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Contents

Five-day Workshop Reports

Chapter 1

Modern Developments in M-Theory (14w5076)

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1.1 Overview of the Field

M-theory originates from string theory, a proposed quantum description of fundamental particles. String theory, in turn, generalises quantum field theory – the most successful description of fundamental physics to date – and reduces to it at low energies. At higher energies, typically those of relevance to quantum phenomena in gravitational systems, string theory departs quite radically from quantum field theory. It provides a specific mechanism to solve the problem of inconsistency at high energies that plagues field-theoretic formulations of gravity.

String theory is consistent only in 10 space-time dimensions but can be easily reduced to a 4-dimensional theory by compactifying it on a suitable manifold. Its formalism is endowed with a deep mathematical beauty that connects to many important results and questions in pure mathematics. Not only does string theory benefit from known theorems in mathematics but mathematics itself has benefited greatly from unexpected connections and unexplored problems suggested by string theory.

When string theory is strongly coupled, its standard description breaks down. In this limit an alternate description becomes available, involving one higher dimension of space. The resulting 11-dimensional theory is called M-theory. One can reduce this theory to string theory by compactifying it on a small circle, however its power and beauty are most evident directly in 11 dimensions. Its low-energy limit is a very special classical field theory: 11-dimensional supergravity. It is notable that supersymmetry is impossible to attain above 11 dimensions, and that under certain minimal assumptions this supergravity is the unique supersymmetric field theory in 11 dimensions.

Just as string theory contains extended excitations: strings and "branes", M-theory too contains extended branes. The mathematics of these branes is a particularly challenging question in view of their strongly coupled nature, inherited directly from the bulk M-theory in which they propagate.

In addition to their potential utility in providing unified theories of fundamental particles and interactions, as well as in stimulating new lines of mathematical research, string and M-theory have come to play a striking new role in the last couple of decades. When they are formulated on (at least asymptotically) anti-de Sitter spacetime, they are dual (i.e. equivalent, though expressed in different variables) to conformal quantum field theories without gravity. In this duality finds that in the quantum field theory, phenomena that would be hard to compute due to strong quantum effects are replaced by a classical, weakly curved gravity description in string or M-theory. This

AdS/CFT duality is therefore considered a potentially useful tool to understand a range of strongly coupled systems including quark-gluon plasma, condensed matter systems and fluids.

While there are many analogies between string theory and M-theory (the presence of extended objects, the possibility of compactification to lower dimensions, the reduction to conventional field theory at low energies, the existence of dualities with conformal field theories and the connection to beautiful mathematical structures) it is almost always the case that M-theory is more difficult to study, largely because of its lack of a small coupling constant in which to perturb. As a consequence, progress in M-theory has tended to proceed at a limited pace. However from time to time, dramatic new results have emerged. This accounts for the special appeal of M-theory to a subset of the string theory community and provides a motivation to hold a focused meeting about it.

1.2 Recent Developments and Open Problems

Since 2007-2008 there have been striking developments in the construction of the previously unknown field theory on multiple membranes in M-theory. Families of field theories of Chern-Simons type were shown by Bagger and Lambert and independently by Gustavsson to posses maximal superconformal symmetries which made them strong candidates for field theories on multiple parallel membranes. This theory relied on a mathematical structure called "3-algebras". Further analysis of this BLG theory by other authors revealed that in fact it can be reduced to ordinary Chern-Simons-type theory albeit in a particular combination that preserves parity. It was argued that BLG theory describes multiple membranes on orbifold spaces where the rank k of the orbifold group is given by the level of the Chern-Simons field theory. At the particular value $k = 1$ the orbifold is absent, and then the theory should describe membranes in flat space. It was also shown that via a novel version of the Higgs mechanism, these theories on the Higgs branch acquire Yang-Mills gauge fields with a fully dynamical gauge field, enabling their comparison with D2-brane theories to which M2-branes reduce in certain limits. Eventually it was realised that BLG theory cannot describe more than two M2-branes and this led to a fresh search for a theory possessing all or most of its relevant properties but allowing for an arbitrary parameter N labeling the number of branes. In a notable breakthrough, Aharony, Bergman, Jafferis and Maldacena, obtained such a theory by reducing the required manifest symmetries. This theory was explicitly proved, via a brane construction, to describe multiple M2-branes. These new developments have illuminated aspects of M-theory and also provided new insights into the dynamics of 2+1 dimensional quantum field theories and their integrability.

Among the open problems involving M-theory membranes, one can list a better understanding of the strongly coupled limit (absence of the orbifold), the construction of compactifications in which these branes arise, as well as verification of the integrability of the field theory and its role within the AdS/CFT context.

Considerable work has also gone into the construction of the M5-brane field theory, but with comparatively less success. In this case, apart from the strongly coupled nature of the field theory, there is the additional issue of a self-dual tensor field. Even at the abelian level such a field does not admit a covariant Lagrangian. Attempts to formulate M5-brane field theories have attempted to circumvent this problem in various ways, for example by using non-self-dual tensor fields and imposing self-duality as an auxiliary condition at a later stage, and/or by relaxing the requirement of manifest Lorentz invariance. Interesting relations have been proposed between M5-branes and the 3-algebra structures that describe M2-branes. A striking conjecture due to Douglas and to Lambert, Papageorgakis and Schmidt-Sommerfeld identifies M5-brane field theory as the strongly coupled limit of supersymmetric Yang-Mills theory in 5 dimensions, locating the extra degrees of freedom that (among other things) render the theory superconformal in 6d within the soliton sector of the 5d theory.

While M2 and M5 branes have been the primary focus of study in recent years, there have been attempts to study M-theory directly in the bulk and these have had some partial success. Attempts to define M-theory non-perturbatively were made over a decade ago using matrices. This led to several related descriptions, the primary one being that of a matrix quantum mechanics based on the D0-brane of type IIA string theory, and others corresponding to 2d matrix string theories or 0d random matrix models. These approaches were later subsumed into the AdS/CFT correspondence but they have their own appeal. One would like to understand degree of validity of such descriptions as well as the symmetries and dynamics of M-theory that follow from them.

Higher-derivative corrections to the low-energy effective action of M-theory have an intricate and beautiful mathematical structure. Much work in recent years has been devoted to the explicit computation of these corrections. Open problems in this area involve not merely computing higher-order corrections, but rather gaining an insight into large classes of computable corrections using profound mathematical tools.

The construction of superconformal quantum field theories in dimension 4 and lower by wrapping M5-branes on Riemann surfaces and other manifolds, dates from the early days of M-theory. The recent work of Gaiotto and others has brought about dramatic progress, illuminating the dualities and other dynamical aspects of a wide variety of SCFT's and providing a powerful way to construct new ones. This subject is growing, with many different perspectives coming from various directions like type IIA string theory and F-theory.

A relatively recent approach to M-theory involves concepts like generalised geometry and doubled field theory, in which the U-duality symmetries of M-theory are manifest. Finding the symmetries, backgrounds and the geometric governing principle behind doubled field theory are all key open problems.

1.3 Presentation Highlights

1.3.1 M2-branes

In the presentation "Exact results and non-perturbative effects in M-theory", Marcos Marino computed the partition function of M2-branes (ABJM theory) on a three-sphere by localization in terms of a matrix integral, resulting in a derivation of the $N^{\frac{3}{2}}$ behavior for a theory of M2-branes. This partition function was found to contain more information including non-perturbative, exponentially small effects at large N. These effects correspond to non-perturbative corrections due to worldsheet and membrane instantons in string theory/M-theory. The resulting expansion highlights the important role of membrane instantons. The corrections due to them can be studied in the Fermi gas approach to the partition function, and are encoded in a system of integral equations of the TBA type. A semi-classical expansion of this system in the ABJM coupling k was studied, corresponding to the strong coupling expansion of the type IIA string. Using these semi-classical results, he verified conjectures for the form of the one-instanton correction at finite k proposed by Hatsuda, Moriyama and Okuyama (HMO), based on a conjectural cancellation of divergences between worldsheet instantons and membrane instantons. Analytic expressions in k were proposed for the full two-membrane instanton correction and for higher-order non-perturbative terms. These pass many consistency checks and provide further evidence for the HMO mechanism. On the mathematical side, the above non-perturbative effects turn out to be connected to topological string theory and its refinements, and to the quantization of algebraic curves.

Stefano Kovacs presented new results on monopole operators in M2-brane theory. Using the AdS/CFT correspondence he presented a proposal for studying the ABJM duality in a genuinely M-theoretic regime. By focussing on a large angular momentum sector, the field theory was studied in a regime in which the gravitational background is eleven-dimensional and the physical states correspond to M2-brane excitations. On the gravity side this sector is well approximated by the pp-wave matrix model, which is weakly coupled. The spectra computed on the two sides were found to agree at leading order, thus verifying the validity of the ABJM duality beyond the previously considered type IIA limit and also providing a new test of the matrix model approach to M-theory.

Bent Nilsson considered topologically gauged BLG: matter/Chern-Simons gauge theory with N = 8 superconformal symmetry coupled to conformal supergravity. His presentation highlighted the discovery of new features like SO(N) gauge groups for any N (instead of the SO(4) in BLG) and Higgsing to topologically massive supergravity and a number of possible "critical" backgrounds. Such results were first found in topologically gauged ABJM/ABJ theory with indications of a "sequential AdS/CFT".

1.3.2 M5-branes

Seok Kim addressed the problem of computing superconformal indices for M5-brane field theories. Starting with maximally supersymmetric Yang-Mills theory in 5d on $CP_2 \times S^1$, he was able to count the BPS local operators of the 6d theory. In a closely related approach, Kimyeong Lee explored the 6d (1,0) and (2,0) superconformal field theories on $R \times S^5/Z_k$ via supersymmetric 5d theories on $CP_2 \times R$. The index computed by these authors agreed with the large-N supergravity index on $AdS_7 \times S^4$ at low energies, and also yielded the negative 'Casimir energy' with an N^3 scaling which was previously calculated from a QFT on S^5.

Costis Papageorgakis examined soliton contributions to perturbative amplitudes in field theory, in the context of the proposed 5d-6d correspondence that conjectures M5-brane field theory to be the strongly coupled limit of 5d Yang-Mills with the desired additional excitations coming from instanton-solitons. This was done by investigating the conditions under which the calculation of a matrix element in the quantum mechanics on the soliton moduli space leads to exponential suppression. In turn, this suggests that the instanton-solitons of 5d supersymmetric Yang-Mills theory will not be suppressed, supporting the proposed correspondence. The same correspondence was discussed by Neil Lambert in a Euclidean context, wherein he proposed that the 5d theory exhibits a hidden time-like dimension.

In a different approach to multiple M5-branes, Chong-Sun Chu put forward a non-abelian self-duality equation in six-dimensions. This led to a proposal for the equation of motion of the 3-form field strength. He discussed how the solutions of these equations have properties that match precisely with the physics of the M5-branes system obtained from other analysis, such as 11 dimensional supergravity and string theory. Dmitri Sorokin presented an alternate approach in which the six-dimensional worldvolume is subject to a covariant split into 3+3 directions by a triplet of auxiliary fields. He discussed the relation of this action to the original form of the M5-brane action and to a Nambu–Poisson 5–brane action based on the Bagger–Lambert–Gustavsson model with the gauge symmetry of volume preserving diffeomorphisms.

1.3.3 Mathematical structures in M-theory

In his presentation "Mathieu moonshine, umbral moonshine and M5-branes", Jeff Harvey related umbral moonshine to the Niemeier lattices: the 23 even unimodular positive-definite lattices of rank 24 with non-trivial root systems. A finite group was attached to each Niemeier lattice by considering a naturally defined quotient of the lattice automorphism group. For each conjugacy class of each of these groups, a vector-valued mock modular form was identified whose components coincide with mock theta functions of Ramanujan in many cases. This then led to the umbral moonshine conjecture, stating that an infinite-dimensional module is assigned to each of the Niemeier lattices in such a way that the associated graded trace functions are mock modular forms of a distinguished nature. These constructions and conjectures include the Mathieu moonshine conjecture that has been of particular interest in the mathematical physics community in recent times. This analysis also highlights a correspondence between genus zero groups and Niemeier lattices. As a part of this relation it was recognised that the Coxeter numbers of Niemeier root systems with a type A component are exactly those levels for which the corresponding classical modular curve has genus zero. In a related development he studied perturbative BPS states in the near-horizon background of two Neveu-Schwarz fivebranes in type IIA superstring theory compactified on $K3 \times S^1 \times R^1$. The brane world-volume wraps the $K3 \times S^1$ factor. He obtained a simple expression for the spacetime helicity supertrace in terms of the completion of the mock modular form $H^{(2)}(\tau)$. This form appears in studies of the decomposition of the elliptic genus of $K3$ surfaces into characters of the $N = 4$ superconformal algebra and manifests a moonshine connection to the Mathieu group M_{24}.

On the same topic, the presentation of Callum Quigley discussed the extension of the Mathieu moonshine conjectures to $N = 2$ string compactifications. In this context it was shown that dimensions of M_{24} representations appear in the new supersymmetric index of heterotic strings on $K3 \times T_2$ and the Gromov-Witten invariants of their type IIA duals. He reported on work in progress to relate these results to the elliptic genus of a wrapped M5-brane. The dimensions of M_{24} representations appear very naturally again in the type IIA context, but now as counting the degeneracies of D4$-$D2$-$D0 bound states (i.e. the Donaldson-Thomas invariants).

1.3.4 Superconformal field theory

The presentation by Leonardo Rastelli: "The superconformal bootstrap program", outlined the modern bootstrap program for four-dimensional theories with extended superconformal symmetry. He found "minibootstrap" equations for supersymmetric quantities, which can be solved analytically, and full-fledged bootstrap equations for non-protected quantities, which can be studied numerically. The entire program relies on general symmetry principles, with no need for "fields" or Lagrangians. The latter part of the talk focused on the numerical results of the $N = 4$ bootstrap and on their interpretation in $N = 4$ supersymmetric Yang-Mills theory. Consistency of the four-point function of the stress-energy tensor multiplet was used to impose significant upper bounds for the scaling dimensions of unprotected local operators as functions of the central charge. At the threshold of exclusion, a particular operator spectrum was singled out by the bootstrap constraints. For large values of the central charge, this was compared and found to be compatible with that of supergravity in $AdS_5 \times S^5$. For finite central charge it was conjectured that the extremal spectrum is that of $N = 4$ SYM at an S-duality invariant value of the complexified gauge coupling.

1.3.5 Higher-spin gravity

In her presentation "Wilson lines in higher spin gravity", Alejandra Castro reviewed the interpretation of Wilson line operators in the context of higher spin gravity in 2+1 dimensional field theories and holography. She showed how a Wilson line encapsulates the thermodynamics of black holes and provides an elegant description of massive particles. This opens a new window of observables which can probe the true geometrical nature of higher spin gravity. Another presentation on higher spins, by Bengt Nilsson, reviewed the coupling of conformal supergravity to CFTs in three dimensions with eight supersymmetries. The so obtained SO(N) models have a new kind of scalar potential that gives rise to a number of possible background geometries. These are specified by a sequence of values for the parameters in the standard topologically massive gravity action that arises after the conformal symmetry breaking. Solutions corresponding to these values were identified, all of which are critical or special in some sense.

1.3.6 Supergravity solutions

Alessandro Tomasiello presented a seminar on all AdS_7 solutions of type- II supergravity. Generalising the important $AdS_7 \times S^4$ solutions (and their orbifolds) in M-theory, he described new AdS_7 supersymmetric solutions in type II supergravity with Romans mass (which does not lift to M-theory). His classification started from a pure spinor approach reminiscent of generalized complex geometry, this determined uniquely the form of the metric and fluxes, up to solving a system of ODE's. His presentation concluded with some work in progress about the CFT_6 duals to these solutions.

1.3.7 Higher-derivative corrections in M-theory

String scattering amplitudes, Feynman diagrams and M- theory and the relations between them were surveyed in the presentation of Michael Green. One class of recent computations involved the determination of explicit expressions for one-loop five-supergraviton scattering amplitudes in type II superstring theories using the pure spinor formalism. The type IIB amplitude was expressed in terms of a doubling of a ten-dimensional super Yang–Mills tree amplitude. A series of terms in the effective action of the schematic form $D^{2k}R^5$ for $0 \leq k \leq 5$ (where R is the Riemann curvature) were evaluated. Comparison with earlier analyses of the tree amplitudes and of the four-particle one-loop amplitude gave rise to an interesting extension of the action of SL(2,Z) S-duality on the moduli-dependent coefficients in the type IIB theory. The investigation also covered closed-string five-particle amplitudes that violate conservation of the U(1) R-symmetry charge and are forbidden in supergravity. Their low energy expansion was found to match the predictions of S-duality. For the six-point function it was shown that the analytic parts of the R^6 and D^4R^6 interactions vanish in the ten-dimensional effective action, but not in lower dimensions.

Anirban Basu presented his results on constraining gravitational interactions in the M-theory effective action. Based on assumptions about the structure of supersymmetry, he was able to obtain the expressions for certain non-BPS operators in the effective action, part of the structure of which is fixed by superstring perturbation theory.

1.4 Outcome of the Meeting

The seminars and deliberations at this meeting were very successful in highlighting the outstanding open problems in the field and proposing new avenues to explore them. Discussions on topics like world-volume formulations of M5-branes, localisation and matrix models for M2-branes, superconformal field theory in 4d, and the mathematics of Mathieu moonshine have led to significant developments during the following year. This meeting was followed up with the "Second Workshop on Developments in M-Theory" held in Gangwon-do, Korea during January 2015.

Participants

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Chapter 2

Theoretical Foundations of Applied SAT Solving (14w5101)

January 19, 2014 - 24, 2014

Organizer(s): Albert Atserias (Universitat Politecnica de Catalunya, Barcelona), Armin Biere (Johannes Kepler University), Samuel Buss (University of California, San Diego), Antonina Kolokolova (Memorial University of Newfoundland), Jakob Nordström (KTH Royal Institute of Technology), Karem Sakallah (University of Michigan and Qatar Computing Research Institute)

2.1 Overview of the Field and Purpose of the Workshop

Proving logic formulas is a problem of immense importance both theoretically and practically. On the one hand, it is believed to be intractable in general, and deciding whether this is so is one of the famous million dollar Clay Millennium Problems [20], namely the P vs. NP problem originating from the ground-breaking work of Cook [12]. On the other hand, today so-called SAT solvers based on conflict-driven clause learning (CDCL) [3, 18, 22] are routinely and successfully used to solve large-scale real-world instances in a wide range of application areas (such as hardware and software verification, electronic design automation, artificial intelligence research, cryptography, bioinformatics, operations research, and railway signalling systems, just to name a few examples — see, e.g., [8] for more details).

During the last two decades, there have been dramatic — and surprising — developments in SAT solving technology that have improved performance by many orders of magnitude. But perhaps even more surprisingly, the best SAT solvers today are still at the core based on relatively simple methods from the early 1960s [14, 15] (albeit with many clever optimizations), searching for proofs in the so-called resolution proof system [9]. While such solvers can often handle formulas with millions of variables, there are also known tiny formulas with just a few hundred variables that cause even the very best solvers to stumble (see, e.g., theoretical work in [10, 17, 28] and experimental results in [19, 29]). The fundamental question of when SAT solvers perform well or badly, and what underlying mathematical properties of the formulas influence SAT solver performance, remains very poorly understood. Other crucial SAT solving issues, such as how to optimize memory management and how to exploit parallelization on modern multicore architectures, are even less well studied and understood from a theoretical point of view.

Another intriguing fact is that although other mathematical methods of reasoning are known that are much stronger than resolution in theory, in particular methods based on algebra [11] and geometry [13], attempts to harness the power of such methods have conspicuously failed to deliver any significant improvements in practical performance. And while resolution is a fairly well-understood proof system, even very basic questions about these stronger algebraic and geometric methods remain wide open.

The purpose of this workshop was to gather leading researchers in applied and theoretical areas of SAT and proof complexity research and to stimulate an increased exchange of ideas between these two communities. To the best of our knowledge, this was the first large-scale workshop aimed specifically at bringing together practitioners and theoreticians from the two fields. We believe that proof complexity can shed light on the power and limitations on current and possible future SAT solving techniques, and that problems encountered in SAT solving can spawn interesting new areas in theoretical research. We see great opportunities for fruitful interplay between theoretical and applied research in this area, and believe that a more vigorous interaction between the two has potential for major long-term impact in computer science and mathematics, as well for applications in industry. Judging from the feed-back from the participants, the workshop provided a powerful stimulus in this direction.

2.2 Presentation Highlights and Workshop Themes

As this workshop brought together different communities many talks at the workshop were designed to be tutorials and surveys, intended to bridge the gaps between the diverse backgrounds of the participants. Specifically, the following five "mini-tutorials" were presented:

1. Marijn Heule: Conflict-driven clause learning (CDCL).
2. Sam Buss: Proof complexity.
3. Matti Järvisalo: Preprocessing.
4. Jakob Nordström Weak proof systems and connections to SAT solving.
5. Albert Atserias: Semialgebraic proof systems.

The presentations by Heule and Järvisalo covered more practical aspects of SAT solver design, the tutorials by Buss and Atserias presented relevant theoretical (proof complexity) background, and the tutorial by Nordström outlined the nature of relationship between the proof complexity and SAT solving.

In addition to the mini-tutorials, there were survey talks on integrating cutting planes/pseudo-Boolean reasoning in CDCL solvers (Daniel Le Berre), parameterized complexity and SAT (Stefan Szeider), satisfiability modulo theories (Albert Oliveras), and QBF solving (Martina Seidl).

The workshop talks and discussions can be grouped into several thematic areas. These include:

- Practical and theoretical issues in the algorithmic design of SAT solvers. A number of the talks discussed the design details of how the most successful SAT solvers are implemented. This included Heule's talk on CDCL, Järvisalo's talk on clause preprocessing, Simon's talk on the power of so-called glue clauses [1], and Biere's talk on the SAT solver Lingeling [6] and other related solvers. The last two presentations were able to delve into implementation details that have not been discussed well in the literature. On the other hand, there was also a general feeling that, in spite of the successes of SAT solvers, we still have a very limited understanding of when and why different techniques work well or poorly. There was a lot of discussion on this topic throughout the week as well as at a special Thursday evening meeting. Many participants expressed the opinion that SAT implementations need better benchmarking and better testing in order to develop an improved understanding of why the techniques currently in use work effectively and how they interact, as well as in order to make future progress on improving SAT solvers.

- Theoretical issues for SAT solvers. Several presentations highlighted gaps between our theoretical understanding of resolution and the implementation of SAT solvers. Since extended resolution is known to be much more powerful than resolution, one much discussed question was how the extension rule can speed up CDCL solvers. Buss's tutorial suggested heuristics for introducing extension variables, Goultiaeva suggested studying whether CDCL SAT solvers without restarts can polynomially simulate resolution, and Van Gelder gave examples of the power of extended resolution for several tautologies. In related topics, Nordström's, Lauria's and Johannsen's talks addressed the memory usage requirements for resolution proofs, and Szeider discussed parameterized complexity of SAT. These measures of proof complexity may also have impact on the effectiveness of SAT algorithms.

- Parallelizability. With the increasing availability of parallel computing, it is natural to try to harness this resource by implementing parallel algorithms for SAT. Sabharwal and Manthey both discussed parallel implementations of satisfiability algorithms and presented a wealth of graphical data analysing their performance. The problems encountered when implementing parallel solvers, especially what concerns choosing branching variables and sharing learned clauses, further highlight the gap between our practical algorithms for satisfiability and our understanding of why different techniques work well. For this reason, there was a lot of discussion on the topics of these talks, both on how sequential algorithms can be parallelized and on how the experiences with parallel algorithms can inform sequential algorithms.

- Non-Boolean SAT solvers. Quite a few talks addressed non-Boolean extensions of SAT solvers. This started with Atserias's tutorial talk on semi-algebraic proof systems. Galesi discussed space complexity of algebraic proof systems. Le Berre and Kullman discussed cutting planes, XOR constraints, and pseudo-Boolean constraints. Kalla spoke on Groebner basis methods. Marques-Silva gave a presentation about using SAT oracles to solve more general problems, such as counting. Beame talked about exact model counting. Olivera and Sinz discussed SMT (satisfiability modulo theories) systems, which are extensions of SAT solvers to more powerful logics. Sakallah discussed how detecting and breaking symmetries can make SAT solving more efficient.

  These extensions to SAT solvers are all very powerful, at least in the right situations. However, for general instances of the SAT problem it still seems that nothing can really beat SAT solvers based on conflict-driven clause learning. The reasons for this are a little mysterious; however, in all implementations to date, the extra power awarded by, e.g., algebraic or pseudo-Boolean reasoning cannot quite compensate for the extra time needed for performing such more advanced reasoning. Nonetheless, there is some prospect that the next major breakthrough in SAT solving may come from some kind of non-Boolean reasoning.

- Quantified Boolean Formulas (QBF). Determining the satisfiability of a quantified Boolean formula is a much harder problem than ordinary satisfiability. In spite of this, recent years have seen surprisingly good progress in this area. Seidl and Narodytska gave talks describing practical implementations of QBF solvers, along with theoretical justifications. Santhanam presented a new asymptotic improvement for QBF solving.

2.3 Open Problems

We solicited open problems from the participants prior to the workshop, and, additionally, held an open problem session during the first evening. Below follows a selection of open problems and conjectures proposed by participants of the workshop.[1]

- Norbert Manthey: An important open problem is that extended resolution is easy in principle to integrate into SAT solver (its a few lines of code for Riss [25], Glucose [16] or MiniSat [21]), but so far it is not used. The reason seems to be that there are no working heuristics known that give a hint which extension to perform, and when to perform it. Good heuristic suggestions would seem to be very valuable, and so if there are some proof related measurements that could be used to decide whether a learned clause should be kept or not (or for guiding the decision heuristic), this would definitely be worth knowing.

- Norbert Manthey: Another open problem is how to generate proofs within parallel SAT solvers. For portfolio-style SAT solvers this problem might be solvable with less effort than for search space splitting parallel SAT solvers. However, currently I do not know any parallel SAT solver that is able to produce an UNSAT proof in any format. Thus, one can also not compare how far current systems are away from actual

[1]Most of the open problems below, as well as several others, can be found in the list of open problem on the pre-workshop webpage `www.csc.kth.se/~jakobn/BIRS_14w5101/`. They have been lightly edited here for context.

(shortest) proof (except considering the number of total learned clauses as the length, and the maximum learned clause size as the width).

- Sharad Malik: It may be helpful for the theory and practice groups to come together to see if they can provide some insight into how modern CDCL locality-based SAT solvers exploit the structure of instances arising in practice. This has been wide open in the community and could benefit from discussion within this diverse group.

- Alasdair Urquhart: Can it be shown for well-known formula families such as the pigeonhole principle (PHP) formulas or Tseitin formulas that regular resolution is optimal? This conjecture seems very plausible to me, but I do not see how to approach it at the moment. More generally, one can ask whether it is possible to give general conditions on a set of clauses that ensure that regular resolution is optimal? In general, the examples separating general and unrestricted resolution have a rather artificial appearance, where we add "spoiler variables" to mess up any regular refutation.

- Karem Sakallah: During the workshop Sakallah presented an empirical study made by himself and Marques-Silva [26] of various SAT heuristics, and asked for theoretical explanations of the observed behaviour.

- Adrian Darwiche: Rather than splitting on variables when making decisions in a SAT solver, one could split on formulas. But does it help? And how to do that in the best way?

- Armin Biere: Current practical successful paradigms for SAT solving all use control-dominated algorithms, like variants of CDCL, WalkSAT, or Look-Ahead based algorithms, and are thus hard to port to highly parallel computing architectures, which require memory locality and thus data-flow orientation. It is a challenge to come up with SAT algorithms which are organized around data-flow.

- Armin Biere: Portfolio based SAT solving is the dominating approach in the parallel application track of the SAT competition [27]. However, the improvements we saw in the last two years are apparently based on using better sharing schemes for learned clauses, thus kind of implicit work splitting. From a practical point of view it is first of all still unclear how much of the success of solvers like Penelope or Plingeling can be attributed to the portfolio idea and how much is due to splitting the work. As the number of compute units is increased it is conjectured that the relative contribution of the portfolio part will saturate. Does this happen and when?

- Armin Biere: The variable scoring scheme VSIDS (variable state independent decaying sum) introduced by Chaff [22] and its modern variants is crucial for the speed of CDCL solvers. There is almost no empirical investigation on how it really works, and further no theoretical explanation why it is working so well.

- Alexandra Goultiaeva: It has been proven that CDCL SAT solvers, viewed appropriately as a proof system, can polynomially simulate resolution [24]. The order of decisions is assumed to be non-deterministic, i.e., the proof shows that (if a short resolution proof exists) there exists a sequence of decisions that would allow the solver to find a short resolution proof. I am very much interested in seeing this extended to heuristics, especially VSIDS. That is, I would like to see a result that either:
  - shows that whenever a short resolution proof exists, there will always be a sequence of decisions that respects VSIDS ordering and allows the solver to find a short resolution proof, or
  - shows a counterexample where a short resolution proof exists but a solver respecting VSIDS ordering (regardless of tie-breaking) can never find a short proof.

- Massimo Lauria: Prove lower (and upper) bounds on proof size in resolution (and stronger proof systems) for k-clique formulas and other combinatorial principles.[2]

- Paul Beame: Could one make SAT solvers learn not just clauses/bad partial assignments but more general residual formulas, or other kinds of "reasons" for formulas being unsatisfiable? What would be good practical "reasons" of this kind?

[2]Code for generating these benchmarks in DIMACS format is available at `github.com/MassimoLauria/cnfgen`.

In addition to the Monday evening open problem session, we also organized a Thursday evening discussion session to provide a period for participants to raise questions, propose problems, and generally discuss and reflect on the issues raised during (the first four days of) the workshop. A selection of topics discussed during the Thursday evening session follows below.

- Karem Sakallah: It is important to increase understanding. The SAT community has done a great job to produce good SAT solvers. It has done a worse job of explaining how they work. Competitions have been very important to drive progree but should now evolve. It is not important to have the fastest solver but to explain why the solver is fast. What happens when the knobs are turned? Which knobs are important? The communities are talking completely different languages. We need to invest in learning to understand each other. Finally, a question: Simple explanations need simple models. From where can we get such models?

- Rahul Santhanam: Can we use a scientific approach to understand hardness as an empirical phenomenon and make falsifiable claims? Possible hypotheses: backdoors, complexity measures, entropy, selection bias towards what works today — what do practitioners think about these hypotheses? What is the most general property Q such that formulas with property Q are easily solvable?

- Moshe Vardi: Here is a list of five central problems:
  - Go beyond resolution for SAT solvers.
  - Go beyond worst-case complexity in the analysis of SAT solver performance (by analogy, think of the smoothed analysis of Spielman-Teng as going beyond worst-case and average-case analysis for the simplex method in linear programming).
  - NP vs PSPACE vs EXPTIME: Is PSPACE really harder than NP?
  - Can we parallelize unit clause propagation / BCP?
  - Exact algorithms / computational complexity: Are any ideas from here relevant for real-world algorithms?

2.4 Opinions About the Workshop

Our impression from interacting with the participants during and after the workshop is that this was a highly successful event. The workshop was even considered significant enough that an editorial in the Communications of the ACM[3] was dedicated exclusively to this "unusual workshop" about which it said: "Of course, one cannot expect robust bridges between two distinct technical communities to be erected in one week, but that should not diminish the tremendous value of such bridge-building workshops."

We also collected feed-back from the participants after the workshop by sending out an e-mail message with questions to which almost half of the workshop participants responded. The questions together with a brief but representative selection of answers follow below.

2.4.1 What were a couple of good aspects of the workshop?

- *Having food together gave lots of opportunities for informal discussion, which was arguably more important than the presentations. The program had a good mix of practical and theoretical results, which started interesting discussion.*

- *My overall opinion of the workshop is very positive. I was able to get input from some of the best theoreticians and practitioners in the area of SAT, and learn about recent work in the area of SAT. The informal setting allowed interactions with many colleagues. Overall I believe this was a great experience!*

- *Most of the talks were very good. I especially enjoyed the tutorials. I also enjoyed the discussion session in which some selected people gave their opinions.*

[3] Available at `cacm.acm.org/magazines/2014/3/172516-boolean-satisfiability/fulltext`.

- *I really liked the tutorials and surveys. I was hoping for an overview of the landscape of SAT solving, and I got exactly that. I also liked the fact that the theorists and practitioners made an attempt to communicate with each other.*

- *The participants where among the best in their fields. The mix of theory and applied people was good, and the discussions between these groups was important. This also revealed some deficiency in the communication between these groups, and identifying a problem is the first step to a solution.*

- *The in-depth discussions, the broad coverage of a range of relevant issues — the agenda was very well planned.*

- *That it brought together people who do not normally get to interact; two communities that could help each other out by collaborating.*

2.4.2 What were some aspects that could have been better?

- *Presentation of open problems in applied SAT, and opportunities from the theory side could have made stronger, and earlier in the week. Communication across the field could have started faster (but I do not have any idea how to achieve this). Maybe, one should have tried to have some task oriented session, where somebody posts a problem, and an idea how to solve it (or without an idea, and another guy comes up with the idea), and then the whole group could decide whether this idea might work or not — again, I am not sure whether something like this would work.*

- *The interaction between the two communities was mainly done through presentations. Maybe some focused discussion on some specific topic would have been fun and productive (modulo a strong moderation).*

- *Maybe the schedule was tight, with not that much time for discussions between talks. But it is difficult to say, since people used to discuss together during breakfast, lunch or dinner.*

2.4.3 Was there any area or topic which was missing or which you would have liked to hear more about?

- *The correlation between the proof complexity and the representation of the problem, hence: encodings, and high-level to low-level problem transformation.*

- *Maybe a little more from the area of algorithms for SAT (exact, parameterized, randomized. . .).*

- *I would have liked to hear more about Random SAT/Survey propagation and BDD-based approaches.*

- *Perhaps more on SMT (but the program was very very good).*

- *Obviously, some areas of proof complexity were not covered, e.g. there were quite a few talks on QBF solving, but nothing on the proof complexity side of it. In general, I believe that proof complexity of logics other than just classical propositional logic are interesting.*

- *I found all relevant topics covered. Maybe the machine learning perspective could have added another aspect.*

- *It would have been helpful to hear more about SAT through divide and conquer. Some of this came up in the discussion on parallel SAT solvers, but this is an important topic in its own right since it deals with information at the interface of problem partitions.*

2.4.4 Was there any area or topic that could have been de-emphasized or skipped?

- *Given the objectives of the workshop, and the audience, I would emphasize overview talks, summarizing relevant recent results, than talks focusing on specific topics or papers, either recently published or to be published. The 50 min talks allow covering a good amount of material, and so it was (and will be) fine to give overviews.*
- *Some of the specialized talks were hard to follow for the other part of the community.*
- *Not as far as I can think of. The program looked quite balanced to me... But, on the other hand, I do not have that much idea about the full plate on the other side. At the risk of offending someone, I thought QBF could be de-emphasized, although not removed.*

2.4.5 Would you personally come again if you were invited to a similar workshop in Banff? In Dagstuhl?

For Banff: 18 "yes" answers, 2 "maybe,", 0 "no." For Dagstuhl: 17 "yes" answers, 3 "maybe,", 0 "no."

2.4.6 And any other comments you might have, of course...

- *I feel like I learned more than at most conferences, maybe all.*
- *I am looking forward to results that originated during the workshop. It seems to be the case that some things already started.*
- *This was the most useful Banff workshop I've attended.*
- *Thank you, I think you did a wonderful job organizing.*
- *I'd like to see even more PhD students at these kind of workshops.*

2.5 Scientific Progress Made

This workshop was intended to foster new collaborations among researchers from the different communities surrounding the SAT problem. The main challenge when bringing together people from such different areas is to help them even understand each other's languages, and it seems clear from the feed-back of the participant that the workshop made a major contribution in this regard. In addition, the workshop also spawned a number of joint research projects, and some of these projects have already produced concrete results. Specifically, participants of the workshop have reported the following papers as resulting from the workshop, or at least being significantly influenced by it:

1. Gilles Audemard and Laurent Simon: Lazy clause exchange policy for parallel SAT solvers [2].
2. Paul Beame and Ashish Sabharwal: Non-Restarting SAT Solvers With Simple Preprocessing Can Efficiently Simulate Resolution [4].
3. Olaf Beyersdorff and Oliver Kullmann: Unified Characterisations of Resolution Hardness Measures [5].
4. Armin Biere, Daniel Le Berre, Emmanuel Lonca and Norbert Manthey: Detecting Cardinality Constraints in CNF [7].
5. Vijay Ganesh, Kaveh Ghasemloo and Jimmy Liang: VSIDS Branching Heuristics in SAT Solvers and Timed Graph Centrality with Smoothing, submitted.
6. Niklas Een, Alex Legg, Nina Narodytska, and Leonid Ryzhyk: SAT-based Strategy Extraction in Reachability Games, accepted to AAAI 2015.

7. Mladen Mikša and Jakob Nordström: Long Proofs of (Seemingly) Simple Formulas [19].

8. Zack Newsham, Vijay Ganesh, Sebastian Fischmeister, Gilles Audemard, and Laurent Simon: Impact of Community Structure on SAT Solver Performance [23].

Many other research project collaborations were initiated as a result of this workshop, although they have not yet led to published papers (we know of at least six such projects, and there are probably more). Several of these projects are between researchers from different communities who met as a result of this workshop.

One concrete project that we want to mention is that João Marques-Silva, Karem Sakallah, and Laurent Simon are conducting a more extensive empirical study of modern CDCL solvers to determine the impact of their many knobs on performance (i.e., a more comprehensive study than the preliminary on in [26] mentioned above). This is still work in progress.

Another ongoing project is that Marijn Heule and Jakob Nordström have initiated a study of combinatorial benchmark formulas and how different SAT solvers perform on these formulas when different SAT solver settings are varied (such as restart frequency or VSIDS decay factor). The goal is to find theoretical explanations for the sometimes dramatic differences in performance discovered so far even with fairly minor changes in parameters, and to draw conclusions that can hopefully guide the design of better SAT solving heuristics.

Additionally, Norbert Manthey designed a CNF formula generator for the clique coloring problem, submitted to the SAT competition 2014 and the Configurable SAT solver challenge 2014, based on the ideas from the workshop presentation by Allen van Gelder titled Elementary short refutations for the clique-coloring principle and for Tseitin odd-charge graph formulas in extended resolution. This is intended to create a reference benchmark for the development of extended resolution in SAT solvers.

2.6 Outcome of the Meeting

The explicit goal of this workshop was to increase the interaction and collaboration between experts in practical SAT solving and theoreticians in the related area of proof complexity. The tutorials and surveys were used to bring both communities on the same page with regards to advances and challenges in SAT solving and available proof complexity techniques that can be used to explain some of the observed behaviour. Thus, a first important outcome of the workshop was to provide both communities with extensive background knowledge of, respectively, theoretical and practical aspects of modern SAT solving.

By organizing two open problem/discussion sessions, we encouraged the participants to present challenges, insights and open problems in their respective areas. There are several collaborations that have started as a result of these discussions, and there are eight papers attributed, at least in part, to this workshop — see the previous section for more details.

Overall, this workshop has given a powerful impetus to a number of world-leading senior practitioners and theoreticians in SAT-related research, as well as to a selection of prominent junior researchers, to collaborate and explore the theoretical foundations of applied SAT solving. We fully anticipate more progress on the development and understanding of SAT solvers over the next several years.

An important next step to further stimulate research in this direction and strengthen the contacts between practitioners and theoreticians will be the Dagstuhl workshop Theory and Practice of SAT Solving in April 2015, explicitly intended as a follow-up on the workshop in Banff. We also hope that it will be possible to organize further workshops on this topic in Banff and/or Dagstuhl in future years to continute to support these developments. We believe that both applied and theoretical researchers stand to benefit greatly from a more vigorous interaction between the two communities, and that this could have a major long-term impact for both academical research and industrial applications.

Participants

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Bibliography

[1] Gilles Audemard and Laurent Simon. Predicting learnt clauses quality in modern SAT solver. In Proceedings of the 21st International Joint Conference on Artificial Intelligence (IJCAI '09), pages 399–404, July 2009.

[2] Gilles Audemard and Laurent Simon. Lazy clause exchange policy for parallel SAT solvers. In Proceedings of the 17th International Conference on Theory and Applications of Satisfiability Testing (SAT '14), volume 8561 of Lecture Notes in Computer Science, pages 197–205. Springer, July 2014.

[3] Roberto J. Bayardo Jr. and Robert Schrag. Using CSP look-back techniques to solve real-world SAT instances. In Proceedings of the 14th National Conference on Artificial Intelligence (AAAI '97), pages 203–208, July 1997.

[4] Paul Beame and Ashish Sabharwal. Non-restarting SAT solvers with simple preprocessing can efficiently simulate resolution. In Proceedings of the 28th AAAI Conference on Artificial Intelligence (AAAI '14), pages 2608–2615, July 2014.

[5] Olaf Beyersdorff and Oliver Kullmann. Unified characterisations of resolution hardness measures. In Proceedings of the 17th International Conference on Theory and Applications of Satisfiability Testing (SAT '14), volume 8561 of Lecture Notes in Computer Science, pages 170–187. Springer, July 2014.

[6] Armin Biere. Lingeling, Plingeling, PicoSAT and PrecoSAT at SAT Race 2010. Technical Report 10/1, FMV Reports Series, Institute for Formal Models and Verification, Johannes Kepler University, August 2010.

[7] Armin Biere, Daniel Le Berre, Emmanuel Lonca, and Norbert Manthey. Detecting cardinality constraints in CNF. In Proceedings of the 17th International Conference on Theory and Applications of Satisfiability Testing (SAT '14), volume 8561 of Lecture Notes in Computer Science, pages 285–301. Springer, July 2014.

[8] Armin Biere, Marijn J. H. Heule, Hans van Maaren, and Toby Walsh, editors. Handbook of Satisfiability, volume 185 of Frontiers in Artificial Intelligence and Applications. IOS Press, February 2009.

[9] Archie Blake. Canonical Expressions in Boolean Algebra. PhD thesis, University of Chicago, 1937.

[10] Vašek Chvátal and Endre Szemerédi. Many hard examples for resolution. Journal of the ACM, 35(4):759–768, October 1988.

[11] Matthew Clegg, Jeffery Edmonds, and Russell Impagliazzo. Using the Groebner basis algorithm to find proofs of unsatisfiability. In Proceedings of the 28th Annual ACM Symposium on Theory of Computing (STOC '96), pages 174–183, May 1996.

[12] Stephen A. Cook. The complexity of theorem-proving procedures. In Proceedings of the 3rd Annual ACM Symposium on Theory of Computing (STOC '71), pages 151–158, 1971.

[13] William Cook, Collette Rene Coullard, and Gyorgy Turán. On the complexity of cutting-plane proofs. Discrete Applied Mathematics, 18(1):25–38, November 1987.

[14] Martin Davis, George Logemann, and Donald Loveland. A machine program for theorem proving. Communications of the ACM, 5(7):394–397, July 1962.

[15] Martin Davis and Hilary Putnam. A computing procedure for quantification theory. Journal of the ACM, 7(3):201–215, 1960.

[16] The Glucose SAT solver. `http://www.labri.fr/perso/lsimon/glucose/`.

[17] Armin Haken. The intractability of resolution. Theoretical Computer Science, 39(2-3):297–308, August 1985.

[18] João P. Marques-Silva and Karem A. Sakallah. GRASP: A search algorithm for propositional satisfiability. IEEE Transactions on Computers, 48(5):506–521, May 1999. Preliminary version appeared in ICCAD '96.

[19] Mladen Mikša and Jakob Nordström. Long proofs of (seemingly) simple formulas. In Proceedings of the 17th International Conference on Theory and Applications of Satisfiability Testing (SAT '14), volume 8561 of Lecture Notes in Computer Science, pages 121–137. Springer, July 2014.

[20] The Millennium Problems of the Clay Mathematics Institute, May 2000. See the webpage `http://www.claymath.org/millennium/`.

[21] The MiniSat page. `http://minisat.se/`.

[22] Matthew W. Moskewicz, Conor F. Madigan, Ying Zhao, Lintao Zhang, and Sharad Malik. Chaff: Engineering an efficient SAT solver. In Proceedings of the 38th Design Automation Conference (DAC '01), pages 530–535, June 2001.

[23] Zack Newsham, Vijay Ganesh, Sebastian Fischmeister, Gilles Audemard, and Laurent Simon. Impact of community structure on SAT solver performance. In Proceedings of the 17th International Conference on Theory and Applications of Satisfiability Testing (SAT '14), volume 8561 of Lecture Notes in Computer Science, pages 252–268. Springer, July 2014.

[24] Knot Pipatsrisawat and Adnan Darwiche. On the power of clause-learning SAT solvers as resolution engines. Artificial Intelligence, 175:512–525, February 2011. Preliminary version appeared in CP '09.

[25] Riss. `http://tools.computational-logic.org/content/riss.php`.

[26] Karem A. Sakallah and João Marques-Silva. Anatomy and empirical evaluation of modern SAT solvers. Bulletin of the EATCS, 103:96–121, 2011.

[27] The international SAT Competitions web page. `http://www.satcompetition.org`.

[28] Alasdair Urquhart. Hard examples for resolution. Journal of the ACM, 34(1):209–219, January 1987.

[29] Allen Van Gelder and Ivor Spence. Zero-one designs produce small hard SAT instances. In Proceedings of the 13th International Conference on Theory and Applications of Satisfiability Testing (SAT '10), volume 6175 of Lecture Notes in Computer Science, pages 388–397. Springer, July 2010.

Chapter 3

Mathematicians and School Mathematics Education: A Pan-American Workshop (14w5128)

January 26 - 31, 2014

Organizer(s): Yuriko Baldin (Universidade Federal de São Carlos), Ed Barbeau (University of Toronto), José Antonio de la Peña (Centro de Investigación en Matemáticas), Patricio Felmer (Universidad de Chile), Solomon Friedberg (Boston College), William McCallum (The University of Arizona)

Background to the Workshop

In January 2012, Patricio Felmer organized a conference in Chile entitled "Mathematicians and School Mathematics Education," bringing together many of the mathematicians involved in the projects described above. The conference had a number of follow-on projects:

- Chile and Mexico collaborated to produce interactive resources that support the books for teacher preparation developed in Chile.
- Mexico developed the online repository ReLaMat.
- Angel Piñeda and José Antonio announced a study on transition from undergraduate to graduate school in Latin America as a result of the Chile meeting.

The participants in the Chile conference agreed that further pan-American collaboration and exchange is desirable, hence this BIRS workshop.

Before describing some of the issues discussed at the workshop, we give a brief overview of work being done in the various participating countries.

In Chile, mathematicians have led the way in writing standards for the preparation of secondary teachers, writing textbooks for teacher preparation courses, and providing professional development for teachers to meet the new standards.

In the United States, mathematicians played a significant role in the writing of the Common Core State Standards for Mathematics, adopted by over 40 states. A mathematician was one of the lead writers and chaired the Work Team, and the presidents of all mathematical societies have endorsed the standards.

In Brazil mathematicians have organized to write vignettes—accounts of modern mathematics for upper secondary teachers—for the Klein Project (see blog.kleinproject.org). The Klein Project (kleinproject.org) is an initiative of the International Mathematical Union and the International Commission on Mathematics Instruction, celebrating the 100th anniversary of the publication of Felix Klein's Elementary Mathematics from an Advanced Standpoint. It promises to be a strong vehicle for bringing the expertise of mathematicians to the school mathematics education enterprise, in a way that gives a voice to both mathematicians and teachers, and promotes productive dialogue. Mathematicians in Brazil have also started to collaborate on constructing virtual repositories of technology based teaching materials. (See, for example, http://portaldoprofessor.mec.gov.br/links.html, http://m3.ime.unicamp.br and http://uff.br/cdme.)

Argentina, Brazil, and Colombia organize Mathematics Olympiads with the active participation of math- ematicians; in Brazil the Olympiad reaches 19 million students through an innovative inclusive model.

In Mexico the Mexican Academy of Sciences developed a professional development program for primary and secondary teachers—Science in Your School—under the direction of a mathematician from the National Autonomous University of Mexico, with both an on-site and on on-line component.

In Brazil, mathematicians have played a key role in replacing a system of sporadic professional devel- opment for high school teachers with a more academic degree for including both research and a deeper understanding of the content, relating abstract concepts and advanced topics to the content of the school cur- riculum. In addition, the Brazilian Mathematical Society initiated in 2011 a purely content-based degree for high school teachers.

In the United States there has been a proliferation of content-based masters' degrees for elementary, middle, and high school teachers. Many of these were developed through federally and state funded Math Science Partnerships, with the active participation of mathematicians. These degrees combine pedagogy courses with mathematics courses, relating the mathematics to what teachers will be teaching.

Canada has a long tradition of mathematicians' involvement in school mathematics education. The Canadian Mathematics Education Study Group was founded by mathematicians and maths educators and plays a major role for mathematics education in Canada and beyond. Mathematicians at the University of Laval started a free mathematics magazine, Accromath, aimed at high school teachers, and a mathematics show for high school students. Mathematicians at York University developed a course to teach further mathematics to current high school teachers.

Highlights of the Presentations

Videos of the presentations and supporting materials such as slides can be seen at the BIRS website. There were panels on the state of mathematics education in the region. There were panels about mathematicians' work in teacher education, both pre-service and in-service, in developing online resources, in curriculum, and in education policy. There were panels about international collaboration and collaboration between mathematicians and education researchers.

The plenary addresses spanned the region and the concerns of the conference:

- Hyman Bass started off the conference with an analysis of the different roles that mathematicians can play in mathematics education.

- Gabriela Gomez Pasquali gave a moving presentation entitled "Paraguay Solves: Aiming High from the Bottom of the Well," about OMAPA, a project that supports both teachers and students in a country with one of the weakest education systems in the region. The project has had remarkable success engaging students in mathematics olympiads and teachers in workshops.

- Jim Lewis talked about how to build local partnerships between mathematicians, educators, and teachers to forge effective continuing education programs for mathematics teachers.

- Carlos Bosch, Universidad Nacional Autónoma de México, gave a presentation on an in-service teacher training course, the last of a series of efforts over the last decade to reach teachers in both urban and distant rural areas of Mexico.

- Patricio Felmer talked about the work of mathematicians to improve school mathematics in Chile, particularly in developing curricula for teacher preparation courses.

Common Concerns Discussed at the Meeting

The last day of the workshop was devoted to group discussions of issues nominated by the participants. Here is a summary of some of those discussions.

Content-based Masters Degrees for Teachers

This discussion centered around the growth of content-based masters degress for teachers, based in departments of mathematics, aimed at increasing teachers' understanding of the mathematics they teach and the mathematics it leads to. Many of those participating in the discussion have been involved in such programs and they wanted to share ideas.

James Madden opened the discussion with a comparison with the medical profession. In 1900 the American Medical Association recognized the lack of professionalism in medical practice, and commissioned the Flexner report. Flexner made a comparison of medical training programs and brought them to public attention, but the resulting changes in the profession where led by the physicians themselves. The question was posed: are we in a similar situation with regard to the training of teachers? Do we have model programs?

Others raised doubts about this analogy, pointing out that we have to consider the national or local context. Some populations of teachers are very mathematically literate, others not. In all cases we want the teachers to be supported by mathematicians in learning mathematics in a way that is condusive to good teaching.

Another point that came up was the relative dearth of such programs compared to the proliferatino of masters degreess offered by colleges of education. The sentiment was expressed that we need more examples of content-rich programs established in mathematics departments before an exercise like the Flexner report.

Some programs are purely content based, with no education research component, such as a program for high school teachers introduced by the Brazilian Mathematical Society in 2011 that serves about 1,000 students per year, or the program at York University, whose intent is simply to teach mathematics to current high school teachers, covering a lot of traditional topics.

Other programs make an effort to integrate the content with mathematics education research. In addition to the Brazilian Mathematical Society program described above, another Brazilian program for high school teachers described by Yuriko Baldin integrates education research, content, and field experience. It relates abstract concepts and advanced topics to the content of the school curriculum. Students engage in research into their teaching, drawing on psychology and education research, and bring it to bear on classroom practice. The program also includes connections between high school and elementary school mathematics.

In Chile there had been a divergence into a content degree and a mathematics education degree around 1979. Now the latter program is being changed into a more content-based degree (for high school teachers).

The program at California State University Fullerton offers core classes in high school content areas and problem solving. Rather than offereing separate courses in teaching methods, instructors in thsi program model the pedagogy of high school in the way that they teach the mathematics.

At Boston College the program goes beyond the masters degree through an induction phase, which systematically provides follow-up and support for the first few years of teaching, incorporating pedagogy, administrative matters, and content.

There are two audiences for a masters degree: experienced teachers of mathematics and finishing undergraduate majors looking to become secondary teachers. The University of Utah has a program for each, and his been thinking of merging them so that the experienced teacher pairs with the more mathematically prepared undergraduate. Louisiana State University has take this approach, but has not yet found the best strategy for bringing about productive contact between the two groups. And, for the CSU Fullerton program mentioned earlier, the enrolment is a mix of high school teachers and community college students or mathematics majors at CSU.

Ed Barbeau offered the following concluding thoughts: a good teacher is a witness (in the evangelical sense) for what is good mathematics. To become such a witness they need to go through some of the struggles of doing mathematics. This can be done with good problems that don't necessarily belong in a topic area. A teacher should be able to orchestrate the use of tools for the students in the way a music teacher leads a band.

How can we support mathematicians in learning to teach mathematics a way that addresses the needs of teachers?

Bernard Hodgson opened with the following question: suppose you are teaching a real analysis course, and all the students are prospective teachers. What kind of analysis course would be good for them? He then suggested that the answer might well include topics not normally taught in such a course: for example, a deep knowledge of how trigonometric functions evolve from ratios of sides of a triangle to functions of a real variable. We need a literature of such examples.

It was pointed out that one way to generate examples is by asking teachers to describe areas where their students ask a question that they cannot give a good answer to, or if there is an area they do not feel quite certain about even though their students don't necessarily ask about it. Problems in courses for teachers should either be problems that help teachers reflect on topics in the curriculum, or problems that help teachers glue these topics together.

This led to a discussion of specific mathematical topics which are often not addressed in undergraduate classes but which secondary school teachers need to know: conic sections, complex numbers, place value, quadratic equations, modeling with calculus. There is also a need to consider the practices of mathematics: for example, what does it mean to have a good mathematical discussion? What does a good mathematical explanation look like?

Jim Lewis enunciated some general principles for courses for teachers. They should

- contain something that informs the curriculum they are teaching, and puts the ideas in that curriculum on a larger framework
- be informed by an awareness that teachers will be advising students about their mathematical future, so they need insights that would help with that
- give teachers a sense of some things that come after the high school mathematics they teach, so that they can judge what is fundamental from what is a side goal.

The session concluded with a discussion of ways of inducting mathematicians into the work of teacher preparation. These included

- asking your colleagues to come and participate in discussion groups with teachers in any venue where there are teachers coming together (courses, teacher circles, evening sessions, problem committees)
- co-presenting with a teacher at workshops, conferences
- co-teaching with someone who is more experienced
- inviting people to observe your class
- observing classes in the school, simply to understand the work of teaching; observinf an entire course; engaging in team teaching with the teacher
- looking at videos of classroom practice is a way of bypassing preconceived ideological positions
- writing and critiquing mathematics problems and looking at student work.

Fostering International Collaboration

The workshop concluded with a discussion of ways of fostering international collaboration.

One goal of collaboration is to develop more systematic practice for the work of mathematicians in mathematics education, rather than isolated local efforts. Furthemore, local efforts can often benefit significantly from the moral support provided by international recognition.

There as some discussion of how countries with more developed programs can help countries with less developed programs. One model is the Visiting Lecture Program started in 2005 in Cambodia by the Centre International de Mathèmatiques Pures et Appliquées (CIMPA). There are not enough Cambodian mathematicians in the country to teach courses for masters' degree programs, so CIMPA arranged for foreign mathematicians volunteer to give these courses.

There is also a hybrid model for such programs, with some semesters running locally and some at a university in the supporting country. The supporting university doesn't need to start a new degree program but provides supporting faculty.

In the discussion of these models it was recognized that there is a tension between the need to develop local capacity versus the need to support a country with little or no local capacity. It was felt that such efforts to be led locally, with outside support.

A case in point is the work in Paraguay that was described at the workshop. Is their initiative something that people from other countries can contribute to, and if so, how?

In general it was agreed that mathematicians from a particular country or region should think about what the barriers are themselves first, before proposing a project. Furthermore, in order to attract funding, we need metrics for what we do.

Participants

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Chapter 4

Positivity of Linear Series and Vector Bundles (14w5056)

February 2 - 7, 2014

Organizer(s): Sándor Kovács (University of Washington, Seattle, USA), Alex Küronya (Budapest University of Technology and Economics, Hungary), Tomasz Szemberg (Pedagogical University of Cracow, Poland)

4.1 Positivity concepts for line and vector bundles

The main focus of the workshop was to study the existing positivity concepts of line bundles and vector bundles with an emphasis on the higher rank case.

There exists a highly developed and widely used theory of positivity for line bundles, which forms one of the fundamental building blocks of modern projective geometry. With the recent shift in emphasis towards birational geometry, there is a heightened interest for the behaviour of big line bundles — as opposed to ample ones, which describe the various birational models of the underlying variety. Both ample and big divisors have numerical, cohomological, and geometric characterizations, which makes for a quite satisfactory theory of positivity for linear series. Also the concept of nef divisors is well understood and commonly applied.

There have been several attempts to extend positivity concepts mentioned above to the case of higher rank vector bundles. In addition to ampleness, bigness and nefness there are various other concepts designed with vector bundles in mind, for instance Viehweg's weak semipositivity, Miyaoka's generic semipositivity and almost everywhere ampleness. These notions play a prominent role for example in the theory of moduli of higher-dimensional varieties, which is an active area of research with very significant recent progress due to Alexeev, Kollár, Kovács, and others.

It has recently come to light in the thesis of Kelly Jabbusch [2] that the two definitions of a big vector bundle put forward by Lazarsfeld and Viehweg, respectively, do not agree. This surprising but simple observation has opened the door to questions regarding the relationship between the various positivity concepts for vector bundles and their geometric consequences. The exploration of how the behaviour of positivity for line bundles extends or branches when considering higher-rank bundles was at the heart of the workshop activities. We explain them in more detail in the next section.

4.2 Various concepts of positivity for vector bundles

Let X be a projective variety and E a vector bundle on X. Let $\pi : \mathbb{P}(E) \to X$ be the projective bundle of one-dimensional quotients of E. Finally, let $\mathcal{O}_{\mathbb{P}(E)}(1)$ be the tautological quotient of $\pi^* E$. The following two notions are well established.

Definition 4.2.1 *A vector bundle E is ample if $\mathcal{O}_{\mathbb{P}(E)}(1)$ is ample.*
Similarly, we say that E is nef, if $\mathcal{O}_{\mathbb{P}(E)}(1)$ is so.

The next positivity notion for line bundles, the bigness does not generalize that easily. Finding the "correct" generalization for vector bundles is one of intriguing problems in this area. We recall several attempts, starting with the most obvious one.

Definition 4.2.2 (L-big, Lazarsfeld weakly big) *A vector bundle E is L-big if $\mathcal{O}_{\mathbb{P}(E)}(1)$ is big. In other words the function*

$$m \to h^0(X, \operatorname{Sym}^m E)$$

has the maximal possible rate of growth.

A stronger property is the following.

Definition 4.2.3 (strongly big) *A vector bundle E is strongly big if it is L-big and*

$$\pi(\operatorname{Bs}(\mathcal{O}_{\mathbb{P}(E)}(1))) \quad \text{is a proper subset of} \quad X,$$

where $\operatorname{Bs}(M)$ denotes the base locus of a line bundle M.

By definition strongly big implies L-big, but the converse implication is false in general.

Studying properties of cotangent bundles Miyaoka [6] introduced in passing the following notion.

Definition 4.2.4 (AEA, almost everywhere ample) *A vector bundle E is almost everywhere ample (AEA, for short), if there exists an ample line bundle A on X, a Zariski closed subset $T \subset \mathbb{P}(E)$, whose projection $\pi(T)$ is a proper subset of X, and a positive number $\varepsilon > 0$ such that*

$$\mathcal{O}_{\mathbb{P}(E)}(1) \cdot C \geq \varepsilon \cdot \pi^*(A) \cdot C$$

for all curves $C \subset \mathbb{P}(E)$ that are not contained in T.

The next notion is due to Viehweg [8].

Definition 4.2.5 (V-big, Viehweg weakly positive) *A vector bundle E is V-big if for all ample line bundles A on X and all positive integers m the bundle*

$$\operatorname{Sym}^{mk} E \otimes A^k$$

is generically spanned for $k \gg 0$.

One can characterize V-bigness by means of asymptotic base loci. We recall first the following basic notion.

Definition 4.2.6 *The base locus of a vector bundle E over X is the set*

$$\operatorname{Bs}(E) := \left\{ x \in X \mid H^0(X, E) \to E(x) \ \text{ is not surjective} \right\}.$$

There are the following two related notions.

Definition 4.2.7 *Let A be an ample line bundle on X and let $A^\vee$ denote its dual. The set*

$$\mathbb{B}_+(E) := \bigcap_{m \geq 1} \operatorname{Bs}(\operatorname{Sym}^m E \otimes A^\vee)$$

is the augmented base locus of E.

The set

$$\mathbb{B}_-(E) := \bigcap_{m \geq 1} \operatorname{Bs}(\operatorname{Sym}^m E \otimes A)$$

is the diminished base locus of E.

Then we have the following result.

Proposition 4.2.8 *A vector bundle E is V-big if and only if $\mathbb{B}_-(E)$ is contained in a proper closed subset $Y \subset X$.*

We conclude this section with another definition which in fact motivated the introduction of augmented and diminished base loci for line bundles.

Definition 4.2.9 *Let E be a vector bundle on X. The set*

$$\mathbb{B}(E) := \bigcap_{m \geq 1} \mathrm{Bs}(\mathrm{Sym}^m E)$$

is the stable base locus of E.

4.3 Relations between positivity concepts for vector bundles

It is clear that one is interested in relations between various notions introduced in the previous section. We point out a couple below.

Problem 4.3.1 *Is AEA vector bundle strongly big and vice versa?*

At present we don't know the answer in general. A series of examined examples suggests that the answer in Problem 4.3.1 might be positive. Discussions during the workshop led to verifying this claim under additional assumption E being nef.

Proposition 4.3.2 *Let E be a nef vector bundle. Then the following conditions are equivalent:*

i) E is AEA;

ii) E is strongly big.

Moreover the strong bigness can be in general characterized by the means of the augmented base locus.

Proposition 4.3.3 *For a vector bundle E the following conditions are equivalent:*

i) E is strongly big;

ii) $\mathbb{B}_+(E) \neq X$.

In the view of this characterization and more generally in order to understand relations between the positivity of a vector bundle E and of a line bundle $\mathcal{O}_{\mathbb{P}(E)}(1)$, it is of interest to study relations between their base loci. We have established the following.

Proposition 4.3.4 *Let E be a vector bundle. Then the stable base loci of E agrees with the projection of the stable base locus of $\mathcal{O}_{\mathbb{P}(E)}(1)$, i.e. there is the equality*

$$\mathbb{B}(E) = \pi(\mathbb{B}(\mathcal{O}_{\mathbb{P}(E)}(1))).$$

It is natural to ask further

Problem 4.3.5 *Is there also the equality*

$$\mathbb{B}_+(E) = \pi(\mathbb{B}_+(\mathcal{O}_{\mathbb{P}(E)}(1))).$$

for augmented base loci?

It is important to know the answer to that problem, in particular since Vojta's preprint [9] defines the augmented base locus of E as the image of the augmented base locus of $\mathcal{O}_{\mathbb{P}(E)}(1)$. However Vojta works under the assumption E being semistable, so his results should be taken with caution in the general framework.

We were able to establish only a weaker but related fact.

Proposition 4.3.6

$$\mathbb{B}_+(E) \supset \mathbb{B}_+(\det(E)).$$

Turning to the diminished base locus, we were able to establish the following property paralleling the well known result for line bundles.

Proposition 4.3.7 *Let E be a vector bundle. The following conditions are equivalent:*

i) E is nef;

ii) $\mathbb{B}_-(E) = \emptyset$.

This implies of course that $\mathbb{B}_-(E)$ and $\mathbb{B}_-(\mathcal{O}_{\mathbb{P}(E)}(1))$ are simultaneously empty or non-empty. However, an analogue of Problem 4.3.5 for diminished base loci remains open.

Problem 4.3.8 *Is there the equality*

$$\mathbb{B}_-(E) = \pi(\mathbb{B}_-(\mathcal{O}_{\mathbb{P}(E)}(1))).$$

for diminished base loci?

Another problem which attracted our attention is to decide whether allowing $\varepsilon = 0$ in Definition 4.2.4 is equivalent to V-bigness.

Problem 4.3.9 *Let E be a vector bundle on X. Let $T \subset \mathbb{P}(E)$ be a proper closed subset, whose projection $\pi(T)$ is a proper subset of X, and such that*

$$\mathcal{O}_{\mathbb{P}(E)}(1) \cdot C \geq 0$$

for all curves $C \subset \mathbb{P}(E)$ that are not contained in T. Does this imply that E is a V-big vector bundle?

It is clear from the discussion above that there are so far more questions than answers and that the positivity of vector bundles will be an area of active research activities in the next future. It is also natural under these circumstances to study the above listed properties on specific families of varieties. Particular attention was devoted to toric vector bundles.

4.4 Toric vector bundles

Let X be a smooth complete toric variety. A toric vector bundle is a locally free $\mathcal{O}_X$-module E of finite rank equipped with a torus action that is compatible with the torus action on X. In other words there exists a torus action on the corresponding geometric vector bundle $V(E) := \mathrm{Spec}(\mathrm{Sym}\, E)$ such that the projection $\pi : V(E) \to X$ is torus equivariant and the torus acts linearly on the fibers of π.

If L is a line bundle on a toric variety, then various positivity properties of L can be read off directly from the convex geometry object, the rational polyhedron P_L associated to L.

In the case of a toric vector bundle E, there is naturally associated set of rational convex polytopes, called the parliament of polytopes for E. This is defined as follows. Let M denote the character lattice of the torus in X and Σ be the fan determining X. There is a finite set $\{v_i\}$ of uniquely determined minimal generators of the rays in Σ. We can view this set as the subset of $\mathrm{Hom}(M, \mathcal{Z})$. By Klyachko's Classification Theorem [3] there is a finite dimensional vector space E_0 associated to E equipped with decreasing filtrations

$$\ldots \supset E_0^{v_i}(j) \supset E_0^{v_i}(j+1) \supset \ldots$$

with $1 \leq i \leq n$ and $j \in \mathcal{Z}$. Then the polytopes P_e in the parliament are defined as

$$P_e := \{u \in M \otimes_{\mathcal{Z}} \mathbb{R} : \ \langle u, v_i \rangle \leq \max(j \in \mathcal{Z} : e \in E_0^{v_i}(j)) \text{ for all } 1 \leq i \leq n\}.$$

The role played by these polytopes in the study of positivity properties of a toric vector bundle E is expressed in the following result.

Proposition 4.4.1 *The lattice points in the parliament of polytopes for E correspond to a torus equivariant generating set of $H^0(X, E)$.*

Of course for a toric line bundle L everything reduces to the aforementioned polytope P_L.

Proposition 4.4.1 implies that base loci of toric vector bundles are torus invariant, which is very convenient for their study. As a sampling result relying on that (expected) observation we have the following.

Theorem 4.4.2 *A toric vector bundle is globally generated if and only if the associated characters correspond to lattice points in the parliament of polytopes and the vectors indexing these polytopes span E_0.*

A natural challenge coming out of the discussions preceding this section is the following.

Problem 4.4.3 *Characterize on toric varieties various notions of positivity for vector bundles introduced in section 4.2 in terms of the parliaments of polytopes.*

It is also interesting to compare positivity properties of line bundles and toric vector bundles. For example, contrary to the rank 1 case, there exist vector bundles which are ample but not globally generated or having an empty base locus (as defined in 4.2.6) and failing to be globally generated. There is a number of other properties which require more detailed study. In particular, the following problem, seems to us quite appealing.

Problem 4.4.4 *Let E be a toric vector bundle on a smooth complete toric variety. Is then the section algebra*

$$\bigoplus_{m \geq 0} H^0(X, \mathrm{Sym}^m(E))$$

finitely generated?

4.5 Newton-Okounkov bodies

Since the pioneering works of Lazarsfeld and Mustaţă on one hand and Kaveh and Khovanskii on the other, there are convex bodies $\Delta(D)$, the Newton-Okounkov bodies, associated to big linear series D on arbitrary normal projective varieties. These bodies are an interesting subject of study quite in their own right. There was a parallel workshop "Convex bodies and representation theory" held at BIRS at the same time. This circumstance has lead to interesting interchanges between both research groups. We shared a couple of lectured. Since the report from the other workshop will surely emphasize on the Newton-Okounkov bodies, we mention here just one path of thoughts particularly interesting from the positivity point of view.

Definition 4.5.1 *A finite collection $\{D_1, \ldots, D_r\}$ of pseudo-effective divisors on a smooth variety X is a Minkowski basis if*

- *For any pseudo-effective divisor D on X there exist non-negative numbers $a_1, \ldots, a_r$ such that*

$$D = \sum a_i D_i \quad \textit{and} \quad \Delta(D) = \sum a_i \Delta(D_i);$$

- *the Newton-Okounkov bodies $\Delta(D_i)$ are indecomposable in the sense of Minkowski sums.*

Minkowski bases were first introduced by Łuszcz-Świdecka in [4] for del Pezzo surfaces. Shortly after Łuszcz-Świdecka and Schmitz [5] realized that using Zariski decompositions the construction carries over to arbitrary surfaces. The key point in this area is the question if Minkowski bases exist on a given variety and if they exist, if there is an explicit way to construct them. An effective algorithm for del Pezzo surfaces was described in [4]. It has been modified and successfully expanded to the case of toric varieties by Pokora, Schmitz and Urbinati [7].

During the workshop two new approaches were discussed. The first one concerns a decomposition of the pseudo-effective cone into Minkowski chambers. This decomposition is obtained as follows. If there is a Minkowski basis element D_i not contained in one of the rays spanning $\overline{\mathrm{Eff}}(X)$ then decompose $\overline{\mathrm{Eff}}(X)$ into subcones spanned by the sides of $\overline{\mathrm{Eff}}(X)$ and the ray spanned by D_i. Repeating this construction one arrives to the point where no

Minkowski basis element lies in the interior of resulting subcones. Then, one can pass to a triangulation of each subcone into simplicial cones without having to add any new rays. The resulting subcones are Minkowski chambers of $\overline{\mathrm{Eff}}(X)$. It is natural to wonder how the decomposition into Minkowski chambers is related to the decomposition into Zariski chambers introduced in [1].

The second problem concerns the global Okounkov body. These objects are far more mysterious than the bodies associated to a single divisor. A general statement obtained in this direction is the following.

Theorem 4.5.2 *Let X be a smooth projective variety such that X admits a Minkowski basis $D_1, \ldots, D_r$ whose corresponding Okounkov bodies, with respect to some fixed admissible flag $Y_\bullet$ are rational polyhedral. Then the global Okounkov body $\Delta(X)$ is rational polyhedral and it is spanned by the following set of vectors*

$$\bigcup \{(x, [D_i]) | x \text{ is a vertex of } \Delta(D_i)\} .$$

This result has a couple of nice consequences. For example

Corollary 4.5.3 *Let X be a toric variety. Then the global Okounkov body $\Delta(X)$ computed with respect to a torus invariant flag is rational polyhedral.*

It is worth to mention that all results listed above have been included in works which originated form the discussions during the workshop or at least were influenced by the workshop. The list of such papers is attached at the end of this report.

Bibliography

[1] Bauer, Th., Küronya, A., Szemberg, T.: Zariski chambers, volumes, and stable base loci, J. Reine Angew. Math. 576 (2004) 209-233

[2] Jabbusch, K.: Notions of positivity for vector bundles. Ph. D. thesis.

[3] Klyachko, A. A.: Equivariant bundles over toric varieties, Izv. Akad. Nauk SSSR Ser. Mat. 53 (1989), no. 5, 1001–1039, 1135 (Russian); English transl., Math. USSR-Izv. 35 (1990), no. 2, 337–375.

[4] Łuszcz - Świdecka, P.: On Minkowski decomposition of Okounkov bodies on a Del Pezzo surface, Annales Universitatis Paedagogicae Cracoviensis, Studia Mathematica 10 (2011), 105–115

[5] Łuszcz - Świdecka, P., Schmitz, D.: Minkowski decomposition of Okounkov bodies on surfaces, Journal of Algebra 414 (2014), 159–174

[6] Miyaoka, Y.: Algebraic surfaces with positive indices. Proc. Symp. Katata/Jap. 1982, Prog. Math. **39** (1983), 281–301.

[7] Pokora, P., Schmitz, D., Urbinati, S.: Minkowski decomposition and generators of the moving cone for toric varieties, preprint arXiv:1310.8505

[8] Viehweg, E.: Quasi-projective moduli for polarized manifolds, Springer 1995

[9] Vojta, P.: Big semistable vector bundles. Preprint, Berkeley 2004

4.6 Presentation Highlights

During the workshop we heard altogether 24 talks. 5 of them were held jointly with the parallel program on ”Convex bodies and representation theory”, partly by the participants from the other workshop.

Some presentations given in the workshop were coupled talks, so that the lectures had the possibility to go into details. This was important for further discussions.

Here we present the list of talks roughly divided in subjects they revolved around. The contest of the talks is described in the preceding sections.

4.6.1 Toric vector bundles.

Sandra Di Rocco, Kelly Jabusch and Greg Smith were speaking on that subject. They went in particular through the construction of parliament of polytopes.

4.6.2 Convex geometric aspects of positivity

There were talks of Klaus Altmann, Alex Küronya, David Schmitz and Tomasz Szemberg devoted to this topic. In particular Minkowski decompositions on surfaces have been discussed in details.

4.6.3 Asymptotic constructions

Ernesto Mistretta, Joaquim Roé and Xin Zhou gave talks related to this subject. In particular various concepts of base loci for vector bundles have been discussed.

4.6.4 Moduli spaces and stability

The talks of Arend Bayer, Aaron Bertram, Daniel Greb and Jack Huizenga were revolving around these concepts. The interest was focused in particular on birational geometry aspects of moduli spaces of higher rank sheaves.

4.6.5 Singularities

They played prominent role in talks of Alberto Chieccio, Sándor Kovács, Karol Palka, Mihnea Popa, Stefano Urbinati. In particular there were many different notions of positivity for Weil divisors discussed in detail.

4.6.6 Revision of established techniques and specific examples

These have motivated talks by Michael Brion, Brian Harbourne, Yusuf Mustopa and Giuseppe Pareschi. In particular there was focus on Ulrich sheaves and splitting of the cotangent bundle on certain types of varieties.

4.7 Outcome of the Meeting

The discussions initialized during the workshop have already lead to a number of interesting preprints. Some ideas are waiting for further investigations. Here is the list of recent preprints which resulted more or less directly from the workshop.

1. Sandra Di Rocco, Kelly Jabbusch, Gregory G. Smith: Toric vector bundles and parliaments of polytope, arXiv:1409.3109

2. Mihnea Popa, Christian Schnell: On direct images of pluricanonical bundles, arXiv:1405.6125

3. Izzet Coskun, Jack Huizenga: The ample cone of moduli spaces of sheaves on the plane, arXiv:1409.5478

4. Thomas Bauer, Sándor J. Kovács, Alex Küronya, Ernesto Carlo Mistretta, Tomasz Szemberg, Stefano Urbinati: On positivity and base loci of vector bundles, arXiv:1406:5941

5. Karol Palka: Cuspidal curves, minimal models and Zaidenberg's finiteness conjecture, arXiv:1405.5346

6. Karol Palka: The Coolidge-Nagata conjecture, part I, arXiv:1405.5917

7. David Schmitz, Henrik Seppänen: On the polyhedrality of global Okounkov bodies, arXiv:1403.4517

8. David Schmitz, Henrik Seppänen: Global Okounkov bodies for Bott-Samelson varieties, arXiv:1409.1857

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Chapter 5

Convex bodies and representation theory (14w5013)

February 2 - 7, 2014

Organizer(s): Megumi Harada (McMaster), Kiumars Kaveh (U Pittsburgh), Askold Khovanskii (U Toronto)

5.1 Introduction and Objectives of the workshop

The theory of toric varieties connects the combinatorics of convex integral polytopes with the geometry of toric varieties. In the case of a toric variety X, its associated polytope Δ coincides with its moment polytope (in the sense of symplectic geometry) and fully encodes the geometry of X, but this is not true in the general case. In ground-breaking work which was originated by Okounkov [17, 18] Kaveh-Khovanskii [8] and Lazarsfeld-Mustata [14] construct polytopes $\Delta(X, \nu)$ (called Newton-Okounkov bodies or Okounkov bodies) with $\dim_{\mathbb{R}} \Delta(X, \nu) = \dim_{\mathbb{C}} X$ associated to a projective variety $X \subseteq \mathbb{P}(V)$ and a valuation ν on its homogeneous coordinate ring, even without the presence of any group action. In fact, this construction in fact works in an even more general setting, associating convex bodies to linear systems on a projective variety. These Okounkov bodies carry interesting geometric information about X: for instance, one can prove a generalization of the Bernstein-Kushnirenko theorem to arbitrary varieties which relates intersection numbers of divisors with the volumes of the corresponding Okounkov bodies. This theory is still quite new (the foundational papers [14] and [8] are from 2008-2009) and the subject is both promising and still wide open. The fundamental question is: What geometric data of X do the combinatorics of these Okounkov bodies encode, and how?

There has been a burst of research activity surrounding Okounkov bodies since their introduction. It is already clear that these convex bodies are related to a wide range of research areas: for instance, Kaveh shows [7] that the *Littelmann-Berenstein-Zelevinsky string polytopes* from representation theory, which generalize the well-known *Gel'fand-Cetlin polytopes*, are examples of $\Delta(X, \nu)$. Also, recent work of Anderson [1] and Kiritchenko-Smirnov-Timorin [12] suggest many connections and possible applications to Schubert calculus. Furthermore, Harada and Kaveh [5] use a toric degeneration associated to $\Delta(X, \nu)$ to construct, in a very general situation, an integrable system on a projective variety; this opens the door to many applications in e.g. symplectic topology. We also mention that, at an MFO Mini-workshop on Okounkov bodies in August 2011, Victor Batyrev suggested that toric degenerations associated to Okounkov bodies may provide new methods for constructing mirror pairs, thus connecting this area also to mirror symmetry.

The main goal of this half-workshop was to bring together (1) researchers active in the area of Newton-Okounkov bodies and (2) mathematicians working in the closely related area of representation theory, particularly with a focus on combinatorial and convex-geometric techniques. By doing so, we were able to foster an active conversation in both directions; people working on Newton-Okounkov bodies gained new perspectives and ideas for future applications, and the researchers working in representation theory were introduced to the relatively new theory of Newton-Okounkov bodies.

As an additional bonus, we had an exciting synergy between our half-workshop and the concurrent half-workshop on “Positivity and linear series”. We held a joint session with them on the Wedsnesday morning of our week-long workshop.

5.2 Schedule of the talks

We had the following schedule of talks.

Monday

9:00-10:00	Askold Khovanskii, Convex bodies and representation theory, Part 1
10:00-10:30	Coffee Break
10:30-11:30	Kiumars Kaveh, Convex bodies and representation theory, Part 2
11:30–13:00	Lunch
14:00-15:00	Susan Tolman, Cohomology of quotients of Hamiltonian loop group actions
15:00-15:30	Coffee Break
15:30-16:30	Nicholas Perrin, Quantum K-theory of homogeneous spaces

Tuesday

7:00–9:00	Breakfast
9:00-10:00	Valentina Kiritchenko, Okounkov polytopes of Bott-Samelson varieties
10:00-10:30	Coffee Break
10:30-11:30	Vladlen Timorin, On the theory of coconvex bodies
11:30–13:30	Lunch
13:30-14:30	Klaus Altmann, Okounkov bodies and versal deformations of toric singularities
14:30-15:00	Coffee Break
15:00-16:00	Boris Kazarnovskii, Exponential sums: Kusnirenko–Bernstein theorem and convex polyhedra in complex space (old and recent results)

Wednesday

Joint session:	(with the parallel half-workshop “Positivity of linear series and vector bundles”)
9:00-9:30	Alex Kuronya, Local positivity in convex geometric terms
9:30-9:45	Break
9:45-10:15	Xin Zhou, Asymptotic Schur decomposition of Veronese syzygy functors
10:15-10:45	Coffee Break
10:45-11:15	Tomek Szemberg, Minkowski decomposition of Okounkov bodies on surfaces

Thursday

9:00-10:00	Jonathan Weitsman, Integrable systems and Berenstein-Zelevinsky polytopes
10:00-10:30	Coffee Break
10:30-11:30	Michel Brion, On linearization of line bundles
11:30–13:30	Lunch
13:30-14:30	Chris Manon, Okounkov bodies and Kaveh-Harada construction for character varieties
14:30-15:00	Coffee Break
15:00-16:00	Jaehyouk Lee, Gosset polytopes and Del Pezzo surfaces

Friday

9:00-10:00	Evgeny Smirnov, Schubert calculus and Gelfand-Zetlin polytopes
10:00-10:30	Coffee Break
10:30-11:30	Informal discussions

5.3 Presentation Highlights

The following are concise synopses of lectures given during the workshop.

Askold Khovanskii: *Convex bodies and representation theory, Part 1*

Khovanskii's was the first lecture of the workshop and served as Part 1 of an introductory series of 2 lectures on the background and context of the main themes of the workshop. In particular, Khovanskii focussed on Newton polyhedra theory. As a motivating question he presented the following. Suppose given a Laurent polynomial $p = \sum_m c_m x^m$ where $m = (m_1, \ldots, m_n)$ is an integer exponent vector, $x = (x_1, \ldots, x_n)$ are the variables, and the coefficients c_m are complex numbers. Let $\Delta(p)$ be the convex hull of $\{m : c_m \neq 0\}$; this is the so-called Newton polytope of p. Given a collection $\Delta(p_1), \ldots, \Delta(p_k)$ of such Newton polyhedra, consider the set of common solutions $X = \{p_1 = \cdots = p_k = 0\}$ in $(\mathbb{C}^*)^k$. The motivating question is: assuming the p_i are sufficiently generic, what invariants of X do the $\Delta(p_i)$ encode? Starting with this question and the 'first' answer along these lines (the Kushnirenko theorem, which deals with the case where all the Newton polytopes are equal, $\Delta(p_i) = \Delta \forall i$ and gives an answer in terms of the Euclidean volume of Δ, Khovanskii gave a broad historical overview of this subject. Topics touched upon included toric varieties, geometric genus, mixed Hodge numbers, f-vectors of simple polytopes, volume polynomials of polytopes, and Hilbert's 16th problem. At the end of the talk, Khovanskii motivated Part 2 of this series of introductory lectures by formulating the non-abelian analogue of the Kushrinenko theorem (i.e. replacing the abelian group $(\mathbb{C}^*)^n$ by a general reductive algebraic group G).

Kiumars Kaveh: *Convex bodies and representation theory, Part 2*

Building on the previous lecture ("Part 1"), Kaveh discussed the generalization to non-abelian groups of many of the themes discussed by Khovanskii. He chose as his starting point a result of Kazarnovskii, which can be interpreted as the non-abelian version of the Kushnirenko theorem. Let G be a reductive algebraic group. Let $\pi : G \to GL(N)$ be a representation and $f_1, \ldots, f_k$ sufficiently generic linear combinations of the matrix entries of π. The Brion-Kazarnovskii theorem then gives a formula for the cardinality of the set of common zeros $\{f_1 = \cdots = f_k = 0\} \subset G$ in terms of an integral over the so-called weight polytope Δ_{wt} of π, which is computed in terms of the set of irreducible representations V_λ appearing in the representation π. The main motivating question for Kaveh's talk was: Can we build a convex polytope $\tilde{\Delta}$ such that the integral over the weight polytope Δ_{wt} can be interpreted (more simply) as the Euclidean volume of $\tilde{\Delta}$? Can we also account for the multiplicities of the representations which occur in π? For some special cases, a clever answer was given by Okounkov in the 1990s. Motivated by Okounkov's results, Kaveh and Khovanskii recently gave a general construction of Newton-Okounkov bodies, which in this context are maximal-dimensional polytopes which account (asympotically) for not only the weights of the representation but also the multiplicities, and a basis for each irreducible representation. Kaveh gave a broad overview of these and related results.

Susan Tolman: *Cohomology of quotients of Hamiltonian loop group actions*

Tolman reported on her joint work with Raoul Bott and Jonathan Weitsman on the computation of the cohomology of quotients of Hamiltonian loop group actions. It is well-known that the theory of Hamiltonian group actions and symplectic quotients is intimately linked with representation theory through Borel-Weil theory and the "quantization commutes with reduction" theorem. One powerful technique in equivariant symplectic geometry is the Kirwan surjectivity theorem, which roughly states that given a Hamiltonian G-space (for G a compact Lie group) (M, ω), there is a natural surjection of cohomology rings $H^*(M) \to H^*(M//G)$ where $M//G$ denotes the symplectic quotient of M by the G-action. This theorem allows one to compute explicitly the cohomology rings of symplectic quotients. Tolman explained her joint work with Bott and Weitsman, which generalizes this Kirwan surjectivity to the case of Hamiltonian loop group quotients, i.e. to the situation when the (infinite-dimensional) loop group LG acts on a symplectic Banach manifold $(\mathcal{M}, \omega)$, under some mild technical conditions. This is also related to the computation of the cohomology of quotients of quasi-Hamiltonian G-spaces.

Nicholas Perrin: *Quantum K-theory of homogeneous spaces*

Nicolas Perrin talked about his joint work with A. Buch, P.-E. Chaput and L. Mihalcea. Let X be a generalized flag variety with Picard groups of rank one. Given a degree d, they consider the Gromov-Witten variety of rational curves of degree d in X that meet three general points. In their joint work, they prove that the product in the small quantum K-theory ring of X is finite and has some positivity properties. One of the main issues is to prove rational connectedness of of the Gromov-Witten variety for all large degreed d.

Valentina Kiritchenko: *Okounkov polytopes and Bott-Samelson varieties*

Kiritchenko reported on her recent work which defines an elementary convex-geometric operation on polytopes which mimics the famous Demazure operators in representation theory and Schubert calculus. These operators are used to construct inductively polytopes that capture Demazure characters of representations of reductive groups. In particular, Gelfand-Zetlin polytopes and twisted cubes of Grossberg-Karshon are obtained in a uniform way. Kiritchenko gave an introduction to her operators, with many examples; in particular, she explained how her operators may be applied to a study of the Okounkov bodies of Bott-Samelson varieties.

Vladlen Timorin: *On the theory of coconvex bodies*

Timorin reported on recent joint work with Askold Khovanskii on the theory of coconvex bodies. If the complement of a closed convex set in a closed convex cone is bounded, then this complement minus the apex of the cone is called a coconvex set. Coconvex sets appear in singularity theory (they are closely related to Newton diagrams) and in commutative algebra. Such invariants of coconvex sets as volumes, mixed volumes, number of integer points, etc., play an important role. Timorin and Khovanskii's joint work aims at extending various results from the theory of convex bodies to the coconvex setting. These include the Aleksandrov-Fenchel inequality and the Ehrhart duality. Timorin gave a well-presented lecture introducing the subject and explaining the basic philosophy behind the theory, as well as the "main theorem" which shows how to prove theorems in co-convex geometry by interpreting co-convex bodies as virtual convex polytopes in the sense of Pukhlikov and Khovanskii.

Klaus Altmann: *Okounkov bodies and versal deformations of toric singularities*

Klaus Altman talked about his old and new works about the notion of versal deformation of toric singularities (i.e. those singularities occurring in toric varieties). The theory of toric varieties assigns to combinatorial objects (such as cones, fans or lattice polytopes) algebraic varieties. Using this construction, cones supported by lattice polytopes correspond to the germs of toric Gorenstein singularities. In a nice earlier paper, Altmann discusses their deformations and in the case in which the singularities are isolated, he gives a complete description of the versal deformation. The basic approach to understanding deformations of toric varieties is to split certain cross cuts of the defining cone into a Minkowski sum of specific polyhedra. In the case of toric Gorenstein varieties, one has to deal with the distinguished cross cut provided by the defining polytope. Its Minkowski summands are parametrized by a convex cone C which determines an affine toric variety itself. The pair consisting of C and the "universal" Minkowski summand C constitutes the material from which the versal deformation is finally built. Altman discussed ideas about possible extensions to a more general setup involving Newton-Okounkov bodies.

Boris Kazarnovskii: *Exponential sums: Kusnirenko–Bernstein theorem and convex polyhedra in complex space (old and recent results)*

Boris Kazarnovskii talked about his older work and some new results on extending the celebrated Bernstein-Kushnirenko theorem to certain classes of analytic functions such as sums of exponential functions (instead of polynomials which are sums of monomials). The Bernstein-Kushnirenko theorem was one of the main motivating results in toric geometry behind the development of the theory of Newton-Okounkov bodies. More specifically, in his talk Kazarnovskii considered the common zero set of n exponential sums in C^n. Because systems of equations he deals with are not algebraic, the number of their solutions can be infinite. Kazarnoskii explained how he studies the asymptotics of the number of solutions within a ball, whose radius he then allows to go to infinity. It turns out that the Newton polyhedra of such exponential sums are responsible for these asymptotics. Much more surprisingly, Kazarnoskii is able to apply methods of modern Algebraic Geometry in the study of this purely transcendental problem.

Alex Kuronya: *Local positivity in convex geometric terms*

Kuronya's talk was both an introduction to the use of theory of Newton-Okounkov bodies in the context of the study of linear systems, and a report on Kuronya's recent joint work with Victor Lozovanu. Kuronya first gave a quick overview of the definition of the (Newton-)Okounkov body $\Delta_{Y.}(D)$ associated to a smooth projective variety X over $\mathbb{C}$, a Cartier divisor D on X, and an admissible flag $Y.$ of subvarieties in X. He reviewed what is known about explicit computations of the Okounkov body $\Delta_{Y.}(D)$ in simple cases, e.g. when X has (complex) dimension 1 and 2, and when X is a toric variety and D and $Y.$ are T-invariant. He explained the main philosophy behind Okounkov-body theory within the context of the study of linear systems, namely, that Okounkov bodies provide a universal family of numerical invariants for D: if D and D' are such that for any admissible flag $Y.$ of subvarieties, $\Delta_{Y.}(D) = \Delta_{Y.}(D')$, then D and D' are numerically equivalent. So roughly speaking, the slogan is that Okounkov bodies encode the numerical invariants of D. As an instance of this philosophy, his recent joint work with Lozovanu shows that D is nef if and only if for all $x \in X$, there exists an admissible flag $Y.$ centered at x such that the origin is contained in $\Delta_{Y.}(D)$. In his talk Kuronya explained this result and gave a sketch of the proof.

Xin Zhou: *Asymptotic Schur decomposition of Veronese syzygy functors*

Xin Zhou discussed his recent results and on-going work join with Mihai Fulger. The syzygies of the d-th Veronese embedding of $\mathbb{P}(V)$ are functors of the complex vector space V. Xin Zhou obtains results about the asymptotic behavior of the Schur functor decomposition of these as d grows. Their result shows that, from a certain perspective, this decomposition is very rich whenever they are not zero. This is deduced from an asymptotic study of related plethysms.

Tomek Szemberg: *Minkowski decomposition of Okounkov bodies on surfaces*

Tomek Szemberg reported on decomposing Okounkov bodies on surfaces with rational polyhedral effective cone into Minkowski sums of some elementary "building bricks". This builds upon recent work of Patrycja Luszcz-Swidecka and David Schmitz (arXiv:1304.4246), where they prove that the Okounkov body of a big divisor with respect to a general flag on a smooth projective surface whose pseudo-effective cone is rational polyhedral decomposes as the Minkowski sum of finitely many simplices and line segments arising as Okounkov bodies of nef divisors.

Jonathan Weitsman: *Integrable systems and Berenstein-Zelevinsky polytopes*

In their influential work, Berenstein-Zelevinsky introduced polytopes whose number of integral points computes the tensor product multiplicities. In his talk, Jonathan Weitsman discussed his work in progress with Lisa Jeffrey and Paul Selick (also with his student Gouri Seal) on constructing integrable systems whose moment map images are the Berenstein-Zelevinsky polytopes. While it is expected that such integrable systems exist (e.g. form the work of Harada-Kaveh) he emphasized that even in the smallest examples such as $SU(3)$ it is not easy to explicitly construct one.

Michel Brion: *On linearization of line bundles*

Michel Brion talked about his recent work on the linearization of line bundles and the local structure of algebraic group actions in the setting of seminormal varieties equipped with an action of a connected linear algebraic group G. He shows that several classical results about normal G-varieties extend to that setting, if the Zariski topology is replaced with the étale topology.

Chris Manon: *Okounkov bodies and Kaveh-Harada construction for character varieties*

Chris Manon talked about constructing families of Newton-Okounkov bodies for the free group character varieties and configuration spaces of any connected reductive group G. The character variety $X(\pi, G)$ associated to a finitely generated group π and a connected reductive group G is defined to be the moduli space of representations of π in G up to inner automorphisms. When π is taken to be the fundamental group of a smooth manifold M , $X(\pi, G)$ is the moduli space of flat, topological principal G bundles on M. His work is related to constructing toric degenerations and integrable systems for character varieties and is an important example of the general approach of Harada-Kaveh for constructing integrable systems on a large class of projective varieties (via toric degenerations).

Jaehyouk Lee: *Gosset polytopes and Del Pezzo surfaces*

Jaehyouk Lee from Ewha Women's University in Korea talked about his past work on the correspondences between the geometry of del Pezzo surfaces and the geometry of corresponding Gosset polytopes. In his talk he introduced main concepts involved such as the definition of a Gosset polytopes. He explained different results on how to read off information about the surface in particular divisor classes in the Picard group from the Gosset polytope. The corresponding leads, for example, to an understanding of Gieser transformations and Bertini transformations on the del Pezzo surface in terms of the symmetry of the Gosset polytope.

Evgeny Smirnov: *Schubert calculus and Gelfand-Zetlin polytopes*

Smirnov reported on joint work with Valentina Kiritchenko and Vladlen Timorin which proposes a new approach to the Schubert calculus on complete flag varieties using the volume polynomial associated with Gelfand-Zetlin polytopes. This approach allows us to compute the intersection products of Schubert cycles by intersecting faces of a polytope. One of their main tools is a construction of Pukhlikov and Khovanskii, which associates to a convex polytope P a graded commutative ring R_P (called the polytope ring). In the case of a smooth toric variety X and its associated polytope P, it is known that the polytope ring R_P is isomorphic to the cohomology ring $H^*(X, \mathcal{Z})$ of the toric variety, and that the product structure in $H^*(X, \mathcal{Z})$ is encoded by the intersections of faces of P. It was observed by Kaveh that the polytope ring of the Gel'fand-Zetlin polytope P_{GZ} is isomorphic to the cohomology ring of the flag variety $GL(n, \mathbb{C})/B)$, which is additively generated by Schubert classes $[X_w]$. Motivated by this, Smirnov, Kiritchenko, and Timorin ask: is there an assignment to each $[X_w]$ a (linear combination of) faces $\mathcal{F}_w$ of P_{GZ} in such a way that multiplication of two such classes $[X_w] \cdot [X_v]$ in the cohomology ring corresponds to taking intersections $\mathcal{F}_w \cap \mathcal{F}_v$? The answer is yes, and involves so-called "reduced Kogan faces" of the Gel'fand-Zetlin polytope. In his talk, Smirnov carefully explained how this works, with many pictures, in the case of $n = 3$.

All lectures were well presented and invited further discussion and collaboration among the workshop participants. Some of this happened already at the workshop itself and we trust that the discussion will continue well after the workshop.

5.4 Developments and scientific progress

During the workshop, there were many promising informal discussions between the participants. We identify some of them here.

- Jonathan Weitsman and Chris Manon realized they are working on very similar problems/ideas regarding constructing integrable systems on varieties appearing in representation theory. In particular, Chris Manon mentioned to Jonathan the connection between their research and the recent results of Harada and Kaveh and they have begun ongoing discussions on this topic.

- Kiumars Kaveh, Chris Manon and Henrik Seppanen started a collaboration on geometric invariant theory and Newton-Okounkov bodies. Seppanen has already posted two preprints on the ArXiv related to these ideas.
- Kiumars Kaveh and J. B. Carrell collaborated on a paper in preparation on lifting the Springer action to equivariant cohomology.
- Kevin Purbhoo and Michel Brion had several discussions on topics related to Brion's talk at the workshop.
- Kiumars Kaveh and Askold Khovanskii collaborated on a paper in preparation on mixed multiplicities of ideals (related to local Newton-Okounkov bodies).
- Valentina Kiritchenko and Kiumars Kaveh discussed some future problems e.g. related to a recent result of Igor Makhlin in Moscow about projections of Gelfand-Zetlin polytopes and character formula for reductive groups.

Participants

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Bibliography

[1] D. Anderson. Okounkov bodies and toric degenerations, January 2010, arXiv:1001.4566.

[2] D. Anderson and A. Kuronya and V. Lozovanu. Okounkov bodies of finitely generated divisors. June 2012, arXiv:1206.2499.

[3] S. Boucksom and H. Chen. Okounkov bodies of filtered linear series, arXiv:0911.2923.

[4] A. Della Vedova and R. Paoletti. Moment maps and equivariant volumes. Acta Math. Sin. (Engl. Ser.) 23 (2007), no. 12, 2155-2188.

[5] M. Harada and K. Kaveh. Integrable systems, toric degenerations, and Okounkov bodies. June 2012, arXiv:1205.5249.

[6] A. Ito. Okounkov bodies and Seshadri constants. February 2012, arXiv:1202.6662.

[7] K. Kaveh. Crystals bases and Newton-Okounkov bodies. January 2011, arXiv:1101.1687.

[8] K. Kaveh and A.G. Khovanskii. Newton-Okounkov bodies, semigroups of integral points, graded algebras and intersection theory, April 2009, arXiv:0904.3350. Ann. of Math. 176 (2012), no. 2, 925–978.

[9] K. Kaveh and A. Khovanskii. Convex bodies associated to actions of reductive groups, April 2010, arXiv:1001.4830. Mosc. Math. J. 12 (2012), no. 2, 369–396, 461.

[10] A. Khovanskii. Newton polyhedra, and the genus of complete intersections. (Russian) Funktsional. Anal. i Prilozhen. 12 (1978), no. 1, 51–61.

[11] A. Khovanskii. Geometry of Formulas. In V.I. Arnold , A.N. Varchenko , A.B. Givental and A.G. Khovanskii, "Singularities of functions, wave fronts, caustics and multidimensional integrals", Soviet Scientific Reviews, Math. Phys. Rev. 4 (1984), 67-91.

[12] V. Kiritchenko and E. Smirnov and V. Timorin. Schubert calculus and Gelfand-Zetlin polytopes. January 2011, arXiv:1101.0278.

[13] A. Kuronya, V. Lozovanu, and C. Maclean. Convex bodies appearing as Okounkov bodies of divisors, August 2010, arXiv:1008.4431.

[14] R. Lazarsfeld and M. Mustata. Convex bodies associated to linear series, May 2008, Ann. Sci. Éc. Norm. Supér. (4) 42 (2009), no. 5, 783–835.

[15] C. Manon. Valuations from representation theory and tropical geometry, June 2010, arXiv:1006.0038.

[16] T. Nishinou, Y. Nohara, and K. Ueda. Toric degenerations of Gelfand-Cetlin systems and potential functions, October 2008, arXiv:0810.3470.

[17] A. Okounkov. Brunn-Minkowski inequality for multiplicities. Invent. Math., 125(3):405–411, 1996.

[18] A. Okounkov. Why would multiplicities be log-concave?. The orbit method in geometry and physics (Marseille, 2000), 329–347, Progr. Math., 213, Birkhäuser Boston, Boston, MA, 2003.

[19] R. Paoletti. The asymptotic growth of equivariant sections of positive and big line bundles. Rocky Mountain J. Math. 35 (2005), no. 6, 2089-2105.

[20] S. Payne. Analytification is the limit of all tropicalizations. Math. Res. Lett. 16, (2009) no 3, 543-556.

[21] D. Rees and R. Sharp On a theorem of B. Teissier on multiplicities of ideals in local rings. J. London Math. Soc. (2) 18 (1978), no. 3, 449-463.

[22] J. Ross, D. Witt Nystrom. Analytic test configurations and geodesic rays, January 2011, arXiv:1101.1612.

[23] Y. Rubinstein and S. Zelditch. Bergman approximations of harmonic maps into the space of Kähler metrics on toric varieties, March 2008, arXiv:0803.1249.

[24] B. Teissier. Sur une inegalité pour les multiplicites. (Appendix to a paper by D. Eisenbud and H. Levine). Ann. Math. 106 (1977), 38-44.

[25] X. Yuan. Volumes of arithmetic Okounkov bodies, January 2012, arXiv:1201.2221.

Chapter 6

Statistical and Computational Theory and Methodology for Big Data Analysis (14w5086)

February 9 - 14, 2014

Organizer(s): Ming-Hui Chen (University of Connecticut), Radu Craiu (University of Toronto), Faming Liang (Texas A&M University), Chuanhai Liu (Purdue University)

6.1 Overview of the Field

The integration of computer technology into science and daily life has enabled the collection of massive volumes of data, such as high-throughput biological assay data, climate data, website transaction logs, and credit card records. However, such big data sets cannot be practically analyzed on a single commodity computer because their sizes are too large to fit in memory or it is too time consuming to process when the current statistical methods are used. To circumvent this obstacle, one may have to resort to parallel and distributed architectures, with multicore and cloud computing platforms providing access to hundreds or thousands of processors. While the parallel and distributed architectures present new capabilities for storage and manipulation of data, from an inferential point of view, it is unclear how the current statistical methodology can be transported to the paradigm of big data. Also, with growing size typically comes a growing complexity of data structures, of the patterns in the data, and of the models needed to account for the patterns. Big data has put a great challenge on the current statistical methodology.

6.2 Recent Developments and Open Problems

There are several algorithms that are recently developed and feasible for statistical inference of big data and workable on parallel machines, including the bag of little bootstraps [1], aggregated estimation equation [2, 3], split-and-conquer algorithms [4], and the subsampling-based stochastic approximation algorithm [5]. The bag of little bootstraps algorithm is designed to assess the quality of an estimator, which functions by averaging the results of bootstrapping multiple small subsets of the original data. The small subsets can be processed in parallel, each on an individual or a very small sets of computer nodes. The aggregated estimation equation and split-and-conquer algorithms are based on the same idea of divide-and-conquer, but focus on different types of problems; the former is for parameter estimation and the latter for variable selection of regression models. In [5], a general principle for big data analysis is proposed: i.e., using Monte Carlo averages, that are calculated from subsamples in parallel, to approximate the quantities that originally need to calculate from the full data. Under this principle, a general parameter estimation approach, maximum mean log-likelihood estimation, is developed in [5] for big data models based on the technique of stochastic approximation.

On the other hand, iterative algorithms have been widely used in the current society of scientific computing. Examples of such iterative algorithms include various Markov chain Monte Carlo (MCMC) algorithms [6, 7, 8], and the EM algorithm [9], which typically require a large number of iterations and a complete scan of the full dataset for each iteration. The MCMC algorithms are rooted in the work of physicists such as Metropolis and von Neumann during the period 1945-55 when they employed modern computers for simulations of some probabilistic problems in atomic bomb designs. After six decades of development, it has proven to be very powerful and typically unique computational tools for analyzing data of complex structures. The EM algorithm represents a hallmark achievement in the history of statistics, and has been widely used in scientific computing for parameter estimation in presence of missing data. Given the successes of the iterative algorithms in modern scientific computing, it would be of great interest to develop some innovative iterative algorithms that are feasible for big data.

There have been significant advances made by the statistical community on big data research. One of open problems is how to generalize and scale up such proposed techniques to the true big data settings. One of the key features of big data is that the statistical methods, which work well on small-scale datasets, usually perform poorly in big data settings. Thus, it is not easy to expect the performance of those statistical methods for the big data problems. The field of neuroimaging has also witnessed big progress made in integratively analyzing imaging data of multiple subjects and multiple modalities, together with genomic data. Other open problems include: (i) to have a better understand of big data and associated statistical issues; (ii) to think more carefully about how to solve big data issues; and (iii) to have a more concrete focus on big data problems. The workshop participant, Christophe Andrieu of the University of Bristol, suggested that an open problem is currently to go beyond "linear regression" and logit type strategies. Since it seems that most of the recent work on big data has been confined to this, is this enough? Should one bother with more complicated models? What would be the gains?

6.3 Presentation Highlights

6.3.1 Day 1: February 10, 2014

The workshop kicked off with the American Statistical Association (ASA) video from the Executive Director, Ron Wasserstein. Ron started with a warm greeting to the workshop participants and then presented the recent ASA activities and initiatives on big data. The morning Session II on February 10 featured two presentations delivered by Hongzhe Li of the University of Pennsylvania and Heping Zhang of the Yale University. Hongzhe's presentation was on "Microbiome, Metagenomics and High Dimensional Compositional Data Analysis". Human gut microbiome plays an important role in human health and disease. Next generation sequencing technologies have made it possible to study all microbes in human gut in an unbiased way. Analysis of such large volumes of reads data, usually in 100s of terabytes, raises many challenges in statistical analysis and computation. He presented several methods for analysis of such data, including model-based methods for quantifying the composition of all bacteria and methods for analysis of high dimensional compositional data. These methods have showed close associations between diets and microbiome composition and microbiome and obesity. Heping's presentation was on "Tree-based Rare Variants Analyses". Heping introduced a tree-based method that adopts a non-parametric disease model and is capable of exploring gene-gene interactions. Their method outperforms the sequence kernel association test (SKAT) in most of our simulation scenarios, and by notable margins in some cases. By applying the tree-based method to the Study of Addiction: Genetics and Environment (SAGE) data, they successfully detected gene CTNNA2 and its 44 specific variants that increase the risk of alcoholism in women. This gene has not been detected in the SAGE data. Post hoc literature search also supports the role of CTNNA2 as a likely risk gene for alcohol addiction. This finding suggests that their tree-based method can be effective in dissecting genetic variants for complex diseases using rare variants data.

Marc A. Suchard of the University of California Los Angeles and Minge Xie of Rutgers University were the presenters in the afternoon Session I on February 10. Marc's presentation was on "When Multi-Core Statistical

Computing Fails for Massive Sample Sizes ...". Much of statistical computing is memory-bandwidth limited, not floating-pointing operation throughput limited as commonly assumed. This often restricts the utility of multi-core computing techniques to improve statistical estimation run-time. Marc explored this conundrum in inference tools for a massive Bayesian model of sea-surface temperatures across the global and further described approaches for computing the data likelihood that exploit fine-scale parallelization for potential scalability to real-time satellite surveillance data. These simple algorithmic changes open the door on using advancing computing technology involving many-core architectures. These architectures provide significantly higher memory-bandwidth and inexpensively afford order-of-magnitude run-time speed-ups. Minge presented "A Split-and-Conquer Approach for Analysis of Extraordinarily Large Data" [4]. If there are extraordinarily large data, too large to fit into a single computer or too expensive to perform a computationally intensive data analysis, what should we do? To deal with this problem, Minge discussed a "split-and-conquer" approach and illustrated it using several computationally intensive penalized regression methods, along with a theoretical support. Specifically, consider a regression setting of generalized linear models with n observations and p covariates, in which n is extraordinarily large and p is either bounded or goes to ∞ at a certain rate of n. They proposed to randomly split the data of size n into K subsets of size $O(n/K)$. For each subset of data, they performed a penalized regression analysis and the results from each of the K subsets are then combined to obtain an overall result. They showed that under mild conditions the combined overall result still retains desired properties of many commonly used penalized estimators, such as the model selection consistency and asymptotic normality. When K is well controlled, they also showed that the combined result is asymptotically equivalent to the result of analyzing the entire data all at once (assuming that there is a super computer that could carry out such an analysis). In addition, when a computational intensive algorithm is used, they showed that the split-and-conquer approach can substantially reduce computing time and computer memory requirement. Furthermore, they demonstrated that the approach has an inherent advantage of being more resistant to false model selections caused by spurious correlations. Similar to what reported in the literature, they established an upper bound for the expected number of falsely selected variables and a lower bound for the expected number for truly selected variables. The proposed methodology was illustrated numerically using both simulation and real data examples.

In the afternoon Session II on February 10, there were three presentations delivered by Ping Li of Rutgers University, Christophe Andrieu of University of Bristol, and Lingsong Zhang of Purdue University. Ping presented "BigData: Efficient Search and Learning Using Sparse Random Projections and Probabilistic Hashing". Modern applications of search and learning have to deal with datasets with billions of examples in billion or even billion square dimensions (e.g., text documents represented by high-order n-grams). Ping first presented the use of very sparse random projections for learning with high-dimensional data. It is evident that the projection matrix can be extremely sparse (e.g., 0.1% or less nonzeros) without hurting the learning performance. For binary sparse data (which are common in practice), however, b-bit minwise hashing turns out to be much more efficient than random projections. In addition, the recent development of one-permutation hashing [10] substantially reduced the processing time of (b-bit) minwise hashing, from (e.g.,) 500 permutations to merely one. There are many other exciting new progresses in the basic research of random projections and hashing, for example, the new work on sign Cauchy random projections for approximating chi-square distances [11] and the work on using stable random projections for very fast and accurate compressed sensing [12]. Christophe's presentation was on "Uniform Ergodicity of the Iterated Conditional SMC and Geometric Ergodicity of Particle Gibbs Samplers" [13]. He discussed the quantitative bounds for rates of convergence and asymptotic variances for iterated conditional sequential Monte Carlo (i-cSMC) Markov chains and associated particle Gibbs samplers. Their main findings are that the essential boundedness of potential functions associated with the i-cSMC algorithm provide necessary and sufficient conditions for the uniform ergodicity of the i-cSMC Markov chain, as well as quantitative bounds on its (uniformly geometric) rate of convergence. Lingsong presented "Scale-Space Inference with Application on Spatial Clustering Detection". He proposed a novel multi-resolution cluster detection (MCD) method to identify irregularly shaped clusters in space and derived the multi-scale test statistic on a single cell based on likelihood ratio statistic for Bernoulli sequence, Poisson sequence and Normal sequence. A neighborhood variability measure is defined to select the optimal test threshold. In his presentation, the MCD method was compared with single scale testing methods controlling for false discovery rate and the spatial scan statistics using simulation and f-MRI data, and the MCD method was shown to be more effective for discovering irregularly shaped clusters. The implementation of his proposed method does not require heavy computation, making it suitable for cluster detection for large spatial data.

6.3.2 Day 2: February 11, 2014

In the morning Session I on February 11, Peihua Qiu of the University of Florida presented "On Nonparametric Profile Monitoring". Quality of a process is often characterized by the functional relationship between a response and one or more predictors. Profile monitoring is for checking the stability of this relationship over time. In the literature, most existing control charts are for monitoring parametric profiles, and they assume that within-profile observations are independent of each other, which is often invalid. In this presentation, he discussed some of their recent research on nonparametric profile monitoring when within-profile data are correlated. He also briefly described the problems of online image monitoring and dynamic disease screening that are closely related to profile monitoring. Hongtu Zhu of the University of North Carolina presented "Functional Analysis of Big Neuroimaging Data". Motivated by recent work on studying massive imaging data in various neuroimaging studies, Hongtu's group proposed several classes of spatial regression models including spatially varying coefficient models, spatial predictive Gaussian process models, tensor regression models, and Cox functional linear regression models for the joint analysis of large neuroimaging data and clinical and behavioral data. Their statistical models explicitly account for several stylized features of neuorimaging data: the presence of multiple piecewise smooth regions with unknown edges and jumps and substantial spatial correlations. They developed some fast estimation procedures to simultaneously estimate the varying coefficient functions and the spatial correlations. They also systematically investigated the asymptotic properties (e.g., consistency and asymptotic normality) of the multiscale adaptive parameter estimates. Their Monte Carlo simulation and real data analysis confirmed the excellent performance of their models in different applications.

In the morning Session II on February 11, Jian Zhang of the University of Kent presented "High-dimensional Inference in Magnetoencephalographic Neuroimaging". Reconstructing neural activities using non-invasive sensor arrays outside the brain is an ill-posed inverse problem since the observed (Magnetoencephalography) MEG sensor measurements could result from an infinite number of possible neuronal sources [14]. MEG data can be complex and of large scale, in particular, when multiple trials and multiple subjects are involved. Should we build a big model for such kinds of large scale data? In this presentation, he focused on a local approach which contains a series of small local models in the source space and is scalable to parallel computing. They proposed a family of procedures called beamformers by using covariance thresholding [15]. A general theory was developed on how their spatial and temporal dimensions determine their performance. Conditions were provided for the convergence rate of the associated beamformer estimation and the implications of the theory were illustrated by simulations and a real data analysis on face-perception MEG data [16]. Momiao Xiong of the University of Texas Health Science Center at Houston discussed "Classification Analysis of Big Image Data". Due to advances in sensors, growing large and complex medical images provides invaluable information for holistic discovery of the genetic and epigenetic structure of disease and has the potential to enhance diagnosis of disease, prediction of clinical outcomes, characterization of disease progression, management of health care and development of treatments, but also pose great methodological and computational challenges. An enormous amount of increasingly larger, more complex and more diverse demand developing unified frameworks and novel statistical methods for cluster and classification analysis of medical image data, which will provide low-cost and powerful tools for early detection and efficient management of complex diseases such as cancers, mental disorders, vascular diseases. The medical images have the ability to visualize the pathology change in the cellular or even the molecular level or anatomical changes in tissues and organs. However, the medical images for the same type of disease from different individuals might be quite similar. As a result, it is a big challenge to extract the key information from a large amount of medical images for early detection of the complex diseases and the prediction of the drug response. To address this issue, he presented an extension of one dimensional functional principal component analysis to the two dimensional functional principle component analysis (2DFPCA). To reduce high dimensional image data to low dimensional space, they developed novel space sufficient dimension reduction methods to select variables. The proposed methods were applied to 250 liver cancer histology image data (99 tumor tissues and 151 normal tissues) and 176 ovarian cancer histology images with the drug response status from TCGA database. For the liver cancer dataset, they obtained almost 84%, 79.8% and 86.8% classification accuracy, sensitivity and specificity, respectively. For the ovarian cancer drug response dataset, classification accuracy, sensitivity and specificity were 80.1%, 85.8% and 71.4%, respectively.

The afternoon on February 11 featured two tutorial and review sessions on the recent developments of statistical methods and computational methods for big data analysis. In the afternoon Session I on February 11, Faming Liang of the Taxes A&M University presented "Recent Developments of Iterative Monte Carlo Methods for Big Data Analysis". Iterative Monte Carlo methods, such as MCMC, stochastic approximation, and EM, have proven to be very powerful tools for statistical data analysis. However, their computer-intensive nature, which typically require a large number of iterations and a complete scan of the full dataset for each iteration, precludes their use for big data analysis. Faming provided an overview of the recent developments of iterative Monte Carlo methods for big data analysis. Chuanhai Liu of the Purdue University presented "Big Data Analysis and Beyond" Based on his current understanding of big data, which essentially says that there is no big data but only bigger data (i.e., data that cannot be analyzed efficiently using a single computer), Chuanhai listed three challenges: (1) modeling - how uncertainly data are related to scientific questions, (2) inference - how data can adequately be converted to knowledge, and (3) computing - how inferential output can be computed from big data. In addition to agreeing with the common recognition that approximate inference can be made by making use of MapReduce, he pointed it out that improved results can be obtained using an iteratveMapReduce-type computational framework, which he developed in R at Purdue for his topic course on massive data analysis. Due to both time limit and overwhelming interest from participants, in the remaining of his presentation he focused on a new inferential framework called inferential models [17, 18, 19, 20]. Unlike all other existing schools of thought, this new framework produces scientifically desirable prior-free and frequency-calibrated probabilistic inference. While it is apparently difficult to introduce such a new framework in 30 minutes to cover its philosophy, theory, computation, and application, Chuanhai delivered a clear message: due to the lack of a solid foundation in statistics, developing such inferential methods is critically important for scientific inference, especially from big data. This calls for attention on research on foundations of statistics, a topic well beyond but fundamentally important in big data analysis.

In the afternoon Session II on February 11, Jun Yan of the University of Connecticut delivered "A Partial Review of Software for Big Data Statistics". Big data brings challenges to even simple statistical analysis because of the barriers in computer memory and computing time. The computer memory barrier is usually handled by a database connection that extracts data in chunks for processing. The computing time barrier is handled by parallel computing, often accelerated by graphical processing units. In this partial review, Jun summarized the open source R packages that break the computer memory limit such as biglm and bigmemory, as well as the academic version of the commercial Revolution R, and R packages that support parallel computing. Products from commercial software will also be sketched for completeness. This review work was a joint effort of Jun Yan, Ming-Hui Chen, Elizabeth Schifano, Chun Wang, and Jing Wu of the University of Connecticut.

6.3.3 Day 3: February 12, 2014

In the morning Session I on February 12, Kun Chen of the University of Connecticut presented "Sparse and low-rank Regression in High Dimensions". The talk discussed the combination of distinct but interrelated dimension reduction techniques in fitting high-dimensional multivariate models. This results in models with some composite low-dimensional structures, which often enjoy enhanced interpretability and improved predictive accuracy. Kun also presented a general methodology and some theoretical results for recovering a sparse and low-rank matrix structure from noisy data, in both unsupervised and supervised learning problems. Linglong Kong of the Purdue University presented "Quantile Regression in Variable Screening". Linglong first introduced a quantile regression framework for linear and nonlinear variable screening with high-dimensional heterogeneous data. Motivated by success of various variable screening methods, especially the quantile-adaptive framework, He discussed how to combine the information from different quantile levels to provide more efficient variable screening procedure. In particular, there are two ways to do so: one is to simply take (weighted) average across different levels of quantile regression; the other one is to use (weighted) composite quantile regression. Asymptotically, these two approaches are equivalent in terms of efficiency. Numerical studies confirm the fine performance of the proposed method for various linear and nonlinear models.

In the morning Session II on February 12, Ying Nian Wu of the University of California at Los Angeles presented "What Is Beyond Sparse Coding?" Many types of data such as natural images admit sparse representations by redundant dictionaries of basis functions (or regressors), and these dictionaries can either be designed or learned from training data. However, it is still unclear how to go beyond sparsity and continue to learn structures behind the sparse representations. Ying Nian reviewed some recent progresses and the major issues and difficulties that need to be addressed. He also presented our own recent work that seeks to learn dictionaries of compositional patterns in the sparse representations. Xiao Wang of the Purdue University presented "Functional Regression and Image Regression" based on his recent papers [21, 22]. Xiao first discussed generalized functional linear models with scalar responses and image predictors. Predicting clinical outcomes on the basis of quantitative image data is quite promising in current psychiatric neuroimaging research. In his talk, he considered prediction with image predictors in the framework of functional linear model and bounded total variation space. The slope image is assumed to belong to the space of bounded total variation. He presented near-optimal guarantee for stable recovery of the slope image using total variation minimization and nonasymptotic error bounds on the excess risk by exploiting various techniques from compressive sensing, as well as the approximation theory. These techniques allows us to obtain finite-sample bounds that hold with high probability, and are specified explicitly in terms of the sample size and the image size.

The afternoon Session I on February 12 featured three presentations delivered by Xiaotong Shen of the University of Minnesota, Xiaojing Wang of the University of Connecticut, and Guanghua Xiao of the UT Southwestern Medical Center. Xiaotong's talk was on "Sentiment Analysis". Sentiment analysis identifies the relevant content as well as determines and understands opinions, from documents or texts, towards a specific event of interest. In this presentation, Xiaotong discussed large margin methods for ordinal classification involving word predictors, where imprecise information is available for prediction regarding linguistic relations among predictors, expressed in terms of a directed graph. Then the methods are used for sentiment analysis, where sentiment function representations of words are derived, on which the imprecise predictor relations are integrated as linear relational constraints over sentiment function coefficients. Computational and theoretical aspects were discussed, in addition to an application to opinion survey. Xiaojing presented "A Bayesian Approach to Subgroup Identification". Xiaojing discussed subgroup identification, the goal of which is to determine the heterogeneity of treatment effects across subpopulations. Searching for differences among subgroups is challenging because it is inherently a multiple testing problem with the complication that test statistics for subgroups are typically highly dependent, making simple multiplicity corrections such as the Bonferroni correction too conservative. In this talk, Xiaojing presented a Bayesian approach to identify subgroup effects, with a scheme for assigning prior probabilities to possible subgroup effects that accounts for multiplicity and yet allows for (pre-experimental) preference to specific subgroups. The analysis utilizes a new Bayesian model selection methodology and, as a byproduct, produces individual probabilities of treatment effect that could be of use in personalized medicine. Xiaojing illustrated the analysis using an example involving subgroup analysis of biomarker effects on treatments. Guanghua presented "Detection of Tumor Driver Genes Using a Fully Integrated Bayesian Approach". DNA copy number alterations (CNAs), including amplifications and deletions, can result in significant changes in gene expression, and are closely related to the development and progression of many diseases, especially cancer. For example, CNA-associated expression changes in certain genes (called tumor driver genes) can alter the expression levels of many downstream genes through transcription regulation, and cause cancer. Identification of such tumor driver genes leads to discovery of novel therapeutic targets for personalized treatment of cancers. Several approaches have been developed for this purpose by using both copy number and gene expression data. In this talk, Guanghua discussed a Bayesian approach to identify tumor driver genes, in which the copy number and gene expression data are modeled together, and the dependency between the two data types is modeled through conditional probabilities. The joint modeling approach can identify CNA and differentially expressed (DE) genes simultaneously, leading to improved detection of tumor driver genes and comprehensive understanding of underlying biological processes. Guanghua also presented simulation studies to evaluate their proposed method and then applied their method to a head and neck squamous cell carcinoma (HNSCC) dataset. Both simulation studies and data application showed that the joint modeling approach can significantly improve the performance in identifying tumor driver genes, when compared to other existing approaches.

The third day (February 12) of the workshop concluded with two featured presentations by Elizabeth D. Schifano of the University of Connecticut on "Online Updating of Statistical Inference in the Big Data Setting" and Nan Lin of the Washington University in St. Louis on "Statistical Aggregation in Massive Data Environment". Elizabeth presented statistical regression methods for big data arising from online analytical processing, where large amounts of data arrive in streams and require fast analysis without storage/access to the historical data. In particular, Elizabeth and her collaborators (Ming-Hui Chen, Jun Yan, Chun Wang, Jing Wu of the University of Connecticut) developed iterative estimating algorithms and statistical inferences for linear models and estimating equations that update as new data arrive. Elizabeth introduced predictive residuals in the online-updated linear model setting that can be used to test the goodness-of-fit of the hypothesized model, as well as a new online-updated estimator under the estimating equation framework that has less bias in finite samples as compared to other online-updated estimators. In simulation studies, their approaches compared favorably with competing approaches in terms of timing and accuracy. Due to their size and complexity, massive data sets bring many computational challenges for statistical analysis, such as overcoming the memory limitation and improving computational efficiency of traditional statistical methods. In Nan's talk, he discussed the statistical aggregation strategy to conquer such challenges posed by massive data sets. Statistical aggregation partitions the entire data set into smaller subsets, compresses each subset into certain low-dimensional summary statistics and aggregates the summary statistics to approximate the desired computation based on the entire data. Results from statistical aggregation are required to be asymptotically equivalent. Statistical aggregation is particularly useful to support sophisticated statistical analyses for online analytical processing in data cubes. Nan detailed its application to two large families of statistical methods, estimating equation estimation and U-statistics.

6.3.4 Day 4: February 13, 2014

In the morning Session I on February 13, Hongyu Zhao of the Yale University could not attend the workshop but sent his presentation slides to all the workshop participants. Hongyu's slides were on "Detecting Genetic Association Signals Leveraging Network Information". Although Genome Wide Association Studies (GWAS) have identified many sceptibility loci for common diseases, these loci only explain a small portion of heritability. It is challenging to identify the remaining disease loci because their association signals are likely weak and difficult to identify among millions of candidates. One potentially useful direction to increase statistical power is to incorporate pathway and functional genomics information to prioritize GWAS signals. In his slides, he first described a method to utilize network information to prioritize disease genes based on the "guilt by association" principle, in which networks are treated as static, and disease associated genes are assumed to locate closer with each other than random pairs in the network. Hongyu then introduced a novel "guilt by rewiring" principle that postulates that disease genes more likely undergo rewiring in disease patients, whereas most of the network is unaffected in disease condition. A Markov random field framework was used for both methods to integrate network information to prioritize genes. Applications in Crohn's disease and Parkinson's disease show that these methods lead to more replicable and biologically meaningful results. Zhang Zhang of the Beijing Institute of Genomics at Chinese Academy of Sciences, China presented "Biocuration in the Era of Big Data". Biology enters the era of big data. More than a dozen biological wikis (bio-wiki) have been constructed to call on community intelligence in big biological data curation. However, one of the major limitations in bio-wikis is insufficient participation from the scientific community, which is intrinsically because of lack of explicit authorship and thus no credit for community-curated contributions. To increase community curation in bio-wikis, Zhang and his collaborators developed AuthorReward [23] to reward community-curated efforts by contribution quantification and explicit authorship. It quantifies researchers' contributions by properly factoring both edit quantity and quality and yields automated explicit authorship according to their quantitative contributions. They also constructed RiceWiki[24] (http://ricewiki.big.ac.cn), a wiki-based, publicly editable, and open-content platform for community curation of rice genes. To test the functionality of AuthorReward, they installed it in RiceWiki. As testified in RiceWiki, AuthorReward is capable of yielding sensible quantitative contributions and providing automated explicit authorship, consistent well with perceptions of all participated contributors. Based on collective intelligence, RiceWiki bears the potential to deal with big data and make it possible to build a rice encyclopedia by and for the scientific community.

In the morning Session II on February 13, Xin Gao of the King Abdullah University of Science and Technology (KAUST) presented "Poly(A) motif prediction using spectral latent features from human DNA sequences" [25]. They propose a novel machine learning method for poly(A) motif prediction by marrying generative learning (hidden Markov models) and discriminative learning (support vector machines). Generative learning provides a rich palette on which the uncertainty and diversity of sequence information can be handled, while discriminative learning allows the performance of the classification task to be directly optimized. They employed hidden Markov models for fitting the DNA sequence dynamics, and developed an efficient spectral algorithm for extracting latent variable information from these models. These spectral latent features were then fed into support vector machines to fine tune the classification performance. The proposed method was evaluated on a comprehensive human poly(A) dataset that consists of 14,740 samples from 12 of the most abundant variants of human poly(A) motifs. Compared with one of previous state-of-art methods in the literature (the random forest model with expert-crafted features), our method reduces the average error rate, false negative rate and false positive rate by 26%, 15% and 35%, respectively. Matthias Katzfuss of the Texas A&M University presented "Statistical Inference for Massive Distributed Spatial Data Using Low-Rank Model" Matthias's talk focused on computationally feasible spatial inference and prediction approaches using spatial low-rank models, for analyzing massive distributed spatial data. The proposed methods adopt the divide-and-conquer strategy to dealing with massive spatial data, which allow local spatial modeling and computations at separated data servers with minimal communication among them. The proposed methods can be very useful in dealing with contemporaneous large-scale spatial-temporal applications.

In the afternoon Session I on February 13, Ruslan Salakhutdinov of the University of Toronto presented "Annealing Between Distributions by Averaging Moments" [26]. Many powerful Monte Carlo techniques for estimating partition functions, such as annealed importance sampling (AIS), are based on sampling from a sequence of intermediate distributions which interpolate between a tractable initial distribution and the intractable target distribution. The near-universal practice is to use geometric averages of the initial and target distributions, but alternative paths can perform substantially better. Ruslan presented a novel sequence of intermediate distributions for exponential families defined by averaging the moments of the initial and target distributions. He discussed and analyzed the asymptotic performance of both the geometric and moment averages paths and derive an asymptotically optimal piecewise linear schedule. AIS with moment averaging performs well empirically at estimating partition functions of restricted Boltzmann machines (RBMs), which form the building blocks of many deep learning models, including Deep Belief Networks and Deep Boltzmann Machines. Alexander Y. Shestopaloff of the University of Toronto presented "MCMC for Non-Linear State Space Models Using Ensembles of Latent Sequences" [27]. Alexander introduced a new MCMC method for non-linear, non-Gaussian state space models using Embedded HMM MCMC and Ensemble MCMC. In contrast to existing methods, which only consider a single state sequence during parameter sampling, their new method considers an enormously large ensemble of latent state sequences at once. This allows making larger proposals while keeping a high acceptance rate, leading to more efficient sampling. He showed that when applied to the problem of Bayesian inference in the Ricker model of population dynamics, their new MCMC method improves performance relative to methods that only look at a single state sequence during sampling. Xiaoyi Min of the Yale School of Public Health presented "Detection of Chromosome Copy Number Variations in Multiple Sequences". Xiaoyi introduced the concept of DNA copy number variation (CNV) and its potential role in human complex diseases. To help identify inherited CNVs which are generally short and common in the population, he introduced an extension to the Screening and Ranking Algorithm [28] which integrates information from multiple samples. In particular, Xiaoyi and his collaborators proposed an adaptive Fisher's method for combining screening statistics across samples, which has a high power regardless of the carrier proportion of the CNV. Furthermore, Xiaoyi gave both theoretical and numerical results to demonstrate that this method performs better than other current methods. Profs. Peihua Qiu, Min-ge Xie, and Hongtu Zhu gave many insightful comments and suggestions from different aspects after his presentation.

The afternoon Session II on February 13 was the last session of this workshop. Lee H. Dicker of the Rutgers University presented "Variance estimation in high-dimensional linear models" and Philip Gautier of the Purdue University presented "Divide & Recombine for Large Complex Data: Likelihood Modelling for Logistic Regression". Lee's talk focused on the role of variance in model fitting procedures for high-dimensional data. Lee provided an overview of popular methods for variance estimation, emphasizing the role of efficiency. The residual variance and the proportion of explained variation are important quantities in many statistical models and model fitting procedures. They play an important role in regression diagnostics, model selection procedures, and in determining the performance limits in many problems. Recently, methods for estimating these and other related summary statistics in high-dimensional linear models have received significant attention. In this talk, Lee discussed some of the various approaches to estimating these quantities (e.g., residual sum-of-squares-based estimators, the method-of-moments) and the conditions required to ensure reliable performance (sparsity, conditions on the predictor covariance matrix). Efficiency was be discussed, along with new estimators that are closely related to ridge regression. Lee also presented an application related to estimating heritability, an important concept in genetics.

There were three thought-provoking points of discussion that came up during and after Lee's talk:

(a) Efficiency and M-estimators. The MLE/ridge estimators described in Lee's talk were derived under a "random β" assumption, but they're interested in their performance in a "fixed β" model. A detailed analysis of the estimators in the random β model is straightforward, by standard likelihood theory. Converting consistency and asymptotic normality results for the random β model into corresponding results for the fixed β model is also fairly straightforward. However, efficiency for the fixed β model seems to be a bit more difficult. One of the comments/suggestions made during Lee's talk was that one could consider efficiency within an appropriate class of M-estimators, and that this might be more tractable than efficiency within the broader likelihood framework. It seems like this may be a very fruitful approach to this problem.

(b) Estimating heritability using "sparse" estimators for σ^2. The main application discussed in Lee's talk was estimating heritability in genetics, i.e. estimating r^2. The methods Lee used were based on "non-sparse" estimators for σ^2 and τ^2 discussed in the talk. However, it also seems feasible to estimate r^2 using "sparse" estimators for σ^2 that have been proposed elsewhere (these estimators require β to be sparse in order to be effective). This approach to estimating r^2 has not been considered in the literature (thus, we would have to derive the sparse estimators for r^2 ourselves, along with their asymptotic distribution), and it would be interesting to compare the performance of the "sparse" and "non-sparse" methods in a real data example.

(c) Towards the end of the talk, someone asked (approximately): "Can you apply these methods in a genomic dataset where $p = 1,000,000$ and $n = 1,000$?" His response during the talk was pretty brief, and the Session Chair, Paul Kvam, basically suggested that this would probably be difficult. However, challenges like this can also be very interesting. To address problems with $p = 1,000,000$ and $n = 1,000$, one might initially seek methods for reducing the ratio p/n (perhaps to around 10-100), before applying methods similar to those proposed in the talk. Reducing p/n could be achieved by either (i) increasing n (this is often not possible) or (ii) decreasing p. Screening-out predictors could be used to decrease p; this could be conducted using only the "X" data and not peeking at the "y" data (e.g. screen out highly correlated predictors, as in the heritability example from the talk). More broadly, Lee was very excited to explore how methods like those proposed in the talk can be used in challenging applications; the comments/feedback he received during and after the talk have provided some great leads for this.

Philip Gautier, a Ph.D. student at Purdue who is working with Professors William Cleveland and Chuanhai Liu, talked about using Divide and Recombine (D&R) as a statistical framework for the analysis of big data. Philip provided context to relate this likelihood-based analysis to previous talks that featured "Split and Conquer" approaches in similar large-data problems. Examples for logistic regression are especially effective in comparing the D&R approach to the simpler "all-data" MLE. Matthias Katzfuss commented that it would be necessary to see how the method I presented (divide & recombine likelihood modelling) would perform on real data sets with many explanatory variables After the talk finished, Nan Lin discussed asymptotics for divide & recombine (a.k.a divide & conquer, split & conquer) methods with the author. The asymptotic results presented earlier by Nan Lin, Minge Xie, and Elizabeth Schifano have the subset size going to infinity. Under these conditions, their estimators were consistent. In real applications, we might expect to be able to collect more data, but the subset size will probably have some upper limit based on our computing environment. The simulations presented showed that, with a fixed subset size and growing number of subsets, bias persists. Philip commented that the focus should be on reducing the size of that bias by pursuing better division and recombination methods, rather than focusing on consistency.

6.4 Scientific Progress Made

Much progress has been made in this workshop. We summarize the comments from some of the workshop participants on this regard.

Christophe Andrieu, School of Mathematics, University of Bristol, UK: It has really helped raise awareness of the multiple facets of what "big data" means. The issues are multiple and not necessarily faced simultaneously (size of the data, computational burden). In Bristol, in collaboration with Warwick, Oxford and Lancaster we have started a reading group to discuss the practical issues faced when using parallel architectures (GPUs and others), and my interest has been raised by the Banff workshop. In terms of computing, the workshop has helped me realise that straightforward parallelisation is not a panacea and there is going to be a two way interaction between computation and statistical modelling and inference (in contrast to what has happened since the advent of cheap and powerful computers, since then computing was ancillary to the inferential task). And this is where statisticians are likely to have the edge, but they need to understand "computation" better. The mix of people with different perspectives on all these issues was really a big + for me.

Minge Xie, Department of Statistics, Rutgers University, USA: First, let me take this opportunity to thank you [the organizers] all for organizing this wonderful workshop. The workshop was a success in every aspect. I had a good time. We all appreciate your handwork and effort for making this an impactful event.

Peihua Qiu, Department of Biostatistics, University of Florida, USA. As I told you [the organizer] during the workshop, this big data workshop is one of the best ones I ever attended. You did an excellent job in organizing the sessions well.

Kun Chen, Department of Statistics, University of Connecticut, USA: I would like to thank the organizers for organizing such a timely and successful workshop on big data. This workshop has greatly facilitated interactions among the statisticians who are currently working on the frontiers of statistical big data research, and also provided great learning opportunities for young researchers who are eager to dedicate to big data research. I believe the workshop will continue to stimulate new ideas on how to conduct statistical big data research and how to better prepare younger generation statisticians to tackle the many challenges we are facing in the big data era.

Guanghua (Andy) Xiao, Quantitative Medical Research Center, Department of Clinical Sciences, University of Texas, Southwestern Medical Center, USA: Thank you [the organizers] very much for giving me the opportunity to attend the workshop. It was a great experience for me at Banff and I have learned a lot from the workshop.

Hongzhe Li, Department of Biostatistics, University of Pennsylvania, USA: Thank you [the organizers] very much for putting together this great workshop and for inviting me to participate. It was a great workshop and all the presentations are very interesting and address many important statistical issues related to big data analysis. The talks and discussions will definitely lead to further works in this very important area of statistical research.

Heping Zhang, Department of Biostatistics, Yale University, USA: It was a very successful and informative meeting. I have learned various important topics related to big data analyses.

Hongtu Zhu, Department of Biostatistics, University of North Carolina, USA: (i) Focus on developing novel statistical and computational methods on integrating imaging-genetic data; and (ii) solve several deep theories associated with our new methods.

Paul Kvam, H. Milton Stewart School of Industrial and Systems Engineering, Georgia Tech, USA: There were a lot of important concepts that I was probably not able to take in during the workshop, but I learned so much about the current state and future direction of the nonparametric methods that are most helpful for big data analysis, my future research is sure to be affected in a great way. I was surely inspired and happy to be there. I am so grateful to you and the hosts for making my experience there possible!

Jian Zhang, School of Mathematics, Statistics and Actuarial Science, University of Kent, UK: It has been one of greatest workshops I attended so far. I have learnt a lot about Big Data Analysis via this workshop.

Xiaojing Wang, Department of Statistics, University of Connecticut, USA: Thank you very much for organizing such a wonderful workshop at Banff! It is really a very interesting workshop and I learned a lot.

Alex Shestopaloff, Department of Statistical Sciences, University of Toronto, CA: As a PhD student attending my first conference outside of Toronto, I must say that it was a very enjoyable and informative experience. I look forward to meeting you (and the others) again! Many thanks for your efforts.

Xiaoyi Min, Yale School of Public Health, USA: From the talks presented at the workshop, I learned a lot about the challenges in "big data" as well as the current developments addressing these challenges. From my personal understanding, the workshop covered recent progresses in three directions. First, many studies deal with the big volume of "big data". The "Divide and Conquer" strategy, for example, is employed in handling data that cannot be stored or computed on a single computer. Second, several talks tackled the computation burden coming from "big data". They use, for example, specific modeling or sampling techniques to allow parallel computing on multiple nodes or even GPUs. Last but not least, many researches focus on the specific data structures arising from different forms of big and complex data such as image data, spatio-temporal data, and genetic and genomic data. To me, furthering and integrating the progresses in all these directions and providing solutions for real data analyses with

"big data" is an important next step. Real data may be large in size, complex in structure, and difficult to compute at the same time. Therefore, an ideal solution should take all these challenges into account. This requires the collaboration of experts in all three aspects. Researchers also need a comprehensive understanding of the problems and the available tools. To this aspect, the workshop provided a great opportunity for researchers to learn from each other, exchange ideas, and start collaboration, which is very beneficial for the future development in the field of big data.
Philip Gautier, Department of Statistics, Purdue University, USA: Thank you for all of your work organizing the conference. The discussions I had with other presenters were very productive.

6.5 Outcome of the Meeting

There are many outcomes of the meeting. The workshop participants learned several new approaches and software for big data analysis. The workshop has initiated potential collaborations. After the workshop, Xiao Wang has obtained image datasets from both Professors Peihua Qiu and Hongtu Zhu. Peihua Qiu and Xiao Wang (two workshop participants) started their collaborative research on statistical process control of images, which is a new research area and involves big data processing and analysis. Hongtu Zhu and Xiao Wang are working on a paper on image classification after workshop. This workshop provided them a great opportunity to communicate with each other. Also, certain methods presented in the workshop, such as the divide-and-conquer method, will be probably used in their research. Minge Xie and Ming-Hui Chen discussed how to combine interval estimates in the steam data setting and they will continue to collaborate after the workshop.

There will be two special issues in Technometrics and Statistics and Its Inference on big data after the workshop. The special issue of Technometrics will publish original high-quality papers that deal with all aspects of the statistical analysis of big data, including but not limited to data visualization and exploratory data analysis, statistical computation, statistical modeling and inferences, and innovative applications. Papers in any application domain that fits within the broad scope of Technometrics will be considered. This special issue is expected to be published in February 2016. The Guest Editorial Board consists of Ming-Hui Chen (University of Connecticut), Radu V. Craiu (University of Toronto), Robert B. Gramacy (University of Chicago), Willis A. Jensen (W. L. Gore and Associates), Faming Liang (Texas A&M University), Chuanhai Liu (Purdue University), William Q. Meeker (Iowa State University), and Peihua Qiu (Editor) (University of Florida).

The special issue of Statistics and Its Inference (SII) will be on "Statistical and Computational Theory and Methodology for Big Data". SII strongly encourages substantive applications and computational developments for analyzing big data in all areas of sciences. High-quality review articles in this emerging new research area are also welcome. The papers, once accepted, will be published together in a future issue of SII. Some of accepted papers may be chosen as invited discussion papers in this special issue. The submission deadline for this SII special issue is November 1, 2014. The Guest Editors for the SII special issue include Ming-Hui Chen (University of Connecticut), Radu V. Craiu (University of Toronto), Faming Liang (Texas A&M University), Chuanhai Liu (Purdue University), and Heping Zhang (Editor-in-Chief) (Yale University).

The potential follow-up workshops were discussed. There were extensive email communications among the workshop participants on developing a textbook for big data after the workshop.

Participants

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Bibliography

[1] A. Kleiner, A. Talwalkar, P. Sarkar and M. I. Jordan, A scalable bootstrap for massive data. Journal of the Royal Statistical Society, Series B (2014). doi:10.1111/rssb.12050.

[2] N., Lin and R. Xi, Aggregated estimating equation estimation. Statistics and Its Interface **4** (2011), 73–83.

[3] R. Xi, N. Lin, and Y. Chen, Compression and aggregation for logistic regression analysis in data cubes. IEEE Transactions on Knowledge and Data Engineering **21**, 479–492.

[4] X. Chen and M. Xie, A split and conquer approach for extraordinarily large data analysis. Statistica Sinica (2014). In press.

[5] F. Liang, Y. Cheng, Q. Song, J. Park, and P. Yang, A resampling-based stochastic approximation method for analysis of large geostatistical data. Journal of the American Statistical Association **108** (2013), 325–339.

[6] M.-H. Chen, Q.-M. Shao, and J.G. Ibrahim, Monte Carlo methods in Bayesian computation, Springer, New York, 2000.

[7] J.S. Liu, Monte Carlo strategies in scientific computing, Springer, New York, 2001.

[8] F. Liang, C. Liu, and R.J. Carroll, Advanced Markov chain Monte Carlo methods: learning from past samples, Wiley, New York, 2010.

[9] A.P. Dempster, N.M. Laird, and D.B. Rubin, Maximum likelihood from incomplete data via the EM algorithm. Journal of the Royal Statistical Society, Series B **39** (1977), 1–38.

[10] P. Li, A. Owen, and C.-H. Zhang, One permutation hashing. Neural Information Processing Systems (NIPS) **25** (2012), 3122–3130.

[11] P. Li, G. Samorodnitsky, and J. Hopcroft, Sign Cauchy projections and Chi-square kernel. Advances in Neural Information Processing Systems **26**, 2013.

[12] P. Li, C.-H. Zhang, and T. Zhang, Compressed counting meets compressed sensing. arXiv:1401.0201v1, 2013.

[13] C. Andrieu, A. Lee, and M. Vihola, Uniform ergodicity of the iterated conditional SMC and geometric ergodicity of particle Gibbs samplers. arXiv:1312.6432, 2013.

[14] R.N., Henson, G. Flandin, K.J. Friston, and J. Mattout, A parametric empirical Bayesian framework for fMRI-constrained MEG/EEG source reconstruction. Human Brain Mapping **31** (2010), 1512–1531.

[15] P. Bickel and E. Levina, E., Covariance regularization by thresholding. Annals of Statistics **36** (2008), 2577–2604.

[16] J. Zhang, C. Liu, and G. Green, Source Localization with MEG Data: A beamforming approach based on covariance thresholding. Biometrics (2013), doi: 10.1111/biom.12123.

[17] R. Martin and C. Liu, Inferential models: a framework for prior-free posterior probabilistic inference. Journal of the American Statistical Association **108** (2013), 301–313.

[18] R. Martin and C. Liu, Comment: foundations of statistical inference. Statistical Science (2014a), in press.

[19] R. Martin and C. Liu, 3. Martin, R. and Liu, C. (2014b). Conditional inferential models: combining information for prior-free probabilistic inference. Journal of the Royal Statistical Society, Series B (2014b), in press.

[20] R. Martin and C. Liu, Marginal inferential models: prior-free probabilistic inference on interest parameters. unpublished manuscript, 2014c.

[21] P. Du and X. Wang, Penalized likelihood functional regression. Statistica Sinca (2013), in press.

[22] X. Wang, P. Du, and J. Shen, (2013). Smoothing splines with varying smoothing parameter. Biometrika **100** (2013), 955–970.

[23] L. Dai, M. Tian, J.Y. Wu, J.F. Xiao, X.M. Wang, J.P. Townsend, and Z. Zhang, AuthorReward: increasing community curation in biological knowledge wikis through automated authorship quantification. Bioinformatics **29** (2013), 1837–1839.

[24] Z. Zhang, J. Sang, L.N. Ma, G. Wu, H. Wu, D.W. Huang, D. Zou, S.Q. Liu, A. Li, L.L. Hao, M. Tian, C. Xu, X.M. Wang, J.Y. Wu, J.F. Xiao, L. Dai, L.-L. Chen, S.N. Hu, and J. Yu, RiceWiki: a wiki-based database for community curation of rice genes. Nucleic Acids Research **42** (2014), D1222–D1228.

[25] B. Xie, B. Jankovic, V. Bajic, L. Song, and X. Gao, Poly(A) motif prediction using spectral latent features from human DNA sequences. Bioinformatics **29** (2013), i316–i325.

[26] R. Grosse, C. Maddison, and R. Salakhutdinov, Annealing between distributions by averaging moments. In Neural Information Processing Systems (NIPS 27), 2013, www.cs.toronto.edu/∼rsalakhu/papers/nips2013_moment.pdf

[27] A.Y. Shestopaloff and R.M. Neal, MCMC for non-linear state space models using ensembles of latent sequences. Technical Report, 2013, http://arxiv.org/abs/1305.0320.

[28] Y.S. Niu and H. Zhang, The screening and ranking algorithm to detect DNA copy number variations. The Annals of Applied Statistics **6** (2012), 1306–1326.

Chapter 7

Multifractal Analysis: From Theory to Applications and Back (14w5045)

February 23 - 28, 2014

Organizer(s): Patrice Abry (CNRS, ENS de Lyon), Stephane Jaffard (Université Paris-Est Créteil), Ursula Molter (Universidad de Buenos Aires), Vladas Pipiras (University of North Carolina)

7.1 Overview of the Field

Multifractals are mathematical objects characterized by unique and interesting scaling properties. Their study is approached commonly from one of the following interrelated perspectives:

- probabilistic modeling, statistics and stochastic processes,
- signal and image processing, and applications at large,
- functional analysis and geometric measure theory.

These perspectives will be referred to below as, respectively, **probability/statistics**, **applications** and **analysis**.

From the **probability/statistics** perspective, (random) processes $X = \{X(t)\}$ are *multifractal* when they exhibit the following scaling behavior:

$$E|T_X(a,t)|^q \sim C_q a^{\lambda(q)}. \tag{7.1.1}$$

Here, $T_X(a,t)$ is some *multiresolution quantity* related to X and corresponding to scale a and time (position) t. For example, $T_X(a,t)$ can be the increments

$$T_X(a,t) = X(t+a) - X(t) \tag{7.1.2}$$

or nth order increments, or the suitably normalized wavelet coefficients

$$T_X(a,t) = c_X(j,k) = \int X(t)2^j\psi(2^jt-k)dt \tag{7.1.3}$$

corresponding to $a = 2^{-j}$, $t = k2^{-j}$, and where ψ is a (mother) wavelet function. Other, more sophisticated choices will be mentioned below. The quantity $E|T_X(a,t)|^q$ is the qth absolute moment of $T_X(a,t)$. The power q is such that $E|T_X(a,t)|^q < \infty$, though this is influenced not only by X but also by the choice of multiresolution quantity itself. $C_q > 0$ in (7.1.1) is a constant, and $\sim$ indicates the asymptotic equivalence as $a \to 0$, that is, at *small scales*. Exponents $\lambda(q)$ are referred to as *(theoretical) scaling exponents*. The focus is on nonlinear exponent functions $\lambda(q)$ which are thought to be associated with true multifractals. The linear case $\lambda(q) = c_1 q$, on the other hand, is thought to be associated with *monofractals*. The classical example of monofractals is that of *self-similar processes* for which there is a self-similarity exponent $H > 0$ such that the laws of the processes $X(ct)$ and $c^H X(t)$ are the same for all $c > 0$.

The class of self-similar processes has been studied quite extensively, including the processes such as Brownian motion, fractional Brownian motion, Rosenblatt processes, stable fractional motions and others (e.g. [49]). Truly multifractal processes include multiplicative cascades [38, 34], compound Poisson cascades [11], infinitely divisible cascades [10], non-scale invariant infinitely divisible cascades [19], multifractal random walks with respect to self-similar processes [8, 1], self-similar processes in multifractal time [39], random wavelet series [7].

From the **applications** perspective, expected values in (7.1.1) are replaced by sample averages, called the *structure function*,

$$S_n(q,a) = \frac{1}{n_a} \sum_{k=1}^{n_a} |T_X(a, t_k(a))|^q, \tag{7.1.4}$$

where n refers to the sample size of X and n_a to the number of multiresolution quantities $T_X(a, t_k(a))$ used in estimation at scale a. Since sample averages are natural estimators of expected values, it is expected in view of (7.1.1) that

$$S_n(q,a) \sim c_q a^{\zeta(q)}, \quad \text{as } a \to 0, n \to \infty. \tag{7.1.5}$$

Note that a different notation $\zeta(q)$ is used for the *(empirical) scaling exponents* in (7.1.5) (cf. (7.1.1)). This is not accidental. It turns out that for most multifractal models of interest,

$$\lambda(q) = \zeta(q), \quad \text{for } q_*^- < q < q_*^+, \tag{7.1.6}$$

but where, for example, $q_*^+ < q_c^+ = \sup\{q > 0 : E|T_X(a,t)|^q < \infty\}$, and the two functions $\lambda(q)$ and $\zeta(q)$ disagree for $q \in (q_*^+, q_c^+)$. With real data, $\zeta(q)$ is typically estimated through a regression of $\log S_n(q,a)$ against $\log a$ across a range of small scales a. Nonlinear estimated $\widehat{\zeta}(q)$ suggests that multifractals is a plausible model for the data at hand.

Data exhibiting multifractal properties arise and multifractal analysis is very popular in a wide range of applications, including those in physics and chemistry (fully developed turbulence, e.g. [17, 24, 38, 50], DNA sequences, e.g. [6]; diffusion-limited aggregation, e.g. [51]), earth and environmental sciences (topography, e.g. [20, 26]; earthquakes, e.g. [27]; river flows, e.g. [43]; rainfall, e.g. [25, 48]; cloud structure, e.g. [47]), image processing (natural images, e.g. [53, 18]; texture, e.g. [35, 57]), medicine and physiology (ECG, human heartbeat, e.g. [28, 52]; medical images, e.g. [44, 22]), computer science (network traffic, e.g. [46, 33, 54]), economics and finance (stock prices, e.g. [39, 9, 15]; volatility, e.g. [16]). This list is by far exhaustive. ScienceDirect alone gives over 4,000 results to the query "multifractal" - most of these in the applied literature.

From the **analysis** perspective, the focus is on the regularity analysis of deterministic functions. For a deterministic function $f = \{f(t)\}$, let

$$A_\alpha = \{t : \text{regularity of } f(t) \text{ at } t \text{ is } \alpha\}, \quad \alpha > 0. \tag{7.1.7}$$

Regularity of f in (7.1.7) is typically measured by using one of the multiresolution quantities $T_f(a,t)$ as in (7.1.2) and (7.1.3). One would say that f has regularity $\alpha = \alpha(t_0)$ at $t = t_0$ if α is the supremum of $h = h(t_0)$ for which

$$|T_f(a, t_0)| \le C a^h. \tag{7.1.8}$$

For multifractal functions f, the sets A_α, $\alpha > 0$, have a nontrivial structure in the sense that their Hausdorff dimension is positive for a range of α. In this case, one talks about the so-called *multifractal spectrum of singularities* of f defined as

$$d(\alpha) = \dim_H(A_\alpha), \tag{7.1.9}$$

where $\dim_H(A)$ indicates the Hausdorff dimension (see, e.g. [23]) of a set A. For deterministic functions, it is still meaningful to consider the corresponding structure function $S_n(q,a)$ in (7.1.4), and

$$\zeta(q) = \liminf_{a\to 0} \frac{\log S_n(q,q)}{\log a}. \tag{7.1.10}$$

It then turns out that, in many cases of interest, the functions d and ζ can be related through the Legendre transformation as

$$d(\alpha) = \inf_{q\neq 0}(1-\zeta(q)+\alpha q) \tag{7.1.11}$$

(1 above is replaced by p in higher dimensions p).

The relation (7.1.11) is often referred to as *multifractal formalism* in the literature. The term "multifractal" refers to a range of exponents α characterizing the signal on various carrier sets A_α. On the functional analysis side, this approach based on regularity of deterministic functions has been advocated by a number of authors, most notably Jaffard [29, 30, 32].

7.2 Recent Developments and Open Problems

Exciting developments have recently been made in connection to all three directions listed in Section 7.1: **probability/statistics**, **applications** and **analysis**. Despite significant progress, however, numerous open questions remain to be addressed.

7.2.1 Recent Developments

For example, originating from the **analysis** direction, *wavelet leaders* [30, 31] have emerged as new and superior multiresolution quantities $T_X(a,t)$ in (7.1.1) to use in multifractal analysis. Wavelet leaders are defined as

$$T_X(a,t) = L_X(j,k) = \sup_{\lambda'\subset 3\lambda} |c_X(j',k')|. \tag{7.2.1}$$

Here, $\lambda = \lambda_{j,k} = [k2^{-j},(k+1)2^{-j})$, $\lambda' = \lambda_{j',k'} = [k'2^{-j'},(k'+1)2^{-j'})$ and $3\lambda = \lambda_{j,k-1}\cup\lambda_{j,k}\cup\lambda_{j,k+1}$. The supremum in (7.2.1) thus consists of the largest wavelet coefficient $c_X(j',k')$ computed at all finer scales $2^{-j'}\le 2^{-j}$ within a narrow time neighborhood, $(k-1)2^{-j}\le k'2^{-j'} < (k+2)2^{-j}$.

The basic idea behind wavelet leaders is that they allow to "look" into scaling exponents for negative values of q. In probabilistic terms, this results from taking the supremum in (7.2.1). With the supremum, the values of wavelet leaders that are close to zero become less likely and hence a higher number of negative moments become available. Even more surprisingly perhaps, wavelet leaders inherit the same scaling behavior (7.1.1) as when using differences or wavelet coefficients. Wavelet leaders have been used for multifractal analysis of real data in [55, 56, 58].

From the **probability/statistics** perspective, for example, significant developments are tied to recent progress in the probabilistic analysis of the so-called branching random walks (e.g. [4, 5]). Branching random walks are closely related to the classical constructions of multifractal measures such as multiplicative cascades. By using this connection, for example, the extremal properties of multiplicative cascades were derived in [40, 14], the multiplicative cascades at the so-called critical regime were studied in [12]. In other directions, probabilistic connections to certain PDEs can be found in [41]. Connections to quantum theory, the KPZ relation, appear in [13, 45]. Statistical inference questions are studied in [42, 36, 37].

Among recent **applications**, multifractal techniques involving wavelet leaders were extended to image analysis [57, 58]. An example concerns the classification of paintings [3]. Recent applications to medicine include those to heart rate variability [2] and fMRI [21]. A number of other applications are related to scaling at large.

7.2.2 Open Problems

At the **analysis** level, the multifractal formalism described in Section 7.1 above provides a potentially powerful tool to measure the multifractal spectrum from real-world data. Yet, a significant number of theoretical questions about its practical use remain open. What appropriate multiresolution quantities, function increments, wavelet coefficients, or more complicated quantities derived from wavelet coefficients such as wavelet leaders, should be used? What function spaces do they correspond to?

The multifractal formalism relies on a Legendre transform and thus on a concavity assumption. What can be done for data that do not fulfill such an assumption? As such, the multifractal formalism does not bring any additional information related to the nature of the singularities that exist in data. How should the formalism be modified to enable the detection of the local regularity of potentially oscillating nature (chirp-type), against the simpler case of non-oscillating (cusp-type) singularities? In several dimensions, how can anisotropy phenomena be analyzed?

At the **probabilisty/statistics** level, the gap between the deterministic definition of the multifractal spectrum and its application to each given sample path of stochastic processes remain to be formalized in a precise manner. Because real-world data are naturally envisaged as realizations of random models by practitioners, bridging that gap would pave the way towards crucial practical issues such as parameter estimation or hypothesis testing performance evaluation.

For example, what are the confidence intervals for given estimates? How can one test formally what model better fits data? Such issues could be addressed on a number of stochastic models designed to serve as reference and benchmark to compare applications to. Along similar lines, the (multi)fractal properties of data are often expected by practitioners to serve as a tool permitting to finely quantify or measure intricate statistical properties of data, such as strong dependencies or subtle departures of data from joint Gaussianity. These properties need to be understood in greater depth for benchmark multifractal processes.

At the **application** level, in many situations, because of the explosion of sensor designs and deployment, the data to analyze no longer consist of univariate signals (or functions). They could either take values in a d-dimensional space (a collection of time series is recorded jointly from one same system) or be indexed by a multiparameter (a field). Notably, there has been a growing interest to incorporate fractal and multifractal analysis into image processing toolboxes, with diverse applications ranging from medicine to satellite imagery. This change in the nature of data to be analyzed raised theoretical and practical issues that have so far been barely addressed.

For example, how should the multivariate multifractal spectrum be defined? How does the notion of anisotropy that naturally comes with images take its place in the multifractal analysis? How could one distinguish between an anisotropic but regular texture that has been superimposed to an isotropic fractal texture from a texture where the anisotropy is truly built-in its (multi)fractal properties? Images can exhibit boundaries (that split them into homogeneous subregions) that may themselves have fractal properties. Can they be distinguished from the fractal properties of the textures? Images may consist of the juxtaposition of fractal and regular patches of textures. How can they be identified?

At the modeling level, practitioners are often facing situations where the outcome of the analysis does not resemble the output of standard theoretical models. It would thus certainly be of interest to design a wide collection of deterministic and stochastic models, whose multifractal properties would be well-understood and could serve as a frame and guideline in the analysis of real-world data. For instance, developing models which incorporate oscillating singularities, or anisotropy, or which display non-concave or non-smooth multifractal spectra would be of great interest.

7.3 Presentation Highlights

The workshop had 18 talks spread over five days and 9 poster presentations in two sessions. One goal of the organizers was to have fewer talks along with unlimited opportunities for poster presentations, so that participants could have ample time for informal discussions. Another goal of the organizers was to gather researchers representing the three perspectives of multifractal analysis discussed above: **probability/statistics**, **applications** and **analysis**.

For example, the first day of the workshop already featured talks in the three directions. Murad Taqqu kicked off the workshop by presenting recent work on the Rosenblatt and related self-similar processes. The talk helped set stage for the workshop by reviewing the basic concepts behind monofractal processes. A highlight of the talk were several intriguing open problems about the marginal distribution of the Rosenblatt process. In a following talk on the same day, on the other hand, Julien Barral started by recalling the fundamental concepts behind multifractal analysis. Among the questions considered was that of the validity of multifractal formalism. An example included a finer behavior of multiplicative cascades in the regimes previously excluded from multifractal analysis. The first day of the workshop was closed with the talk of Herwig Wendt on wavelet leaders for multifractal analysis, touching upon not only their applied but also theoretical aspects.

Related to **probability/statistics**, two other talks were on anisotropic scaling of random fields. Gustavo Didier presented recent work on the structure of self-similar anisotropic, possibly vector random fields. Interesting points were made on the interplay between domain and range properties of such fields. One of the main messages was that a number of interesting issues arise even in the case of self-similarity (monofractality). Some of this was echoed in the talk by Beatrice Vedel. But in a significant step further, Beatrice Vedel also discussed ways of combining multifractality and anisotropy.

Paul Balança presented his recent work on oscillating singularities for Lévy processes. The existence of such singularities for any class of common stochastic processes has been a long standing problem. Paul Balança has made the first real progress in addressing this question, within the large family of Lévy processes. Edward Waymire spoke on the convergence of normalized multiplicative cascades in the so-called strong disorder. Using the results on branching random walks recently derived in the probability literature, not only the convergence could be proved but the limit could also be characterized in revealing ways.

In the poster sessions, the talk of Murad Taqqu was nicely complemented and extended by Shuyang Bai. Julien Hamonier's poster concerned estimation issues in the so-called linear multifractional stable motion. Nikolai Leonenko presented work on the construction of multifractal processes through products of geometric stationary processes, and on detection of multifractality under heavy tails. Peter Morter's poster considered the condensation phenomenon in the Kingman's model.

Other talks on **applications** were by: Shaun Lovejoy who spoke on scaling and multifractals in geophysics; Franklin Mendivil on fractal image processing; Philippe Ciuciu on multifractal modeling of fMRI signals; Ken Kyono on modeling heart rate variability; Alain Arneodo on scaling in genomics; and Patrick Flandrin on data-driven methods of scale invaraince analysis.

In the poster sessions, Patrice Abry presented his work on using multifractals for drawing classification. Joan Bruna advocated the use of scattering moments in multifractal analysis. The poster of Stephanie Randon de la Torre concerned applications to financial markets. Finally, Roberto Leonarduzzi considered the automatic selection of scaling range in multifractal analysis.

On the **analysis** side, Jun Kigami spoke on the multifractal structures arising with diffusions in inhomogeneous media, with a surprising role payed by a metric chosen in the multifrcatal analysis. Ka-sing Lau's talk focused on spectral properties of self-similar sets and measures, describing the recent progress made in this challenging research direction. Stephane Seuret spoke on p–exponents and p–multifractal spectrum of some lacunary Fourier series, with fascinating connections to number theory, harmonic analysis and dynamical systems.

Yang Wang revisited the celebrated Cantor set by raising surprising open questions and providing partial answers. Michel Zinsmeister spoke on the multifractality of whole-plane SLE. Finally, in a poster session, Céline Esser revisited the so-called S^{ν} spaces with wavelet leaders to detect non concave and non increasing spectra.

7.4 Scientific Progress Made and Outcome of the Meeting

The organized workshop has met its main objective of bringing together experts in fractals and multifractals from three different areas of research:

- probabilistic modeling, statistics and stochastic processes,
- signal and image processing, and applications at large,
- functional analysis and geometric measure theory.

Since workshops gathering researchers from these three communities are rare, the meeting was unique in this sense.

In bringing together these research areas, cross-fertilization between communities was fostered, easing transfers of theoretical results to real applications, as well as relevant applied questions to theoretical formalizations. The meeting provided an excellent overview of the field, from the three perspectives described above. It generated, often lively, discussions on open and crucial issues in multifractal analysis. The meeting also served as the starting point of new collaborations between researchers with different cultures and backgrounds in order to go towards the resolution of these issues.

Participants

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Bibliography

[1] Abry, P., P. Chainais, L. Coutin and V. Pipiras (2009). Multifractal random walks as fractional Wiener integrals, IEEE Transactions on Information Theory, 55(8), 3825-3846.

[2] Abry, P., H. Wendt, S. Jaffard, H. Helgason, P. Goncalves, E. Pereira, C. Gharib, P. Gaucherand and M. Doret (2010), Methodology for multifractal analysis of heart rate variability: From LF/HF ratio to wavelet leaders, Engineering in Medicine and Biology Society (EMBC), 2010 Annual International Conference of the IEEE.

[3] Abry, P., S. Jaffard and H. Wendt (2013). When Van Gogh meets Mandelbrot: Multifractal classification of painting's texture, Signal Processing, 93(3), 554-572.

[4] Aïdékon, E. (2013). Convergence in law of the minimum of a branching random walk, The Annals of Probability, 41(3A), 13621426.

[5] Aïdékon, E. and Z. Shi (2014). The SenetaHeyde scaling for the branching random walk, The Annals of Probability, 42(3), 959993.

[6] Arneodo, A., B. Audit, N. Decoster, J.-F. Muzy and C. Vaillant (2002). Wavelet based multifractal formalism: Application to DNA sequences, satellite images of the cloud structure and stock market data. In *The Science of Disasters: Climate Disruptions, Heart Attacks, and Market Crashes* (A. Bunde, J. Kropp and H. J. Schellnhuber, eds.), pp. 26-102. Springer Verlag, Berlin.

[7] Aubry, J.-M. and S. Jaffard (2002). Random wavelet series, Communications in Mathematical Physics, 227, 483-514.

[8] Bacry, E., J. Delour and J. F. Muzy (2001). Multifractal random walk, Physical Review E, 64, 026103.

[9] Bacry, E., J. Delour and J. F. Muzy (2001-2). Modelling financial time series using multifractal random walks, Physica A, 299, 84-92.

[10] Bacry, E. and J. F. Muzy (2003). Log-infinitely divisible multifractal processes, Communications in Mathematical Physics, 236, 449-475.

[11] Barral, J. and B. B. Mandelbrot (2002). Multifractal products of cylindrical pulses, Probability Theory and Related Fields, 124, 409-430.

[12] Barral, J., A. Kupiainen, M. Nikula, E. Saksman and C. Webb (2014). Critical Mandelbrot cascades, Communications in Mathematical Physics, 325(2), 685711.

[13] Benjamini, B. and O. Schramm (2009). KPZ in one dimensional random geometry of multiplicative cascades, Communications in Mathematical Physics, 289, 653-662.

[14] Bramson, M. and O. Zeitouni (2009). Tightness for a family of recursion equations, The Annals of Probability, 37(2), 615-653.

[15] Calvet, L. E. and A. Fisher (2002). Multifractality in asset returns: theory and evidence, The Review of Economics and Statistics, 84(3), 381-406.

[16] Calvet, L. E. and A. Fisher (2008). *Multifractal Volatility: Theory, Forecasting, and Pricing*, Academic Press.

[17] Castaing, B., F. Y. Gagne and E. J. Hopfinger (1990). Velocity probability density functions of high Reynolds number turbulence, Physica D, 46, 177-200.

[18] Chainais, P. (2007). Infinitely divisible cascades to model the statistics of natural images, IEEE Transactions on Pattern Analysis and Machine Intelligence, 29(12), 2105-2119.

[19] Chainais, P., R. Riedi and P. Abry (2005). On non-scale-invariant infinitely divisible cascades, IEEE Transactions on Information Theory, 51(3), 1063-1083.

[20] Cheng, Q. and F. P. Agterberg (1996). Multifractal modeling and spatial statistics, Mathematical Geology, 28(1), 1-16.

[21] Ciuciu, P., P. Abry, C. Rabrait and H. Wendt (2009). Log wavelet leaders cumulant based multifractal analysis of EVI fMRI time series: evidence of scaling in ongoing and evoked brain activity, IEEE Journal of Selected Topics in Signal Processing, 2(6), 929-943.

[22] Derado, G., K. Lee, O. Nicolis, F. D. Bowman, M. Newell, F. F. Rugger and B. Vidakovic (2008). Wavelet-based 3-D multifractal spectrum with applications in breast MRI images. In *Bioinformatics Research and Applications*, Lecture Notes in Computer Science, Volume 4983 (I. Mandoiu, R. Sunderraman, and A. Zelikovsky, eds.), pp. 281-292. Springer-Verlag Berlin Heidelberg.

[23] Falconer, K. J. (2003). *Fractal Geometry. Mathematical Foundations and Applications*, John Wiley & Sons, Inc., Hoboken, New Jersey.

[24] Frisch, U. (1991). From global scaling, a la Kolmogorov, to local multifractal scaling in fully developed turbulence, Proceedings: Mathematical and Physical Sciences, Turbulence and Stochastic Process: Kolmogorov's Ideas 50 Years On, 434(1890), 89-99.

[25] Gupta, V. K. and E. Waymire (1990). Multiscaling properties of spatial rainfall and river flow distributions, Journal of Geophysical Research, 95(D3), 1999-2009.

[26] Gagnon, J.-S., S. Lovejoy and D. Schertzer (2006). Multifractal earth topography, Nonlinear Processes in Geophysics, 13, 541-570.

[27] Hirabayashi, T., K. Ito and T. Yoshii (1992). Multifractal analysis of earthquakes, Pure and Applied Geophysics, 138(4), 591-610.

[28] Ivanov, P. C., L. A. N. Amaral, A. L. Goldberger, S. Havlin, M. G. Rosenblum, Z. R. Struzik and H. E. Stanley (1999). Multifractality in human heartbeat dynamics, Nature, 399, 461-465.

[29] Jaffard, S. (1997). Multifractal formalism for functions. I. Results valid for all functions, SIAM Journal on Mathematical Analysis, 28(4), 944-970.

[30] Jaffard, S. (2004). Wavelet techniques in multifractal analysis. In *Fractal Geometry and Applications: a Jubilee of Benoît Mandelbrot, Part 2*, Proc. Sympos. Pure Math., 72, pp. 91-151. Amer. Math. Soc., Providence, RI.

[31] Jaffard, S., B. Lashermes and P. Abry (2006). Wavelet leaders in multifractal analysis. In *Wavelet Analysis and Applications* (T. Qian, M. I. Vai and X. Yuesheng, eds.), pp. 219-264. Birkhäuser Verlag, Basel, Switzerland.

[32] Jaffard, S. (2009). Wavelet methods for multifractal analysis of functions. In *Scaling, Fractals and Wavelets* (P. Abry, P. Gonçalves, and J. Lévy Véhel, eds.), pp. 103-137. Wiley.

[33] Krishna, P M., V. M. Gadre and U. B. Desai (2003), *Multifractal Based Network Traffic Modeling*, Springer.

[34] Kahane, J.-P. and J. Peyriere (1976). Sur certaines martingales de Benoit Mandelbrot, Advances in Mathematice, 22(2), 131-145.

[35] Levy Vehel, J., P. Mignot and J.-P. Berroir (1992). Multifractals, texture, and image analysis, Proceedings of 1992 IEEE Computer Society Conference on Computer Vision and Pattern Recognition, 661-664.

[36] Ludena, C. (2008). Lp-variations for multifractal fractional random walks, The Annals of Applied Probability, 18(3), 1138-1163.

[37] Ludena, C. (2009). Confidence intervals for the scaling function of multifractal random walks, Statistics & Probability Letters, 79(1), 1186-1193.

[38] Mandelbrot, B. B. (1974). Intermittent turbulence in self-similar cascades: divergence of high moments and dimension of the carrier, Journal of Fluid Mechanics, 62(2), 331-358.

[39] Mandelbrot, B. B. (1999). A multifractal walk down Wall Street, Scientific American, February 1999, 70-73.

[40] Muzy, J. F., E. Bacry and A. Kozhemyak (2006). Extreme values and fat tails of multifractal fluctuations, Physical Review E, 73, 066114.

[41] Ossiander, M. (2005). A probabilistic representation of solutions of the incompressible Navier-Stokes equations in R3, Probability Theory and Related Fields, 133, 267-298.

[42] Ossiander, M. and E. C. Waymire (2000). Statistical estimation for multiplicative cascades, The Annals of Statistics, 28(6), 1533-1560.

[43] Pandey, G. (1998). Multifractal analysis of daily river flows including extremes for basins of five to two million square kilometres, one day to 75 years, Journal of Hydrology 208, 62-81.

[44] Reljin, I. S. and B. D. Reljin (2002). Fractal geometry and multifractals in analyzing and processing medical data and images, Archive of Oncology, 10(4), 283-293.

[45] Rhodes, R. and V. Vargas (2011). KPZ formula for log-infinitely divisible multifractal random measures, ESAIM Probab. Stat. 15, 358371.

[46] Riedi, R. H., M. S. Crouse, V. J. Ribeiro and R. G. Baraniuk (1999). A multifractal wavelet model with application to network traffic, IEEE Transactions on Information Theory, 45(3), 992-1018.

[47] Roux, S. G., A. Arneodo and N. Decoster (2000), A wavelet-based method for multifractal image analysis. III. Applications to high-resolution satellite images of cloud structure, The European Physical Journal B, 15, 765-786.

[48] Roux, S. G., V. Venugopal, K. Fienberg, A. Arneodo and E. Foufoula-Georgiou (2009), Evidence for inherent nonlinearity in temporal rainfall, Advances in Water Resources, 32, 41-48.

[49] Samorodnitsky, G. and M. S. Taqqu (1994). *Stable Non-Gaussian Random Processes. Stochastic Models with Infinite Variance*. Stochastic Modeling, Chapman & Hall, New York.

[50] She, Z.-S. and E. Leveque (1994). Universal scaling laws in fully developed turbulence, Physical Review Letters, 72(3), 336-339.

[51] Stanley, H. E. and P. Meakin (1988). Multifractal phenomena in physics and chemistry, Nature, 335, 405-409.

[52] Stanley, H. E., L. A. N. Amaral, A. L. Goldberger, S. Havlin, P. C. Ivanov and C.-K. Peng (1999). Statistical physics and physiology: Monofractal and multifractal approaches, Physica A, 270, 309-324.

[53] Turiel, A. and N. Praga (2000). The multifractal structure of contrast changes in natural images: from sharp edges to textures, Neural Computation, 12, 763-793.

[54] Veitch, D., N. Hohn and P. Abry (2005). Multifractality in TCP/IP traffic: the case against, Computer Networks, 48, 293-313.

[55] Wendt, H., P. Abry and S. Jaffard (2007). Bootstrap for empirical multifractal analysis, IEEE Signal Processing Magazine, 24(4), 38-48.

[56] Wendt, H. and P. Abry (2007). Multifractality tests using bootstrapped wavelet leaders, IEEE Transactions on Signal Processing, 55(10), 811-820.

[57] Wendt, H., P. Abry, S. Jaffard, H. Ji and Z. Shen (2009). Wavelet Leader multifractal analysis for texture classification, 16th IEEE International Conference on Image Processing (ICIP), 3829-3832.

[58] Wendt, H., S. G. Roux, S. Jaffard and P. Abry (2009). Wavelet leaders and bootstrap for multifractal analysis of images, Signal Processing, 89(6), 1100-1114.

Chapter 8

Advances in Scalable Bayesian Computation (14w5125)

March 2 - 7, 2014

Organizer(s): Luke Bornn (Harvard University), Nando de Freitas (University of British Columbia), Christian Robert (Ceremade - Université Paris-Dauphine), Scott Schmidler (Duke University)

8.1 Workshop Objectives

As the statistical models used to understand complex systems grow, the methods used to fit these models must scale accordingly. While advanced computational methods are being developed to fit these complex models, their speed and memory requirements often demand tremendous computational power via large clusters. This approach of relying on ever larger computational resources is quickly becoming unsustainable, particularly for practitioners for whom these resources are not available. As such, there is a large and growing need for statistically efficient methods which scale in terms of speed and memory while being straightforward to implement and communicate.

Several communities are currently working on methods for Bayesian computation which are scalable; however, interaction between these communities has been limited and as such significant cross-community learnings are being missed. As the communities grow and diverge, it is important to bridge the gap at this crucial stage in the development of scalable methods.

Currently, the exchanges between the Monte Carlo (including MCMC, SMC, and ABC), INLA, optimization, and other communities remain surprisingly limited. With each group having their own workshops and conferences, and little work being done to compare and educate between the various approaches, this workshop strived to:

(1) Gather people from different research communities and foster links between these communities. (2) Expose the various communities to the state of the art in scalable Bayesian computation methods, including MCMC, SMC, ABC, INLA, optimization, and other methods. (3) Classify the advantages, limitations, and possibilities from each class of methods, and equip all participants with the knowledge to bridge the existing gap in scalable Bayesian computation. (4) Create a venue to encourage innovation through the synthesis and development of new approaches by combining existing, currently disjoint, approaches to Bayesian computation.

In reaching out to statisticians, computer scientists, mathematicians, and others working in Bayesian computation as potential participants, the desire for such a workshop was overwhelming. To quote several of the contacted participants, a fantastic and very timely conference topic, sounds incredibly interesting and highly pertinent, a particularly timely topic, and a great opportunity to see what others are doing.

8.2 Overview of the Field

While linear models under the assumption of Gaussian noise were the hallmark of early 20th century statistics, the past several decades have seen an explosion in statistical models which produce complex and high-dimensional density functions for which simple, analytical integration is impossible. This growth was largely fueled by renewed interest in Bayesian statistics accompanying the Markov chain Monte Carlo (MCMC) revolution in the 1990s. With the computational power to explore the posterior distributions arising from Bayesian models, MCMC allowed practitioners to build models of increasing size and complexity.

Though advanced MCMC methods are being actively developed to fit the extreme scale data arising in fields ranging from sociology to climatology, their speed and memory requirements often demand tremendous computing power. This approach of relying on ever larger computational resources is quickly becoming unsustainable, particularly for practitioners for whom these resources are not available. As such, there is a persistent and growing need for statistically efficient methods which scale in terms of speed and memory while also allowing for straightforward implementation and communication.

In response to the computational cost associated with MCMC, the machine learning community has steadily moved towards variational inference, which approximates the original complex model with a simple, tractable model. While such approximations lead to the development of quick, simple solvers, they are known to systematically underestimate uncertainty, and it is notoriously difficult to judge the accuracy of the implicit approximation in general situations.

8.3 Presentation Highlights

8.3.1 Day 1

This was the first day of our workshop Advances in Scalable Bayesian Computation and the theme was probabilistic programming. Indeed, both Vikash Mansinghka and Frank Wood gave talks about this concept, Vikash detailing the specifics of a new programming language called Venture and Frank focussing on his state-space version of the above called Anglican. This is a version of the language Church, developed to handle probabilistic models and inference.

The other talks of Day 1 were of a more classical nature with Pierre Jacob explaining why non-negative unbiased estimators were impossible to provide in general, including an interesting objective Bayes example. Then Sumeet Singh presented a joint work with Nicolas Chopin on the uniform ergodicity of the particle Gibbs sampler with a nice coupling proof. And Maria Lomeli gave an introduction to the highly general Poisson-Kingman mixture models as random measures, which encompasses all of the previously studied non-parametric random measures, with an MCMC implementation that included a latent variable representation for the alpha-stable process behind the scene, representation that could be (and maybe is) also useful in parametric analyses of alpha-stable processes.

We also had an open discussion in the afternoon that ended up being quite exciting, with a few of us voicing out some problems or questions about existing methods and others making suggestions or contradictions.

Speaker: **Mansinghka, Vikash** (MIT)
Title: *Probabilistic computing for Bayesian inference*
Abstract: Although probabilistic modeling and Bayesian inference provide a unifying theoretical framework for uncertain reasoning, they can be difficult to apply in practice. Inference in simple models can seem intractable, while more realistic, flexible models can be difficult to specify, let alone implement correctly. My talk will describe three prototype probabilistic computing systems — including probabilistic programming languages, a Bayesian database system, and intentionally stochastic hardware — designed to mitigate these challenges.

I will focus on Venture, a new, open-source, Turing-complete probabilistic programming platform that aims to be sufficiently expressive, extensible and efficient for general-purpose use. Venture programmers specify models via executable code, where random choices correspond to latent variables; this approach can yield a 100x reduction in code size for state-of-the-art models. Multiple scalable, computationally universal inference algorithms are provided, based on MCMC, conditional SMC and mean field variational techniques. Unlike probabilistic programming tools like BUGS or Church, users can also reprogram the inference strategy for each application and easily

implement novel approximation schemes. I will review applications of Venture to text modeling with millions of observations; 2D and 3D computer vision problems; and structured inverse problems in geophysics.

I will also touch on the ways the ideas behind Venture fit together into a mathematically coherent software and hardware stack for Bayesian inference.

This talk includes joint work with Daniel Roy, Eric Jonas, Daniel Selsam and Yura Perov.

Speaker: **Jacob, Pierre** (University of Oxford)
Title: *On non-negative unbiased estimators*
Abstract: I will talk about performing exact inference using Monte Carlo methods, that is, estimating an integral in such a way that the error goes to zero when the computational effort increases to infinity. This is in general possible when the target probability density function can be unbiasedly estimated pointwise, as in the pseudo-marginal approach. However it requires almost surely non-negative unbiased estimators which are not always available. In this talk I will talk about schemes providing unbiased estimators and about the sign problem, leading to a general result stating the non-existence of schemes yielding non-negative unbiased estimators. I will discuss the consequences of that result in some statistical settings.

Speaker: **Lomeli, Maria** (Gatsby Unit, University College London)
Title: *Marginal Sampler for σ-Stable Poisson-Kingman Mixture Models*
Abstract: Bayesian nonparametric mixture models reposed on random probability measures like the Dirichlet process allow for flexible modelling of densities and for clustering applications where the number of clusters is not fixed a priori. Our understanding of these models has grown significantly over the last decade: there is an increasing realisation that while these models are nonparametric in nature and allow an arbitrary number of components to be used, they do impose significant prior assumptions regarding the clustering structure which may or may not conform to actual prior beliefs.

In recent years, there is a growing interest in extending modelling flexibility beyond the classical Dirichlet process first proposed by Ferguson. Examples include Pitman-Yor processes, normalized inverse Gaussian processes, and normalized random measures. With each process, additional flexibility comes with additional developments in characterizing properties of each process. These characterizations are useful to develop tractable Markov chain Monte Carlo posterior simulation algorithms.

In this talk we explore the use of a very wide class of random probability measures, called σ-stable Poisson-Kingman processes or Gibbs-type priors with positive indices, for Bayesian nonparametric mixture modelling. This class of processes encompasses all known tractable random probability measures proposed in the literature so far. We argue that it forms a natural class in which to study. We propose a number of characterizations of the process which allow the development of tractable inference algorithms. Specifically, we develop an efficient marginal sampler which can be used for posterior simulation for the whole class of nonparametric priors.

(Joint work with Stefano Favaro and Yee Whye Teh)

Speaker: **Singh, Sumeetpal** (Unievrsity of Cambridge)
Title: *On Particle Gibbs Sampling*
Abstract: The particle Gibbs sampler is a Markov chain Monte Carlo (MCMC) algorithm to sample from the full posterior distribution of a state-space model. It does so by executing Gibbs sampling steps on an extended target distribution defined on the space of the auxiliary variables generated by an interacting particle system. This paper makes the following contributions to the theoretical study of this algorithm. Firstly, we present a coupling construction between two particle Gibbs updates from different starting points and we show that the coupling probability may be made arbitrarily close to one by increasing the number of particles. We obtain as a direct corollary that the Particle Gibbs kernel is uniformly ergodic. Secondly, we show how the inclusion of an additional Gibbs sampling step that reselects the ancestors of the Particle Gibbs extended target distribution, which is a popular approach in practice to improve mixing, does indeed yield a theoretically more efficient algorithm as measured by the asymptotic variance. Thirdly, we extend Particle Gibbs to work with lower variance resampling schemes. A detailed numerical study is provided to demonstrate the efficiency of Particle Gibbs and the proposed variants.

This is joint work with Nicolas Chopin.

Speaker: **Wood, Frank** (University of Oxford)
Title: *A new approach to probabilistic programming inference*
Abstract: Probabilistic programming languages hold the promise of dramatically accelerating the development of both new statistical models and inference strategies. In probabilistic programs, variables can take on random values at run time and inference is performed by calculating expectation values over all execution traces that are in agreement with a set of observed data. This allows statistical models to be represented in a concise and intuitive manner, enabling more rapid iteration over model variants. Inference schemes, when implemented as a backend to a programming framework, can easily be tested on a large collection of models, enabling a much more systematic comparison of the efficacy of inference strategies.

We introduce the use of particle Markov chain Monte Carlo to perform probabilistic programming inference. Our approach is simple to implement, easy to parallelize, and supports accurate inference in models that make use of complex control flow, including stochastic recursion. It also includes primitives from Bayesian nonparametric statistics. Our experiments show that this approach can be more efficient than previously introduced single-site Metropolis-Hastings methods.

Joint work with Brooks Paige, Jan Willem van de Meent, and Vikash Mansingkha

8.3.2 Day 2

The main theme of the second day was about brains In fact, Simon Barthelms research originated from neurosciences, while Dawn Woodard dissected a brain (via MRI) during her talk! Simons talk was quite inspiring, using Tibshirani et al.s trick of using logistic regression to estimate densities as a classification problem central to the method and suggesting a completely different vista for handling normalising constants. Then Raazesh Sainudiin gave a detailed explanation and validation of his approach to density estimation by multidimensional pavings/histograms, with a tree representation allowing for fast merging of different estimators. Raaz had given a preliminary version of the talk at CREST last Fall, which helped with focussing on the statistical aspects of the method. Chris Strickland then exposed an image analysis of flooded Northern Queensland landscapes, using a spatio-temporal model with changepoints and about 18,000 parameters, still managing to get an efficiency of O(np) thanks to two tricks. Then it was time for the group photograph outside in a balmy -18 and an open research time that was quite profitable.

In the afternoon sessions, Paul Fearnhead presented an auxiliary variable approach to particle Gibbs, which again opened new possibilities for handling state-space models, but also connecting to Xiao-Li Mengs reparameterisation devices. Questions were asked whether or not the SMC algorithm was that essential in a static setting, since the sequence could be explored in any possible order for a fixed time horizon. Then Emily Fox gave a 2-for-1 talk, mostly focussing on the first talk, where she introduced a new technique for approximating the gradient in Hamiltonian (or Hockey!) Monte Carlo, using second order Langevin. She did not have much time for the second talk, which intersected with the one she gave at BNPski in Chamonix, but focussed on a notion of sandwiched slice sampling where the target density only needs bounds that can get improved if needed. A cool trick! And the talks ended with Dawn Woodards analysis of time varying 3-D brain images towards lesion detection, through an efficient estimation of a spatial mixture of normals.

Speaker: **Simon Barthelmé** (University of Geneva)
Title: *LATKES in Space: flexible models for spatial sequences*
Abstract:

Most questions that arise in the analysis of spatial data are some variant of the following: “Why are there more X in area A than in other places?”. In epidemiology for example, the question pertains to disease cases, in ecology, to some particular plant or animal, and in astrostatististics, to galaxies. Point process models try to answer these questions by relating the intensity of a phenomenon in a certain region of space to a set of spatial covariates that might explain the data.

An interesting application of point process models is to eye movements, where the goal is to understand why people look in certain places more often than others. In applications of spatial statistics to eye movements the *temporal* dimension also plays an important role: where the eyes move to depends on where they were before.

In this talk I will outline an extension of point process models to spatial sequences, based on *Log-Additive Transition Kernels* (LATKES).

I will show that the "logistic regression trick" used for non-parametric density modelling, can be extended to sequences of dependent data. A consequence is that inference in LATKES models can be transformed into logistic regression problem, at the cost of some Monte Carlo error. I will discuss links with the Poisson-multinomial transform, variational bounds on the likelihood, and inference in unnormalised statistical models, a set of topics which turn out to be closely related.

Speaker: **Sainudin, Raazesh** (University of Canterbury)
Title: *Statistical Regular Pavings for Bayesian Non-parametric Density Estimation*
Abstract: We present a novel method for averaging a sequence of histogram states visited by a Metropolis-Hastings Markov chain whose stationary distribution is the posterior distribution over a dense space of tree-based histograms. The computational efficiency of our posterior mean histogram estimate relies on a statistical data-structure that is sufficient for non-parametric density estimation of massive, multi-dimensional metric data. This data-structure is formalized as statistical regular paving (SRP). A regular paving (RP) is a binary tree obtained by selectively bisecting boxes along their first widest side. SRP augments RP by mutably caching the recursively computable sufficient statistics of the data. The base Markov chain used to propose moves for the Metropolis-Hastings chain is a random walk that data-adaptively prunes and grows the SRP histogram tree. We use a prior distribution based on Catalan numbers and detect convergence heuristically. The L1-consistency of the the initializing strategy over SRP histograms using a data-driven randomized priority queue based on a generalized statistically equivalent blocks principle is proved by bounding the Vapnik-Chervonenkis shatter coefficients of the class of SRP histogram partitions. The performance of our posterior mean SRP histogram is empirically assessed for large sample sizes simulated from several multivariate distributions that belong to the space of SRP histograms.

We also present arithmetical capabilities of the SRPs, including tree-based algorithms and structures for marginalization, conditional density extraction, fast look-up of product likelihood in validation, uniform approximation of other density estimates as SRP histograms and more general arithmetic operations. These operations are used in an SRP-based ABC method and in fast cross-validation for prior-selection.

This is joint work with Dominic Lee, Jennifer Harlow and Gloria Teng.

Speaker: **Christopher Strickland** (UNSW)
Title: *A scalable Bayesian changepoint methodology for large space-time data sets*
Abstract: A scalable Bayesian changepoint methodology is developed to analyse large space-time data sets, which allows for an unknown number of change points in the common components of a hierarchical space-time model. The computational cost scales linearly with the sample size, across both space and time, and the methodology is simulation efficient. The methodology is used to assess the impact of extended inundation on the ecosystem of the Gulf Plains bioregion in northern Australia. Our data set consists of nearly 5 million observations, and our methodology is sufficiently efficient to conduct a full Bayesian analysis in tens of minutes, despite the complexity of the proposed model.

Speaker: **Fearnhead, Paul** (Lancaster University)
Title: *Reparameterisations for Particle MCMC*
Abstract: Consider inference for a state-space model with unknown parameters. Standard implementation of Particle MCMC involves using an MCMC kernel to propose a new value for the parameters, and then a particle filter to propose a new value for the path of the state process conditional on this value for the parameters. However alternative approaches are possible. For example we could use the particle filter to update some of the parameters (as well as the state). This reduces the dependence in the MCMC update, but at the expense of greater Monte Carlo error when running the particle filter. We consider generalisations of this approach, based on introducing pseudo observations. This allows us to run the particle filter conditional on part of the information about the current set of parameters and state path.

We give examples of how this approach can improve the mixing in particle Gibbs, and help with the initialisation of the particle filter.

Speaker: **Fox, Emily** (University of Washington)
Title: *2-for-1: Stochastic Gradient Hamiltonian Monte Carlo and Bayesian Learning of DPP Kernels*
Abstract: In this talk, we will present two separate vignettes on Bayesian computation. One is stochastic gradient Hamiltonian Monte Carlo (HMC). HMC methods provide a mechanism for defining distant proposals with high acceptance probabilities in a Metropolis-Hastings framework, enabling more efficient exploration of the state space than standard random-walk proposals. However, a limitation of HMC methods is the required gradient computation for simulating the Hamiltonian dynamical system—such a computation is infeasible in problems involving a large sample size or streaming data. We instead consider the impacts of a noisy gradient estimate computed from a subset of the data. Surprisingly, the natural implementation of the stochastic approximation can be arbitrarily bad. To address this problem we introduce a variant that uses second-order Langevin dynamics with a friction term that counteracts the effects of the noisy gradient, maintaining the desired target distribution as the invariant distribution.

In our second vignette, we consider learning the kernel parameters of determinantal point processes (DPPs), a class of repulsive point processes. While DPPs have many appealing properties, such as efficient sampling, learning the parameters of a DPP is still considered a difficult problem due to the non-convex nature of the likelihood function. We explore a set of Bayesian methods to learn the DPP kernel parameters even in large-scale and continuous DPP settings when the exact form of the eigendecomposition is unknown.

The HMC work is in collaboration with Tianqi Chen and Carlos Guestrin. The DPP work is joint with Raja Hafiz Affandi, Ryan Adams, and Ben Taskar.

Speaker: **Woodard, Dawn** (Cornell University)
Title: *Model-Based Image Segmentation / Efficiency of MCMC in Parametric Models*
Abstract: I will discuss two topics. First, I discuss an improved method for spatial model-based clustering, and apply it to segment three-dimensional Dynamic Contrast Enhanced Magnetic Resonance (DCE-MR) images. The approach extends an existing Monte Carlo Expectation-Maximization method for Markov random field mixture models, and is guaranteed to converge to a local maximum of the likelihood. The first extension is to show how to incorporate cluster weight parameters in a computationally tractable way; these parameters are needed to accurately capture small features in the image. Secondly, we incorporate a covariance decomposition to allow control over geometric characteristics of the segmentation. Thirdly, we give a consistent approximation to the observed-data likelihood.

In the second part of the talk I discuss work analyzing the efficiency of Markov chain Monte Carlo (MCMC) methods used in Bayesian computation. While convergence diagnosis is used to choose how long to run a Markov chain, it can be inaccurate and does not provide insight regarding how the efficiency scales with the number of parameters or other quantities of interest. We instead characterize the number of iterations of the Markov chain (the running time) sufficient to ensure that the approximate Bayes estimator obtained by MCMC preserves the property of asymptotic efficiency. We show that in many situations where the likelihood satisfies local asymptotic normality, the running time grows linearly in the number of observations n.

8.3.3 Day 3

The theme running through day three was industry, as the three speakers spoke of problems and solutions connected with Google, Facebook and similar companies. First, Russ Salakhutdinov presented some of the video hierarchical structures on multimedia data, like connecting images and text, with obvious applications at Google. The first part described Boltzman machines with impressive posterior simulations of characters and images. Then Steve Scott gave us a Google motivated entry to embarrassingly parallel algorithms. One of the novel things in the talk (for me) was the inclusion of BART in this framework, with the interesting feature that using the whole prior on each machine was way better than using a fraction of the prior, as predicted by the theory! And Joaquin Quinonero Candela provided examples of machine learning techniques used by Facebook to suggest friends and ads in a most efficient way.

Speaker: **Salakhutdinov, Ruslan** (University of Toronto)
Title: *Learning Structured, Robust, and Multimodal Models*
Abstract: Building intelligent systems that are capable of extracting meaningful representations from high-dimensional

data lies at the core of solving many Artificial Intelligence tasks, including visual object recognition, information retrieval, speech perception, and language understanding. In this talk I will first introduce a broad class of hierarchical probabilistic models called Deep Boltzmann Machines (DBMs) and show that DBMs can learn useful hierarchical representations from large volumes of high-dimensional data with applications in information retrieval, object recognition, and speech perception. I will then describe a new class of more complex models that combine Deep Boltzmann Machines with structured hierarchical Bayesian models and show how these models can learn a deep hierarchical structure for sharing knowledge across hundreds of visual categories, which allows accurate learning of novel visual concepts from few examples. Finally, I will introduce deep models that are capable of extracting a unified representation that fuses together multiple data modalities. I will show that on several tasks, including modelling images and text, video and sound, these models significantly improve upon many of the existing techniques.

Speaker: **Scott, Steve** (Google)
Title: *Bayes and Big Data: The Consensus Monte Carlo Algorithm*
Abstract: A useful definition of "big data" is data that is too big to comfortably process on a single machine, either because of processor, memory, or disk bottlenecks. Graphics processing units can alleviate the processor bottleneck, but memory or disk bottlenecks can only be eliminated by splitting data across multiple machines. Communication between large numbers of machines is expensive (regardless of the amount of data being communicated), so there is a need for algorithms that perform distributed approximate Bayesian analyses with minimal communication. Consensus Monte Carlo operates by running a separate Monte Carlo algorithm on each machine, and then averaging individual Monte Carlo draws across machines. Depending on the model, the resulting draws can be nearly indistinguishable from the draws that would have been obtained by running a single machine algorithm for a very long time. Examples of consensus Monte Carlo are shown for simple models where single-machine solutions are available, for large single-layer hierarchical models, and for Bayesian additive regression trees (BART).

Speaker: **Darren Wilkinson** (Newcastle University))
Title: *Parallelisation strategies for Monte Carlo algorithms*
Abstract: An overview will be presented of parallelisation strategies for Monte Carlo algorithms such as ABC, SMC, MCMC, and pMCMC, with particular emphasis on the problem of inference for intractable Markov process models. Different algorithms have differing degrees of amenability to parallelisation, leading to trade-offs with statistical efficiency. A hybrid approach will be discussed, which attempts to effectively utilise multicore systems. The potential benefits of functional programming languages, immutable data structures and "monadic" algorithm design for scalable Bayesian computation will also be examined.

8.3.4 Day 4

Still looking for a daily theme, parallelisation could be the right candidate, even though other talks this week went into parallelisation issues, incl. Steves talk Wednesday. Indeed, Anthony Lee gave a talk this morning on interactive sequential Monte Carlo, where he motivated the setting by a formal parallel structure. Then, Darren Wilkinson surveyed the parallelisation issues in Monte Carlo, MCMC, SMC and ABC settings, before arguing in favour of a functional language called Scala. In the afternoon session, Sylvia Frhwirth-Schnatter exposed her approach to the (embarrassingly) parallel problem, in the spirit of Steves, David Dunsons and Scotts. Marc Suchard mostly talked about flu and trees in a very pleasant and broad talk, he also had a slide on parallelisation to fit the theme! Although unrelated with parallelism, Nicolas Chopins talk was on sequential quasi-Monte Carlo algorithms, and was full of exciting stuff. Similarly, Alex Lenkoski spoke about extreme rain events in Norway with no trace of parallelism, but the general idea behind the examples was to question the notion of the calibrated Bayesian (with possible connections with the cut models).

Speaker: **Lee, Anthony** (University of Warwick)
Title: *On the role of interaction in sequential Monte Carlo algorithm*
Abstract: Motivated largely by issues surrounding parallel implementation of particle filters, we introduce a general form of sequential Monte Carlo (SMC) algorithm defined in terms of a parameterized resampling mechanism.

We find that a suitably generalized notion of the Effective Sample Size (ESS), widely used to monitor algorithm degeneracy, appears naturally in a study of its convergence properties. We are then able to phrase sufficient conditions for time-uniform convergence in terms of algorithmic control of the ESS, in turn achievable by adaptively modulating the interaction between particles. This leads us to suggest novel algorithms which are, in senses to be made precise, provably stable and yet designed to avoid the degree of interaction which hinders parallelization of standard algorithms. As a by-product we prove time-uniform convergence of the popular adaptive resampling particle filter. The resulting scheme provides some indication of how one can achieve scalable SMC algorithms in practice.

This is joint work with Nick Whiteley and Kari Heine.

Speaker: **Quinonero Candela, Joaquin** (Facebook)
Title: *Examples and Lessons from Machine Learning at Facebook*
Abstract: The problem of selecting what information to present users is prevalent at Facebook. In this talk I will give a couple of examples of machine learning applied to rank Facebook content. I will also describe a couple of simple tricks to operate at scale. Finally, I will share some practical lessons learnt from ranking ads, the area I have been working on the past year and a half.

Speaker: **Chopin, Nicolas** (ENSAE-CREST)
Title: *Sequential Quasi-Monte Carlo*
Abstract: We develop a new class of algorithms, SQMC (Sequential Quasi Monte Carlo), as a variant of SMC (Sequential Monte Carlo) based on low-discrepancy points. The complexity of SQMC is O(N log N) where N is the number of simulations at each iteration, and its error rate is smaller than the Monte Carlo rate $O(N^{-1/2})$. The only requirement to implement SQMC is the ability to write the simulation of particle x_t^n given x_{t-1}^n as a deterministic function of x_{t-1}^n and uniform variates. We show that SQMC is amenable to the same extensions as standard SMC, such as forward smoothing, backward smoothing, unbiased likelihood evaluation, and so on. In particular, SQMC may replace SMC within a PMCMC (particle Markov chain Monte Carlo) algorithm. We establish several convergence results. We provide numerical evidence in several difficult scenarios than SQMC significantly outperforms SMC in terms of approximation error.

(Joint work with Mathieu Gerber)

Speaker: **Frühwirth-Schnatter, Sylvia** (WU Vienna University of Economics and Business)
Title: *Merging parallel MCMC output for horizontally partitioned data*
Abstract: Horizontally partitioned data frequently occur when different entities cannot pool or share their data, either due to privacy protection, or if data are too large to be analyzed within a single analysis due to the computational burden. One way to handle this problem is to partition the data and perform independent manageable analyzes in parallel on each partition. Somewhat surprisingly, combining and merging the independently obtained results to obtain overall Bayesian inference for the whole sample is far from trivial.

The first part of the talks reviews and comments on several methods that have been proposed recently in this context, such as embarrassingly parallel MCMC, the consensus Monte Carlo algorithm, and parallel MCMC via Weierstrass sampler. However, none of the existing methods applies a fully Bayesian analysis based on MCMC sampling for each of the sub-samples and merging the draws into a single sample from the joint posterior distributions given all data.

The second part of the talk discussed two approaches to construct such a merged sample directly from the MCMC sub samples obtained for partitioned data. The first approach uses naive reweighting of the observations of one sample with the estimated posterior density of the other. The second approach applies an independence Metropolis-Hastings-algorithm to merge two samples from different partitions into one sample from the joint posterior. This algorithm is based on using one of the posteriors as proposal which leads to quite a simple acceptance rate for the draws from this posterior. Both procedure are applied sequentially over all sub samples.

We evaluate the performance of both approaches for various examples of univariate Bayesian inference and discuss how to extend these approaches to multivariate Bayesian inference and hierarchical models.

(Joint work with Alexandra Posekany.)

Speaker: **Lenkoski, Alex** (Norsk Regnesentral/Norwegian Computing Center)
Title: *Hierarchical Bayesian Methods in Modern Industrial Statistics*
Abstract: The reliance on computationally intensive hierarchical methods and the (re-)emergence of the Bayesian paradigm is now thoroughly established in academic statistical research. Further, through the parallel development of machine learning methods, innumerable techniques have been developed to handle a variety of problems faced by information-oriented technology companies. However, in the more staid domain of industrial statistics, uptake of computationally intensive methods has been somewhat more subdued. This talk will present four applications across the industrial realm where advanced Bayesian methods either have been, or should be, used to good effect. These applications include: Mapping regional heterogeneity of extreme precipitation levels in Norway, issuing a calibrated prediction that an insurance claim is fraudulent, creating temporally coherent predictive distributions of wind power production in Germany and using bid-ask curve data to form distributional electricity price forecasts in the Nordic region. In the course of each project, a host of questions came up regarding the appropriate implementation and ultimate usefulness of modern, cutting-edge methods over more standard statistical routines. We will highlight these issues and hopefully discuss how to truly integrate current research into industrial solutions.

Speaker: **Suchard, Marc** (UCLA)
Title: *Scaling Bayesian models for large-scale infectious disease surveillance*
Abstract: Influenza viruses undergo continual antigenic evolution allowing mutant viruses to evade host immunity. Antigenic phenotype is often assessed through pairwise measurement of cross-reactivity between influenza strains using the hemagglutination inhibition (HI) assay. Large-scale experimentation is generating HI measurements between thousands of strains. Semi-parametric clustering of these measurements guides annual influenza vaccine selection, but current methods fail to account for uncertainty in cluster identification and the unobserved shared evolutionary history between strains. We propose a semi-parametric Bayesian model that uses multidimensional scaling to map pairwise measurements into a latent low-dimensional space. Viral coordinates in this space identify clusters and the viruses' shared history provides a prior distribution over coordinates through a Browian diffusion process along the history. Central to the success of this model lies a novel sum-product algorithm that transforms an $O(N^3K^3)$ into an $O(NK^2)$ computation for the Brownian diffusion, where N counts the number of viruses and K counts the dimension of the phenotypes in the database. The algorithm exploits the directed acyclic graph structure of the shared history and opens the door for joint inference of multiple, high-dimensional phenotypes. We show that seasonal influenza A/H3N2 evolves faster and in a more punctuated fashion than other influenza lineages. [Joint work with Trevor Bedford, Andrew Rambaut and Philippe Lemey]

Participants

Barthelm, Simon (University of Geneva)
Bornn, Luke (Simon Fraser University)
Chopin, Nicolas (ENSAE)
Craiu, Radu (University of Toronto)
Fearnhead, Paul (Lancaster University)
Fox, Emily (University of Washington)
Fruhwirth-Schnatter, Sylvia (Wirtschaftsuniversitat Wien)
Girolami, Mark (The University of Warwick)
Jacob, Pierre (National University of Singapore)
Lee, Anthony (University of Warwick)
Lenkoski, Alex (Norwegian Computing Center)
Lomeli, Maria (University College London)
Mansinghka, Vikash (Massachusetts Institute of Technology)
Murray, Lawrence (CSIRO)
Pudlo, Pierre (Universit Montpellier 2)
Quinonero Candela, Joaquin (Facebook)
Robert, Christian (Universit Paris-Dauphine)

Rue, Hvard (Norwegian University of Science and Technology Trondheim)
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Salakhutdinov, Russ (University of Toronto)
Schmidler, Scott (Duke University)
Scott, Steve (Google)
Singh, Sumeetpal (University of Cambridge)
Strickland, Chris (University of New South Wales)
Suchard, Marc (University of California at Los Angeles)
VanDerwerken, Doug (Duke University)
Wilkinson, Darren (Newcastle University)
Wood, Frank (Oxford)
Woodard, Dawn (Cornell University)

8.4 Outcome of the Meeting

The meeting provided a great opportunity for many researchers from around the world to come together and discuss different approaches to making Bayesian computation scale to modern problems. It was a uniform success, with many excellent discussions between research groups which had previously not communicated, and a dissemination of ideas across fields which has opened many avenues for future research. To quote one participant, Simon Barthelmé (University of Geneva),

> Attending the workshop has been tremendously valuable. I was able to get an overview of the state-of-the-art in the field, and interact closely with some of its best researchers. What made it especially interesting for me is that I work in a neighbouring field and cannot easily keep myself abreast of all the latest developments. I've received excellent feedback on my own work, and I've come home with many new ideas as well as excellent memories of the workshop.

Current research in Bayesian computation seeks innovation through one of three mechanisms: adaptation, parallelization, or model simplification. The first, adaptation, strives to have the algorithm tune itself as it runs. The second, parallelization, seeks to cleverly distribute computation across clusters and modern graphical processing units. While these techniques generally improve performance, the $O(N^{-1/2})$ convergence of Monte Carlo methods remains.

In contrast, to exploit the idea of model simplification, the machine learning community is actively developing fast and efficient variational methods. Unfortunately, however, it can be difficult to gauge the quality of the approximation made by these methods. Efforts are being made to improve and better understand these approximations, though generally such improvements are model-specific, and as such there lacks a unified, yet efficient, computational framework for Bayesian modeling.

This workshop bridged these two communities, and has opened doors for building hybrid methods which avoid the inherent pitfalls of existing approaches.

Chapter 9

Geometric Tomography and Harmonic Analysis (14w5085)

March 9 - 14, 2014

Organizer(s): Alexander Koldobsky, (University of Missouri), Dmitry Ryabogin, (Kent State University), Vladyslav Yaskin, (University of Alberta), Artem Zvavitch, (Kent State University)

Geometric Tomography is the area of Mathematics where one investigates properties of solids based on the information about their sections and projections. It shares ideas and methods from many fields of Mathematics, such as Differential Geometry, Functional Analysis, Harmonic Analysis, Combinatorics and Probability. But the most significant overlap is with Convex Geometry and in particular with the classical Brunn-Minkowski theory. The workshop brought together a number of top researchers as well as students and postdocs with the aim of discussing most recent developments in the area.

The topics of the workshop included harmonic analysis on the sphere, spherical operators and special classes of bodies, geometric inequalities, discrete geometry, probability and random matrices.

We start the description with a harmonic analysis type result proved by Wolfgang Weil and his collaborators. Goodey, Yaskin and Yaskina in 2009 introduced certain operators I_p on $C^\infty(S^{n-1})$ by means of the Fourier transform. These operators turned out to be useful for various applications. Goodey and Weil used these operators I_p for the study of k-th mean section bodies. Informally speaking, $M_k(K)$, the k-the mean section body of a convex body K in $\mathbb{R}^n$ is the Minkowski sum of all its sections by k-dimensional affine planes. Until recently it was unknown (up to some particular cases) whether convex bodies are uniquely determined by their k-th mean section bodies. Goodey and Weil proved that this is indeed true. Moreover, they established an interesting connection between the support function of $M_k(K)$ and the $(n+1-k)$-th surface area measure of K, which involves a combination of operators I_p mentioned previously. Further research in this direction led Goodey, Hug and Weil to a new Crofton-type formula for area measures and also to a local version of the Principal Kinematic Formula.

Mathieu Meyer presented recent results obtained in collaboration with Carsten Schütt and Elisabeth Werner on affine points. An *affine invariant point* on the class of convex bodies $\mathcal{K}^n$ in $\mathbb{R}^n$, endowed with the Hausdorff metric, is a continuous map from $\mathcal{K}^n$ to $\mathbb{R}^n$ which is invariant under one-to-one affine transformations $\mathbb{R}^n$. This concept was introduced by Grünbaum. Well known examples of affine invariant points are the centroid and the Santalo point.

Earlier the authors established a number of results about affine points. In particular, they answered in the negative a question by Grünbaum who asked if there exists a finite basis of affine invariant points. They gave a positive answer to another question by Grünbaum about the size of the set of all affine invariant points.

More recently, the authors introduced a new concept of a dual affine point q of an affine invariant point p. It is defined by the formula $q(K^{p(K)}) = p(K)$ for every $K \in \mathcal{K}^n$, where $K^{p(K)}$ denotes the polar of K with respect to the point $p(K)$.

The authors answered a number of questions. In particular, does every affine invariant point p have a dual? The answer is negative. They also show that if a dual affine invariant point exists, it is unique. A reflexivity principle for affine invariant points is established, namely that the double dual point of p equals p. Furthermore, new examples of affine invariant points are presented.

Vitali Milman gave a talk on characterizing summations of convex sets. Details of the proof were presented by Liran Rotem in his subsequent lecture. This work continues a series of studies of fundamental concepts in convex geometry by means of the corresponding characterization theorems. It is a classical result of Minkowski that volume is polynomial with respect to the Minkowski addition.

One can consider other summations, in place of the Minkowski summation. One of the important examples is the p-summation: $h_{A+_pB} = (h_A^p + h_B^p)^{1/p}$, where h is the corresponding support function. Each summation $\bigoplus$ defines an induced homothety $\bigodot$ as follows: for $m \in \mathbb{N}$,

$$m \bigodot A = A \bigoplus \cdots \bigoplus A \ \ (m \text{ times}).$$

Two of the main questions are the following. Does the homothety recovers the summation? What sums have the polynomiality property for the volume functional? Answers to these questions were given in the talk. If there is a function $f : \mathbb{N} \to \mathbb{R}_+$ such that $m \bigodot A = f(m)A$, then certain conditions guarantee when the corresponding sum is a corresponding p-sum.

It is also shown that if the summation is polynomial (and satisfies certain natural conditions), then the summation is either the Minkowski summation or the ∞-summation that is defined by $A +_\infty B = \text{conv}(A \cup B)$.

Liran Rotem gave a talk on "Isotropicity with respect to a measure". Recall that a measure μ is called *isotropic* if $\int_{\mathbb{R}^n} \langle x, \theta \rangle^2 d\mu(x)$ is independent of the unit vector θ. For every measure μ there exists a linear transformation $T \in SL(n)$ such that the push-forward of μ by T is isotropic. If C is a body in $\mathbb{R}^n$, define $\mu_C(A) = \mu(A \cap C)$. C is said to be isotropic with respect to μ if μ_C is isotropic.

The following questions are studied:

1) Given C and μ, does there exist $T \in SL(n)$ such that TC is isotropic with respect to μ.

2) If "yes", which properties will C have in such a position?

Regarding question 1, it was shown earlier by Bobkov that this is true in the case of the Gaussian measure on $\mathbb{R}^n$.

The following result is obtained: TC is isotropic with respect to a rotation invariant measure μ if and only if T is a critical point of a certain functional J. Some other related questions were also discussed.

Franz Schuster spoke about Cosine and Radon Transforms in the Theory of Minkowski Valuations.

Let $\mathcal{K}^n$ be the set of convex bodies in an $\mathbb{R}^n$. A map $\phi : \mathcal{K}^n \to \mathbb{R}$ is called a (real valued) *valuation* if

$$\phi(K) + \phi(L) = \phi(K \cup L) + \phi(K \cap L)$$

whenever K, L, $K \cup L \in \mathcal{K}^n$.

Valuations on convex bodies have been actively studied. A famous classical result in this area is Hadwiger's classification of rigid motion invariant real valued continuous valuations as linear combinations of the intrinsic volumes.

A map $\Phi : \mathcal{K}^n \to \mathcal{K}^n$ is called a Minkowski valuation if

$$\Phi(K) + \Phi(L) = \Phi(K \cup L) + \Phi(K \cap L)$$

whenever K, L, $K \cup L \in \mathcal{K}^n$.

A problem is to describe the set $\text{MVal}^{SO(n)}$ of continuous Minkowski valuations that are translation invariant and $SO(n)$-equivariant.

Open problem 1. For $\Phi \in \text{MVal}^{SO(n)}$, are there $\Phi_i \in \text{MVal}_i^{SO(n)}$ such that

$$\Phi = \Phi_0 + \Phi_1 + \cdots + \Phi_n?$$

Here, $\text{MVal}_i^{SO(n)} = \{\Phi \in \text{MVal}^{SO(n)} : \Phi(\lambda K) = \lambda^i \Phi(K)\}$.

Open problem 2. Find a classification/description of $\text{MVal}_i^{SO(n)}$.

Regarding the description of $\mathrm{MVal}_i^{SO(n),\infty}$ (there is some natural notion of smoothness), Schuster has show that if $\Phi_i \in \mathrm{MVal}_i^{SO(n),\infty}$, $2 \le i \le n-2$, is even, then there is a unique smooth $O(i) \times O(n-i)$-invariant measure μ on the sphere such that

$$h(\Phi_i(K), \cdot) = \mathrm{vol}_i(K|\cdot) * \mu.$$

The measure μ is called the Crofton measure of Φ_i.

Jointly with Wannerer, Schuster proved that if a measure μ is the Crofton measure of an even $\Phi_i \in \mathrm{MVal}_i^{SO(n),\infty}$, then there exists $L \in \mathcal{K}^n$ such that

$$(C\mu)(u) = \int_{S^{n-1}} |\langle u, v\rangle| d\mu(v), \qquad u \in S^{n-1}.$$

They also obtained the following description. If $\Phi_i \in \mathrm{MVal}_i^{SO(n),\infty}$, $1 \le i \le n-1$, is even, then there exists a unique function $g \in C^\infty([-1,1])$ such that

$$h(\Phi_i K, u) = \int_{S^{n-1}} g(\langle u, v\rangle) dS_i(K, u), \qquad u \in S^{n-1}.$$

The function g is called the generating function of Φ_i.

They also obtained a relation between μ and g in terms of the Radon transform on the Grassmanian and the inverse spherical cosine transform.

Astrid Berg presented a joint work with L. Parapatits, F. Schuster and M. Weberndorfer titled "Log-concavity properties of Minkowski valuations". The classical Brunn-Minkowski inequality for intrinsic volumes asserts that for convex bodies K and L in $\mathbb{R}^n$, $1 < i \le n$ and $0 < \lambda < 1$, the following holds

$$V_i((1-\lambda)K + \lambda L) \ge V_i(K)^{1-\lambda} V_i(L)^\lambda.$$

Let $MVal_j$ denote the class of continuous, translation invariant, $SO(n)$-equivariant and j-homogeneous Minkowski valuations. The authors studied the following question. Fix $\Phi_j \in MVal_j$. Does the family of inequalities

$$V_i(\Phi_j((1-\lambda)K + \lambda L)) \ge V_i(\Phi_j K)^{1-\lambda} V_i(\Phi_j L)^\lambda$$

hold? For which i does it hold?

The authors proved the following.

Theorem 9.0.1 *Let $1 \le i \le n$ and let $\Phi_j \in MVal_{j,i-1}$, $2 \le j \le n-1$, be non-trivial. If K and L are convex bodies (with non-empty interior), then for $\lambda \in (0,1)$,*

$$V_i(\Phi_j((1-\lambda)K + \lambda L)) \ge V_i(\Phi_j K)^{1-\lambda} V_i(\Phi_j L)^\lambda,$$

with equality if and only if K and L are translate of each other.

Christos Saroglou gave a talk titled "Remarks on the conjectured log-Brunn-Minkowski inequality".

Böröczky, Lutwak, Yang and Zhang recently conjectured a certain strengthening of the Brunn-Minkowski inequality for symmetric convex bodies, the so-called log-Brunn-Minkowski inequality.

Conjecture. If K and L are centrally symmetric convex bodies, then for $\lambda \in (0,1)$,

$$V(\lambda K +_0 (1-\lambda)L) \ge V(K)^\lambda V(L)^{1-\lambda}.$$

Here

$$\lambda K +_0 (1-\lambda)L = \{x \in \mathbb{R}^n : \langle x, u\rangle \le h_K^\lambda(u) h_L^{1-\lambda}(u),\ \forall u \in S^{n-1}\}.$$

The author proved the following result.

Theorem 9.0.2 *Let K and L be unconditional convex bodies (with respect to the same orthonormal basis) in $\mathbb{R}^n$ and $\lambda \in (0,1)$. Then*

$$V(\lambda K +_0 (1-\lambda)L) \geq V(K)^{\lambda} V(L)^{1-\lambda}.$$

Equality holds in the following case: whenever $K = K_1 \times \cdots \times K_m$, for some irreducible unconditional convex sets K_1,..., K_m, then there exist positive numbers such that $L = c_1 K_1 \times \cdots \times c_m K_m$.

Applications of this result are discussed. Moreover, it is shown that the log-Brunn-Minkowski inequality is equivalent to the (B)-Theorem for the uniform measure of the cube (this has been proven by Cordero-Erasquin, Fradelizi and Maurey for the gaussian measure instead).

Florian Besau presented his joint work with Franz Schuster on Binary Operations in Spherical Convex Geometry. This is in some respect related to Vitali Milman's talk since the goal is similar: to characterize binary operations. There is a result of Gardner, Hug and Weil that characterizes the Minkowski addition among binary operations on $\mathcal{K}^n$. The geometry of spherical convex sets is much less understood. Is there an analogue of the Minkowski addition on the sphere?

The authors define the operation of projection of a convex set on the sphere. They also define the spherical support function, using a geometric construction analogous to that in the Euclidean space.

Let $K_u^p(S^n)$ be the set of spherical convex bodies contained in S_u^+ (the open hemisphere with centre u). Consider $K^p(S^n) = \cup_{u \in S^n} K_u^p(S^n)$.

Let $u \in S^n$. An operation $* : K_u^p(S^n) \times K_u^p(S^n) \to K_u^p(S^n)$ is called u-projection covariant if for all k-spheres S, $0 \leq k \leq n$ with $u \in S$, we have

$$K|S * L|S = (K * L)|S$$

for all K, $L \in K_u^p(S^n)$.

An operation $* : K^p(S^n) \times K^p(S^n) \to K^p(S^n)$ is called projection covariant if it is u-projection covariant for all $u \in S^n$.

The authors proved the following results.

Theorem 9.0.3 *Let $C = \cup_{u \in S^n}(K_u^p(S^n) \to K_u^p(S^n))$. An operation $* : C \to K^p(S^n)$ is projection covariant if and only if*

$$K * L = \mathrm{conv}(K \cup L) \quad \text{or} \quad K * L = -\mathrm{conv}(K \cup L)$$

or it is trivial (i.e. projection on the first or the second component, maybe with a minus sign).

Theorem 9.0.4 *An operation $* : K^p(S^n) \times K^p(S^n) \to K^p(S^n)$ is projection invariant and continuous if and only if it is trivial.*

Several presenters talked about new developments in the theory of random matrices. In particular, Susanna Spektor gave a talk based on the joint work with Alexander Litvak on Quantitative version of a Silverstein's result.

Let $w_{i,j}$ be i.i.d. copies of a random variable w with $\mathbb{E}w = 0$ and $\mathbb{E}w^2 = 1$. Consider the $p \times n$ matrix

$$W_n = \{w_{i,j}\}_{i \leq p, j \leq n}, \quad p = p(n),$$

and its sample covariance matrix

$$\Gamma_n = \frac{1}{n} W_n W_n^T.$$

The rows of W_n are denoted by X_i, $i \leq p$.

A theorem of Silverstein asserts the following. Assuming that $p(n)/n \to c > 0$ as $n \to \infty$, $\|\Gamma_n\|_{op}$ converges in probability to a non-random quantity (which is $(1+\sqrt{c})^2$) if and only of $n^4 \mathbb{P}(|w| \geq n) = o(1)$.

The authors' goal was to quantify Silverstein's result. Namely, they proved the following:

Theorem 9.0.5 *Let $\alpha \geq 2$, $c_0 > 0$. Let w be a random variable satisfying $\mathbb{E}w = 0$ and $\mathbb{E}w^2 = 1$ and*

$$\forall t \geq 1, \qquad \mathbb{P}(|w| \geq t) \geq \frac{c_0}{t^{\alpha}}.$$

Let W_n, X_j, Γ_n be as above. Then for every $K \geq 1$,

$$\mathbb{P}(\|\Gamma_n\|_{op} \geq K) \geq \mathbb{P}(\max_{i \leq p} |X_i| \geq \sqrt{Kn}) \geq \min\left\{\frac{c_0 p}{4n^{(\alpha-2)/2}K^{\alpha/2}}, \frac{1}{2}\right\}.$$

Another talk on random matrices was given by Alexander Litvak, with the title "Approximating the covariance matrix with heavy tailed columns and RIP", joint work with O. Guédon, A. Pajor, N. Tomczak-Jaegermann.

Let A be a matrix whose columns $X_1, \ldots, X_N$ are independent random vectors in $\mathbb{R}^n$. Assume that p-th moments of $\langle X_i, a\rangle$, $a \in S^{n-1}$, $i \leq N$, are uniformly bounded. For $p > 4$ the authors proved that with high probability A has the Restricted Isometry Property (RIP) provided that Euclidean norms $|X_i|$ are concentrated around $\sqrt{n}$ and that the covariance matrix is well approximated by the empirical covariance matrix provided that

$$\max_i |X_i| \leq C(nN)^{1/4}.$$

They also provided estimates for RIP when

$$\mathbb{E}\,\phi\left(|\langle X_i, a\rangle|\right) \leq 1$$

for $\phi(t) = (1/2)\exp(t^\alpha)$, with $\alpha \in (0, 2]$.

The theme of random matrices was continued in the talk "Small ball probabilities for linear images of high dimensional distributions" by Mark Rudelson (joint work with Roman Vershynin)

The main object of the study is a random vector $X = (X_1, ..., X_n)$ in $\mathbb{R}^n$ with independent coordinates X_i. Given a fixed $m \times n$ matrix A, the authors study the concentration properties of the random vector AX. They establish results of the following type:

If the distributions of X_i are well spread on the line, then the distribution of AX is well spread in space.

In particular, they extend the bound obtained by Paouris for log-concave measures to random vectors with independent coordinates.

Theorem 9.0.6 *Let $X = (X_1, ..., X_n) \in \mathbb{R}^n$ be a vector with independent coordinates and let the densities of X_i be bounded by K. If A is an $m \times n$ matrix, then*

$$\mathcal{L}(AX, t\|A\|_{HS}) \leq \left(\frac{CKt}{\sqrt{\varepsilon}}\right)^{(1-\varepsilon)r(A)}, \qquad \textit{for all} t, \varepsilon > 0.$$

Here, $r(A)$ is the stable rank of A, and $\mathcal{L}$ is the Levy concentration function.

Eric Grinberg gave a talk on "The Torus Transform on Symmetric Spaces of Compact Type", joint work with Steven Jackson. In a 1913 paper Paul Funk proved that a suitable function on the sphere S^2 is odd if and only if its integrals over great circles (closed geodesics) vanish, and that an even function is determined by such integrals. The authors replace the sphere S^2 by a symmetric space of compact type, e.g. a Grassmann manifold, and great circles by maximal totally geodesic at tori, and consider the transform that integrates over these. They showed that, when the symmetric space is the "universal covered space" in its class, the torus transform is injective, and otherwise the transform is non-injective, with a kernel that is directly linked to deck transformations of the appropriate symmetric cover. This gives one of the direct extensions of Funk's transform and its injectivity properties.

The talk of Yves Martinez-Maure focused on the question "Can hedgehogs be useful for Geometric Tomography?" Hedgehogs are geometrical objects that describe the Minkowski differences of arbitrary convex bodies in $\mathbb{R}^n$. For a function $h \in C^2(S^{n-1})$ the corresponding hedgehog can be parameterized as

$$x_h = h(u)u + \nabla h(u), \quad u \in S^{n-1}.$$

One can extend many classical notions to hedgehogs, such as its curvature function R_h, algebraic area, algebraic volume, projection hedgehog, hedgehog of constant width etc.

One of the interesting (and powerful) applications of hedgehogs to convex geometry concerns an old conjecture due to A. D. Aleksandrov, which states that if $S \subset \mathbb{R}^3$ is a closed convex surface of class C^2_+ such that

$$(k_1 - c)(k_2 - c) \leq 0,$$

with $c = \text{const}$, where k_1 and k_2 are the principal curvatures, then S must be a sphere of radius $1/c$.

It has an equivalent formulation in terms of hedgehogs. If $H_h \subset \mathbb{R}^3$ is a hedgehog such that $R_h \leq 0$, then H_h is a point. Martinez-Maure constructed a counterexample to the latter conjecture.

Matthieu Fradelizi spoke about Functional versions of L_p-affine surface area and entropy inequalities, which is a joint work with U. Caglar, O. Guéedon, J. Lehec, C. Schütt and E. Werner. Let us recall the definition of the L_p-affine surface area of a convex body. Let K be a convex body, containing the origin in its interior and $p \in \mathbb{R} \cup \{+\infty\}$, $p \neq -n$. Then the *L_p-affine surface area* of K is

$$as_p(K) = \int_{\partial K} \left(\frac{\kappa_K(x)}{\langle x, N_K(x)\rangle^{n+1}} \right)^{\frac{p}{n+p}} \langle x, N_K(x)\rangle dx,$$

where $N_K(x)$ is the unit normal to K at x and $\kappa_K(x)$ is the Gauss curvature.

This concept has been actively studied in recent years. In this work the authors introduce a functional version of the affine surface area. Let $\psi : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ be a convex function and $\lambda \in \mathbb{R}$. Define

$$as_\lambda(\psi) = \int_{\{\psi < +\infty\}} e^{(2\lambda-1)\psi(x) - \lambda\langle x, \nabla\psi(x)\rangle} \left(\det \nabla^2\psi(x)\right)^\lambda dx.$$

It has many properties that hold for the usual affine surface area. Moreover, the latter can be obtained from the definition above by letting $\psi = \frac{1}{2}\|\cdot\|^2$ and $\lambda = \frac{p}{p+n}$.

There is also a duality relation similar to that for the usual L_p affine surface area, namely

$$as_\lambda(\psi) = as_{1-\lambda}(\psi^*),$$

where ψ^* is the Legendre transform of ψ.

They also established functional functional versions of affine isoperimetric inequalities.

Theorem 9.0.7 *If $\int x e^{-\psi(x)} dx = 0$ and $\lambda \in [0, 1]$, then*

$$as_\lambda(\psi) \leq (2\pi)^{\lambda n} \left(\int e^{-\psi(x)} dx \right)^{1-2\lambda},$$

with equality if and only if $\psi(x) = \langle Ax, x\rangle + c$. The inequality is reversed if $\lambda < 0$.

The theorem, in particular, allows to recover the affine isoperimetry for convex bodies.

Fradelizi also discussed the following reverse log-Sobolev inequality. Let $\psi : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ be a convex function such that $\int e^{-\psi(x)} dx = 1$. Then

$$S(\psi_0) - S(\psi) \geq \frac{1}{2} \int \log(\det \nabla^2\psi) e^{-\psi} dx,$$

with equality if and only if $\psi(x) = |Ax|^2 + bx + c$. Here, $S(\psi)$ is the entropy of $e^{-\psi}$ and $S(\psi_0)$ is the entropy of the Gaussian.

The inequality is due to Artstein, Klartag, Schütt and Werner. In the present work the authors relaxed the smoothness hypotheses, established the equality case and gave a new proof.

A related theme was discussed in the talk by Elisabeth Werner on "Equality characterization and stability for entropy inequalities", joint work with T. Yolcu. Caglar and Werner recently proved the following result.

Theorem 9.0.8 *Let $f : (0, \infty) \to \mathbb{R}$ be a concave function. Let $\psi : \mathbb{R}^n \to R$ be a convex function that is in $C^1(\mathbb{R}^n)$. Then*

$$\int f\left(e^{2\psi - \langle \nabla\psi, x\rangle} \det(\nabla^2\psi) \right) d\mu < f\left(\frac{\int_{\mathbb{R}^n} e^{-\psi^*} dx}{\int d\mu} \right) \int d\mu. \tag{9.0.1}$$

If f is convex, the inequality is reversed. Here, ψ^* is the Legendre transform of ψ.

Up to now there was no characterization of equality in the latter theorem. It can be shown that in the case of f being either strictly convex or strictly concave, equality holds in (9.0.1) if and only if ψ satisfies the Monge-Ampère equation

$$\det(\nabla^2\psi(x)) = \frac{\int e^{-\psi^*}dx}{\int e^{-\psi}dx} e^{-2\psi+\langle\nabla\psi(x),x\rangle}, \quad x \in \mathbb{R}^n. \tag{9.0.2}$$

Using methods from mass transport, due to Brenier and Gangbo-McCann, the authors show the uniqueness of the solution of (9.0.2).

Theorem 9.0.9 *Let f be a strictly convex, respectively concave, function. Then $\psi(x) = \frac{1}{2}\langle Ax, x\rangle + c$ is the unique solution of (9.0.2) and moreover equality holds in (9.0.1) if and only if $\psi(x) = \frac{1}{2}\langle Ax, x\rangle + c$. Here, c is a positive constant and A is an $n \times n$ positive definite matrix.*

The authors then give stability versions of (9.0.1), as well as for a reverse log Sobolev inequality and for the L_p-affine isoperimetric inequalities for both, log concave functions and convex bodies. In the case of convex bodies such stability results have only been known in all dimensions for $p = 1$ and for $p > 1$ only for 0-symmetric bodies in the plane.

Joseph Lehec gave a talk titled "Bounding the norm of a log-concave vector via thin-shell estimates", a joint work with Ronen Eldan. Chaining techniques show that if X is an isotropic log-concave random vector in R^n and Γ is a standard Gaussian vector then

$$\mathbb{E}\|X\| < Cn^{1/4}\mathbb{E}\|\Gamma\|$$

for any norm $\|\cdot\|$, where C is a universal constant.

Using a completely different argument the authors establish a similar inequality relying on the thin-shell constant

$$\sigma_n = \sup(\sqrt{var(|X|)} : X \text{ is isotropic and } \log-\text{concave on } \mathbb{R}^n).$$

In particular, they show that if the thin-shell conjecture $\sigma_n = O(1)$ holds, then $n^{1/4}$ can be replaced by $\log(n)$ in the inequality. As a consequence, they obtain certain bounds for the mean-width, the dual mean-width and the isotropic constant of an isotropic convex body. In particular, they give an alternative proof of the fact that a positive answer to the thin-shell conjecture implies a positive answer to the slicing problem, up to a logarithmic factor.

Ronen Eldan presented his work titled "A Two-Sided Estimate for the Gaussian Noise Stability Deficit". *The Gaussian noise-stability* of a set $A \subset \mathbb{R}^n$ is defined by

$$S_\rho(A) = \mathbb{P}(X \in A \;\&\; Y \in A)$$

where X, Y are standard jointly Gaussian vectors satisfying $\mathbb{E}[X_iY_j] = \delta_{ij}\rho$. Borells inequality states that for all $0 < \rho < 1$, among all sets $A \subset \mathbb{R}^n$ with a given Gaussian measure, the quantity $S_\rho(A)$ is maximized when A is a half-space.

Eldan gave a novel short proof of this fact, based on stochastic calculus. Moreover, he proved an almost tight, two-sided, dimension-free robustness estimate for this inequality: by introducing a new metric to measure the distance between the set A and its corresponding half-space H (namely the distance between the two centroids), he shows that the deficit $S_\rho(H) - S_\rho(A)$ can be controlled from both below and above by essentially the same function of the distance, up to logarithmic factors. As a consequence, he also established the conjectured exponent in the robustness estimate proven by Mossel-Neeman, which uses the total-variation distance as a metric. In the limit $\rho \to 1$, he obtained an improved dimension-free robustness bound for the Gaussian isoperimetric inequality. The estimates are also valid for a more general version of stability where more than two correlated vectors are considered.

The Ball as a Pessimal Shape for Packing was the topic of Yoav Kallus' talk. It was conjectured by Ulam that the ball has the lowest optimal packing fraction out of all convex, three-dimensional solids. A naive motivation is that the sphere is the most symmetric solid and therefore also the least free: in placing a sphere in space there are only three degrees of freedom, compared to five in the case of any other solid of revolution, and six in the case of any other solid.

On the plane the situation is different. It is known that the circle is not even a local pessimum (the opposite of an optimum). There are origin-symmetric shapes arbitrarily circular (the outradius and inradius both being arbitrarily close to 1) that cannot be packed as efficiently as circles. Ulam's conjecture implies that this would not be the case in three dimensions. The question then is in which dimensions, if in any, the ball is a local pessimum.

Here the author proved that any origin-symmetric convex solid of sufficiently small asphericity can be packed at a higher efficiency than balls. The author shows that the ball is not a local pessimum in dimensions 4, 5, 6, 7, 8, and 24. On the other hand, in the three-dimensional case the ball is proved to be a local pessimum.

Galyna Livshyts spoke about her work on "Maximal surface area of a convex set in $\mathbb{R}^n$ with respect to log-concave rotation invariant measures". Recall that the *Minkowski surface area* of a convex set Q with respect to the measure γ is defined to be

$$\gamma(\partial Q) = \liminf_{\varepsilon \to 0^+} \frac{\gamma(Q + \varepsilon B_2^n) \setminus Q}{\varepsilon}$$

Let $\mathcal{K}^n$ be the set of all convex bodies in $\mathbb{R}^n$. It was shown by K. Ball that in the case when γ is the standard Gaussian measure, $\sup_{Q \in \mathcal{K}^n} \gamma(\partial Q)$ is finite and does not exceed $4n^{1/4}$. F. Nazarov showed that this order is actually the right one, and in fact,

$$0.28n^{1/4} < \sup_{Q \in \mathcal{K}^n} \gamma(\partial Q) < 0.64n^{1/4}.$$

The author establishes a similar result for all rotation invariant log-concave probability measures. It is shown that the maximal surface area with respect to such measures is of order

$$\frac{\sqrt{n}}{\sqrt[4]{Var|X|}\sqrt{\mathbb{E}|X|}},$$

where X is a random vector in $\mathbb{R}^n$ distributed with respect to the measure.

Peter Pivovarov spoke on "Volume of the polar of random sets and shadow systems", joint work with D. Cordero-Erausquin, M. Fradelizi , G. Paouris. The speaker discussed inequalities for the volume of the polar of random sets, generated for instance by the convex hull of independent random vectors in Euclidean space. Extremizers are given by random vectors uniformly distributed in Euclidean balls. This provides a randomized extension of the Blaschke-Santaló inequality. In particular, they prove the following.

Theorem 9.0.10 *Let N, $n \geq 1$. In the class of N-tuples $(X_1, ..., X_N)$ of independent random vectors in $\mathbb{R}^n$ whose laws have a density bounded by one, the expectation of the volume of the set*

$$(\mathrm{conv}\{\pm X_1, ..., \pm X_N\})^\circ$$

is maximized by N independent random vectors uniformly distributed in the Euclidean ball $D_n \subset \mathbb{R}^n$ of volume one.

This theorem, in particular, implies the classical Blaschke-Santaló inequality for convex bodies.

Luis Rademacher gave a talk titled "The More, the Merrier: the Blessing of Dimensionality for Learning Large Gaussian Mixtures", based on joint work with J. Anderson, M. Belkin, N. Goyal and J. Voss. He discussed recent developments in high dimensional geometric statistical inference. The problems included the reconstruction of polytopes from uniformly random points and the estimation of parameters of Gaussian Mixture Models. The main questions were the stability of the estimation and the design of efficient algorithms. The techniques involved provably correct and stable versions of the method of moments and more general harmonic analysis. The main original result is a somewhat unexpected "blessing of dimensionality", where it was shown that the problem of estimating the parameters of a Gaussian Mixture Model is generically easy in high dimension, while it is generically hard in low dimension.

Konstantin Tikhomirov spoke on the distance of polytopes with few vertices to the Euclidean ball. Let n, N be natural numbers satisfying $n + 1 \leq N \leq 2n$, B_2^n be the unit Euclidean ball in $\mathbb{R}^n$ and $P \subset B_2^n$ be a convex n-dimensional polytope with N vertices and the origin in its interior. He proved that

$$\inf\{\lambda \geq 1 : \, B_2^n \subset \lambda P\} \geq cn/\sqrt{N-n},$$

where $c > 0$ is a universal constant (this solves a conjecture of Gluskin and Litvak). As an immediate corollary, for any covering of S^{n-1} by N spherical caps of geodesic radius ϕ, $\cos(\phi) \le C\sqrt{N-n}/n$ for an absolute constant $C > 0$. Both estimates are optimal up to the constant multiples c, C.

Pierre Youssef spoke about "Almost orthogonal contact points". Let $K \subset \mathbb{R}^n$ be a convex body in John's position. The aim is to find a "large" number of contact points which is almost equivalent to an orthonormal basis of l_2.

Recall that a sequence of unit vectors $\{y_j\}_{j\le k} \in \mathbb{R}^n$ is said to be C-equivalent to the canonical basis of ℓ_2^k if there exists $\alpha, \beta > 0$ such that $C = \beta/\alpha$ and for any scalars $\{a_j\}_{j\le k}$

$$\alpha\left(\sum_{j\le k} a_j^2\right)^{1/2} \le \left\|\sum_{j\le k} a_j y_j\right\|_2 \le \beta\left(\sum_{j\le k} a_j^2\right)^{1/2}.$$

The author proves the following.

Theorem 9.0.11 *Let $\varepsilon \in (0,1)$, there exists $r = r(\varepsilon)$ such that the following is true. Let $n \in \mathbb{N}$ and K a convex body in $\mathbb{R}^n$ such that B_2^n is the ellipsoid of maximal volume contained in K. There exists a basis of $\mathbb{R}^n$ formed by contact points x_1,..., x_N and there is a partition of $[n]$ in r sets σ_1,..., σ_r such that $\forall i \le r$, $\{x_j\}_{j\in\sigma_j}$ is $(1+\varepsilon)$-equivalent to the canonical basis of $\ell_2^{\sigma_i}$.*

This is proved as a consequence of a more general result which asks about extracting a well conditioned block inside a given matrix.

Carsten Schütt gave a talk on "Order statistics" (joint work with S. Kwapien). The expression $\underset{1\le i\le n}{\text{k-min}}\, a_i$ denotes the k-smallest of all the numbers $a_1, \dots, a_n$.

Let $M = (M_1, \dots, M_n)$ be an n-tuple of increasing maps from $[0,\infty)$ onto itself. Then for all $x \in \mathbb{R}^n$ we define

$$\|x\|_M = \inf\left\{\rho \left| \sum_{i=1}^n M_i\left(\frac{x_i}{\rho}\right) \le 1\right.\right\}.$$

Theorem 9.0.12 *There is a universal constant C such that for all independent, positive and uniformly subregular sequences of random variables $\xi_1, \dots, \xi_n$ with continuous distribution functions $F_1, \dots, F_n$*

$$\mathbb{E}\left(\underset{1\le i\le n}{\text{k-min}}\,\xi_i\right) \sim \text{med}\left(\underset{1\le i\le n}{\text{k-min}}\,\xi_i\right) \sim \frac{1}{\|(1,\dots,1)\|_{\frac{F}{k-\frac{1}{2}}}}.$$

Petros Valettas gave a talk on "Neighborhoods on the Grasmannian of marginals with bounded isotropic constant", joint work with G. Paouris.

Recall that the isotropic constant of a centered log-concave probability measure on $\mathbb{R}^n$ is defined as

$$L_\mu = \|\mu\|_\infty^{1/n}\left[\det\left(\int_{\mathbb{R}^n} x_i x_j d\mu(x)\right)\right]^{1/(2n)},$$

where $\|\mu\|_\infty = \|f_\mu\|_\infty$ and f_μ is the density function of μ.

If μ is isotropic, then $L_\mu = \|\mu\|_\infty^{1/n}$. The hyperplane conjecture can be formulated in the form: there exists a constant $C > 0$ such that for all n and any μ log-concave isotropic probability measure on $\mathbb{R}^n$, we have $L_\mu < C$.

The authors proved a theorem in the spirit of Klartag's isomorphic version of the hyperplane conjecture. Consider the following distance on the Grassmanian. For $E, F \in Gr(n,k)$, let

$$d(E,F) = \inf\{\|I-U\|_{op} : U \in O(n),\ U(E) = F\}.$$

The main result is as follows.

Theorem 9.0.13 *Let μ be an isotropic log-concave probability measure on $\mathbb{R}^n$ and let $1 \leq k \leq \sqrt{n}$. For every $\varepsilon > 0$ and any $E \in Gr(n, k)$ there exists $F \in Gr(n, k)$ with $d(E, F) < \varepsilon$ such that*

$$L_{\pi_F \mu} \leq C/\varepsilon,$$

where $C > 0$ is an absolute constant. Additionally, if L_μ is bounded, then one can take $1 \leq k \leq n - 1$.

Patrick Spencer presented "A note on intersection bodies and Lorentz balls in dimensions greater than 4".

Let K be an origin-symmetric star body in $\mathbb{R}^n$. A star body L is called the intersection body of K if

$$\rho_L(\xi) = |K \cap \xi^\perp|, \quad \xi \in S^{n-1},$$

where $\rho_L(\xi)$ is the radius of L in the direction of ξ and $\xi^\perp$ is the hyperplane through the origin perpendicular to ξ.

The closure (in the radial metric) of the class of intersection bodies of star bodies is called the class of intersection bodies.

Let $w = (a_1, ..., a_n) \in \mathbb{R}^n$ be such taht $a_1 \geq a_2 \geq \cdots \geq a_n \geq 0$. Define a norm on $\mathbb{R}^n$ as

$$\|x\|_{w,q} = (a_1(x_1^*)^q + \cdots a_n(x_n^*)^q)^{1/q},$$

where x_1^*,..., x_n^* is the non-increasing permutation of $|x_1|$,..., $|x_n|$.

The space $\ell_{w,q}^n = (\mathbb{R}^n, \|\cdot\|_{w,q})$ is called the Lorentz space. The following result is proved.

Theorem 9.0.14 *Let $n \geq 5$ and $q > 2$. The function $\|x\|_{w,q}^{-p}$ represents a positive definite distribution if and only if $p \in [n - 3, n)$.*

In particular, the unit ball of $\ell_{w,q}^n$ is not an intersection body for $q > 2$ and $n \geq 5$.

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Chapter 10

Global/Local Conjectures in Representation Theory of Finite Groups (14w5024)

March 16 - 21, 2014

Organizer(s): Gunter Malle (TU Kaiserslautern), Gabriel Navarro (University of Valencia), Pham Huu Tiep (University of Arizona)

10.1 Overview of the Field

Group Theory is essentially the theory of symmetry for mathematical and physical systems, with major impact in diverse areas of mathematics. The Representation Theory of Finite Groups is a central area of Group Theory, with many fascinating and deep open problems, and significant recent successes. In 1963 R. Brauer [3] formulated a list of deep conjectures about ordinary and modular representations of finite groups. These conjectures have led to many new concepts and methods, but basically all of his main conjectures are still unsolved to the present day. A new wealth of difficult problems, relating global and local properties of finite groups, was opened up in the seventies and eighties (of the 20th century) by subsequent conjectures of J. McKay [Mc], J. Alperin [A2], M. Broué [Br], and others, all remain open up to date.

The classification of finite simple groups raised the hope that one should be able to reduce some of the aforementioned conjectures to statements about simple groups, and subsequenly establish these statements by exploring deep knowledge about simple groups provided by the Deligne-Lusztig theory and other recent fundamental results in group theory. This hope has recently materialized when the first three of the above mentioned conjectures have been reduced to questions about finite simple groups (see M. Isaacs, Malle, and G. Navarro [IMN], Navarro and P.H. Tiep [NT2], Navarro and Späth [NSp], and B. Späth [Sp2, Sp3]). Since then, further substantial progress on some of the remaining steps towards proving these conjectures has been achieved.

10.2 Recent Developments and Open Problems

In the meeting, we concentrated on recent progress on the following famous and longstanding global/local conjectures, some of which is discussed in more detail below. If G is a finite group, we denote by $\mathrm{Irr}(G)$ the set of irreducible complex characters of G and by $\mathrm{Irr}_{p'}(G)$ its subset consisting of characters having degree not divisible by p.

10.2.1 The Alperin-McKay Conjecture and refinements

The McKay conjecture [Mc] from 1972 is at the center of the representation and character theory. It is the origin, together with the Alperin Weight Conjecture, of the more far-reaching Dade conjecture as well as the Broué Conjecture (see below). If p is a prime and G is a finite group, then the McKay conjecture asserts that

$$|\mathrm{Irr}_{p'}(G)| = |\mathrm{Irr}_{p'}(\mathbf{N}_G(P))|\,,$$

where P is a Sylow p-subgroup of G and $\mathbf{N}_G(P)$ its normalizer. That is to say, a certain fundamental information on G is encoded in some local subgroup of G, namely the Sylow normalizer. Some time later, Alperin [A1] extended the statement to include Brauer blocks. This generalization is now known as the Alperin-McKay conjecture. Later, Isaacs, Navarro, and A. Turull [IN2, 81, Tu] discovered several refinements of the conjecture and these have contributed significantly to a further understanding of the problem.

A significant breakthrough was achieved by Isaacs, Malle and Navarro in 2007 in [IMN] where they reduced the McKay conjecture to a question on simple groups, the so-called *inductive McKay condition*. The latter has been established for important families of simple groups by Malle and Späth [Ma1, Sp1], relying heavily on the Deligne-Lusztig theory [27], and has led to interesting and difficult questions on automorphism groups of simple groups of Lie type. Ongoing work of Broué, P. Fong, and B. Srinivasan aims at proving the McKay conjecture and its refinements for finite reductive groups (in cross characteristic). Very recently, M. Cabanes and Späth [CS1, CS2] have proved the inductive McKay condition for some further families of simple groups of Lie type, and some of these results were presented by Cabanes at the meeting, see Section 3 for details. [1]

10.2.2 The Alperin Weight Conjecture

If the McKay Conjecture counts characters of p'-degree, then the Alperin Weight Conjecture (AWC), as formulated by R. Knörr and one of our main intended speakers G. R. Robinson [KR], counts characters with maximal p-part, the so called defect zero characters. Specifically, a character $\chi \in \mathrm{Irr}(G)$ has defect zero if $\chi(1)_p = |G|_p$. Alperin's original 1986 formulation [A2] is given by the formula

$$l(G) = \sum_Q z(\mathbf{N}_G(Q)/Q)\,,$$

where Q runs over representatives of conjugacy classes of p-subgroups in G; furthermore, $z(X)$ is the number of defect zero characters of the group X, and $l(G)$ is the number of p-regular classes of G. By using Möbius inversion, it is then possible to describe $z(G)$ in terms of local subgroup information. E. Dade's Conjecture extends the Knörr–Robinson formulation of AWC, and suggests a way to count the characters of G of any defect in terms of the local subgroup structure. It therefore generalizes both the McKay Conjecture and the Alperin Weight Conjecture. Dade's Conjecture was proved for p-solvable groups by Robinson [R].

In 2011 Navarro and Tiep [NT2] reduced the Alperin Weight Conjecture to a question on simple groups, the so-called *inductive AWC condition*. (L. Puig also announced another reduction of AWC to simple groups). This inductive AWC condition has now been established by work of Navarro–Tiep, Malle, J. An and H. Dietrich for many families of finite simple groups. Following the work of Navarro and Tiep [NT2], Späth [Sp2] has proved a reduction theorem for the stronger blockwise version of the Alperin Weight Conjecture. In the basic case of cyclic defect blocks, these inductive conditions (also for the Alperin-McKay conjecture) have been established recently by Koshitani and Späth [4] and presented at the meeting.

10.2.3 The Brauer Height Zero Conjecture

The Height Zero Conjecture, a fundamental problem on blocks of finite groups formulated in 1955 by Brauer, lead to many interesting and challenging questions on characters of finite groups. If B is a p-block with defect group D, then Brauer conjectured that all irreducible characters in B have height zero if and only if D is abelian. In particular, a positive solution would exhibit another connection between local and global invariants, providing, for

[1] Dr. B. Späth was one of the main invited speakers. Due to unexpected circumstances, she could not attend the meeting.

example, an extremely simple method to detect from a group's character table whether its Sylow p-subgroup is abelian. The p-solvable case of the Height Zero Conjecture is already an impressive result by D. Gluck and T. Wolf [GW00].

In the last two years, several breakthrough results have been proved concerning this conjecture. First, the solution of the Brauer Height Zero Conjecture for 2-blocks of maximal defect by two of the proposers, Navarro and Tiep, in [NT1]. Next, R. Kessar [2] and another proposer, Malle, completed in [KM] the proof of the "if" direction of the conjecture, relying in particular on the Berger-Knörr reduction [BK], as well as established the "only if" implication for the quasisimple groups. In another direction, Navarro and Tiep [NT3] have been able to prove the odd-p analogue of the aforementioned theorem of Gluck and Wolf, and therewith remove one of the main obstacles towards establishing the remaining, "only if" direction of the Height Zero Conjecture. Navarro and Späth [NSp] in 2012 succeeded in proving a reduction theorem for this direction of the conjecture to the inductive Alperin–McKay condition. Thus progress on the aforementioned Alperin–McKay Conjecture will ultimately also lead to a full proof of Brauer's conjecture.

10.2.4 The Broué Conjecture

The Alperin-McKay conjecture asserts that if B is a Brauer block of a finite group, then B and its First Main Theorem correspondent b have the same number of height zero characters. The block b is a uniquely determined block of the local subgroup $\mathbf{N}_G(D)$, where D is the defect group of B. Now, blocks are algebras, and Broué [Br] conjectured that the algebras B and b have intimate structural connections that should imply the desired facts on height zero characters and much more. Currently, the Broué Conjecture is only stated for D abelian, and it remains a challenge to find the correct formulation when the defect group is non-abelian.

In the landmark paper [CR1] J. Chuang and Rouquier have given a proof of the Broué Abelian Defect Conjecture for symmetric groups. More recently, D. Craven and Rouquier [CR2] have been exploring an interesting connection between cohomology of Deligne-Lusztig varieties and the Broué Conjecture for unipotent blocks of finite groups of Lie type. This approach already proves Broué's conjecture in some new cases and helps determine the previously unknown structure of the Brauer tree for some blocks with cyclic defect. Furthermore, at the meeting Craven announced a reduction theorem for the case of principal blocks of the Broué conjecture.

10.2.5 Future Directions

Recent progress on all these fundamental conjectures raises the hope that complete proofs of some of them may be possible in the not too distant future. Further significant progress will be achieved once we can resolve a number of basic questions on representations of finite groups of Lie type. With many experts in the Deligne-Lusztig theory present at the meeting, we had a discussion session on Thursday afternoon to draw a roadmap towards possible solutions of some of these principal obstacles.

10.3 Presentation Highlights

Now that reduction theorems for many basic conjectures have been proved, major efforts are concentrated in establishing the resulting inductive conditions for various families of finite simple groups. The opening lecture was given by M. Cabanes, in which he reported about his recent joint work with B. Späth establishing the inductive McKay conditions for finite simple groups of Lie type A (projective special linear and unitary groups over finite fields). Building on this, they also showed how one can verify the more involved conditions on the inductive Alperin-McKay conditions.

In a related direction, recent work of S. Koshitani and Späth is devoted to proving the inductive Alperin-McKay and blockwise Alperin weight conditions for cyclic defect blocks. Koshitani spoke at the meeting about this result.

When the block in question has a relatively small defect group, it is possible to prove some of the basic conjectures for this block directly, without using reduction theorems and the classification of the finite simple groups. In his talk, B. Sambale presented a new result establishing the Alperin–McKay Conjecture for blocks with

[2] Prof. R. Kessar was one of the main invited speakers. Unfortunately, due to visa issues, she was not able to make the trip.

metacyclic, minimal non-abelian defect groups. These are precisely the metacyclic groups whose derived subgroup have order p. In the special case $p = 3$, he also verified the Alperin Weight Conjecture for these defect groups.

M. Linckelmann spoke about his joint work with R. Kessar and Navarro. The starting point is a result by M. Isaacs, showing that a finite group G is p-nilpotent if and only if the highest power of p dividing the sum of the squares of the characters of degree prime to p is equal to the index of the p-focal subgroup in a Sylow p-subgroup of G. They showed that this statement admits a blockwise version which gives a characterization of nilpotent blocks. They also stated a variation of Brauer's Height Zero Conjecture for hyperfocal subalgebras.

For special classes of finite groups, the putative bijection in the McKay conjecture can indeed be constructed in a canonical way. This is the case for finite groups G with the property that $N_G(P) = PC_G(P)$ for a Sylow p-subgroup P and $p > 2$. At the meeting, C. Vallejo discussed her joint work with G. Navarro and P. H. Tiep, in which they proved that there is a natural correspondence between the irreducible characters of G of degree not divisible by p in the principal block and those of $N_G(P)$. In particularly, their result yields a natural McKay bijection for groups with self-normalizing Sylow p-subgroups. In fact, for these groups, Navarro's refinement of the McKay conjecture implies that there is a way to read off from the character table of G whether a Sylow p-subgroup of G is self-normalizing. This is indeed the case when $p > 2$, by a result of Navarro, Tiep, and A. Turull [NTT]. The case $p = 2$ of this question remains open, and A. Schaeffer Fry's talk discussed the reduction of that problem to simple groups.

Another highlight was O. Dudas' lecture, discussing his joint work with Malle on new techniques to compute decomposition numbers for finite groups of Lie type in non-defining characteristic. These techniques are based on modular analogues of Lusztig's results on the cohomology of Deligne-Lusztig varieties, some of which are still conjectural. Potential applications of these techniques include (i) a definition of families for representation in positive characteristic, (ii) an approach to showing unitriangular shape of the decomposition matrix, and (iii) bounds on the number of (Morita classes of) unipotent blocks depending only on the rank of the underlying algebraic group.

More generally, further progress in both complex and cross characteristic representation theories of finite groups of Lie type depends on better understanding of character sheaves, a class of perverse sheaves on a connected reductive algebraic group G as introduced by Lusztig in 1985. Given a Steinberg endomorphism $F : G \to G$, each F-stable character sheaf admits a class function of the finite group G^F. Determining the values of these class functions is of central importance to the determination of the ordinary character table of the finite group G^F. In his talk, J. Taylor presented a recent result which gives the restriction of each such class function to the set of unipotent elements. He then described how this fits into a larger goal of understanding Kawanaka's generalised Gelfand-Graev representations and the decomposition numbers of G^F in non-defining characteristic.

Harish-Chandra series of Brauer characters in groups of Lie type have been introduced more than 20 years ago. By work of Geck, the unipotent Brauer characters of the finite unitary groups $\mathsf{GU}_n(q)$ are labelled by partitions of n. The question of describing the division of the unipotent Brauer characters of the unitary groups into Harish-Chandra series is still open in general. G. Hiss' talk presented a series of conjectures relating this division with crystal graphs of certain integrable highest weight modules of the quantum group corresponding to a suitable affine Lie algebra of type A, and gave some evidence for these conjectures.

Broué, Malle and Michel [BMM] gave a bijection between between characters in a block of a general linear or classical group on one hand, and characters of a corresponding complex reflection group on the other hand. In her talk, B. Srinivasan gave a description of that connection, as arising from two equivalent representations of a Heisenberg algebra acting on a Fock space. She also made some remarks on the ℓ-decomposition numbers of $\mathrm{GL}_n(q)$ for large ℓ, again using the Fock space.

Given the recent progress on the Brauer Height Zero Conjecture, characters of positive defect in p-blocks of finite groups have started to gain more attention. In particular, a conjecture of Eaton and Moreto states that, whenever the defect group of a block is non-abelian, the smallest non-zero height in the block and in its defect group are the same. O. Brunat spoke about his joint work with Malle, where they verified this conjecture for all principal 2-blocks of finite quasi-simple groups, for all blocks of groups of Lie type when the prime is the defining characteristic and for all covering groups of symmetric and alternating groups.

Many years ago, Brauer and Feit proved that the irreducible characters in a block of defect $d \geq 2$ have height at most $d - 2$. Their argument used Brauer's notion of "subsections". It turns out the same result can be obtained using vertices and sources, as shown in M. Geline's talk.

D. Craven presented his recent joint work with R. Rouquier on the Broué conjecture. With the classification of Brauer trees for unipotent blocks of groups of Lie type being completed, they aim to investigate what happens in the non-cyclic defect group case. In particular, Craven discussed the techniques needed to solve the Brauer tree case, which of these techniques can extend, and how the derived category of a unipotent ℓ-block of $G(q)$ is independent not only of q, but also of ℓ.

Although being in the focus of intensive study for more than two decades, verifying the Broué conjecture for many of the 26 sporadic finite simple groups is still very challenging, both theoretically and computationally. J. Müller talked about his joint work with Koshitani and Noeske (Aachen), in which they showed how a combination of theoretical strategies and techniques from computational representation theory can be pursued to prove the Abelian Defect Group Conjecture of Broué for some of the sporadic simple groups.

Broué's perfect isometries are the shadow at the level of characters of derived equivalences between blocks of finite groups. In 1988, Michel Enguehard proved that two blocks of symmetric groups with the same weight are perfectly isometric. J.-B. Gramain discussed his recent joint work with O. Brunat, in which they generalize this result to many families of groups, such as alternating groups, double covers of symmetric and alternating groups, Weyl groups of types B and D, and certain wreath products.

An important step in the celebrated Chuang–Rouquier proof of the Broué conjecture for symmetric groups in characteristic p is a theorem of Chuang and Kessar establishing a Morita equivalence between the wreath product of the principal block of the symmetric group $\mathfrak{S}_p$ with $\mathfrak{S}_w$ and a certain special block of weight w of a symmetric group, called RoCK block (or Rouquier block), for $w < p$. In an effort to generalise this result to the case $w \geq p$ (i.e. to blocks of non-abelian defect), Turner conjectured that in this general case the same wreath product is Morita equivalent to a certain idempotent truncation of the RoCK block. A. Evseev's talk outlined a proof of Turner's conjecture, which also gives a new (and more explicit) proof of the Chuang–Kessar theorem.

Given any finite group G and any prime p, it is interesting to ask which ordinary irreducible representations of G remain irreducible in characteristic p. This question was solved for the symmetric groups several years ago, by the work of G. James and others. In his talk, M. Fayers addressed the case of the alternating group when p is odd. He explained how one can translate the question to one about representations of the symmetric group and thus ultimately answer it.

Motivated by the Broué conjecture and splendid Rickard equivalences, R. Boltje and P. Perepelitsky introduced the notion of p-permutation equivalences between p-blocks. In his talk at the meeting, Boltje discussed their joint work where they proved that a p-permutation equivalence between two blocks A and B preserves important invariants of the blocks A and B. Namely, such an equivalence induces (i) an isomorphism between defect groups and fusion systems, (ii) p-permutation equivalences on the local levels and an isotypy between A and B, (iii) Morita equivalences between the Brauer correspondents of A and B. It also preserves the 2-cohomology classes on the inertia groups and also the Külshammer–Puig classes for corresponding centric subgroups of the defect groups. They also determined restrictive properties of the shape of a p-permutation equivalence, and showed that the group of p-permutation auto-equivalences of a block is finite, and determined its structure in very simple cases.

Yet another highlight was B. Elias's lecture about his joint work with G. Williamson on Soergel bimodules and the p-canonical basis. In 1990, Soergel introduced a monoidal category SBim of bimodules over a polynomial ring, which encapsulates category O for the complex semisimple Lie algebra attached to a given semisimple algebraic group G. In 2000, he showed that this same monoidal category, but now defined over a field k of finite characteristic, encapsulates the rational representation theory of the algebraic group $G(k)$ "around the Steinberg weight." Both the characteristic zero and characteristic p versions have Grothendieck group isomorphic to the Hecke algebra H of the Weyl group, and the symbol of an object, when expressed in the standard basis of H, encodes certain multiplicities. In characteristic zero, Elias and Williamson have (re)proved the Soergel conjecture, which states that the symbols of indecomposable bimodules yield Kazhdan–Lusztig's canonical basis of H. In characteristic p, the symbols of indecomposable bimodules yield a basis called the p-canonical basis; its computation is an interesting and difficult open problem. In a more recent joint work, extending earlier work of Libedinsky and Elias–Khovanov, they established a presentation of (a monoidal subcategory of) SBim by generators and relations. This allows for a direct algebraic approach to the computation of the p-canonical basis, an approach which has already led to Williamson's recent disproof of the Lusztig conjecture.

A celebrated theorem of C. Jordan states that, for any d there exists a constant C such that any finite subgroup G of $GL_d(\mathbb{C})$ has an abelian subgroup $A \leq G$ of index at most C, and A can be generated by at most d elements. While the theorem is about finite linear groups, a number of analogues of it have been proposed. In his talk, A. Turull discussed his joint work with I. Mundet i Riera in which some of these conjectures are reduced to simpler questions. These joint results are used by Mundet to prove a conjecture of É. Ghys on manifolds without odd cohomology.

10.4 Scientific Progress Made and Outcome of the Meeting

10.4.1 General Comments

The meeting featured 20 talks, given by well-known experts in the area as well as many younger participants (including postdocs and a Ph. D. student !) The main theme of the meeting was to discuss recent important progress on several old and famous conjectures in modular representation theory, like the McKay conjecture, the Alperin weight conjecture, and the Brauer Height Zero Conjecture.

Aside from the officially scheduled talks, ample time was allocated to informal discussions. As mentioned above, a discussion session took place on Thursday afternoon to draw a roadmap towards possible solutions of some of these principal obstacles on the way to complete proofs of these conjectures. Many participants commented that the workshop "was a very fruitful and inspiring meeting due to the presence of almost all experts of the field, plus some other experts in neighboring subjects." Some of the younger participants also said that "meeting all the renowned experts in the field was very inspirational" and "through this workshop they had fruitful discussions which will be determining for their future research". Let us also quote Paul Fong, another participant, who said "I thought the recent Banff workshop one of the best of its kind. The theme of the workshop was well-served by the depth and breadth of the talks, by the insightful questions that followed many talks, and by the discussion sections Thursday afternoon. I liked the mixture of old and new faces. That so many young mathematicians are pushing the frontiers of the field is really encouraging. The relaxed atmosphere of the workshop gave ample opportunities for participants to have exchanges on the known and unknown."

10.4.2 Collaboration Started or Continued During the Meeting

Numerous additional discussions between the meeting's participants led to further collaborations and new results and projects; we reproduce some of the comments on these outcomes given by participants below.

Boltje: "It was a wonderful experience to be at BIRS. The following developments would not have happened (at all or as quickly) without the visit to Banff: (1) After my talk, Jürgen Müller and Susanne Danz approached me with the suggestion to write a computer program that would allow to compute and analyze p-permutation equivalences and more generally p-permutation modules. We met for about 3 hours, discussed possible algorithms, and have now an initial concept to work on. (2) There is a logical hierarchy between different types of equivalences of blocks of finite groups. Discussions with Jeremy Rickard and Markus Linckelmann gave me new ideas how to construct p-permutation equivalences that do not come from the stronger notion of a splendid Rickard equivalence. Examples of this type are currently unknown. (3) In collaboration with Susanne Danz we continued to complete a paper that we started more than a year ago on the quasi-heredity of certain category algebras."

Cabanes: "With Tiep I discussed the possibility of proving certain stabilizer statements in the case of finite symplectic groups from the existing literature he knows well. With Brunat, following Gramain's talk on their joint work, I discussed the possible applications of the representation theory of wreath products and the related Morita equivalences to the proof of more equivalences between blocks of Weyl groups or Hecke algebras of classical types. I had many discussions with Paul Fong about the relevance of his joint work with Broué and Srinivasan on Dade's conjecture in the case of unipotent blocks of finite reductive groups, especially in view of recent results by Späth producing a reduction theorem for that conjecture."

Danz: "Inspired by Robert Boltje's talk on Tuesday, he, Jürgen Müller, and I started to discuss possible strategies for investigating p-permutation equivalences between blocks of finite groups computationally. During the problem session on Thursday afternoon we developed some concrete ideas, and we now plan to meet again this summer to pursue our joint project. Moreover, during the free afternoon on Wednesday, Boltje and I had the chance to make significant progress on another joint project (on quasi-hereditary twisted category algebras), which we had started several months ago, but were not able to complete just via email or skype correspondence."

Denoncin: "Through this workshop I had fruitful discussions in particular with Brunat, Chuang, Gramain and Olsson which will be determinant for my future research. In particular I believe that I have all the tools to prove that the extension of Enguehard's isometry I constructed between two blocks of double cover of symmetric groups in characteristic 2 is perfect. The next goal is to do the same with double covers of alternating groups, thus completing the recent work of Brunat–Gramain."

Eaton: "Here are some fruitful interactions I had during the conference: (i) Initiation of research with Benjamin Sambale on invariants of 2-blocks with elementary abelian defect groups. This is in its early stages, but we have made some progress. (ii) Discussion on upper bounds of Loewy lengths of blocks with Shigeo Koshitani. We were able to discuss at length my ideas for these bounds. (iii) Discussions with Markus Linckelmann on two topics: centres of blocks; and subrings of blocks defined by irreducible characters of height zero. The former is leading to a new line of enquiry for my PhD student, involving the projective centre of a block and stable equivalences; the latter is related to his talk at BIRS and relates to my past research on generalised perfect isometries, and I will be looking into this. (iv) I had the opportunity to tell David Gluck at length about my work with Alex Moreto on minimal non-zero heights in blocks. There is an open problem arising from this research to do with p-solvable groups, which David is very well equipped to tackle."

Fong: "I found myself fielding questions from Suzanne Dansk related to defect groups of blocks in classical groups, getting in turn references from Joe Chuang on extensions of derived equivalences between $SL_2(q)$ and a Sylow p-normalizer, catching up with the state of some of Britta Späth's current work on the inductive conjectures from Marc Cabanes, and puzzling still over a question by Jay Taylor related to Brauer trees in classical groups."

Geck: "I enormously enjoyed my stay at BIRS; the workshop was very inspiring for me. Besides getting a great overview on current developments and meeting and discussing with people whom I haven't seen for a while, I found particularly useful the problem session/discussion, in which a variety of problems (from major directions to important obstacles of a mere technical nature) were explained and possible ways discussed on how to overcome them. This certainly provided some fresh insights for me which – I hope – may even lead to some new research projects and collaborations."

Gluck: "G. Navarro mentioned a problem to me in August, 2013. At Banff, we had a useful discussion about this problem, and I am thinking about it now. Also at Banff, C. Eaton mentioned another interesting problem, which I may work on in the future."

Koshitani: "(1) I discussed interesting subjects in the modular representation theory of finite groups from global-local point of view with Charles Eaton. This could be new joint work. (2) I discussed at length with Caroline Lassueur a problem coming from endo-trivial modules which show up quite often in many important and interesting situations in representation theory of finite groups. Thanks to our stay at BIRS, we have been able to start our joint work and hopefully it would be completed soon. (3) I discussed integral representation theory of finite groups with Michael Geline, especially the so-called Knörr lattices. "

Külshammer: "I personally profited, in particular, from discussions with M. Geline, M. Linckelmann and A. Turull on vertices of simple modules and characters. R. Kessar, M. Linckelmann and I are in the course of preparation of a manuscript on this topic which will hopefully be available in a few weeks or perhaps months."

Lassueur: "As a young postdoc the workshop has been an excellent opportunity to meet and ask questions to the researchers working in my area and getting a better idea of who is doing what... I also used the week in Banff to work on a collaboration started two weeks earlier with Koshitani on the computation of Green correspondence for blocks with Klein-four defect group. We have proved a first result in Banff and could also put together a schedule for our future work. I also realized from discussions with J. Müller that the work I have recently done on computing Green correspondence of simple modules going upstairs for the sporadic groups could be a good starting point for future work on Broué's conjecture for some blocks of the sporadic groups in characteristic 5 or 7."

Müller: "In the aftermath of Robert Boltje's talk on p-permutation equivalences, together with him and Susanne Danz we started to discuss ideas how these might be examined computationally. This seems desirable to obtain a better understanding, as currently there is a lack of interesting substantial examples, in particular of p-permutation equivalences which do not already come from splendid derived equivalences. Actually, we will meet later this year again to pursue this."

Navarro: "I have started a new line of research with M. Linckelmann about characterizing nilpotent blocks, which is a possible continuation of one of my recent papers. Also, with my co-organizer P. H. Tiep, we have started a possible refinement of McKay in groups with nilpotent Hall subgroups. At the meeting, my student C. Vallejo gave her first important international talk, and she already received an invitation to visit Kaiserlautern with Gunter Malle for some months to join his team working on the McKay conjecture. I also spoke with Gluck about my conjecture with Gunter about characterizing nilpotent blocks."

Schaeffer Fry: "Following my talk, there were some very good recommendations and discussions, for example with G. Malle, G. Navarro, and J. Taylor, which may help my progress on one of my current problems. I also had the opportunity to speak with G. Malle and P.H. Tiep about possibilities for future directions for my research involving the inductive Alperin-McKay and Blockwise AWC conditions, as well as S. Koshitani about new ways to simplify some arguments in my earlier work on the inductive conditions, which will be quite helpful in my future research. The workshop has also produced the exciting possibility of visiting the institutions of others involved in the workshop in the coming year, namely M. Geline and G. Malle."

Srinivasan: "I had discussions with several participants, including Marc Cabanes, Joe Chuang, Olivier Dudas and Anton Evseev. One lecture in particular by Olivier Dudas on work he was doing with Gunter Malle was especially interesting for me and gave me insight into my research. Among new contacts I would specially mention Ben Elias, a young mathematician who is doing cutting edge research."

Tiep: "During my stay at BIRS, I was able to start a new research project with my collaborator Gabriel Navarro, as well as continue our collaboration on ongoing projects that aim to resolve some basic questions on representations of finite groups. Together with Gunter Malle and Frank Lübeck (and in discussion with Jean-Baptiste Gramain and Olivier Brunat), I had started another new research project with the aim to answer a question of R. M. Guralnick concerning representations of finite quasisimple groups. I also had discussions with other participants, including Marc Cabanes, Gerhard Hiss, Klaus Lux, Bhama Srinivasan, and Amanda Schaeffer Fry."

Turull: "While at Banff, I enjoyed productive mathematical discussion on these and related topics with a number of researchers, including Michael Geline, David Gluck, and Burkhard Külshammer. These and other informal exchanges affected a number of papers on these conjectures that I am in the process of writing, and suggested new promising avenues of research. It was an excellent and productive experience all around."

10.4.3 Conclusion

All the workshop's participants agreed that Banff lived up to its promises of a quiet, inspiring and very comfortable place to make mathematics. We are all very grateful to the BIRS for providing such excellent facility for discussing and doing mathematics, and hope to return some time in the future.

Participants

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Bibliography

[A1] J. L. ALPERIN, The main problem of block theory. Pp. 341–356 in: Proceedings of the Conference on Finite Groups, Univ. Utah, Park City, Utah (1975), Academic Press, New York, 1976.

[A2] J. L. ALPERIN, Weights for finite groups. Pp. 369–379 in: The Arcata Conference on Representations of Finite Groups, Arcata, Calif. (1986), Proc. Sympos. Pure Math. **47**, Part 1, Amer. Math. Soc., Providence, 1987.

[BK] T. R. BERGER AND R. KNÖRR, On Brauer's height 0 conjecture. Nagoya Math. J. **109** (1988), 109–116.

[B] R. BRAUER, Representations of finite groups. Pp. 133–175 in: Lectures on Modern Mathematics **1**, Wiley New York, 1963.

[Br] M. BROUÉ, Rickard equivalences and block theory. Pp. 58–79 in: Groups '93 Galway/St. Andrews, London Math. Soc. Lecture Note Series **211**, Cambridge Univ. Press, 1995.

[BMM] M. BROUÉ, G. MALLE, AND J. MICHEL, Generic blocks of finite reductive groups. Reprsentations unipotentes génériques et blocs des groupes réductifs finis. Astérisque No. **212** (1993), 7–92.

[CS1] M. CABANES AND B. SPÄTH, Equivariant bijections in finite reductive groups with connected centre, Math. Z. **275** (2013), 689–713.

[CS2] M. CABANES AND B. SPÄTH, On the inductive Alperin-McKay condition for simple groups of type A. ArXiv e-prints. (1403.4708), (submitted).

[CR1] J. CHUANG AND R. ROUQUIER, Derived equivalences for symmetric groups and sl_2-categorification. Ann. of Math. (2) **167** (2008), 245–298.

[CR2] D. A. CRAVEN AND R. ROUQUIER, Perverse equivalences and Broué conjecture. Adv. Math. **248** (2013), 1–58.

[GW] D. GLUCK AND T. R. WOLF, Brauer's height conjecture for p-solvable groups. Trans. Amer. Math. Soc. **282** (1984), no. 1, 137–152.

[IN2] I. M. ISAACS AND G. NAVARRO, New refinements of the McKay conjecture for arbitrary finite groups. Ann. of Math. (2) **156** (2002), 333–344.

[IMN] I. M. ISAACS, G. MALLE AND G. NAVARRO, A reduction theorem for the McKay conjecture. Invent. Math. **170** (2007), 33–101.

[KM] R. KESSAR AND G. MALLE, Quasi-isolated blocks and Brauer's height zero conjecture. Ann. of Math. **178** (2013), 321–384.

[KR] R. KNÖRR AND G. R. ROBINSON, Some remarks on a conjecture of Alperin. J. London Math. Soc. (2) **39** (1989), 48–60.

[KS] S. KOSHITANI AND B. SPÄTH, The inductive Alperin-McKay and blockwise Alperin weight conditions for blocks with cyclic defect groups, (submitted).

[L] G. LUSZTIG, 'Characters of Reductive Groups over a Finite Field', Annals of Math. Studies **107**, Princeton Univ. Press, Princeton, 1984.

[Ma1] G. MALLE, Height 0 characters of finite groups of Lie type. Represent. Theory **11** (2007), 192–220.

[Mc] J. MCKAY, Irreducible representations of odd degree. J. Algebra **20** (1972), 416–418.

[N] G. NAVARRO, The McKay conjecture with Galois automorphisms. Ann. of Math. **160** (2004), 1129–1140.

[NSp] G. NAVARRO AND B. SPÄTH, On Brauer's height zero conjecture. J. Europ. Math. Soc. (to appear).

[NT1] G. NAVARRO AND PHAM HUU TIEP, Brauer's height zero conjecture for the 2-blocks of maximal defect. J. Reine Angew. Math. **669** (2012), 225–247.

[NT2] G. NAVARRO AND PHAM HUU TIEP, A reduction theorem for the Alperin weight conjecture, Invent. Math. **184** (2011), 529–565.

[NT3] G. NAVARRO AND PHAM HUU TIEP, Characters of relative p'-degree over normal subgroups. Ann. of Math. **178** (2013), 1135–1171.

[NTT] G. NAVARRO, PHAM HUU TIEP, AND A. TURULL, p-rational characters and self-normalizing Sylow p-subgroups. Represent. Theory **11** (2007), 84–94.

[R] G. R. ROBINSON, Dade's projective conjecture for p-solvable groups. J. Algebra **229** (2000), no. 1, 234–248.

[Sp1] B. SPÄTH, The McKay conjecture for exceptional groups of Lie type and odd primes. Math. Z. **261** (2009), no. 3, 571–595.

[Sp3] B. SPÄTH, A reduction theorem for the Alperin-McKay conjecture. J. Reine Angew. Math. **680** (2013), 153–189.

[Sp2] B. SPÄTH, A reduction theorem for the blockwise Alperin weight conjecture. J. Group Theory **16** (2013), 159–220.

[Tu] A. TURULL, Strengthening the McKay conjecture to include local fields and local Schur indices. J. Algebra **307** (2007), no. 1, 300–305.

Chapter 11

Parameterized Morse Theory in Low-Dimensional and Symplectic Topology (14w5119)

March 23 - 28, 2014

Organizer(s): David Gay (University of Georgia), Michael Sullivan (University of Massachusetts-Amherst)

11.1 Overview and highlights of workshop

Morse theory uses generic functions from smooth manifolds to $\mathbb{R}$ (Morse functions) to study the topology of smooth manifolds, and provides, for example, the basic tool for decomposing smooth manifolds into elementary building blocks called handles. Recently the study of parameterized families of Morse functions has been applied in new and exciting ways to understand a diverse range of objects in low-dimensional and symplectic topology, such as Morse 2–functions in dimension 4, Heegaard splittings in dimension 3, generating families in contact and symplectic geometry, and n–categories and topological field theories (TFTs) in low dimensions. Here is a brief description of these objects and the ways in which parameterized Morse theory is used in their study:

A **Morse** 2**–function** is a generic smooth map from a smooth manifold to a smooth 2–dimensional manifold (such as $\mathbb{R}^2$). Locally Morse 2–functions behave like generic 1–parameter families of Morse functions, but globally they do not have a "time" direction. The singular set of a Morse 2–function is 1–dimensional and maps to a collection of immersed curves with cusps in the base, the "graphic". Parameterized Morse theory is needed to understand how Morse 2–functions can be used to decompose and reconstruct smooth manifolds [20], especially in dimension 4 when regular fibers are surfaces, to understand uniqueness statements for such decompositions [21], and to use such decompositions to produce computable invariants.

A **Heegaard splitting** of a 3–manifold is a decomposition into two solid genus g handlebodies, and the existence of Heegaard splittings follows directly from Morse theory. Heegaard splittings are unique up to a certain stabilization procedure, a fact which is proved with standard Cerf theory. Parameterized Morse theory arises much more subtly when comparing two Heegaard splittings and asking how many stabilizations are needed to make them the same. The two Heegaard splittings are replaced with two Morse functions, or sweepouts, and these give a map to $\mathbb{R}^2$ which, generically, is a Morse 2–function as discussed above. For example, Johnson [27] built on ideas of Rubinstein and Scharlemann [36] and used a careful understanding of the graphic of critical values to get bounds on the number of stabilizations needed.

To understand **generating families**, consider a cotangent bundle with the standard symplectic structure, or a one-jet space with the standard contact structure. Using an N-dimensional Cerf theory, Viterbo showed how to generate any Lagrangian submanifold in the cotangent bundle with an N-parameter family of functions, where N might be arbitrarily large [48]. In this context, the N-parameter family is called a "generating family." For a similarly-defined generating family of any Legendrian submanifold in a one-jet space, a certain relative Morse homology is called the submanifold's generating homology. Traynor and her collaborators have a number of computations demonstrating the homology's applicability [33, 39, 40], while Fuchs and Rutherford show that this homology is the same as a certain linearization of the Chekanov-Eliashberg differential graded algebra (DGA) for Legendrian knots in standard contact R^3 [18].

An n**–category** is something for which the prototypical example is given by cobordisms between cobordisms between cobordisms and so on, for n levels. For example, the 2–category of surfaces has objects which are points, morphisms which are 1–dimensional cobordisms between points, and 2–morphisms which are 2–dimensional cobordisms between 1–dimensional cobordisms between points. A **TFT** is a functor from a cobordism n–category to an n–category of algebraic objects, such as vector spaces, giving invariants of manifolds computable by cutting up into n–category cobordisms. Just as ordinary Morse functions give decompositions into elementary cobordisms, i.e. handles, n–families of Morse functions and Morse n–functions can give decompositions in the n–category sense, and introducing further parameters can give relations amongst such decompositions. Schommer-Pries [44] has carried out this program to get a complete set of generators for the 2–category of surfaces.

The study of each of these objects naturally uses very similar tools in parameterized Morse theory, but the broad fields in which the study of these objects live are often seen as quite far apart, so that researchers in these fields are not necessarily aware of the overlaps. This workshop brought together these researchers to learn from each other, develop common terminology, and share tools. As people working in one field gained a clearer picture of how parameterized Morse theory is being used in other fields, they came away with new techniques to use in their own fields as well as new ideas for how their own techniques may contribute to the other fields.

For those readers who would like to watch some of the recorded videos from the workshop, our week was structured as follows: Monday was devoted to four introductory talks, on 3–manifolds, 4–manifolds, TFTs, and symplectic topology. Tuesday morning focused on 3–manifolds, Tuesday afternoon focused on 4–manifolds, and Tuesday evening was devoted to a group discussion of open problems in 3– and 4–dimensional topology. Wednesday morning focused on TFTs, Wednesday afternoon was free, and Wednesday evening we discussed open problems related to TFTs. Thursday focused on symplectic and contact topology, ending with an open problem session Thursday evening. Friday morning featured one more 4–manifold talk and one more contact topology talk.

We would like to highlight two specific talks as representative of the impact and diversity of the workshop. Jamie Vicary introduced a room full of topologists to some fascinating ideas in computer science, ranging from quantum teleportation to encrypted communication, that are beautifully tied to low-dimensional topology and Morse theory. Yakov Eliashberg gave the first public announcement of a ground breaking result (with coauthors Emmy Murphy and Strom Borman) extending Eliashberg's well known existence and uniqueness results for overtwisted contact structures in dimension 3 to arbitrary odd dimensions.

The evening problem sessions were not recorded on video but careful notes were produced. The bulk of this report describes the problems which arose during these sessions.

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11.2 Problems

This next section describes problems (many of which were open to the conference participants as of March 2014) posed during the evening problem sessions. The person listed at the beginning of each problem is the one who posed it to the other participants. After some of the problems follows a list of remarks that were discussed in response.

11.2.1 3– and 4–dimensional manifolds

Problem 11.2.1 *(Johnson and Baker) Characterize fibred tunnel number one knots.*

Remark: Rathbun [35] has shown the tunnel can be isotoped to lie in the fiber.

Problem 11.2.2 *(Baker) Does there exist an infinite family of fibred knots in S^3 such that the same surgery produces the same manifold?*

Remark: Osoinach [34] introduced a way to create infinite families of knots for which the same surgery produces the same manifold, but it appears only finitely many knots in such families will be fibered.

Problem 11.2.3 *(Baker) Classify tunnel number one knots with lens space surgeries.*

Remark: All knots in S^3 known to admit a lens space surgery (the Berge knots) have tunnel number one.

Problem 11.2.4 *(Baker) Must a knot in S^3 with a lens space surgery have tunnel number one?*

Remark: This is weaker than the Berge conjecture, which is that such knots are tunnel one and doubly-primitive.

Problem 11.2.5 *(Baker) Which strongly quasipositive knots (SQP) are fibred?*

Remarks: Given an SQP knot in an SQP presentation, is there an efficient way to determine if the knot is fibred? Is there a monotonic simplification within SQP presentation to easily determine if a knot is fibred?

A knot is strongly quasipositive if it has a braid presentation as a product of the braids $\sigma_{i,j} = (\sigma_i \ldots \sigma_{j-2})\sigma_{j-1}(\sigma_i \ldots \sigma_{j-2})^{-1}$ where σ_i is the standard braid generator.

Lee Rudolph [37] introduced quasipositive knots in his study of complex algebraic curves, and strongly quasipositive knots arise from links of singularities. Hedden [26] has shown that fibered SQP knots are precisely the fibered knots in S^3 whose open books support the tight contact structure, and any knot in S^3 with a positive surgery to a Heegaard Floer L-space must be a fibered SQP knot.

Problem 11.2.6 *(Baker) Let K_1 and K_2 be a pair of homotopic knots in a 3-manifold M and K_1^*, K_2^* be a pair of homotopic knots in M^* such that for some non-trivial slope r, $K_i(r)$ (filling) is homeomorphic to M^* with surgery dual K_i^*. Because they're homotopic, it makes sense to talk about the same surgery slope for both K_1 and K_2. Must one of the pairs K_1, K_2 or K_1^*, K_2^* be isotopic? Perhaps up to an orientation-preserving automorphism of M or M^*.*

Remark: Specializing to $M = S^3$, this asks the following. If r surgery on each of a pair of distinct knots produces the same manifold M^*, then must the surgery duals to these knots be in distinct free homotopy classes modulo orientation-preserving homeomorphisms of M^*? An affirmative answer would, for example, resolve the Berge Conjecture.

Problem 11.2.7 *(Budney) Let $K_n = \{f : \mathbb{R} \to \mathbb{R} \times \mathbb{R}^{n-1}, f(x) = (x, 0)\ \forall x \notin [-1, 1]\}$. The maps f are required to be C^∞-smooth embeddings, and we give the space K_n the C^∞-topology. The inclusion $\mathbb{R}^n \to \mathbb{R}^{n+1}$ gives an inclusion $K_n \to K_{n+1}$. A classical argument all topologists are familiar with is that all smooth embeddings $S^1 \to S^4$ are isotopic. In this context, that argument provides two null-homotopies of the inclusion $K_n \to K_{n+1}$. The first null-homotopy comes from perturbing the knot in the positive orthogonal direction $\mathbb{R}^n \times \{0\} \subset \mathbb{R}^{n+1}$ and then applying the straight-line homotopy in the $\mathbb{R}^n \times \{0\}$ factor. The second null-homotopy comes from using the negative of that bump function. The two maps together give a map*

$$K_n \to \Omega K_{n+1}$$

Is this map null-homotopic? i.e. are the two ways of trivializing knots from K_n in K_{n+1} distinct?

Remark: If it is null-homotopic, can you find two canonical ones? And does the map $K_n \to \Omega^2 K_{n+1}$ induce an isomorphism on the lowest-dimensional homotopy group? The first non-trivial homotopy group of K_n is in dimension $2n - 6$, and is isomorphic to $\mathbb{Z}$ for $n \geq 4$.

Problem 11.2.8 *(Gay) Given a Morse function $f : X^4 \to \mathbb{R}$ on a 4–manifold X, find a lower-boundon the complexity of the Cerf graphic connecting f to $-f$ in terms of the combinatorial data in f.*

Remark: In [25] it was shown that for some 3–manifolds M, g births and deaths were needed where g is the genus of the Heegaard surface for f; [27] for a combinatorial version.

Problem 11.2.9 *(Melvin) The surgery number of a* 3*-manifold* Y *is defined to be the smallest* n *such that the* Y *can be realized as integer surgery on an* n *component link in the* 3*-sphere. Compute the surgery numbers of lens spaces. In particular, which lens spaces have surgery number* 2*?*

Remark: Note that the lens spaces of surgery number 1 have been characterized by Josh Greene [24]; they are precisely those that arise from surgery on Berge knots.

Problem 11.2.10 *(Auckly) Given a cusped hyperbolic* 3*-manifold* M*, all but finitely-many fillings are hyperbolic, and for all but finitely many fillings, the filled manifold* M' *has an isometry group which embeds in the isometry group of* M*, i.e.* $Isom(M') \subset Isom(M)$*. Find examples of exceptional surgeries where* $Isom(M')$ *does not embed in* $Isom(M)$*.*

Let M and N be homotopy equivalent (or homeomorphic, after Freedman) closed oriented simply-connected smooth 4-manifolds. Since Wall [49], we know that M and N are stably-diffeomorphic, i.e., they become diffeomorphic after connect summing both M and N with n copies of $S^2 \times S^2$ for large enough n. However, there is no known a priori upper bound on n.

Furthermore, it was shown in [11] that all *known* ways to construct infinite families of exotic (i.e. pairwise homeomorphic but not diffeomorphic) simply-connected 4-manifolds up to date always produce 4-manifolds which become diffeomorphic after one stabilization, that is, $n = 1$. The same result for knot surgery (remove a $T^2 \times B^2$, and glue in a knot complement cross S^1) was obtained earlier by Auckly [5] and Akbulut [2] using Kirby calculus.

Problem 11.2.11 *(Auckly): Are there any pairs* M *and* N *as above for which at least* n *stabilizations are needed for them to become diffeomorphic, with* $n > 1$*? Are there pairs for which* n *is arbitrarily large?*

Remark: Similar stabilization problems and analogous results for embeddings of surfaces are studied in [6] and in [12]. In the latter paper, exotic embeddings (topologically isotopic but not smoothly) of surfaces in 4-manifolds are shown to be stably smoothly isotopic where stabilization means a pairwise connected sum with (S^4, T^2). Again, for all known constructions, one stabilization is enough to get smoothly isotopic surfaces.

Recall that a logarithmic transform is the surgery operation in dimension 4 analogous to Dehn surgery in dimension 3: take out the tubular neighborhood of an embedded self-intersection zero 2-torus and glue it back in possibly with a twisted boundary diffeomorphism.

In [11], it was shown that between any two homeomorphic (in general, not necessarily simply-connected!) M and N as above, there is a cobordism from M to N which consists of round 2-handles only. As a corollary, one can pass from M to N after a sequence of n logarithmic transforms. If M and N are diffeomorphic after 1 stabilization with $S^2 \times S^2$, then one can pass from M to N after at most 2 integral logarithmic transforms, and conversely, if one can pass from M to N after 1 integral logarithmic transform, then M and N are diffeomorphic after 1 stabilization.

Hence, since almost all constructions of exotic 4-manifolds involve generalized logarithmic transforms along tori, it would be good to consider the following re-formulation of the problem above — with the obvious shift by 1 in mind.

Problem 11.2.12 *(Stern): Are there any pairs* M *and* N *as above for which at least* n *logarithmic transforms are needed to pass from* M *to* N*, with* $n > 1$*? Are there pairs for which* n *is arbitrarily large?*

Problem 11.2.13 *(Kirby) If a simply connected 4-manifold does not admit an almost-complex structure, is it a connected sum? Possible counterexamples are given in Problem 4.97 of [28].*

Problem 11.2.14 *(Budney) If a* 3*-manifold* M *embeds smoothly in* S^4*, it decomposes the* 4*-sphere into two* 4*-manifolds* V_1 *and* V_2 *having* M *as their common boundary. Can one ensure, after possibly re-embedding* M *in* S^4 *that* $\pi_1 V_1$ *and* $\pi_1 V_2$ *have solvable word problems?*

Remark: There are explicit examples of 3-manifolds in S^4 where either (or both) $\pi_1 V_1$ and $\pi_1 V_2$ have unsolvable word problems. See Dranishnikov and Repovs [14]. There are also examples due to Gompf for $M = S^3$ where V_1 has trivial fundamental group, yet the presentation from the standard height function on S^4 is not known to be Andrews-Curtis trivializable [23].

Problem 11.2.15 *(Teichner) Does every closed, smooth, oriented 4-manifold have a Heegaard splitting in the sense that it is a twisted double of a handlebody made with 0-, 1- and 2-handles?*

Problem 11.2.16 *(Baykur) Does every simply-connected smooth 4-manifold admit an involution with 2-dimensional fixed-point set?*

Problem 11.2.17 *(Budney) Is there an algorithm to recognize a triangulated S^4?*

Remark: In dimension 3 there is the Rubinstein-Thompson algorithm [46]. There is no algorithm to recognize all connected sums of $S^2 \times S^2$ [30]. In dimension $n \geq 5$ it is not an algorithmically-solvable problem (Nabutovsky).

Problem 11.2.18 *(Budney) Is there a reasonable theoretical criterion for a smooth 4-manifold to fibre over S^1?*

Remark: In dimension 3 there are two such theorems; Stallings' theorem states that all one needs is an epimorphism $\pi_1 M^3 \to \pi_1 S^1$ with finitely-presented kernel, and Schleimer's dissertation gives an algorithm to decide (assuming M has a triangulation). In high dimensions there is the Farrell fibering theorem, which uses the language of surgery theory.

Problem 11.2.19 *(Budney) If a 3-manifold embeds smoothly in a homotopy 4-sphere, does it embed smoothly in S^4?*

Remark: Replace 3 and 4 by n and $n+1$ and the answer is affirmative for all $n \neq 3$. If the answer to this question appears to be negative, it could provide a strategy to recognize non-standard homotopy 4-spheres.

In the next four problems Morse 2-functions and trisections of 4-manifolds are mentioned. A Morse 2-function $f : X^n \to \Sigma^2$ is a generic smooth map to an orientable surface, often B^2 or S^2 [21]. When $\Sigma = B^2$, f can be homotoped so that if B^2 is a pie with three slices, then f^{-1} of each slice is diffeomorphic to a connected sum of k copies of $S^1 \times B^3$, whose boundary has a Heegaard splitting of genus g; thus $f^{-1}(0)$ is a surface of genus g [22]; When g is minimal, g is the trisection genus of X^4.

Problem 11.2.20 *(Zupan) Use Morse 2-functions [21] to find a notion of thin position for 4-manifolds.*

Problem 11.2.21 *(Gay) Compute a trisection genus of a 4-manifold that is 3 or larger.*

Remark: This represents the problem of trying to find computable lower-bounds on the trisection genus.

Problem 11.2.22 *(Scharlemann) If a homology 4-ball with boundary S^3 can be described as $2/3$ of a trisection diagram, is this enough to conclude that the 4-manifold is the standard PL B^4?*

Remarks: One can view $2/3$ of a trisection as a Heegaard union, as introduced in [43][Section 3]: Two 4-dimensional handlebodies J_1, J_2, of genus $\rho_1 \leq \rho_2$, are glued together along a 3-dimensional handlebody H so that in each of $\partial J_1, \partial J_2$ the complement of H is also a 3-dimensional handlebody. In [43][Prop. 3.3] it is shown that if a homology 4-ball W with $\partial W = S^3$ is a Heegaard union, then the weak generalized Property R conjecture (for a link of ρ_1 components) implies $W \cong B^4$. (The proof shows slightly more, namely that we can restrict attention to links with tunnel number $\leq \rho_2$. This last observation may just be a distraction, but it was useful in [42], because at the time Property R had only been proven for knots of tunnel number 1 [41].)

The problem itself is motivated by one approach to the Schoenflies Conjecture: given a standard Kearton-Lickorish embedding of S^3 in S^4, try to iteratively reimbed the complementary components X and Y in a level-preserving way so that ultimately one or the other (say X) has middle level a 3-dimensional handlebody. If this can be accomplished (as Fox's reimbedding theorem gently suggests might be possible), then X has the structure of a Heegaard union, so a solution to the problem above would show that X is D^4.

Problem 11.2.23 *(Johnson) What 3-manifolds occur as boundaries of $2/3$ of a trisection diagram?*

Remark: "$2/3$ of a trisection diagram" means gluing together two 4-dimensional handlebodies along a 3-dimensional handlebody which is half of a Heegaard splitting of each boundary (which is the connect-sum of $S^1 \times S^2$'s).

The answer to this question is "all". Here is a sketch of a proof which relies on a good understanding of [22] where the argument is only implicit. Observe that if a sector (1/3 of a trisection) is B^4 with the genus 1 Heegaard splitting of the bounding S^3, then the sector has one fold curve with a cusp, and the cusp is associated with a Dehn twist in the T^2 along the $1-1$ curved which takes meridian to longitude. In general a cusp corresponds to a Dehn twist along a curve in the Heegaard surface. (It also corresponds to adding a 2-handle to one 3-dimensional handlebody to obtain another 3-dimensional handlebody.) Now write our closed, orientable 3-manifold as a Heegaard splitting with a diffeomorphism d of the Heegaard surface, realize d as a product of Dehn twists, and realize the Dehn twists as cusps in fold curves.

Problem 11.2.24 *(Baykur) Find an exotic family of simply-connected 4-manifolds X_n with broken genus of X_n arbitrarily large, as n gets large. Determine the broken genus of the remaining standard simply-connected 4-manifolds, i.e. connected sums of copies of $S^2 \times S^2$ and $K3$.*

Remark: A simplified broken Lefschetz fibration for X^4 is a Lefschetz fibration over S^2 but with at most one fold circle which is embedded with all Lefschetz singularities on one side. The broken genus is the minimal genus of a fiber (on the higher side of the fold circle) over all possible broken Lefschetz fibrations [9][10].

A related notion is an indefinite Morse 2-function to $X^4 \to S^2$ with one indefinite embedded fold with cusps [50]; the cusps can be replaced by Lefschetz singularities which turns it into a simplified broken Lefschetz fibration.

Problem 11.2.25 *(Auckly) Find more accurate lower-bounds on the Martelli complexity [31][4] of smooth 4-manifolds.*

Problem 11.2.26 *(Eliashberg) Given an almost-symplectic M^4, $\omega \in H^2 M$ with $\omega^2 \neq 0$ with an almost-complex structure, does there exist a surface $\Sigma \subset M$ such that $\Sigma^* \in H^2 M$ is a multiple of ω, and a branched cover of (M, Σ) admits a symplectic structure such that Σ is a symplectic surface in the cover?*

Remark: This is the algebraically symplectic implies virtually symplectic problem.

Problem 11.2.27 *(Baker) Is there a useful generalization of A'Campo's links of divides to higher dimensions?*

Remark: Studying real Morsifications of complex plane curve singularities led A'Campo [1] to the notion of a divide and the link of a divide. A divide P is the image of a generic relative immersion of a disjoint union of r arcs into the unit disk in $\mathbb{R}^2$. Viewing S^3 as the unit sphere in $T\mathbb{R}^2$, the link of a divide P is the link in S^3 of r components $L(P) = \{(x, v) \in T\mathbb{R}^2 \colon x \in P, v \in T_x P, |x|^2 + |v|^2 = 1\}$. Links of connected divides with δ double points are oriented fibered links with fibers of genus $r - 1 + \delta$ whose monodromy is a product of $r - 1 + 2\delta$ positive Dehn twists. If $r = 1$ so that $L(P)$ is a knot, then both its gordian number and 4–ball genus is δ. There are several generalizations of links of divides that encompass a greater variety of knots and links in 3–manifolds.

Are there higher dimensional analogues? For example, with S^5 as the unit sphere in $T\mathbb{R}^3$, one may ask about the link of a generic relative immersion of a disk in the unit 3-ball. This however leads to an immersion of S^3 into S^5 rather than an embedding.

11.2.2 Topological Field Theories

An introduction by Paul Melvin, one of the facilitators for the TFT evening session:

- I worked on quantum invariants in the early days. Several at this conference have asked: What is the point of Topological Quantum Field Theory (TQFT)? We've seen at this conference how it relates to mathematics, computer science and physics. A good starting point for understanding the latter is Baez's paper on its role in framing a theory of quantum gravity [8].

- On page 136 of Turaev's book [47], he formulates the properties of an arbitrary quantum invariant $\tau(M)$ of closed n-manifolds needed for it to be promoted to a TQFT T : nCob $\to$ Hilb. The main condition is the 'splitting axiom'. Maybe this is a 'cheat' but I always found it interesting.

Problem 11.2.28 *(Auckly) Are all Chern-Simons theories for $(G, \text{level } k)$ determined by finitely many BPS states?*

Remark: See Auckly and Koshkin's monograph [3] for further details. It appears that there might exist a 3-manifold invariant taking the form $Z_M(a,q)$ such that:

- It gives the rank N level k Chern-Simons invariant of M for $a = q^N$, $q = e^{2\pi i/(k+N)}$.
- It has the structure $Z_M(a,q) = \sum Z_d(q)a^d$
- The coefficients of Taylor expansion of $Z_d(q)$ about $q = 0$ are integers.
- The function $Z_d(-e^{iu})$ has an asymptotic expansion at $u = 0$ along the positive reals.
- The functions $Z_d(q)$ satisfy some funky modularity properties as evidenced by Hikami and others.
- It is determined by a finite number of integer BPS invariants.

Problem 11.2.29 *(Not recorded) Is there a 4-dimensional TFT (necessarily not unitary by the work of Mike Freedman et al [17]) that distinguishes smooth structures?*

Remark: Known invariants that distinguish smooth structures, such as Seiberg-Witten invaraints, are not known to be TFT's. To date we have used PDE's to distinguish smooth structures. But we know in dim 4 that Diff = PL, so we know there should be something combinatorial. An application of the cobordism hypothesis would be a combinatorial model.

Problem 11.2.30 *(Gay) What are the obstructions to finding generators and relations for Bord$_{1,2,3,4}$?*

Remark: According to Douglas and Schommer-Pries, there is no fundamental obstruction, just hard work; they did a bunch of calculations on this, working out 3-Morse theory singularities $M^4 \to \mathbb{R}^3 \to \mathbb{R}^2 \to \mathbb{R}$. It seems to give a whole stack of relations and it may be too difficult to simplify these relations. Better would be to have tools to say, for example, "These singularities are not necessary," perhaps a version of Igusa's theorem. Teichner points out that if you just do 2-3-4 then it's much harder, you need to throw in the surface with all its diffeomorphisms; not just the mapping class group but π_0 and π_1. You can't cut the surface up anymore.

Problem 11.2.31 *(Not recorded) What are the possible applications of the presentation of Bord$_{123}$ to the study of 3-dimensional manifolds?*

Remark: Suggestions include: recognizing S^3; proving some known restrictions on π_1 of 3–manifolds (eg. show that no 3-manifold has fundamental group $\mathbb{Z}_2 \times \mathbb{Z}_2$); showing that an orientable 3-manifold is parallelizable; deriving complexity measures on 3-manifolds; deciding if a 3-manifold has an essential torus or not. One difficulty is that Funar has recently proved [19] that Reshetikhin-Turaev TQFT's cannot distinguish certain torus bundles over the circle, and [13] shows that all TQFT's are of RT type. However, perhaps in a different target 2-category they may be distinguishable. There is also the information flow from topology to algebra. For instance, [13] shows how the Radford theorem on the square of the antipode in a Hopf algebra follows from $\pi_1 SO(3) = \mathbb{Z}_2$. This uses a trivial fact from 3-manifold topology to prove something interesting in algebra. Maybe more nontrivial 3-manifold facts will lead to even more interesting results in algebra.

Problem 11.2.32 *(Douglas) Do all 3D quantum invariants come from quantum groups?*

Problem 11.2.33 *(Kirby) What is the nicest reference for understanding the cobordism hypothesis of Baez and Dolan?*

Remark: The survey by Dan Freed [16].

11.2.3 Symplectic geometry

Problem 11.2.34 *(Sabloff) Characterize the smooth knot types that have a Legendrian representative with a Lagrangian filling.*

Remark: A sufficient condition is that the knot type is positive. A necessary condition is that it is quasi-positive. One conjectured necessary and sufficient condition is quasi-positive and sharp HOMFLY.

Problem 11.2.35 *(Sabloff) Classify the geography for non-loose Legendrian n-spheres in standard contact R^{2n+1}. That is, what range of tb and r can be realized by such?*

Remark: Murphy showed that there is no restriction for loose Legendrians [32]. If the non-loose Legendrian has a Lagrangian filling, then probably $r = 0$.

Problem 11.2.36 *(Sullivan) If a k-dimensional sphere of loose Legendrian submanifolds in standard contact R^{2n+1} has no formal obstruction to being contractible, can it be contracted to a single Legendrian?*

Remark: Murphy proves that obstructions to isotopying loose Legendrians are purely formal [32]. She does this using an h-principal and removing certain wrinkle and fold singularities. The k-parametric h-principal exists [15]. The removal of singularities, while not immediate, should be doable.

Problem 11.2.37 *(Eliashberg) Consider a Weinstein manifold constructed by surgery along a loose knot. Does it have a presentation using surgery along only non-loose knots? Similarly, can attaching along a single non-loose knot yield a flexible Weinstein manifold?*

Problem 11.2.38 *(Eliashberg) Characterize flexible Weinstein manifolds in terms of Lefschetz fibrations for dimension ≥ 6.*

Problem 11.2.39 *(Not recorded) Characterize all Legendrian submanifolds that have generating families.*

Remark: They must be non-loose, but that is not a sufficient condition.

Problem 11.2.40 *(Traynor) Compare generating homology (Morse theory) with linearized Legendrian contact homology (pseudo-holomorphic curves) for a Legendrian submanifold in one-jet spaces.*

Remark: For Legendrian knots in R^3, every generating homology is some linearization of contact homology. Lisa Traynor, Josh Sabloff and Paul Melvin are trying to work on the other direction. For Legendrian surfaces, Dan Rutherford and Mike Sullivan have work in progress that shows that a Legendrian has a generating homology if and only if it has a linearized contact homology, although the homologies a priori might be different. Frederic Bourgeois is developing a larger hybrid theory in any dimension which should “degenerate” in two ways to produce the two homology theories.

Problem 11.2.41 *(Sullivan) There are two maps from the homotopy groups of the based space of Legendrian submanifolds $\mathcal{L}$ (in one-jet spaces) to a certain group of endomorphisms: Sabloff and Sullivan construct one using generating homology $\pi_k(\mathcal{L}; L) \to End_{k-1}(GH(L))$ [38]; Bourgeois and Bronnle construct using linearized Legendrian contact homology $\pi_k(\mathcal{L}; L) \to End_{k-1}(LCH(L))$. Are these the same? As a follow-up, do any of these preserve structures such as the Whitehead product $\pi_k \times \pi_l \to \pi_{k+l-1}$?*

Remark: A comparison of the two maps may result from Bourgeois' work in the previous problem. As for the follow-up, it seems likely when l (or k) is 1, and unlikely otherwise, from dimensionality reasons. (Somehow, these maps see more at the homological level, where such a product, if defined, is uninteresting if $l, k > 1$.)

Problem 11.2.42 *(Sullivan) Do Legendrian fronts constitute a bordism category? Can Lurie's cobordism hypothesis apply and simplify computations of generating homology, for example?*

Remark: Here objects would be Legendrian points, 1-morphisms would be Legendrain tangles, etc. It seems promising, given that Schommer-Pries' Cerf-theory approach [44] to the cobordism hypothesis for 2-categories resembles Legendrian front projections.

Problem 11.2.43 *(Gay) When constructing generating families, why use R^N as the fiber? Are there benefits to changing the fiber?*

Remark: This would work for Legendrians in $J^1 M$ for $M \neq R^n$. For example, if $M = S^1$ and the fiber is S_1, a birth followed by a death can produce a a non-trivial Legendrian knot. This works for $M = S^2$, etc, as well. A follow-up (vague) question was whether or not this can put into a more general theory.

Problem 11.2.44 *(Hutchings) Can we apply symplectic geometry to solve the Schonflies conjecture? Can we deform any S^3 to be pseudo-convex?*

Problem 11.2.45 *(Bourgeois)How do overtwisted disks presented by Eliashberg for high-dimensional contact manifolds compare to others in the literature? More specifically, take the contact manifold (M, ξ) with an open book given by a Dehn twist on ST^*S^n. Is this overtwisted in Eliashberg's sense?*

Remark: One difficulty in answering this question is that Eliashberg's theorem is not constructive, so the disk is hard to "see."

Problem 11.2.46 *(Wehrheim) What do Lagrangians look like in moment polytopes?*

Remark: Apparently this relates to work by Denis Auroux and his student.

Problem 11.2.47 *(Eliashberg) Are holomorphic curves the only way to detect symplectic/contact rigidity results? More concretely, consider the Arnold Conjecture in T^*M. The number of intersections of a Hamiltonian deformation of the zero-section O with O is bounded from below by the stable morse number of O. This follows from generating families. Can the bound be improved? Can holomorphic curves prove this bound?*

Remark: In some cases, the stable Morse number bound might follow from the bifurcation analysis proofs of Floer invariance in [45] or [29].

Problem 11.2.48 *(Eliashberg) Prove flexibility results for symplectic 6-manifolds and 4-manifolds of general type.*

Problem 11.2.49 *(Wehrheim) Prove an h-cobordism like theorem for Floer homology.*

Remark: A key step would be to replicate Milnor's cancelling disk trick.

11.3 Abstracts for talks

This section lists the titles and abstracts of the talks, in alphabetical order of the speakers' last names.

Speaker: **Bruce Bartlett**
Title: *Three-dimensional bordism representations via generators and relations*
Abstract: The three-dimensional oriented bordism bicategory has closed 1-manifolds as objects, 2-dimensional cobordisms as 1-morphisms, and diffeomorphism classes of 3-dimensional cobordisms as 2-morphisms. We use higher Morse theory to find a simple generators-and-relations presentation of it. Dropping a certain relation leads to a "signature" central extension of the oriented bordism bicategory. The presentation allows for an elementary proof that a representation of this bicategory (i.e. a "123 TQFT") corresponds in a 2-1 fashion to a modular category, which must be anomaly-free in the oriented case. J/w Chris Douglas, Chris Schommer-Pries, Jamie Vicary.

Speaker: **Stefan Behrens**
Title: *Singular Fibrations on 4-Manifolds*

Abstract: The last 15 years of 4-manifold theory have seen a revival of the study of smooth maps to surfaces. While this subject had already enjoyed popularity in the third quarter of the 20th century, the current developments were motivated by work of Donaldson and Gompf on symplectic 4-manifolds and Lefschetz pencils as well as Taubes's work on the Seiberg-Witten invariants of near-symplectic 4-manifolds. In this talk I will begin with a brief historical overview and then go on to describe the basic structure of generic maps from 4-manifolds to surfaces and 1-parameter families thereof. I will point out relations to 3- and 4-dimensional Morse theory and the theory of (broken) Lefschetz fibrations. Finally, I will describe how this "surface valued Morse theory" leads to pictorial descriptions of 4-manifolds in terms of curve configurations on surfaces. If time permits, I will discuss some (potential) applications and open problems.

Speaker: **Ryan Budney**
Title: *Triangulating 4-manifolds and a table of knots in homotopy 4-spheres.*
Abstract: I will update the group on an ongoing project which creates a census of triangulated smooth 4-manifolds. The ultimate goal of the project is to see how computationally useful triangulations of 4-manifolds can be, as compared to with 3-manifold theory. The table of knot exteriors in homotopy 4-spheres is nearing completion, this has included the discovery of a new 2-knot type.

Speaker: **Yasha Eliashberg**
Title: *All manifolds are contact except those which are obviously not.*

Speaker: **M. Brad Henry**
Title: *A combinatorial differential graded algebra for Legendrian knots from generating families*
Abstract: We outline recent work that assigns a differential graded algebra (DGA) to a Legendrian knot in the standard contact structure on $\mathbb{R}^3$. The definition of the DGA is motivated by considering Morse-theoretic data from a generating family. A generating family f_x for a Legendrian knot is a 1-parameter family of functions whose Cerf diagram is a projection of the knot. Generating family homology is a useful invariant of Legendrian knots extracted from the generating family. The new DGA is defined combinatorially using the Cerf diagram and handleslide data from f_x. Although defined combinatorially, the differential of the DGA is geometrically motivated by a conjectured extension of generating family homology using gradient flow trees. We will discuss this motivation and how it informs the combinatorial definition of the DGA, and relate the new DGA to the Chekanov-Eliashberg DGA. This work is joint with Dan Rutherford (University of Arkansas).

Speaker: **Jesse Johnson**
Title: *Minsky Models and Morse two-functions on three-manifolds*
Abstract: Morse two-functions have recently become popular in three-dimensional topology via the closely related of a (Rubinstein-Scharlemann) graphic. In this talk, I will describe how a Morse two-function on a three-dimensional manifold encodes topological and geometric information about the three-manifold via a combinatorial structure called a Minsky model.

Speaker: **Daniel Rutherford**
Title: *Cellular computation of Legendrian contact homology and generating families*
Abstract: This is joint work with Mike Sullivan. We consider a Legendrian surface, L, in $\mathbb{R}^5$ (or more generally in the 1-jet space of a surface). Such a Legendrian, L, can be conveniently presented via its front projection which is a surface in $\mathbb{R}^3$ that is immersed except for certain standard singularities.

We associate a differential graded algebra (DGA) to L by starting with a cellular decomposition of the base projection (to $\mathbb{R}^2$) of L that contains the projection of the singular set of L in its 1-skeleton. A collection of generators is associated to each cell, and the differential is determined in a formulaic manner by the nature of the singular set above the boundary of a cell. Our motivation is to give a cellular computation of the Legendrian contact homology DGA of L. In this setting, the construction of Legendrian contact homology was carried out by Etnyre-Ekholm-Sullvan with the differential defined by counting holomorphic disks in $\mathbb{C}^2$ with boundary on the Lagrangian projection of L. In work in progress, we hope to establish equivalence of our DGA with LCH using work of Ekholm on gradient flow trees.

As an application we discuss connections between the cellular DGA and generating families. Here, augmentations arise from Morse complexes and bifurcation data appearing in 2-parameter families of functions.

Speaker: **Hyam Rubinstein**
Title: *Parametrised Morse theory for 3-manifolds*
Abstract: The first part of the talk will be a quick survey on the homotopy type of the group of Diffeomorphisms of a 3-manifold. Pioneering work was done by Hatcher and Ivanov in the late 70s and early 80s, computing this for Haken 3-manifolds and famously the Smale conjecture. Following Thurston, the natural question is whether Diff is homotopy equivalent to the group of isometries, for geometric 3-manifolds. Gabai showed this is true in the hyperbolic case. McCullough and others studied Seifert fibred spaces and many spherical classes of examples.

In the second part, I will talk about Heegaard splittings, a natural view of Morse theory for 3-manifolds. Casson-Gordon in the mid 1980s introduced a key idea of strong irreducibility and this was extended by Scharlemann-Thompson to telescoping. There have subsequently been many developments, including classification of splittings for all 7 non hyperbolic geometries of Thurston. Comparing splittings was introduced by Scharlemann and I, and distance of splittings by Hempel. If time permits the relationship with hyperbolic geometry will be sketched.

Speaker: **Josh Sabloff**
Title: *Families of Legendrian Submanifolds via Generating Families*
Abstract: I will introduce a framework to investigate families of Legendrian submanifolds using generating family homology through an application of the families theory to the analysis of a loop of Legendrian n-spheres in the standard contact space that is contractible in the smooth, but not Legendrian, category; this is joint work with Mike Sullivan. The computation of generating family homology necessary for the application comes from joint work with on Lagrangian cobordisms withFrederic Bourgeois and Lisa Traynor.

Speaker: **Martin Scharlemann**
Title: *The Schönflies Conjecture and its spin-offs*
Abstract: We briefly review the resolution of the Schnflies Conjecture in all dimensions other than four, discuss why the remaining conjecture is important, and the classic approach to its resolution. This approach has spawned much beautifully pictorial mathematics, without actually succeeding. An underlying theme is that, although the conjecture has not yet been settled, it interlocks with and has inspired much interesting topology in dimensions three and four.

Speaker: **Chris Schommer-Pries**
Title: *From the cobordism hypothesis to higher Morse theory*
Abstract: This talk will survey some recent developments in our understanding of extended topological field theories and their classification. This includes the cobordism hypothesis and related results. In the course of this talk we hope to make clear the role of higher Morse theory in this story.

Speaker: **Lisa Traynor**
Title: *An Introduction to Symplectic and Contact Topology and the Technique of Generating Families*
Abstract: I will give a brief introduction to some of the major objects in symplectic and contact topology: symplect and contact manifolds, Lagrangian and Legendrian submanifolds, and symplectic and contact diffeomorphisms. Then I will describe the technique of generating families: this is a way to encode a Lagrangian or Legendrian submanifold by a parameterized family of functions. Morse-theoretic constructions then lead to generating family (co)homology groups for a Legendrian submanifold and wrapped generating family (co)homology groups for a Lagrangian cobordism. I will also describe how from a Lagrangian cobordism with a generating family, one obtains a cobordism map that satisfies some of the typical properties of a TQFT.

Speaker: **Jamie Vicary**
Title: *Computations with topological defects*
Abstract: I will show how some fundamental computational processes, including encrypted communication and quantum teleportation, can be defined in terms of the higher representation theory of defects between 2d topological

cobordisms, giving insight into fundamental questions in classical and quantum computation. No knowledge of computer science will be required to understand this talk.

Speaker: **Katrin Wehrheim**
Title: *How to extend 2+1 (symplectic but not quite) field theories to 2+1+1*
Abstract: In previous work with Chris Woodward, we gave constructions of 2+1 NQFT's (not quite field theories) via dimensionally reduced gauge theories and the symplectic 2-category. More precisely, these are functors from the category of connected 2+1 bordisms to Symp, composed with a natural functor from Symp to Cat. Using Morse 2-functions on 4-manifolds, I will explain that/how such theories naturally extend to 2+1+1 NQFT's under a single nontrivial axiom. And I hope to find help for translating this into the more algebraic TFT language during the workshop.

Speaker: **Jonathan Williams**
Title: *Weak Floer A-infinity algebras for smooth 4-manifolds*
Abstract: I will talk about how to apply constructions of Lipshitz and Akaho-Joyce to a certain class of maps from 4-manifolds to the 2-sphere to yield possibly new diffeomorphism invariants for general smooth, closed oriented 4-manifolds, and discuss future directions.

Speaker: **Alexander Zupan**
Title: *Knots with compressible thin levels*
Abstract:Thin positions theories have played a prominent role in 3-manifold topology over the last several decades, beginning with Gabai's definition of thin position for knots in the 3-sphere and proceeding up to Johnson's axiomatic thin position, which encompasses most existing adaptations. Modern notions of thin position are highly technical but exhibit the natural property that for a thin presentation of a knot or a 3-manifold, all thin surfaces are essential. This motivates the question, "For a knot in Gabai thin position, are all thin levels essential in the knot exterior?" We give a negative answer to this question, exhibiting an infinite family of knots whose thin positions have compressible thin levels. This is joint work Ryan Blair.

11.4 Feedback from some participants

This section records some of the post-conference feedback emailed to the conference organizers.

- Christopher Douglas: I just wanted to thank you for organizing the Banff workshop — I had a fabulous week. Really, it's been years since I enjoyed a math workshop or conference as much as I did this past week. It was engaging, informative, productive, inspiring, and fun to boot!

- Chris Schommer-Pries: Thanks for the great workshop. I definitely got several things from the conference. One of them was a better understanding of what the other approaches to 2-Morse theory do and do not do. For example I got a better feeling for the difference that occur when you consider being transverse to a foliation, such as in the tqft work.

  I think an important question that was raised is what is the analog of a framed generalised 2-Morse function? One requirement is that the space of these should be contractible in a suitable sense. This could have lots of important applications to tqfts and is also perhaps natural to consider in geometric contexts as well.

  One thing that was raised during the problem session was the question of whether there are results about 3-manifolds that can be proven or reproven using the presentations from tqfts. A similar reverse question would be to look at standard 3-manifold facts and then ask what do these mean when applied to a particular target n-category. For example I mentioned that one of the simplest 3-dimensional facts, that there is an immersed surface in R^3 connection the twice twisted circle to the untwisted circle (i.e. $\pi_1 SO(3) = Z/2$) leads, via extened tqfts, to interesting an important facts about tensor categories (representations of finite quantum groups/Hopf algebras). What happens when we take other facts about 3-manifolds? what do these topological results tell us about these algebraic categories? I hadn't yet considered taking important results in 3-manifolds and transporting them to this other situation.

- Jamie Vicary: Let me say thanks again for an excellent workshop. I had a really great and productive time. Particular highlights: - Discovering the open questions lying at the boundary between my own work and other fields, e.g. symplectic/contact topology - Discovering that topologists are interested in what I'm doing!

- Katrin Wehrheim: Thanks for a wonderful conference! Banff is always productive for me, but this meeting has been exceptional. I learned a lot of TFT and was able to pretty much fully translate my results into an abstract result that mixes geometric "blob-complex-like" input with a cobordism hypothesis type result. And I was thrilled to find that the TFT specialists found this interesting, surprising, and yet believable - after several long discussions which allowed us to learn each others' language.

  I also have a very concrete new project and collaborator out of this week - we conjecturally constructed a new combinatorial 4-manifold invariant. I'd be prepared to say more if in ca 10 weeks I'll have heard from another specialist that it is believable and doesn't step on other people's toes.

- Hyam Rubinstein: I got a lot out of the conference as did my student David In particular I have two new ideas in mind One is to relate trisections of 4-manifolds to triangulations Dave Gay asked me about this and I also talked to Rob I am working on a project with Stephan Tillman on triangulations and Heegaard splittings of 3-manifolds and believe our methods apply in dimension 4 and most likely extend to higher dimensions as well Secondly after Ryan Budneys talk and also some informal conversations have some ideas for algorithms for 4-manifolds I have a project on normal 3-manifolds in triangulated 4-manifolds and have some new ideas for more interesting applications

- Josh Sabloff: First, thank you for organizing such an interesting and productive conference. It was great to interact with people I would not normally see, as well as those I donormally see.

  I got three main things from the conference:

  1. I got to talk with some of the TQFT folks about some algebraic structures that come up in Legendrian Contact Homology, and they had some helpful ideas about where else similar structures have appeared. I hope to use this in an ongoing project – in a sense, it gives me a target to aim for.

  2. Inspiration, once again from the TQFT people, about the structure into which generating family homology and the families framework fit.

  3. Frederic, Lisa, and I also made progress on an old project, and it was good to be in the same place at the same time to have some intensive discussions. This also goes for an old project with Joan.

- Paul Melvin: It was a great conference, superbly run! Sorry I had to leave early (and in particular, to miss the contact/symplectic day).

  For me, the most interesting outcome was a better appreciation of the unifying role of topological quantum field theories in low dimensional topology, as well as its application to other areas of mathematics. I can see many possibilities for increased impact of this perspective on my future research. I also benefited from discussions with Dave Auckly releated to our joint work on stable isotopy in 4-manifolds; in particular we made progress on generalizing some of the cork-constructions that we have developed to a wider family of corks arising from symmetric ribbon knots.

  Thanks again to you and Dave for organizing a terrific conference.

- M. Brad Henry:

  1. Dan Rutherford and I began a new project to understand Legendrian invariants in the 1-jet space of the circle. We made very nice progress and left Banff with a clear intuition as to how to proceed.

  2. Dan Rutherford, Lisa Traynor, Paul Melvin, Josh Sabloff, and I discussed an on-going project related to constructing and distinguishing generating families.

  3. Stefan Behrens provided Paul Melvin with three references that may be of important use to the project from 2. above.

4. This was my first exposure to symmetric monoidal 2-categories. Legendrian submanifolds may fit into this algebraic framework in a natural way.

5. Lisa Traynor, Ziva Myer and I discussed Ziva's graduate research in Legendrian graph theory.

6. Perhaps most importantly, I have a greater sense for the broad tapestry that all of the topics discussed are woven into.

- Marty Scharlemann: David Gay, Rob Kirby, Abby Thompson and I began discussing a prospective FRG proposal at the Banff workshop, and the setting was a definite plus for this activity. I had a good number of very helpful conversations, most memorably with Yasha Eliashberg about hopes and attempts at proving the Schonfliess Conjecture coming out of geometry. All in all a very nice conference - thanks for the invitation.

- Robion Kirby: This conference worked better than any conference I can remember. Well perhaps the one on 4-manifolds in Durham in 1982 just after both Freedman and Donaldson's great works was more exciting. But that is a very high standard. Banff had a lot of back and forth between the speakers and the audience which is always a good sign, so much better than a quiet zombie like audience that asks no questions. The organizers were either excellent choosers of participants, or plenty lucky!

Participants

Auckly, David (Kansas State University)
Baker, Ken (University of Miami)
Bartlett, Bruce (University of Oxford)
Baykur, Inanc (University of Massachusetts)
Behrens, Stefan (Max Planck Institute for Mathematics)
Bourgeois, Frdric (Universit Paris-Sud)
Bryant, Kathryn (Bryn Mawr College)
Budney, Ryan (University of Victoria)
Castro, Nick (University of Georgia)
Douglas, Christopher (Oxford University)
Eliashberg, Yakov (Stanford University)
Frohman, Charles (University of Iowa)
Gay, David (University of Georgia)
Hass, Joel (UC Davis)
Hayano, Kenta (Osaka University)
Henry, M. Brad (Siena College)
Hutchings, Michael (University of California)
Johnson, Jesse (Oklahoma State University)
Kirby, Robion (University of California - Berkeley)
Kirszenblat, David (University of Melbourne)
Koytcheff, Robin (Unviversity of Victoria)
Li, Jiayong (Massachusetts Institute of Technology)
Licata, Joan (Australian National University)
Lowell, Mark (University of Massachusetts)
Melvin, Paul (Bryn Mawr College)
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Zupan, Alex (University of Nebraska-Lincoln)

Bibliography

[1] A'Campo, Norbert. Generic immersions of curves, knots, monodromy and Gordian number. Inst. Hautes Etudes Sci. Publ. Math., 88 (1998), 151–169 (1999).

[2] Akbulut. Selman. Variations on Fintushel-Stern knot surgery on 4-manifolds. Turkish J. Math. , 26 (2002), 81–92.

[3] Auckly, David. Families of four-dimensional manifolds that become mutually diffeomorphic after one stabilization. Topology Appl., 127 (2003), 277–298.

[4] Auckly, David. The number of smooth 4-manifolds with a fixed complexity. Int. Math. Res. Not. IMRN, 17 (2007), no. 17, Art. ID rnm054, 19 pp.

[5] Auckly, David. Families of four-dimensional manifolds that become mutually diffeomorphic after one stabilization. In Proceedings of the Pacific Institute for the Mathematical Sciences Workshop "Invariants of Three-Manifolds" (Calgary, AB, 1999). Topology Appl., 127 (2003), 277–298.

[6] Auckly, David; Kim, Hee Jung; Melvin, Paul; Ruberman, Daniel. Stable isotopy in four dimensions. In preparation.

[7] Auckly, David; Koshkin, Sergiy. Introduction to the Gopakumar-Vafa large N duality. http://arxiv.org/abs/math/0701568.

[8] Baez, John. Higher-dimensional algebra and Planck scale physics. http://math.ucr.edu/home/baez/planck/.

[9] Baykur, R. İnanç. Topology of broken Lefschetz fibrations and near-symplectic 4-manifolds. Pacific J. Math., 240 (2009), 201–230.

[10] Baykur, R. İnanç. Broken Lefschetz fibrations and smooth structures on 4-manifolds. Geom. & Topol. Monographs, 12 (2012), 9–34.

[11] Baykur, R. İnanç; Sunukjian, Nathan. Round handles, logarithmic transforms and smooth 4-manifolds. J. Topol., 6, (2013), 49?-63.

[12] Baykur, R. İnanç; Sunukjian, Nathan. Exotic embeddings of surfaces in 4-manifolds and stabilizations In preparation.

[13] Douglas, Chris; Schommer-Pries Chris; Snyder, Noah. Dualizable tensor categories http://arxiv.org/abs/1312.7188.

[14] Dranišnikov, A. N.; Repovš, D., Embeddings up to homotopy type in Euclidean space, Bull. Austral. Math. Soc., 47, 1993, 145–148

[15] Eliashberg, Yakov; Mishachev Nikolai. Introduction to the h-principle, Graduate Studies in Mathematics, AMS (2002).

[16] Freed, Dan. The cobordism hypothesis. http://arxiv.org/abs/1210.5100.

[17] Freedman, Michael; Kitaev, Alexei; Nayak, Chetan; Sligerland, Johannes; Walker, Kevin; Wang, Zhenghan. Universal manifold pairings and positivity. http://arxiv.org/abs/math/0503054.

[18] Fuchs, Dmitry; Rutherford, Dan. Generating families and Legendrian contact homology in the standard contact space. J. Topol. 4 (2011), no. 1, 190226.

[19] Funar, Louis. Torus bundles not distinguished by TQFT invariants, http://arxiv.org/abs/math/1101.0509.

[20] Gay, David T.; Kirby, Robion. Reconstructing 4-manifolds from Morse 2-functions. In Proceedings of the Freedman Fest, Geometry & Topology Monographs (18) 2012.

[21] Gay, David T.; Kirby, Robion. Indefinite Morse 2-functions; broken fibrations and generalizations. arXiv:1102.0750.

[22] Gay, David T.; Kirby, Robion. Trisecting 4-manifolds. arXiv:1205.1565.

[23] Gompf, Robert. Killing the Akbulut-Kirby 4-sphere, with relevance to the Andrews-Curtis and Schoenflies problems, Topology, 30, (1991) 97–115.

[24] Greene, Josh. The lens space realization problem. Ann. of Math.. 177 (2013), 449-511).

[25] Hass, Joel; Thompson, Abigail; Thurston, William. Stabilization of Heegaard splittings. Geom. Topol. 13 (2009), 2029–2050.

[26] Hedden, Matthew. Notions of positivity and the Ozsvth-Szab concordance invariant. J. Knot Theory Ramifications, 19 (2010), 617–629.

[27] Johnson, Jesse. Bounding the stable genera of Heegaard splittings from below. Journal of Topology, 3(2010) no. 3, 668–690.

[28] Kirby, Robion. Problems in Low-dimensional Topology. Geometric topology (Athens, GA, 1993), AMS/IP Stud. Adv. Math. vol. 2, part 2, pages 35–473, Amer. Math. Soc., Providence, RI, 1997.

[29] Lee, Yi-Jen. Reidemeister Torsion in Floer–Novikov Theory and Counting Pseudo-holomorphic Tori, I, J. Symplectic Geom. Volume 3, Number 2 (2005), 221–311.

[30] Markov, A. A. Unsolvability of homeomorphy problem. Proc. ICM, Edinburgh, 1958, Cambridge Univ. Press, 1960, 300–306.

[31] Martelli, Bruno. Links, two-handles, and four-manifolds. Int. Math. Res. Not. 58,(2005) 3595–3623.

[32] Murphy, Emmy. Loose Legendrian embeddings in high dimensional contact manifolds arXiv:1201.2245 (2012).

[33] Ng, Lenhard; Traynor, Lisa. Legendrian solid-torus links. J. Symplectic Geom. 2 (2004), no. 3, 411–443.

[34] Osoinach, John K., Jr. Manifolds obtained by surgery on an infinite number of knots in S^3. Topology, 45 (2006), 725–733.

[35] Rathbun, Matthew. Tunnel one, fibered links. Pacific Journal of Mathematics, 259-2 (2012), 473–481.

[36] Rubinstein, Hyam; Scharlemann, Martin. Comparing Heegaard splittings of non-Haken 3-manifolds. Topology, 35:1005–1026, 1996.

[37] Rudolph, Lee. Quasipositivity and new knot invariants. Rev. Mat. Univ. Complut. Madrid, 2 (1989), 85–109.

[38] Sabloff, Josh and Sullivan, Michael. Families of Legendrian via generating families. Quant. Topol. to appear.

[39] Sabloff, Joshua M.; Traynor, Lisa. Obstructions to the existence and squeezing of Lagrangian cobordisms. J. Topol. Anal. 2 (2010), no. 2, 203–232.

[40] Sabloff, Joshua M.; Traynor, Lisa. Obstructions to Lagrangian Cobordisms between Legendrian Submanifolds. arXiv:1109.5660

[41] Scharlemann, Martin. Tunnel number one knots satisfy the Poenaru conjecture. Topology Appl.. 18 (1984), 235–258.

[42] Scharlemann, Martin. The four-dimensional Schoenflies conjecture is true for genus two imbeddings. Topology. 23 (1984), 211–217.

[43] Scharlemann, Martin. Generalized Property R and the Schoenflies Conjecture, Comm. Math. Helv., 83 (2008), 421–449.

[44] Schommer-Pries, Christopher. The Classification of Two-Dimensional Extended Topological Field Theories, PhD thesis (2008).

[45] Sullivan, Michael. K-theoretic invariants for Floer homology Geom. Funct. Anal., 12, (2002), 810–872.

[46] Thompson, Abigail. Thin position and the recognition problem for S^3, Math. Res. Lett., 5, (1994), 613–630.

[47] Turaev, Vladimir. Quantum invariants of knots and 3-manifolds, De Gruyter Studies in Mathematics **18**, 2010.

[48] Viterbo, Claude. Generating functions, symplectic geometry, and applications. Proceedings of the International Congress of Mathematicians, Vol. 1, 2 (Zürich, 1994), 537–547, Birkhäuser, Basel, 1995.

[49] Wall, C. T. C. On simply-connected 4-manifolds. J. London Math. Soc., 39, (1964) 141–149

[50] Williams, Jonathan. The h-principle for broken Lefschetz fibrations. Geom. Topol. , 14 (2010), 1015–1061.

Chapter 12

Specialization of Linear Series for Algebraic and Tropical Curves (14w5133)

March 30 - April 4, 2014

Organizer(s): Matthew Baker (Georgia Institute of Technology), Lucia Caporaso (University of Rome: Roma Tre), Maria Angelica Cueto (Columbia University), Eric Katz (University of Waterloo), Sam Payne (Yale University)

12.1 Overview of the Field

Recent developments in tropical geometry have opened the possibility of significant applications to the classical study of linear series and projective embeddings of algebraic curves. These developments take the form of "specialization lemmas" that control how curves with special linear series behave in degenerating families [5, 8]. Here, algebraic curves are 1-dimensional algebraic varieties and linear series are certain vector spaces of functions on these curves. The technique of degeneration involves considering a family of algebraic curves that may become singular and to deduce properties of the smooth members of the family from that of the singular ones. The specialization lemma allows one to use degenerations more pathological than those considered before and to understand the smooth members in terms of the combinatorics of the singular members, specifically in the study of their dual graphs.

Our technical setup is as follows. We fix a curve X and consider a regular, generically smooth, semi-stable curve $\mathcal{X}$ over a discrete valuation ring R with generic fiber X. The special fiber $\mathcal{X}_k$ is a reduced nodal curve over the residue field k of R. For simplicity, we assume k is algebraically closed. We let $\bar{G} = (G, w)$ be the (weighted) dual graph of $\mathcal{X}_k$, whose vertices v correspond to irreducible components C_v of the curve $\mathcal{X}_k$ and whose (multi)-edges (u, v) are in one-to-one correspondence with the components of pairwise intersections $C_u \cap C_v$. The weight function $w\colon V(G) \to \mathbb{Z}_{\geq 0}$ associates to every vertex v of G, the geometric genus of the component C_v.

Classically, the study of such degenerations was essentially limited to degenerations of "compact type", where the dual graph of the special fiber is a tree and the Jacobian of the special fiber is compact. Eisenbud and Harris developed their theory of "limit linear series" to describe the linear series on components of the special fiber obtained as limits of special linear series on the general fiber, in degenerations of compact type, and used it to prove many new results in the geometry of curves [28]. Among them, we can mention three contributions: the full symmetric action of monodromy on Weierstrass points of a general curve [29], the fact that M_g is of general type for g at least 24 [27], and new simple proofs of the Brill-Noether and Gieseker-Petri Theorems [26]. The later are the core of classical Brill-Noether theory which studies the behavior of linear series on a general curve, that is curves outside a subset of positive codimension in the moduli space.

Figure 12.1: A curve and its dual graph.

Tropical geometry, on the other hand, is most naturally suited to study "maximal degenerations" of curves – the opposite of compact type degenerations – where the dual graph of the special fiber has the largest possible first Betti number (equal to the genus of the generic fiber) and the Jacobian of the special fiber is affine. In its most basic form, the theory of tropical linear series studies the possible ways in which the degree of a special divisor in the generic fiber can be distributed over the components of the special fiber. There is a certain tension between combinatorics and algebraic geometry: when the dual graph of the special fiber has simple combinatorics, the algebraic geometry of the components may be complicated; when the components are simple, the combinatorics of distributing degrees among points of the dual graph becomes complicated and rich. This combinatorial information is surprisingly powerful; it has already led to new proofs of the Brill-Noether Theorem [23] and the Gieseker-Petri Theorem [12, 38]. Similar methods have been used by Castryck–Cools [21], and Kawaguchi [41, 42] to compute the gonality of the generic curve with a given Newton polygon. All of these proofs rely on the original, prototypical specialization lemma, due to Baker [8]. Remarkably, to prove a result about generic curves, it suffices to prove a combinatorial statement for a single suitably-chosen example.

Several more advanced specialization lemmas have been proved since Baker's original version, allowing non-maximal degenerations and degenerations with singular components, taking into account the genus of components of the special fiber, and permitting the divisors, as well as the curves, to move in families. Most recently, Amini and Baker [4] have used Berkovich's machinery for nonarchimedean analytic geometry to develop a specialization lemma for "tropical limit linear series." This new perspective takes into account both the distribution of degrees on components of the special fiber and also the linear series that can appear on these components. Their results apply to semistable curves which are not necessarily of compact type

An important remark is that combinatorial information on dual graphs does not suffice to develop this new enriched theory. For this purpose, Amini-Baker developed the notion of a metrized complex of an algebraic curve X which arises from the data of special fiber $\mathcal{X}_k$ together with a metric structure on its dual dgraph. The metric is determined by the speed with which the nodes form in the degeneration. These metrized complexes satisfy a specialization lemma as in [5, 8], and a Riemann–Roch Theorem which generalizes both the classical Riemann-Roch theorem and its graph-theoretic and tropical analogues due to Baker-Norine [10], Gathmann-Kerber [33], and Mikhalkin-Zharkov [53].

In the compact type case, Amini and Baker exactly recover the Eisenbud-Harris theory of limit linear series, while in the maximally degenerate case this new theory is strictly stronger than any previous tropical specialization lemma. These more refined specialization lemmas rely on the tropical concept of lifting. A natural question arises in this context. Given a piece of combinatorial data on the dual graph of a singular curve, for example, a tropical divisor, can we extend it to an algebraic geometric object on a smoothing of the given singular curve? More restrictive conditions on lifts lead to better specialization lemmas.

This workshop brought together leading experts and young researchers from tropical geometry and the classical theory of linear series on algebraic curves. The meeeting provided the first opportunity to bridge these communities and advance the state of the art on both sides. The three primary goals set up for the meeting were achieved:

- **Objective 1** Create an opportunity for tropical geometers and researchers in the classical theory of linear series to learn the state of the art and fundamental techniques on both sides, and foster mutual understanding across these two disciplines.

- **Objective 2.** Explore possibilities for combining classical and tropical techniques to resolve outstanding problems on both sides, such as those mentioned above.

- **Objective 3.** Help advanced graduate students and recent PhDs working in these two areas to connect with peers and experts across these two subjects, and encourage an understanding of the rigorous connections between tropical geometry and classical linear series. Participants included 4 PhD students and 10 postdocs.

As explained above, new specialization lemmas in tropical geometry simultaneously generalize both the classical theory of limit linear series, due to Eisenbud and Harris, as well as the original tropical specialization lemma, due to Baker. Both approaches lead to proofs of the Brill–Noether and Gieseker–Petri Theorems, and the extent to which combining the two approaches may lead to significant new results is not yet known, but experts on both sides are very interested in exploring the possibilities as a result of discussions that occurred during the meeting. The workshop included an evening open problem session presenting the some of the outstanding open questions in these areas, including the Maximal Rank Conjectures and the Kodaira dimension of M_{23}. We discuss these topics in Section 12.2.

12.2 Recent Developments and Open Problems

There are a number of open questions in linear systems on algebraic curves that may be approachable by the methods of tropical geometry. Some of these were surveyed by Brian Osserman in his talk. The Maximal Rank Conjecture concerns the behavior of an embedding given by a symmetric power of a linear system. It is phrased in terms of the rank of a particular linear map between symmetric powers of spaces of sections of a line bundle. A refinement of this conjecture, the Strong Maximal Rank Conjecture, predicts the dimension of the locus in the Picard variety of a general curve parametrizing line bundles where these linear maps drop rank. One particular case of this conjecture would imply that the moduli space of curves of genus 23 is of general type. Prescribed ramification involves a series of questions about extending Brill-Noether theory from sections of a line bundle to section of a line bundle with prescribed ramification. Indeed, Brill-Noether theory involves the existence of a linear system with prescribed degree and rank on a generic curve when it is predicted by a dimension count. This can be generalized to ask about the existence of a linear systems with prescribed ramification sequences at particular points. This is known by work of Eisenbud-Harris is characteristic 0, but is open in characteristic p smaller than the degree. One may also want to know how many linear systems there are if the expected dimension is 0. Another variant of these questions is the real case where much is open when the genus is greater than 0.

The tools used in tropical geometry are not completely understood, and there are many open questions regarding their nature. The precise algebraic geometric interpretation of some of the most important tropical invariants of divisors, including the "rank" that appears in Baker's specialization lemma, remain mysterious. In [17], Caporaso introduced the notion of algebraic rank and conjectured that it behaves as a minimax formula over curves and line bundles. Although the conjecture fails in general by work of Caporaso, Len and Melo [18], it is true in a large number of cases. While there are combinatorially defined total spaces of linear systems and Brill Noether loci, their relationship to their classical analogues is still unexplored. Many open questions in tropical geometry centre on the question of <u>lifting</u>, that is, given a combinatorial object can one find a algebraic geometric object that specializes to it. For example, one may try to lift a tropical divisor of a particular rank to a classical divisor of the same rank. This is important in practice as the bound given by the tropical rank function may not be sharp because it is considering divisors that do not lift. In fact, there is a hierarchy of lifting conditions coming from extending divisors to a family. Progress on these issues should give insight into lifting tropical linear systems, allowing refinements to the specialization lemma and further applications to the classical theory.

A particular gap in applying tropical geometry to questions in linear systems stems from an insufficiently-developed theory of ranks of linear maps in tropical geometry. Indeed, a number of conjectures in linear systems such as the maximal rank conjecture or Green's conjecture are phrased in terms of the ranks of particular linear maps between vector spaces of sections of line bundles. However, there is not a suitable Abelian category in tropical geometry to allow one to talk about kernels and cokernels of linear maps. A recent, important development is the proof of the Geiseker-Petri theorem due to Jensen-Payne [38] which used tropical techniques to show that a particular multiplication map is injective. This was done by using an explicit basis to study the multiplication map.

This paper opens the possibility of using tropical techniques to study the ranks of linear maps considered in these open problems.

12.3 Presentation Highlights

The talks reviewed techniques in the subject, introduced the audience to open problems, and announced new results. Rather than presenting them in chronological order, we group them by topic.

Background material was surveyed to bridge the backgrounds of the participants coming from different research communities during the first morning of the workshop. **Farbod Shokrieh** explained the Baker-Norine theory of linear systems of graphs and its main result: the Riemann–Roch Theorem for graphs and tropical curves. Rather than presenting the original proofs of [10], he gave an alternative proof as in [6] based on the burning algorithm due to Dhar. This approach is more suited for effective computations of these ranks. Finally, he discussed another approach to this result by means of monomial initial ideals, lattice binomial ideals and Alexander Duality developed by Manjunath and Sturmfels in [51].

Melody Chan introduced Baker's specialization lemma as a powerful technique for bounding the rank of a divisor on a curve by using combinatorics of the dual graph of a degeneration of a curve. In addition to providing a proof of this foundational result, she discussed illuminating examples regarding Specialization of Weierstrass points on smooth plane quartics, setting the context for the tropical proof of Brill–Noether Theorem [23].

Brian Osserman surveyed the most relevant open problems in linear series, concentrating on the maximal rank conjecture, prescribed ramification, and real linear series, described in detail in Section 12.2.

Questions about the nature of the Baker-Norine rank were discussed in talks by Yoav Len, Shu Kawaguchi and Dustin Cartwright. The Baker-Norine rank gives an upper bound for the rank of divisors on curves with particular specialization. One may ask when this bound is sharp. **Shu Kawaguchi** gave a complete answer in the genus 3 and hyperelliptic cases: in these cases he gave necessary and sufficient combinatorial conditions for the upper bound in the specialization lemma to be tight, following [43, 44]. **Dustin Cartwright** presented examples where this bound is never sharp. These examples were constructed using realizability techniques from matroid theory: indeed, by relating these linear systems to combinatorial ones, he relates the lifting question to the realization of certain matroids; interesting counterexamples come from non-representable matroids. **Yoav Len** discussed the notion of algebraic rank of divisors on tropical curves as defined by Caporaso in [17]. It is defined in terms of a minimax formula in terms of curves and divisors with particular specialization. Although this notion differs from the Baker-Norine rank, it has many desirable properties. In particular, his lecture presented interesting examples where both ranks differ, as shown in [18].

A new application of linear systems on graphs to linear systems was discussed by **David Jensen**. His presentation was twofold. On one hand, he surveyed the tropical perspective of Brill–Noether theory and presented tropical proofs of the Brill–Noether theorem, following [23]. Second, he discussed tropical multiplication maps and gave a tropical criterion for a curve over a valued field to be Gieseker–Petri general, thus providing a tropical proof of the Gieseker–Petri Theorem, as in [38]. Significantly, this proof is able to use linear algebraic genericity techniques that have previously resisted translation into tropical geometry.

Extensions of line bundles to degenerate curves were discussed by Jesse Kass and Eduardo Esteves. Notably, these questions are nontrivial because the naïve moduli spaces of line bundles fail to be compact when the dual graph of the degeneration is not a tree. One must expand the moduli spaces to include some non-classical objects. **Jesse Kass** compared two candidate compactifications, the Néron model and the moduli space of stable sheaves proving that they are the same [**?**].

Eduardo Estevez presented work in progress on new perspectives for limit linear series, attempting to merge previous approaches to construct a variety of limit linear series. First, Eisenbud–Harris work for curves of compact type [27, 28]. Second, L. Caporaso's approach by construction a relative compactification $\overline{P_g^d}$ of M_g of the relative Jacobian. Third, L. Maino's construction of a moduli space E_g of enriched curves over $\overline{M_g}$ that captured the essence of the inseparability of the relative Jacobian [50]. And fourth, Osserman's approach to the subject that incorporated the data coming from degenerations of linear series in order to construct meaningful varieties $G_d^r(X)$ of limit linear series for two-component curves X of compact type [55]. The goal of his talk was to build a projective variety over $\overline{P_g^d}$ whose fibers parameterize Maino-style enriched structures and their degenerations, and whose general points parameterize Osserman-style limit linear series.

Applications of tropical geometry to studying moduli problems were discussed by Renzo Cavalieri and Dan Abramovich. **Renzo Cavalieri** discussed Hurwitz numbers which are weighted counts of branched covers of curves. He related the piecewise polynomiality of Hurwitz numbers, a phenomenon proved by Goulden-Jackson-Vakil in [35] to wall-crossing in the enumeration of tropical covers of curves, as proven in [13]. **Dan Abramovich** discussed tropical geometry and skeletons of analytic spaces associated to toroidal embeddings (in the sense of Thuillier [56]) as basic techniques for constructing combinatorial models of moduli problems from a given stratification of the input spaces. In addition to presenting joint work with Caporaso and Payne on the tropicalization of the moduli space of curves, he presented work in progress on how to address the well-known phenomenon of superabundance[1] of tropical curves described in [52], by studying the moduli space of log stable maps from the tropical perspective.

Another topic discussed at the workshop was the application of specialization lemmas and tropical geometry to number theory. **David Zureick-Brown** explained his recent results with Eric Katz [40] on the Chabauty-Coleman method for bounding the number of rational points on curves of low Mordell-Weil rank. When the curves are of bad reduction at a given prime, one may obtain sharper bounds by using the theory of linear series on metrized complexes of curves. **Janne Kool** presented her recent work with Gunther Cornelissen and Fumiharu Kato on the combinatorial Li-Yau inequalities [25]. In the classical case, these inequalities relate the degree of a map with the smallest nonzero eigenvalue of the Laplace operator and the volume of the curve [47]. Using the Laplacians of the dual graph they provide bounds the gonality of a curve over a given non-Archimedean field. This in turn yields a finiteness statement for the number of rational points of low degree. She concluded her talk by presenting applications to Drinfeld modular curves in analogy with Dan Abramovich's results lower bounds on the gonality of modular curves in the classical case [1].

Filip Cools gave an overview talk on combinatorial methods applied to gonality of curves that are general with respect Newton polygons, surveying many of the results from [21]. By working with linear pencils that are visible from the geometry of the Newton polygon, he explained how this gonality as well as Clifford's index are encoded. As a further application of this method, he presented a concrete way to write down generators of the canonical ideal of the curve, and suggested an approach to producing potential counterexamples to Green's Conjecture, using this result. He explained that, with 7 exceptions, every gonality pencil on (the smooth projective model of) a curve that is general with respect to Newton polygon is combinatorial, a result obtained independently by Kawaguchi [41, 42] and Castryck–Cools [21]. He also explained the 7 exceptions in detail, and computed the gonality in each case. He furthermore presented lower bounds on the gonality of using near-gonality pencils and presented explicit formulas for the Clifford index and the Clifford dimension, as in [21, 41, 42]

Marc Coppens presented the main result of [24], namely Clifford Theorem for metric graphs. He gave a complete, detailed proof of this important result, based on the Riemann–Roch Theorem for graphs, the Abel-Jacobi map for tropical curves [53] and the algorithm for computing rank of divisors on tropical curves given in [6].

Omid Amini discussed work in progress on the limit behaviour of Weierstrass points when specializing from a curve to a graph. He studied a degenerating family of curves equipped with a line bundle and asked how the Weierstrass points of powers of the line bundle specialize to the central fiber of the family. His result can be viewed as the non-Archimedean analogue of a theorem of Mumford-Neeman [9]: he showed that such points are equidistributed with respect to Zhang's measure on the dual graph.

12.4 Outcome of the Meeting and Scientific Progress Made

As mentioned in Section 12.1, this conference brought together leading experts and young researchers from two communities that seldom have the opportunity to discuss new ideas and learn from each other. Having a mixture of Ph.D. students, several postdocs and researchers in tropical geometry and the classical theory of linear series on algebraic curves from Europe, Japan and North America provided an ideal environment for exchanging perspectives and start new collaborations.

[1] A map $f : C \to \mathbb{TP}^n$ is called superabundant if the dimension of the space of deformations of the pair (C, f) is strictly larger than that predicted by naïve dimension counts.

The overall impression was that this was one of the best conferences ever attended, for most of the participants. The open problem session, together with the discussions and collaborations it initiated throughout the week proved to be one of the most successful activities of the conference. The ample time between the lectures was used by smaller groups to give spontaneous presentations and to do mathematics together.

Intangible benefits, such as building a community, establishing mathematical as well as personal connections, and of course, disseminating knowledge, were widely mentioned. We also got feedback from several participants about very concrete results from the workshop. These range from new projects conceived at the conference to existing projects completed and papers made ready for publication. Here is a sample of such results.

1. Matt Baker, Yoav Len and Nathan Pflueger were able to take steps towards completing an ongoing research project on bitangents of tropical plane quartic curves. The paper was posted shortly after the end of the BIRS workshop as `arXiv:1404.7568`.

2. M. Angelica Cueto and Martin Ulirsch had a long discussion on how to relate non-Archimedean skeleta of toroidal embeddings to geometric tropicalization, and are currently planning to collaborate in order to work out this connection in detail.

3. Martin Ulirsch discussed with Dustin Cartwright, Eric Katz, and Sam Payne several aspects of a current joint project with M.-W. Cheung, L. Fantini and J. Park on the faithful realizability of tropical curves. This project started as a group project in a Mathematical Research Community Summer School in 2013, under the guidance of Sam Payne. Thanks to the discussion he had at BIRS (especially conversations with D. Cartwright) he came around on how to resolve the missing step in one of the main results of the aforementioned project.

4. Filip Cools and Jan Draisma have started collaborating on a paper in which they aim to prove that the locus of metric graphs of (tree) gonality less than expected has exactly the same codimension as in the classical case.

5. Jan Draisma and Anton Leykin started working on signature-based Gröbner bases in the context of equivariant Gröbner bases. By now, they have settled the relevant Noetherianity of first syzygies, in collaboration with Robert Krone.

6. Marc Coppens, Shu Kawaguchi and Kazuhiko Yamaki started collaborating on a lifting of divisors and gonalities, two ideas that grew out of Kawaguchi's presentation.

We end this report with some of the testimonies gathered after the meeting (in alphabetical order):

Marc Coppens said: "I had a very good time at the conference in BIRS and it was very helpful to me. Since I am not attending conferences that often, it was a nice occasion for me to meet some people whose work I have studied and/or used in the past. As an older participant, the conference gave me a new perspective on linear systems on curves. I am especially interested in both the similarities and the differences between linear systems on curves and on graphs and I would like to find out how the study of linear system on graphs can give new information on linear systems on smooth complex and/or real curves. A lot of talks were extremely useful from that point of view. In addition, I had several conversations with Shu Kawaguchi and Kazuhiko Yamaki related to the topic of the talk of Kawaguchi. They asked me some relevant questions on linear systems on algebraic curves to aim at generalizing their results on the subject. This inspired me to search for families of graphs could manifest such generalizations. During the conference, Sam Payne already gave an example of a trigonal graph having infinitely many trigonal pencils. Thus, generalizing their results to all trigonal graphs is impossible, but it might still be achievable for hyperelliptic graphs. By considering these graphs I also found that a lot of nice behaviour of linear systems on curves does not hold for other types of graphs.

After a conversation with Dave Jensen and Sam Payne, I learned that a way to define a weak form of adding a fixed point to a divisor on a graph does not seem to work (this is a pity of course). From Spencer Backman I learned a new way to describe the rank of a divisor on a metric graph using orientations and allowed changes of them. This gives rise to another proof of the Riemann–Roch Theorem for graphs. He also explained how to use this method to try to obtain a more conceptual proof for the complete Clifford Theorem for curves, much more complete that the one I presented in my talk. I started discussing with him and some other participants regarding generalizations of Clifford's Theorem known in curve theory and not yet known for graphs.

In Melody Chan's talk there was a very easy but interesting example showing differences between ranks on the graph and the curve in a degeneration that is due to the fact that in a dual graph one loses information about how components intersect. A Ph.D. student of Filip Cools and myself is currently investigating similarities between results concerning gonality of curves with plane models and the gonality of natural corresponding graphs. In her talk, Chan also observed a similar phenomenon.

From conversations with Matthew Baker I learned that he is currently developping a very refined definition of limit linear pencils on metrized complexes of curves. The aim of this project is to solve the differences that occur in the example given in Chan's talk. My hope is that this refined definition will help solves the differences occuring in the work of my student. If this were the case, then it would indicate that the similarity between the situation of those curves with plane models and the one corresponding to metrized complexes of curves (with rational curves at the vertices) is better observed than by just using metric graphs.

Also during the conference (probably caused by the "atmosphere") I got some new idea for obtaining new results on the gonality of interesting special types of curves using degenerations to graphs. I hope to find time in the near future to think more intensively on it."

Ethan Cotterill said: "I would like to remark five interesting exchange of ideas I had at the BIRS workshop. First, with Eric Katz and Sam Payne, we discussed the problem of characterizing the tropicalizations of singular rational curves; note that this is a variation on a theme already studied by Alicia Dickenstein, Hannah Markwig, Evgeny Shustin, and Luis Tabera (amongst others) in the context of hypersurfaces. Second, Nathan Pflueger explained to me the content of his thesis, in which he studies (the codimension of) Weierstrass-type loci inside the moduli space of curves. Codimension is predicted to be computed by the weight of the associated semigroup, but in many instances this fails and one needs to produce a substitute combinatorial invariant, which he calls the effective weight. In joing work with L.F. Abrantes and R.V. Martins I have been studying how to bound the codimension of (embedded) singular rational curves according to the semigroups of their singularities. Again the codimension is expected to be computed by the weight. It would be interesting to see how far this analogy can be pushed.

Third, Spencer Backman explained to me how to view divisors on a (metric) graph as partial orientations, and how to compute the rank of these according to this point of view. Fourth, Diane Maclagan explained to me her recent work with Felipe Rincon, in which they make the scheme-theoretic tropicalization due to Noah and Jeffrey Giansiracusa effective. It seems this has good potential for proving liftability/realization results for tropical subvarieties, e.g. curves in surfaces or lines in threefolds. Finally, Eric Katz explained to me the basic philosophy underlying log geometry, and how it serves as a tool for proving correspondence theorems in tropical geometry."

Jan Draisma said: "In addition to starting two new research projects with other participants of this BIRS workshop, I had been many stimulating discussions with M. Angelica Cueto (on faithful tropicalizations), with Gunther Cornelissen and with Sam Payne. Finally, I had interesting conversation with Janne Kool, in which I encourage her to apply for a postdoctoral position in the Networks program in the Netherlands."

Eduardo Esteves said: "Thank you very much for having organized the meeting. It was very interesting for me. I had discussions with Jesse Kass about his approach to proving autoduality for compactified Jacobians by means of the Néron model interpretation. I enjoyed discussing with Filippo Viviani about the approach to limit linear series I presented in my talk. And most of all I profited a lot from discussing with Omid Amini and comparing his tropical approach to limit linear series against my joint project on limit linear series with Brian Osserman."

Jesse Kass said: "The workshop was a great opportunity to meet with researchers, both in my field and in neighboring fields. I had the opportunity to discuss recent work of mine on autoduality with Filippo Viviani and Eduardo Esteves, two people who have done important work on the topic. The feedback they provided was very helpful! Listening to Renzo Cavalieri's talk gave me some new ideas for a project on intersection theory that I have been working with Nicola Pagani. Renzo and I had many interesting discussions at the workshop, which I hope will advance both our research programs."

Nathan Pflueger said: "I spoke at length with Ethan Cotterill about different problems we are both studying concerning numerical semigroups in algebraic geometry. We found that we both have unpublished ideas that could help the other's research, and I will very likely travel to meet with him and collaborate in the following year. In addition, the methods Dave Jensen described in his talk made me realize that some of the techniques I have developed to study classical limit linear series could be very useful in studying the Brill–Noether theory of tropical curves. This led to many fruitful discussions with Sam Payne and David Jensen about further directions of work, which could have significant applications for both tropical and algebraic curves. ”

Martin Ulirsch said: “As a graduate student I immensely profited from being able to discuss my research projects with established and junior researchers in this workshop.”

Ravi Vakil said: “I came in the hopes of making new connections. And as a result, I think I may embark on a whole new theme of research (with Matt Baker). So I am very glad to have come.”

Kazuhiko Yamaki said: “I had conversations with several participants about trigonal curves and trigonal graphs among other things. One of these discusions gives me a nice perspective about rank-preseving liftability of divisors from graphs to curves. This would contribute to my research on the relation between graphs and curves. Another discussion enabled me with new techniques to find interesting examples of graphs and curves in which the rank of divisors might behaves well, a significantly new viewpoint that I have never found before. Even after the workshop, I am in correspondence with some of the participants on lifting of divisors, gonalities, and so on. This workshop will certainly enrich my future research.”

Participants

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Bibliography

[1] D. Abramovich, A linear lower bound on the gonality of modular curves, Internat. Math. Res. Not. **1996** (1996), no. 20, 1005–1011.

[2] D. Abramovich, L. Caporaso and S. Payne, The tropicalization of the moduli space of curves, preprint, arXiv:1212.0373.

[3] O. Amini, Reduced divisors and embeddings of tropical curves, Trans. Amer. Math. Soc. **365** (2013), no. 9, 4851–4880.

[4] O. Amini and M. Baker, Linear series on metrized complexes of algebraic curves, preprint, arxiv:1204.3508.

[5] O. Amini and L. Caporaso, Riemann–Roch theory for weighted graphs and tropical curves, Adv. Math. **240** (2013), 1–23.

[6] Y. An, M. Baker, G. Kuperberg and F. Shokrieh, Canonical Representatives for Divisor Classes on Tropical Curves and the Matrix-Tree Theorem, preprint, arXiv:1304.4259.

[7] M. Aprodu and G. Farkas, Koszul cohomology and applications to moduli," In Grassmannians, moduli spaces and vector bundles, 25–50, Clay Math. Proc., **14**, Amer. Math. Soc., Providence, RI, 2011.

[8] M. Baker, Specialization of linear systems from curves to graphs, Algebra Number Theory **2** (2008), no. 6, 613–653.

[9] M. Baker and X. Faber, Metric properties of the tropical Abel–Jacobi map, J. Algebraic Combin. **33** (2011), no. 3, 349–381.

[10] M. Baker, S. Norine, Riemann–Roch and Abel–Jacobi theory on a finite graph, Adv. Math. **215** (2007), no. 2, 766–788.

[11] M. Baker, S. Payne and J. Rabinoff, Nonarchimedean geometry, tropicalization, and metrics on curves, preprint, arXiv:1104.0320.

[12] V. Baratham, D. Jensen, C. Mata, D. Nguyen and S. Parekh, Towards a tropical proof of the Gieseker–Petri Theorem, Collectanea Mathematica **65** (2014), no. 1, 17–27.

[13] A. Bertram, R. Cavalieri and H. Markwig, Polynomiality, Wall Crossings and Tropical Geometry of Rational Double Hurwitz Cycles, J. Combin. Theory Ser. A **120** (2013), no. 7, 1604–1631.

[14] L. Caporaso, Algebraic and Tropical Curves: Comparing their Moduli Spaces. In Handbook of Moduli, edited by Farkas and Morrison; (2011).

[15] L. Caporaso, Linear series on semistable curves, Int. Math. Res. Not. **13** (2011), 2921–2969.

[16] L. Caporaso, Algebraic and combinatorial Brill–Noether theory. In Compact moduli spaces and vector bundles, 69–85, Contemp. Math., **564**, Amer. Math. Soc., Providence, RI, 2012.

[17] L. Caporaso, Rank of divisors on graphs: an algebro-geometric analysis. In A celebration of Algebraic Geometry, Volume in honor of Joe Harris, 45–65, Clay Math. Proc. **18**, Amer. Math. Soc., Providence, RI, 2013.

[18] L. Caporaso, Y. Len and M. Melo, Algebraic and combinatorial rank of divisors on finite graphs, preprint, arXiv:1401.5730.

[19] D. Cartwright, Tropical complexes, preprint, arXiv:1308.3813.

[20] D. Cartwright, D. Jensen and S. Payne, Lifting divisors on a generic chain of loops," preprint, arXiv:1404.4001.

[21] W. Castryck and F. Cools, Newton polygons and curve gonalities, J. Algebr. Comb. **35** (2012), no. 3, 345–366.

[22] M. Chan, Combinatorics of the tropical Torelli map, Algebra Number Theory **6** (2012), no. 6, 1133–1169.

[23] F. Cools, J. Draisma, S. Payne, and E. Robeva. A tropical proof of the Brill–Noether Theorem, Adv. Math. **230** (2012), 759–776.

[24] M. Coppens, Clifford's Theorem for metric graphs, preprint, arXiv:1304.6101.

[25] G. Cornelissen, F. Kato and J. Kool, A combinatorial Li-Yau inequality and rational points on curves, preprint, arxiv:1211.2681.

[26] D. Eisenbud and J. Harris, A simpler proof of the Gieseker–Petri theorem on special divisors, Invent. Math. **74** (1983), no. 2, 269–280.

[27] D. Eisenbud and J. Harris, Limit linear series, the irrationality of M_g, and other applications, Bull. Amer. Math. Soc. (N.S.) **10** (1984), no. 2, 277–280.

[28] D. Eisenbud and J. Harris, Limit linear series: Basic theory, Invent. Math. **85** (1986), 337–371.

[29] D. Eisenbud and J. Harris, The monodromy of Weierstrass points, Invent. Math. **90** (1987), no. 2, 333–341.

[30] E. Esteves, Linear systems and ramification points on reducible nodal curves, Math. Contemp. **14** (1998), 21–35.

[31] G. Farkas, The geometry of the moduli space of curves of genus 23, Math. Ann. **318** (2000), no. 1, 43–65.

[32] G. Farkas and M. Popa, Effective divisors on M_g, curves on $K3$ surfaces, and the slope conjecture, J. Algebraic Geom. **14** (2005), no. 2, 241–267.

[33] A. Gathmann and M. Kerber, A Riemann–Roch theorem in tropical geometry, Math. Z. **259** (2008), no. 1, 217–230.

[34] D. Gieseker, Stable curves and special divisors: Petri's conjecture, Invent. Math. **66** (1982), no. 2, 251–275.

[35] I.P. Goulden, D.M. Jackson and R. Vakil, Towards the geometry of double Hurwitz numbers, Adv. Math. **198** (2005), no. 1, 43–92.

[36] P. Griffiths and J. Harris, "On the variety of special linear systems on a general algebraic curve," Duke Math. J. **47** (1980), no. 1, 233–272.

[37] C. Haase, G. Musiker and J. Yu, Linear systems on tropical curves, Math. Z. **270** (2012), nos. 3–4, 1111–1140.

[38] D. Jensen and S. Payne, Tropical multiplication maps and the Gieseker–Petri Theorem, preprint, arXiv:1401.2584.

[39] J. Kass, Two ways to degenerate the Jacobian are the same, Algebra & Number Theory **7** (2013), no. 2, 379–404.

[40] E. Katz and D. Zureick-Brown, The Chabauty-Coleman bound at a prime of bad reduction and Clifford bounds for geometric rank functions, preprint, arXiv:1204.3335.

[41] R. Kawaguchi, The gonality conjecture for curves on certain toric surfaces, Osaka J. Math. **45** (2008), no. 1,113–126.

[42] R. Kawaguchi, The gonality conjecture for curves on toric surfaces with two $\mathbf{P}^1$-fibrations, Saitama Math. J. **27** (2010), 35–80.

[43] R. Kawaguchi, Ranks of divisor classes on hyperelliptic curves and graphs under specialization, preprint, arXiv:1304.6979, to appear in Int. Math. Res. Not. (2013).

[44] R. Kawaguchi, Algebraic rank on hyperelliptic graphs and graphs of genus 3, preprint arXiv:1401.3935

[45] S. Kleiman and D. Laksov, On the existence of special divisors, Amer. J. Math. **94** (1972), 431–436.

[46] R. Lazarsfeld, Brill–Noether–Petri without degenerations, J. Differential Geom. **23** (1986), no. 3, 299–307.

[47] P. Li and S.T. Yau, A new conformal invariant and its applications to the Willmore conjecture and the first eigenvalue of compact surfaces, Invent. Math. **69** (1982), no. 2, 269–291.

[48] C. M. Lim, S. Payne and N. Potashnik, A note on Brill–Noether theory and rank-determining sets for metric graphs, Int. Math. Res. Not. **2012** (2012), no. 23, 5484–5504.

[49] Y. Luo, Rank-determining sets of metric graphs, J. Combin. Theory Ser. A **118** (2011), no. 6, 1775–1793.

[50] L. Maino, Moduli Space of Enriched Stable Curves. Ph.D. Dissertation, Harvard University.

[51] M. Manjunath and B. Sturmfels, Monomials, binomials, and Riemann–Roch, J. Algebr. Comb. **37** (2013), no. 4, 737–756.

[52] G. Mikhalkin, Enumerative tropical algebraic geometry in $\mathbb{R}^2$, J. Amer. Math. Soc. **18** (2005), no. 2, 313–377.

[53] G. Mikhalkin and I. Zharkov, Tropical curves, their Jacobians and theta functions, In Curves and abelian varieties, Contemp. Math., **465**, 203–230, Amer. Math. Soc., Providence, RI, 2008.

[54] A. Neeman, The distribution of Weierstrass points on a compact Riemann surface, Ann. of Math. **120** (1984), 317–328

[55] B. Osserman, A limit linear series moduli scheme, Ann. Inst. Fourier **56** (2006), no. 4, 1165–1205.

[56] A. Thuillier, Géométrie toroïdale et géométrie analytique non archimédienne. Application au type d'homotopie de certains schémas formels, Manuscripta Math. **123** (2007), no. 4, 381–451.

Chapter 13

Complex Monge-Ampère equations on Compact Kähler manifolds (14w5033)

April 6 - 11, 2014

Organizer(s): Sébastien Boucksom (CNRS & IMJ, Paris, France), Philippe Eyssidieux (IUF & Institut Fourier, Grenoble, France), Vincent Guedj (IUF& Institut Mathématiques Toulouse, France)

13.1 Overview of the Field

The workshop focused on analytic methods in complex algebraic and Kähler geometry, with a special emphasis on complex Monge-Ampère equations. From a PDE point of view the latter are fully non-linear and possibly degenerate second order elliptic equations, and are quite ubiquitous in complex geometry and analysis, most strikingly in the context of Kähler geometry.

Indeed on the one hand the complex Monge-Ampère operator is closely related to intersection theory since it can be seen as the top degree self-intersection operator on closed positive $(1,1)$-currents. On the other hand the Ricci curvature of a Kähler metric is expressed in terms of the complex Monge-Ampère operator of the Kähler potential, which explains why the existence problem for Kähler-Einstein metrics and the study of the Kähler-Ricci flow boil down to the study of a complex Monge-Ampère equation and the associated parabolic evolution equation.

An impressive number of works have been devoted to the existence, uniqueness and regularity of solutions to complex Monge-Ampère equations, both on compact manifolds and on domains. These problems were settled for Kähler-Einstein equations of negative and zero curvature by Yau's resolution of the Calabi conjecture in the late 70's [Yau78]. Getting a geometric understanding of the existence of Kähler-Einstein metrics on higher dimensional Fano manifolds and more generally of constant scalar curvature Kähler metrics on polarized manifolds is a more delicate problem and a very active research area.

Roughly at the same time as Yau's result, Bedford and Taylor's fundamental work on degenerate Monge-Ampère equations in domains [BT82] opened new research directions in several complex variables and pluripotential theory. Let us mention notably the work of Kolodziej [Kol05].

It is interesting to note that until very recently the differential-geometric and potential-theoretic sides have developed rather independently, mostly because of a lack of common vocabulary and interest.

Complex geometry allows to build a bridge between complex analysis and pluripotential theory on the one hand, and complex differential and algebraic geometry on the other hand. This was well illustrated by [Dem93], [DP04] where Monge-Ampère equations were used to obtain the first general results in the direction of Fujita's conjecture and to get a numerical characterization of the Kähler cone respectively.

13.2 Recent Developments and Open Problems

One of the most famous problems in Kähler geometry is that of finding when Kähler-Einstein metrics exist on Fano manifolds. Since Kähler-Einstein metrics can also be viewed as the stationary points of the Kähler-Ricci flow, this problem is the same as the one of the convergence of this flow. Its relation with the Monge-Ampère equation is particularly strong, since the Kähler-Ricci flow is just a parabolic version of the Monge-Ampère equation.

Perelman's work [SeT08] has created new tools for the study of the Kähler-Ricci flow [TZ07, PSSW08, ST09], while the recent breakthrough of Birkar, Cascini, Hacon and McKernan [BCHM10] in the Minimal Model Program has motivated the study of Kähler-Einstein metrics on singular varieties [EGZ09, BEGZ10, ST12].

Campana's birational classification scheme [Camp11], which aims at understanding the hyperbolicity properties of complex varieties, also calls for Kähler-Einstein metrics on geometric orbifolds. Birational geometry of higher dimensional varieties more generally leads to consider complex Monge-Ampère equations in more degenerate situations:

-the cohomology classes involved are no longer Kaehler,

-the measures to be considered are no longer volume forms,

-the solutions are merely weak (non-smooth, possibly unbounded).

These additional complications require the use of fine tools from complex analysis, pluripotential theory and algebraic geometry.

It thus appears that the study of complex Monge-Ampere equations in a context general enough to fit with the birational classification schemes calls for a whole range of very diversified techniques.

The last decade has witnessed an explosive growth in the subject, which has opened up entire new venues for investigation. Let us stress important progress on

-developing new methods for solving Monge-Ampère equations (algebraic approximation [PS06], variational methods [20, BBGZ13])

-regularity properties of degenerate solutions [DZ10, EGZ11],

-extensions of Bando-Mabuchi uniqueness theorem [CT08, Ber09, Ber11],

-conical Kähler-Einstein metrics [Don11, CGP11, JMR11],

-limits of Kähler-Einstein manifolds [DS12, BBEGZ11, CDS12a, CDS12b, CDS13, Tian12].

A strong motivation for all these works comes from the Yau-Tian-Donaldson conjecture (see [PS10]) which states that the existence of constant scalar curvature Kähler metrics in a Hodge class is equivalent to a suitably modified version of GIT stability of the underlying polarized manifold. This influential conjecture has recently attracted great interest among algebraic geometers (see e.g. [Oda12]).

Kähler geometry has recently known dramatic progress through the resolution, in an important special case (the "anticanonically polarized" case), of this conjecture. The diversity of techniques involved, extending across algebraic geometry, complex analysis, fully non-linear partial differential equations, pluripotential theory, and the Riemannian geometry of possibly singular spaces, makes it a very challenging task to understand in detail all aspects of the proof. At the same time it is clear that the new methods introduced are bound to play a major role in the forthcoming developments of Kähler geometry, as was well illustrated by the talks and informal discussions during our workshop.

13.3 Presentation Highlights

13.3.1 The Yau-Tian-Donaldson conjecture

The study of special Kähler metrics on compact Kähler manifolds, pioneered by Calabi in the 1950's, has been a guiding question in the field ever since, which led to an impressive number of remarkable developments, among which the solution by Yau of the Calabi conjecture in the late 1970's [Yau78] was one of the crowning achievements. The latter settled the existence and uniqueness problem for Kähler-Einstein metrics of negative or zero curvature, which amounts to the resolution of certain complex Monge-Ampère equations.

The case of Kähler-Einstein metrics of positive curvature turned out to be of a very different nature. Besides being non-unique in general (in fact, precisely in the presence of holomorphic vector fields according to a result of

Bando and Mabuchi [BM87]), obstructions to their existence were also constructed, first in terms of holomorphic vector fields (Futaki invariants), before being generalized by Tian through the introduction of the notion of K-stability in the late 90's [Tia97]. The latter was given an algebro-geometric interpretation by Donaldson around 2000, which led to the precise formulation of the Yau-Tian-Donaldson conjecture: the equivalence between the existence of positively curved Kähler-Einstein metrics (or, more generally, of constant scalar curvature Kähler metrics) and K-(poly)stability. One remarkable feature of this conjecture is the possibility to encode in a purely algebro-geometric condition the exact obstruction to solving certain fully non-linear elliptic PDE's.

A proof of this fundamental conjecture has recently been announced by Chen-Donaldson-Sun and by Tian, independently [CDS12a, CDS12b, CDS13, Tian12]. The method relies on a continuity method where the parameter is the cone angle of a Kähler metric with singularities along a smooth complex hypersurface. A crucial ingredient is Gromov's compactness theorem for Riemannian manifolds with Ricci curvature bounded below, which allows to consider Gromov-Hausdorff limits of such manifolds. Such limits are typically very singular compact metric spaces, and understanding the structure of these limit spaces is the subject of the subtle Cheeger-Colding theory. A particularly remarkable step in the proof of the Yau-Tian-Donaldson establishes that Gromov-Hausdorff limits of positively curved Kähler-Einstein manifolds of fixed volume are actually projective algebraic varieties with fairly mild singularities (to be described within the Minimal Model Program in birational geometry), endowed with a singular Kähler-Einstein metric.

Several talks of the workshop were directly connected to this major breakthrough. *M.Paun* surveyed recent developments around conical Kähler-Einstein metrics, *S.Paul* explained how the notion of (semi)stable pair is equivalent to the existence of Kähler-Einstein metrics on Fano manifolds with finite automorphism group, *G.Szekelyhidi* proved a partial C^0-estimate along the classical continuity method, *X.Wang* showed that any two toric n-manifolds can be joined in Gromov-Hausdorff topology by a continuous path of conical Kähler-Einstein toric manifolds, and *X.Zhu* studied the Gromov-Hausdorff convergence of almost Kähler-Ricci solitons.

13.3.2 Kähler-Ricci flow and the Minimal Model Program

From a general perspective, the Kähler-Ricci flow is obtained by specializing Hamilton's Ricci flow to Kähler manifolds; however, the corresponding PDE reduces in the Kähler case to a parabolic complex Monge-Ampère equation, and has therefore been studied quite independently from the general Riemannian case.

Along the flow, the cohomology class of the Kähler form evolves linearly towards the canonical class, and its positivity is in fact the only obstruction to the existence of the flow. The existence time can therefore be described by a purely cohomological condition, which turns out to fit exactly the procedure used to set up one step of the Minimal Model Program (MMP) in birational geometry.

Building on this important fact, Song and Tian have developed a program [87] viewing the Kähler-Ricci flow as a metric version of the MMP, each step of the MMP corresponding to a surgery that is used to repair a finite time singularity of the flow and start it over again. Moreover, they have been able to analyze the long time behavior of the flow at the final stage of the MMP, where the variety has become minimal.

However, most of the convergence results obtained so far stay away from the singularities themselves, proving C^∞ convergence on compact sets away from the singularities. Understanding the global behavior of the flow in the Gromov-Hausdorff topology is a fundamental and very challenging problem. The recent work of Chen-Donaldson-Sun and Tian has considerably improved our knowledge of Gromov-Hausdorff limit of algebraic Kähler-Einstein manifolds. Recently, in [CD11] Chen and Donaldson have revisited and improved some of the results of Cheeger-Colding-Tian. Moreover Colding, Cheeger and Naber have also given new information about non collapsed Gromov-Hausdorff limit of manifolds with a lower bound on the Ricci curvature [CN13, CN12].

Several lectures of the workshop concerned this interplay between the MMP and the Kähler-Ricci flow. *F.Campana* explained how the solution of the Abundance conjecture in dimension 3 can be adapted to the Kähler setting. *T.Collins* showed that finite time singularities of the Kähler-Ricci flow always form along analytic subvarieties. *J.Song* studied Calabi-Yau varieties with crepant singularities, identifying the metric completion of the Kähler-Einstein metric space constructed by Eyssidieux-Guedj-Zeriahi. *A.Zeriahi* developed the first steps of a viscosity theory in order to study the Kähler-Ricci flow on mildly singular varieties.

13.3.3 Degenerations of Kähler-Einstein manifolds

In algebraic geometry, degenerations are used to study points at infinity in moduli spaces. In the special case of K3 surfaces and, more generally, Calabi-Yau manifolds, the choice of a polarization (ample line bundle or Kähler cohomology class) uniquely determines a Ricci-flat Kähler metric, and it is a central problem to investigate the metric behavior of polarized Calabi-Yau manifolds approaching the boundary of the moduli space.

While the case of arbitrary degenerations seems completely out of reach at the moment, the case of maximal degenerations, also known as 'large complex structure limits', has attracted a lot of attention recently. Indeed, a remarkable conjecture of Kontsevich-Soibelman [KS01] and Gross-Siebert predicts that the Gromov-Hausdorff limit should be found as the dual complex of a relative minimal model of the degeneration, equipped with a metric of Monge-Ampère type, a real analogue of a complex Ricci flat metric. This conjecture originates from the Strominger-Yau-Zaslow picture of mirror symmetry, involving special Lagrangian fibrations that are only expected to exist in such large complex structure limits.

The Kontsevich-Soibelman version of the picture actually suggests to look for the limit metric using non-Archimedean geometry, building on the fact that the dual complex embeds in a natural way in the Berkovich space attached to the degenerations. Recent progress has been accomplished [MN12, NX13] on the algebro-geometric aspects of this conjecture, which connect in an exciting way the Minimal Model Program and non-Archimedean geometry.

An apparently more managable problem consists in analyzing the metric behavior as the cohomology class of the metric approaches the boundary of the Kähler cone of a fixed Calabi-Yau manifold. As shown by Tosatti and Zhang, an important feature of this situation is the existence of an a priori bound on the diameter. Combined with the fundamental Gromov compactness theorem, this guarantees the existence, up to a subsequence, of a limit in the Gromov-Hausdorff topology.

In the non-collapsed case, the limit class has positive volume and is the pull-back of a Kähler class by a birational contraction to a Calabi-Yau variety with canonical singularities. Combining [RoZh13, RuZh11] with the fondamental result of Donaldson-Sun [DS12], the limit is known to be given by the corresponding Ricci-flat metric on this singular Calabi-Yau variety.

In the collapsed case, the limit class is the pull-back of a class on the base of a fibration, and the limit metric is conjecturally the unique metric in this class with Ricci curvature equal the Weil-Petersson metric. This was pioneered by Gross and Wilson in the case of K3 surfaces [GW00]. In higher dimensions, [Tos10] proves $C^{1,\alpha}$ convergence away from the singular fibers; C^∞ convergence away from the singular fibers is established in [GTZ13a] for abelian fibrations, and Gromov-Hausdorff convergence is obtained in [GTZ13b] when the base is further assumed to be one-dimensional.

The lectures by *V.Tosatti* surveyed his recent works with Gross and Zhang on this theme. *H.Guenancia* explained his construction (joint work with Berman) of Kähler-Einstein metrics on stable varieties, an important step towards understanding the compactification of the moduli space of Kähler-Einstein manifolds of negative curvature.

Working with pairs impose to consider similar questions on quasi-projective manifolds. *H.Auvray* reviewed the construction of Poincaré type metrics in this context, *M.Haskins* studied complete Ricci flat Kähler manifolds that are asymptotic to cylinders at infinity, *H.C.Lu* solved degenerate Calabi-type equations of quasi-projective varieties.

13.3.4 Other talks

C.Arezzo explained how to construct constant scalar curvature Kähler metrics on blow-ups and desingularization of orbifolds with isolated quotient singularities.

S.Dinew reviewed the local regularity theory of complex Monge-Ampère equations, while *C.Li* studied the critical solvability exponents of the latter.

J.Ross gave detailed asymptotics of the partial Bergman Kernels, *B.Weinkove* developed Calabi-Yau type theorems for Gauduchon and balanced metrics, *D.Witt-Nyström* established local regularity results for geodesic rays in the space of Kähler potentials.

13.4 Outcome of the Meeting

The objective of the workshop was to bring together an international group of leading experts with complementary backgrounds from each above mentioned field, to report on and discuss recent progress and open problems in the area and thus foster interaction and collaboration between researchers in diverse subfields.

The workshop was timely, since the bulk of the progress described above took place in the last three or four years. It is remarkable that major contributions came from researchers from all over the world. Thus the workshop has also provided a unique opportunity for interaction between different groups who would normally reside in several distinct continents.

We had thirty-eight participants, including some of the main researchers in the fields of interest, coming from eleven different countries (Canada, China, France, Germany, Italy, Japan, Korea, Poland, Sweden, UK, USA). It was important for us that the workshop provide an opportunity for postdocs and graduate students to interact with experts. We have been quite successful in that respect, having five graduate students attending (from the Universities of Columbia, Grenoble, Paris, Purdue and Roma) and eight postdocs (from the Ecole Normale Supérieure and the Universities of Cambridge, Göteborg, Leibniz, McMaster, Stony Brook and Waterloo).

The workshop stimulated a number of fruitful discussions and collaborations. S.Dinew and H.C.Lu took the opportunity to finish their paper on mixed Hessian inequalities (arXiv April 2014), so did P.Eyssidieux, V.Guedj and A.Zeriahi with their study of weak Kähler-Ricci flows (arXiv June 2014). The discussions following Paun's lecture lead him to provide another proof of his main result (which he is presently writing up). S.Boucksom, T.Hisamoto and M.Jonsson took advantage of the free wednesday afternoon to have a lengthy discussion and start a joint project.

The participants were very enthusiastic about the scientific content of the workshop. The warm hospitality and professionalism of the staff were very much appreciated, the beautiful scenery and the great facilities helped make the workshop a success.

Participants

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Bibliography

[BM87] S. Bando, T. Mabuchi: Uniqueness of Einstein Kähler metrics modulo connected group actions, in Algebraic geometry, Sendai, 1985 (T. Oda, Ed.), Adv. Stud. Pure Math. **10**, Kinokuniya, 1987, 11–40.

[BT82] E. Bedford, B. A. Taylor: A new capacity for plurisubharmonic functions. Acta Math. **149** (1982), no. 1-2, 1–40.

[Ber10] R. Berman: A thermodynamical formalism for Monge-Ampère equations, Moser-Trudinger inequalities and Kähler-Einstein metrics. Adv. Math. 248 (2013), 1254–1297.

[Ber12] R.Berman: K-polystability of $\mathbb{Q}$-Fano varieties admitting Kähler-Einstein metrics. Preprint (2012) arXiv:1205.6214.

[BerBo10] R. Berman, S. Boucksom: Growth of balls of holomorphic sections and energy at equilibrium. Invent. Math. **181** (2010).

[BBGZ13] R. Berman, S. Boucksom, V. Guedj, A. Zeriahi: A variational approach to complex Monge-Ampère equations. Publ. Math. Inst. Hautes Etudes Sci. 117 (2013), 179–245.

[BBEGZ11] R. Berman, S. Boucksom, P. Eyssidieux, V. Guedj, A. Zeriah: Kähler-Einstein metrics and the Kähler-Ricci flow on log Fano varieties. Preprint (2011) arXiv:1111.7158.

[BBWN11] R. Berman, S. Boucksom, D. Witt-Nyström: Fekete points and convergence towards equilibrium measures on complex manifolds. Acta Math. (2011) 207, no. 1, 1–27.

[Ber09] B. Berndtsson: Curvature of vector bundles associated to holomorphic fibrations. Ann. Math. **169** (2009), no.2, 531-560.

[Ber11] B. Berndtsson: A Brunn-Minkowski type inequality for Fano manifolds and the Bando-Mabuchi uniqueness theorem. Preprint (2011) arXiv:1103.0923.

[BCHM10] C.Birkar, P.Cascini, C.Hacon, J.McKernan: Existence of minimal models for varieties of log general type. J. Amer. Math. Soc. **23** (2010), no. 2, 405-468.

[BEGZ10] S. Boucksom, P. Eyssidieux, V. Guedj, A. Zeriahi: Monge-Ampère equations in big cohomology classes. Acta Math. **205** (2010), 199–262.

[CC02] E. Calabi and X.X.Chen: The space of Kähler metrics. II. J. Differential Geom. 61 (2):173-193, 2002.

[Camp11] F. Campana: Special geometric orbifolds and bimeromorphic classification of compact Kähler manifolds. J. Inst. Math. Jussieu **10** (2011), no. 4, 809-934.

[CGP11] F. Campana, H. Guenancia, M. Paun: Metrics with cone singularities along normal crossing divisors and holomorphic tensor fields. Preprint (2011) arXiv:1104.4879v2.

[CCT02] J. Cheeger, T. H. Colding, G. Tian: On the singularities of spaces with bounded Ricci curvature. Geom. Func. Anal. 12 (2002), 873–914.

[CN13] J. Cheeger, A. Naber: Lower Bounds on Ricci Curvature and Quantitative Behavior of Singular Sets. Inventiones Math. 191 (2013), 321–339.

[CT05] J. Cheeger, G. Tian: Anti-self-duality of curvature and degeneration of metrics with special holonomy, Commun. Math. Phys. 255 (2005) 391–417.

[CT06] J. Cheeger, G. Tian: Curvature and injectivity radius estimates for Einstein 4-manifolds. J. Amer. Math. Soc. 19 (2006), no. 2, 487–525.

[CD11] X. X. Chen, S. K. Donaldson: Integral bounds on curvature and Gromov-Hausdorff limits. Preprint (2011) arXiv :1112.1594.

[CDS12a] X.X. Chen, S. K. Donaldson, S. Sun: Kähler-Einstein metrics on Fano manifolds, I: approximation of metrics with cone singularities. Preprint (2012) arXiv:1212.4566.

[CDS12b] X.X. Chen, S. K. Donaldson, S. Sun: Kähler-Einstein metrics on Fano manifolds, II: limits with cone angle less than 2π. Preprint (2012) arXiv:1212.4714.

[CDS13] X.X. Chen, S. K. Donaldson, S. Sun: Kähler-Einstein metrics on Fano manifolds, III: limits as cone angle approaches 2π and completion of the main proof. Preprint (2013) arXiv:1302.0282.

[CT08] X.X.Chen, G.Tian: Geometry of Kähler metrics and foliations by holomorphic discs. Publ. Math. I.H.E.S. **107** (2008), 1-107.

[CN12] T. H. Colding, A. Naber: Sharp Hölder continuity of tangent cones for spaces with a lower Ricci curvature bound and applications. Annals of Math. 176 (2012), Issue 2, 1173–1229.

[CHNP] A. Corti, M. Haskins, J. Nordström, T. Pacini: G_2-manifolds and associative submanifolds via semi-Fano 3-folds. Preprint (2012) arXiv:1207.4470.

[Dem93] J. P. Demailly: A numerical criterion for very ample line bundles. J. Differential Geom. **37** (1993), no. 2, 323-374.

[DP04] J.P.Demailly, M.Paun: Numerical characterization of the Kähler cone of a compact Kähler manifold. Ann. Math. (2004).

[DZ10] S. Dinew, Z. Zhang: On stability and continuity of bounded solutions of degenerate complex Monge-Ampère equations over compact Kähler manifolds. Adv. Math. **225** (2010), 367–388.

[Don11] S. K. Donaldson: Kähler metrics with cone singularities along a divisor. Preprint arXiv (2011).

[DS12] S. K. Donaldson, S. Sun: Gromov-Hausdorff limits of Kähler manifolds and algebraic geometry. arXiv:1206.2609.

[EGZ09] P. Eyssidieux, V. Guedj, A. Zeriahi: Singular Kähler-Einstein metrics. J. Amer. Math. Soc. **22** (2009), 607-639.

[EGZ11] P. Eyssidieux, V. Guedj, A. Zeriahi: Viscosity solutions to degenerate Complex Monge-Ampère equations. Comm.Pure & Appl.Math **64** (2011), 1059–1094.

[GTZ13a] M. Gross, V. Tosatti, Y. Zhang: Collapsing of abelian fibered Calabi-Yau manifolds. Duke Math. J. 162 (2013), no. 3, 517–551.

[GTZ13b] M. Gross, V. Tosatti, Y. Zhang: Gromov-Hausdorff collapsing of Calabi-Yau manifolds. Preprint (2013) arXiv:1304.1820.

[GW00] M. Gross, P. M. H. Wilson: Large complex structure limits of K3 surfaces. J. Differential Geom. 55 (2000), no. 3, 475-546.

[Hei12] H.-J. Hein: Gravitational instantons from rational elliptic surfaces. J. Amer. Math. Soc. 25 (2012), 355–393.

[HC13] H.-J. Hein, R. Conlon: Asymptotically conical Calabi-Yau manifolds, I. Preprint arXiv:1205.6347, to appear in Duke Math. J.

[HN14] H.-J. Hein, A. Naber: New logarithmic Sobolev inequalities and an ε-regularity theorem for the Ricci flow. To appear in CPAM.

[JMR11] T.D. Jeffres, R. Mazzeo, Y.A. Rubinstein: Kähler-Einstein metrics with edge singularities. arXiv:1105.5216.

[Joy00] D. Joyce : Compact manifolds with special holonomy. Oxford Mathematical Monographs, Oxford University Press, Oxford, 2000.

[Kol05] S.Kolodziej: The complex Monge-Ampère equation and pluripotential theory. Mem.A.M.S. **178** (2005), no. 840, 64 pp.

[KS01] M. Kontsevich, Y. Soibelman: Homological mirror symmetry and torus fibrations. Symplectic geometry and mirror symmetry (Seoul, 2000), 203–263, World Sci. Publ., River Edge, NJ, 2001.

[KT00] M. Kontsevich and Y. Tschinkel: Non-Archimedean Kähler geometry. Preliminary notes (2000).

[Kov03] A. Kovalev: Twisted connected sums and special Riemannian holonomy. J. Reine Angew. Math. 565 (2003), 125–160.

[MN12] M. Mustata, J. Nicaise: Weight functions on non-archimedean analytic spaces and the Kontsevich-Soibelman skeleton. Preprint (2012) arXiv:1212.6328.

[NX13] J. Nicaise, C. Xu: The essential skeleton of a degeneration of algebraic varieties. Prpublication (2013) arXiv:1307.4041.

[Oda12] Y. Odaka: The GIT stability of polarized varieties via discrepancy, Annals of Math., to appear.

[PS06] D. H. Phong, J. Sturm: The Monge-Ampère operator and geodesics in the space of Kähler potentials. Invent. Math. **166** (2006), no. 1, 125-149.

[PSSW08] D. H. Phong, J. Song, J. Sturm, B. Weinkove: The Kähler-Ricci flow with positive bisectional curvature. Invent. Math. **173** (2008), no. 3, 651-665.

[PS10] D. H. Phong, J. Sturm: Lectures on stability and constant scalar curvature. Handbook of geometric analysis, No. 3, 357436, Adv. Lect. Math. (ALM), 14, Int. Press (2010).

[RoZh13] X.Rong, Y. Zhang: Degenerations of Ricci-flat Calabi-Yau manifolds. Communications in Contemporary Mathematics 15 (2013), no. 4, 1–8.

[Ru99] W. D. Ruan: On the convergence and collapsing of Kähler metrics. J. Differential Geom. 52 (1999), no. 1, 1–40.

[RuZh11] W.D.Ruan, Y. Zhang: Convergence of Calabi-Yau manifolds. Adv. in Math. 228 (2011) 1543–1589.

[SeT08] N.Sesum, G.Tian: Bounding scalar curvature and diameter along the Kähler-Ricci flow (after Perelman). J. Inst. Math. Jussieu **7** (2008), no. 3, 575-587.

[ST12] J. Song, G. Tian: Canonical measures and Kähler-Ricci flow. J. Amer. Math. Soc. **25** (2012), no. 2, 303-353.

[ST09] J. Song, G. Tian: The Kähler-Ricci flow through singularities. Preprint (2009) arXiv:0909.4898.

[SSW13] J. Song, G. Székelyhidi, B. Weinkove: The Kähler-Ricci flow on projective bundles. Int. Math. Res. Not. IMRN 2013, no. 2, 243–257.

[SW] J. Song, B. Weinkowe: Contracting exceptional divisors by the Kähler-Ricci flow. Duke Math. J. 162 (2013), no. 2, 367–415.

[SY] J. Song, Y. Yuan: Metric flips with Calabi ansatz. Geom. Funct. Anal. 22 (2012), no. 1, 240–265.

[Tian90] Tian, G.: On a set of polarized Kähler metrics on algebraic manifolds. J. Differential Geom. 32 (1) (1990), 99–130.

[Tia97] G. Tian: Kähler-Einstein metrics with positive scalar curvature. Inv. Math. 130 (1997), 239–265.

[Tian12] G. Tian: K-stability and Kähler-Einstein metrics. Preprint (2012) arXiv:1211.4669.

[TZ07] G. Tian, X. Zhu: Convergence of Kähler-Ricci flow. J. Amer. Math. Soc. **20** (2007), no. 3, 675–699.

[Tos09] V. Tosatti: Limits of Calabi-Yau metrics when the Kähler class degenerates. J. Eur. Math. Soc. (JEMS) 11 (2009), no. 4, 755–776.

[Tos10] V. Tosatti: Adiabatic limits of Ricci-flat Kähler metrics. J. Differential Geom. 84 (2010), no. 2, 42–453.

[Yau78] S. T. Yau: On the Ricci curvature of a compact Kähler manifold and the complex Monge-Ampère equation. I. Comm. Pure Appl. Math. **31** (1978), no. 3, 339–411.

Chapter 14

Subfactors and Fusion Categories (14w5083)

April 13 - 18, 2014

Organizer(s): Vaughan Jones (Vanderbilt University), Scott Morrison (Australian National University), David Penneys (UCLA), Emily Peters (Northwestern University), Noah Snyder (Indiana University)

Classifying subfactors and fusion categories

Vaughan Jones, Scott Morrison, David Penneys, Emily Peters, and Noah Snyder

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1 Introduction

This workshop brought together mathematicians studying subfactors, fusion categories, and Hopf algebras. The majority of the participants were from Canada and the US, but we also had many international participants, including mathematicians from Argentina, Australia, Colombia, Denmark, France, Great Britain, Israel, Japan, and the Netherlands. Seven women and 33 men participated. Seven graduate students and four postdocs attended.

This is a very exciting time for these fields, as it's only recently been appreciated how many of the techniques and ideas from each field can be fruitfully applied in the others. Many new classification results have appeared in the last few years, and the change of perspective offered by thinking about old questions using the techniques of another field have suggested many new approaches, and new problems.

In order to facilitate collaborations between researchers in different areas, we scheduled a smaller number of research talks than in a typical conference, and set up focused discussion groups in the afternoons. After each morning of talks, we all came together to propose ideas for working groups for the afternoon, and then divided up the conference amongst a few smaller groups. Sometimes this groups worked as intensive tutorials led by an expert in one field, and other times the groups worked together on new problems. Some of the most exciting sections involved discussions of the material of a morning talk, with participants realizing new applications of the ideas in their own subject.

We really enjoyed organizing the conference in this format, and we highly recommend it to other organizers! It requires a certain amount of planning, direction from the organizers on the day, and care to ensure that everyone has an interesting group to join, but we think that the outcomes justify this extra work.

The remainder of this report consists of the following subsections:

(1) Exciting new developments reported in the lectures

(2) Advances made by small group discussions

(3) Open problems

2 New developments reported in lectures

2.1 The Asaeda-Haagerup subfactor

One of the most exciting results discussed at the conference was the current work of Grossman-Izumi-Snyder on the Asaeda-Haagerup subfactor. Until this work, the Asaeda-Haagerup subfactor was among the least well understood subfactors of the currently known examples.

It was first constructed by Asaeda and Haagerup [AH99], by a very direct construction that does not seem very enlightening! The possibility of its existence was first noticed by Haagerup [Haa94], in the first project to exhaustively describe possible principal graphs for small index subfactors. Thus the Asaeda-Haagerup subfactor, along with the "extended Haagerup" subfactor, was considered quite exotic!

This new result of Grossman-Izumi-Snyder shows how the Asaeda-Haagerup subfactor is naturally associated with the family of 3^G subfactors. These subfactors are natural generalizations of the Haagerup subfactor at index $\frac{5+\sqrt{13}}{2}$. A 3^G subfactor has principal graph a spoke graph with all arms having length 3. The even bimodules consists of a group G of invertible bimodules together with one other G-orbit of simple bimodule. Such fusion categories were constructed by Izumi in [Izu01], and later, more were constructed by Evans-Gannon [EG11].

These 3^G subfactors are not completely understood. While it seems likely that there will be an infinite family of 3^G subfactors, they have only been constructed in specific cases for $|G| \leq 19$. Each construction requires solving a system of polynomial equations, which scales poorly as the size of the group increases.

In [GS12b], Grossman-Snyder found the quantum subgroups of the Haagerup $3^{\mathbb{Z}/3}$ subfactor, i.e., all Frobenius algebra objects in the even half. They were able to determine the Brauer-Picard groupoid, whose objects are the Frobenius algebras, and whose morphisms are invertible bimodules in the category. In a subsequent article [GS12a], they studied the Brauer-Picard groupoid of the Asaeda-Haagerup subfactor, but were left with some open cases.

In this recent work, Grossman-Izumi-Snyder complete the open cases to show that the even half of the Asaeda-Haagerup subfactor is Morita equivalent to a generalized Haagerup category, obtained by a de-equivariantization of the even half of a $3^{\mathbb{Z}/4\times\mathbb{Z}/2}$ subfactor. Thus the Asaeda-Haagerup subfactor fits into the family of 3^G subfactors together with (de-)equivariantizations and Morita equivalences.

Further, their work on the $3^{\mathbb{Z}/4\times\mathbb{Z}/2}$ subfactors allows them to completely describe the centre of the Asaeda-Haagerup subfactor, including its S and T matrices.

2.2 Computing centers of quadratic categories

A quadratic fusion category is a fusion category with a non-invertible simple object X such that every simple object is either invertible or is isomorphic to X tensored with an invertible object. Most known examples of fusion categories that do not come from finite groups or quantum groups are Morita equivalent to quadratic fusion categories. The quantum doubles, or Drinfeld centers, of quadratic fusion categories provide interesting examples of modular tensor categories.

These quantum doubles can be explicitly described, and invariants such as S and T

matrices computed, using two ideas of Izumi. The first idea is that many quadratic fusion categories can be represented as categories of endomorphisms of (von Neumann algebra closures of) Cuntz algebras. The second idea is that the Cuntz algebra representations of these fusion categories allow for an explicit description of their tube algebras.

The tube algebra of a unitary fusion category $\mathcal{C}$ is, as a vector space, the direct sum of the intertwiner spaces $\mathrm{Hom}(XY, YZ)$ where X, Y, and Z range over representatives of the simple objects of $\mathcal{C}$. This vector space is then endowed with an associative multiplication and an involution. The minimal central projections of the tube algebra are in bijection with the simple objects of the quantum double, and the half-braidings and S and T matrices can also be described in terms of the tube algebra.

For a quadratic fusion category represented as endomorphisms of a Cuntz algebra, one can often choose a basis for the tube algebra where the intertwiners are words in the Cuntz algebra (together with labels for the intertwiner space), and the tube algebra multiplication is given by a combination of multiplications in the Cuntz algebra and endomorphisms of the Cuntz algebra. The structure constants for the tube algebra can thus be written down explicitly in terms of a certain basis. However, this description of the tube algebra does not reveal its simple summands or indicate a formula for finding matrix units.

To actually find matrix units for the tube algebra, one first looks at components of the tube algebra of the form $\mathrm{Hom}(g-, -g)$, where g is invertible. Such components are easy to understand using the structure of the group of invertible objects. Then to understand components of the form $\mathrm{Hom}(X-, -X)$, with X noninvertible, one first looks at the intertwiner spaces $\mathrm{Hom}(g-, -X)$ to find the projections of $\mathrm{Hom}(X-, -X)$ which have nontrivial intertwiners to projections in $\mathrm{Hom}(g-, -g)$ for invertible objects g. The remaining parts of $\mathrm{Hom}(X-, -X)$ are typically harder to describe and usually require some computer linear algebra. Once one has matrix units for the tube algebra, the half-braidings and modular data can be computed and analyzed.

Izumi worked out a number of examples in his seminal papers [Izu00, Izu01], including near-group categories and generalized Haagerup categories associated to groups of odd order. Further examples of these two types were computed and studied by Evans and Gannon [EG11, EG14], who also analyzed the modular data of these quadratic categories and found striking patterns and relations to modular data of finite groups. Their work persuasively argues that these quadratic fusion categories are not exotic but rather fit into larger families. More recently, Grossman-Izumi-Snyder announced that the even parts of the Asaeda-Haagerup subfactor are Morita equivalent to three quadratic categories, including a de-equivariantization of a generalized Haagerup category for a group of even order, which allowed for the computation of the quantum double by similar methods.

2.3 Rank finiteness for modular tensor categories

A long standing open conjecture in the study of modular tensor categories is rank-finiteness, namely that there are only finitely many equivalence classes of MTCs in each rank (the rank is simply the number of simply objects). A proof of this conjecture was announced shortly before the conference, by Bruillard-Ng-Rowell-Wang [BNRW13], and Eric Rowell gave the first public lecture on their argument at the conference. This lecture was then followed by an afternoon discussion section which went through some of the more technical details.

Unfortunately the bounds provided by this proof seem to be very large, and hard to make effective, but it is still extremely exciting to have a solution to this puzzle!

The method of proof relies heavily on modularity, but nevertheless a group at the conference had ideas for extending the result to spherical braided fusion categories.

It is tempting to dream of proving rank-finiteness at the level of fusion categories, as well!

2.4 A new sequence of subfactors from the E_{N+2} quantum subgroup of $SU(N)$

Jones' index rigidity theorem classified the possible indices of II_1 subfactors to the range

$$\{4\cos^2(\pi/n)|n \geq 3\} \cup [4, \infty)$$

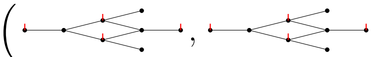
In the same article, he constructed an example with each allowed index. The subfactors arising from the discrete series in his article come from $SU_q(2)$ at a root of unity. Soon afterward, Ocneanu announced the complete classification of subfactors with index less than 4, resulting in an ADE classification. In more detail, the principal graph of a subfactor with index less than 4 must be one of A_n, D_{even}, E_6, and E_8. Interestingly, D_{odd} and E_7 do not occur. There is a unique subfactor with each allowed type A or D principal graph, and a pair of complex conjugate subfactors for both E_6 and E_8.

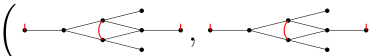
This result can be understood as a classification of all quantum subgroups of $SU(2)$. A type I quantum subgroup of a fusion category $\mathcal{C}$ can be thought of in two ways: a commutative Frobenius algebra object $A \in \mathcal{C}$, or equivalently the category of A-bimodules in $\mathcal{C}$. It is well known that finite-depth subfactors are in 1-to-1 correspondence with Frobenius algebra objects in unitary fusion categories, so quantum subgroups correspond to certain subfactors. For $SU(2)$ at roots of unity, the non-trivial quantum subgroups exactly correspond to the D_{2n} and E_6 and E_8 subfactors.

In [Ocn02], Ocneanu gave the complete list of quantum subgroups of $SU(3)$ and $SU(4)$. He also proved some general facts about quantum subgroups. There is always a D-series which arises from a $\mathbb{Z}/n\mathbb{Z}$-equivariantization corresponding to the dimension 1 representations. He also claimed that there are only finitely many exceptional quantum subgroups for any fixed $SU(N)$.

In his talk in the Wednesday morning session, Ostrik gave an expository talk in which he outlined the proof that there are only finitely many exceptional quantum subgroups for $SU(2)$. Of course, this is known from the classification of subfactors of index less than 4, but this proof could hopefully generalize to the higher $SU(N)$. The details have not yet been completely worked out, and it would be highly important and worthwhile for someone to do this. One of the most interesting and exciting small group discussions focused on extending this proof to $SU(3)$ (see §3.2).

In recent work, Zhengwei Liu has constructed the E_{N+2} quantum subgroup of $SU(N)$ for all N. Motivated by the recent classification article of Liu-Morrison-Penneys [LMP14] which constructs subfactors with principal graphs

$\mathcal{S} = \Big($  $\Big)$ or

$\mathcal{S}' = \Big($  $\Big)$.

using a 'twisted' version of a braiding, Liu gives a uniform construction for an infinite family of related subfactors.

Liu constructs these examples using a partial braiding, as is the case for quantum subgroups corresponding to commutative algebra objects. Moreover, he gives a complete classification of singly-generated Yang-Baxter planar algebras. A Yang-Baxter planar algebra is generated by 2-boxes such that one triangle can be simplified in terms of the other triangle and lower order terms.

2.5 Connections to conformal field theory

Subfactors and fusion categories are intimately connected to conformal field theory. It is conjectured that the infinite family of subfactors that Liu constructed also comes from an infinite family of conformal inclusions. Also, it is conjectured (by Kawahigashi) that every modular tensor category arises from conformal field theory. This is an important open question in the field.

Kawahigashi, together with Longo and Bischoff proved a conjecture due to Kong-Runkel. Starting with a non-local extension of a chiral CFT $\mathcal{A}$, one can construct a full CFT based on $\mathcal{A}$ via boundary CFT, which gives a natural subfactor. One can also describe the non-local extension in terms of a non-commutative Frobenius algebra object, and perform the 'full center' construction to obtain another natural subfactor. Bischoff-Kawahigashi-Longo proved these subfactors are canonically isomorphic. Thus they showed that there is a bijective correspondence between Morita-equivalence classes of non-local extensions of $\mathcal{A}$ and equivalence classes of full CFT's based on $\mathcal{A}$.

2.6 Quantum Computation

Quantum computation is an exciting field of research, as it offers the tantalizing possibility of redefining 'hard' and 'not hard' problems in computer science. For example, Shor's algorithm [Sho99] gives a way to factor integers in polynomial time using a quantum computer.

However, quantum computers are a long way from being able to do these calculations in practice: despite decades of research, the largest verified quantum computer ever built had only 14 qubits.

Quantum 'qubits' are hard to maintain for long enough to do even simple computations. While Shor, Steane, and Kitaev have independently discovered fault tolerance schemes for quantum computation, the decoherence rate in present implementations is still too high.

A proposed workaround to the fragility of quantum systems, due to Freedman and Kitaev, is to use topology to make the system robust to decoherence. The group at Microsoft Station Q is studying topological phases of matter in connection to developing a topological quantum computer.

Topological phases of matter are quantum systems whose ground state space has dimension greater than 1, and whose eigenvalues have a spectral gap that survives in the limit as the number of particles increases. The assignment of ground states to surfaces in this case is a 2-dimensional topological quantum field theory. Since the ground state has dimension greater than 1, quasiparticles/anyons can be manipulated within this ground state. They are protected from jumping to other states via the spectral gap.

To perform quantum computations, we start with a certain finite gate set of unitary $2^n \times 2^n$ matrices for varying ns. A quantum circuit is a composite of tensor powers of elements of our gate set. We perform a quantum computation by starting with a state, applying the quantum circuit, and measuring the the final state. We arrange the circuit such that the probability of observing some particular state is close to one when the answer ought to be 'yes', and otherwise this probability is close to zero.

Now the idea behind topological quantum computing is that a certain braid of anyons should correspond to a quantum gate. There are analogous notions of tensor products and composition of braids of anyons. The computation is then performed by braiding the anyons to create the corresponding quantum circuit, and measuring the output.

We are immediately led to the question of which quantum gates and circuits are possible to realize. A gate set is called universal for quantum computation if we can approximate any unitary matrix as a composite of tensor products of elements from our gate set (with the number of gates polynomial in the precision of the approximation).

In the topological computation approach, the anyons correspond to simple objects in a unitary modular category (UMC). The unitary modular category is called universal for quantum computation if given an object x, the image of the braid group in $\mathrm{End}(x^{\otimes N})$ is dense in $PSU(2^N)$ for all N. It is known that the Ising theory (the A_3 UMC) is not universal, whereas the Fibonacci theory (the A_4 UMC) is universal [FLW02].

In fact, the A_3 UMC has Property (F): the images of the braid groups are finite for every object. This relates to an important conjecture of Rowell that Property (F) is equivalent to weak integrality, i.e., all objects have dimensions which are square roots of integers. Property (F) should be thought of as the polar opposite to universality.

3 Small group discussions

3.1 Cuntz algebras for beginners and intermediates

As mentioned above, Cuntz algebras play an important role in the construction of 3^G subfactors, and a Cuntz algebra construction of a subfactor makes its center easier to compute. Gannon's talk included some extremely hands-on examples of how to do computations with Cuntz algebras, and emphasized the point that there should be many, many more subfactors than we know about. He observed that every construction technique we know has allowed us to 'shine a flashlight in one direction' and see some new subfactors, but there are still many undiscovered ones waiting in the dark.

In light of this, there was enthusiasm among many participants to practice these Cuntz algebra construction techniques ourselves. This group began with a discussion, led by Izumi, about which subfactors one should expect Cuntz algebra techniques to succeed with; the group then reproduced many calculations (which already appear in the literature) with the goal of understanding the role, in the subfactor, of each of the equations being solved.

3.2 Exceptional quantum subgroups of $SU(3)$

As stated before, Ostrik presented a proof that there are finitely many exceptional quantum subgroups of $SU(2)$. On one hand, this result due to Ocneanu is old. But the proof technique Ostrik presented was new to many experts in the field. During one of the afternoon sessions, about a dozen of us worked on extending the proof Ostrik presented that there are only finitely many exceptional quantum subgroups of $SU(2)$ to the case of $SU(3)$.

The main hurdle to extending this proof was the fact that the fusion rules for $SU(3)$ are more complicated than $SU(2)$. In more detail, as N grows, the fusion graph with respect to the standard representation forms an N-simplex, and writing down the explicit rules for fusion between any two objects becomes complicated.

Some participants were able to modify the technique to prove that 'any non-A_∞ subfactor with index less than 4.07 is at most 20-supertransitive'. This result follows already from classification techniques, and apparently cannot generalize to higher indices, but it is nevertheless exciting as it is the first direct bound on supertransitivity.

3.3 Weakly integral modular categories

During one of the break-out sessions at the workshop, it was suggested to study weakly integral modular categories, with the goal of classifying them in low rank. These are modular categories with integral categorical dimension, and include those categories whose objects have integer dimensions. An easy example is the Ising modular category, which has 3 simple objects with dimensions 1,1 and $\sqrt{2}$. The group included Z. Wang, C. Galindo, E. Rowell, J. Plavnik and S.-H. Ng. At the end of the Banff workshop they had made some nice progress, including an idea of how to classify modular categories of dimension $4p$ where p is prime. The working group had several more occasions to meet in 2014 (adding P. Bruillard to the group) and have now classified all weakly integral modular categories of rank 6 and 7, as well as all modular categories of dimension $4m$ where m is odd and square-free. Integral modular categories of rank at most 7 are all pointed, with the first non-pointed example in rank 8 being the familiar representation category of the double of the symmetric group S_3. Building upon this work, the cases of ranks 8 and 9 have now been completed under the assumption that some object has non-integral dimension (so-called "strictly weakly integral"), by a slightly different group of researchers. The current goal is to show that all strictly weakly integral modular categories of rank at most 11 can be obtained via direct products of $\mathbb{Z}_2$-de-equivariantization of Tambara-Yamagami categories and pointed categories. There is an example in rank 12 that is not of this form, which motivates this goal.

3.4 Computing S and T matrices

Terry Gannon gave a talk on calculating the S and T matrices for the center of a fusion category, leveraging the representation theory of the modular group. After this talk, Terry Gannon, Scott Morrison, and David Evans began work on the center of the extended Haagerup subfactor. This built on an article posted to the arXiv during the Banff conference by Scott Morrison and Kevin Walker [MW14], which used a combinatorial technique to prove that the center of the extended Haagerup subfactor has 22 simple objects.

3.5 Gannon's new proof on the bound on the Frobenius-Schur exponent

Gannon pointed out a new way to bound the Frobenius-Schur exponent N of a modular category in terms of the rank r: look at the minimum dimension m of a faithful representation of $SL(2, \mathbb{Z}_{p^k})$ (which is bounded below in terms of p^k). If $m > r$ then p^k does not divide N. This should improve the current best bound.

3.6 Various smaller groups

During the small group sessions, many mathematicians chose to collaborate in smaller groups. For instance, Brothier and Yamashita reported having a fruitful discussion on infinite depth subfactors, and Kawahigashi and Wang discussed modular tensor categories, anyons, and topological phases of matter.

3.6.1 The generator conjecture for 3^G subfactor planar algebas

At this point, planar algebra techniques have not been as successful as Cuntz algebra techniques for analyzing quadratic categories. The first step to analyzing these 3^G subfactor planar algebras is to find the formulas for the low weight rotational eigenvectors at depth 4 which generate the subfactor planar algebra. We know from [JP11, BP14, MP12] that the jellyfish algorithm can be used to construct such subfactors by finding them inside the graph planar algebra of the principal graph. However, one must know the formula for the generators in the graph planar algebra, and one must be able to compute the requisite 2-strand jellyfish relations. From the previous work [Jon12, Pet10, MP12, PP13], Penneys had conjectured a formula for the low weight rotational eigenvectors in the 3^G subfactor planar algebra. Liu and Penneys proved this conjecture for the case $|G|$ odd during the workshop.

3.6.2 MTC with dimension $4p$

Shortly after the workshop, the group of Bruillard (not present at this conference), Galindo, Ng, Plavnik, Rowell, and Wang classified modular categories of dimension $4p$ with p prime, generalizing p to any odd square-free number. They also extended the classification of weakly integral modular categories to rank 7.

4 Open Problems

(1) Give a complete proof of Ocneanu's theorem on finiteness of exception quantum subgroups of SU(N).

(2) Can the finite results for quantum subgroups of $SU(N)$ be adapted to give supertransitivity bounds for subfactors? High supertransitivity subfactors appear to be very rare, yet our inability to control supertransitivity makes classifications very difficult.

(3) (Kawahigahi) Does every unitary modular tensor category arise as the representation category of a conformal net?

(4) Can one classify the quantum subgroups of $U_q(\mathfrak{g})$ for simple Lie algbras $\mathfrak{g}$ outside of type A? The exceptional group G_2 in particular may be tractable [EP14].

(5) Does weakly integral imply weakly group theoretical for fusion categories?

(6) (Liu) What is the skein theory of subfactors from conformal inclusions, in particular, the ones in a family?

(7) (Rowell) Which modular categories have trivial Galois group? This remains open, and seems hard.

(8) (Rowell) Extend rank-finiteness to spherical braided fusion categories. (Plavnik, Galindo, Ng, Rowell, Wang and Bruillard have an approach to this.)

(9) (Rowell) The Property F conjecture for braided fusion categories. This remains open.

(10) What is the list of unitary fusion categories of rank 4? (The classification in the modular case is already known [RSW09].)

(11) For how large of value of D can one classify all fusion rings with global dimension at most D? ($D \sim 12$ is certainly feasible, but it may be possible to go much further.)

(12) The modular data for the Haagerup subfactor appears to be 'grafted' together out of simpler pieces [EG11]. Are there constructions making this precise?

(13) The even part of the 4442 subfactor appears to be a 'non-graded extension' of $RepA_4$. (That is, it has the form $\mathcal{C} \oplus \mathcal{M}$ where $\mathcal{C} = RepA_4$ and $\mathcal{M}$ is $\mathcal{C}$ as a module over itself, but the tensor product structure on $\mathcal{M}$ itself is more complicated.) Is there a construction making this precise?

(14) Compute the center and the S and T matrices of the extended Haagerup subfactor.

References

[AH99] Marta Asaeda and Uffe Haagerup, *Exotic subfactors of finite depth with Jones indices* $(5+\sqrt{13})/2$ *and* $(5+\sqrt{17})/2$, Comm. Math. Phys. **202** (1999), no. 1, 1–63, arXiv:math.OA/9803044 MR1686551 DOI:10.1007/s002200050574.

[BNRW13] Paul Bruillard, Siu-Hung Ng, Eric C. Rowell, and Zhenghan Wang, *On modular categories*, 2013, arXiv:1310.7050.

[BP14] Stephen Bigelow and David Penneys, *Principal graph stability and the jellyfish algorithm*, Math. Ann. **358** (2014), no. 1-2, 1–24, MR3157990 DOI:10.1007/s00208-013-0941-2 arXiv:1208.1564.

[EG11] David E. Evans and Terry Gannon, *The exoticness and realisability of twisted Haagerup-Izumi modular data*, Comm. Math. Phys. **307** (2011), no. 2, 463–512, arXiv:1006.1326 MR2837122 DOI:10.1007/s00220-011-1329-3.

[EG14] ———, *Near-group fusion categories and their doubles*, Adv. Math. **255** (2014), 586–640, arXiv:1208.1500 MR3167494 DOI:10.1016/j.aim.2013.12.014.

[EP14] David E. Evans and Mathew Pugh, *Spectral measures for g_2 II: finite subgroups*, 2014, arXiv:1404.1866.

[FLW02] Michael H. Freedman, Michael Larsen, and Zhenghan Wang, *A modular functor which is universal for quantum computation*, Comm. Math. Phys. **227** (2002), no. 3, 605–622, MR1910833 DOI:10.1007/s002200200645 arXiv:quant-ph/0001108v2.

[GS12a] Pinhas Grossman and Noah Snyder, *The Brauer-Picard group of the Asaeda-Haagerup fusion categories*, 2012, arXiv:1202.4396.

[GS12b] ———, *Quantum subgroups of the Haagerup fusion categories*, Comm. Math. Phys. **311** (2012), no. 3, 617–643, arXiv:1102.2631 MR2909758 DOI:10.1007/s00220-012-1427-x.

[Haa94] Uffe Haagerup, *Principal graphs of subfactors in the index range $4 < [M : N] < 3 + \sqrt{2}$*, Subfactors (Kyuzeso, 1993), World Sci. Publ., River Edge, NJ, 1994, MR1317352, pp. 1–38.

[Izu00] Masaki Izumi, *The structure of sectors associated with Longo-Rehren inclusions. I. General theory*, Comm. Math. Phys. **213** (2000), no. 1, 127–179, MR1782145 DOI:10.1007/s002200000234.

[Izu01] ———, *The structure of sectors associated with Longo-Rehren inclusions. II. Examples*, Rev. Math. Phys. **13** (2001), no. 5, 603–674, MR1832764 DOI:10.1142/S0129055X01000818.

[Jon12] Vaughan F. R. Jones, *Quadratic tangles in planar algebras*, 2012, arXiv:math/1007.1158 MR2972458 DOI:10.1215/00127094-1723608, pp. 2257–2295.

[JP11] Vaughan F. R. Jones and David Penneys, *The embedding theorem for finite depth subfactor planar algebras*, Quantum Topol. **2** (2011), no. 3, 301–337, arXiv:1007.3173 MR2812459 DOI:10.4171/QT/23.

[LMP14] Zhengwei Liu, Scott Morrison, and David Penneys, *1-supertransitive subfactors with index at most $6\frac{1}{5}$*, Comm. Math. Phys. (2014), arXiv:1310.8566, DOI:10.1007/s00220-014-2160-4.

[MP12] Scott Morrison and David Penneys, *Constructing spoke subfactors using the jellyfish algorithm*, 2012, arXiv:1208.3637, to appear in Transactions of the American Mathematical Society.

[MW14] Scott Morrison and Kevin Walker, *The centre of the extended Haagerup subfactor has 22 simple objects.*, 2014, arXiv:1404.3955.

[Ocn02] Adrian Ocneanu, *The classification of subgroups of quantum* SU(N), Quantum symmetries in theoretical physics and mathematics (Bariloche, 2000), Contemp. Math., vol. 294, Amer. Math. Soc., Providence, RI, 2002, MR1907188, pp. 133–159.

[Pet10] Emily Peters, *A planar algebra construction of the Haagerup subfactor*, Internat. J. Math. **21** (2010), no. 8, 987–1045, arXiv:0902.1294 MR2679382 DOI:10.1142/S0129167X10006380.

[PP13] David Penneys and Emily Peters, *Calculating two-strand jellyfish relations*, 2013, arXiv:1308.5197.

[RSW09] Eric Rowell, Richard Stong, and Zhenghan Wang, *On classification of modular tensor categories*, Comm. Math. Phys. **292** (2009), no. 2, 343–389, MR2544735 arXiv:0712.1377 DOI:10.1007/s00220-009-0908-z.

[Sho99] Peter W. Shor, *Polynomial-time algorithms for prime factorization and discrete logarithms on a quantum computer*, SIAM Rev. **41** (1999), no. 2, 303–332 (electronic), arXiv:quant-ph/9508027v2 MR1684546 DOI:10.1137/S0036144598347011.

Chapter 15

Women in Numbers 3 (14w5009)

April 20 - 25, 2014

Organizer(s): Ling Long (Lousiana State University), Rachel Pries (Colorado State University), Kate Stange (University of Colorado)

Women in Numbers 3

Ling Long (Lousiana State University),
Rachel Pries (Colorado State University),
Kate Stange (University of Colorado)

April 21-25, 2014

1 Conference at BIRS

1.1 Rationale and Goals

There has been a recent surge of activity in number theory, with major results in the areas of algebraic, arithmetic and analytic number theory. This progress has impacted female number theorists in contradictory ways. Although the number of female number theorists has grown over the past fifteen years, women remain virtually invisible at high profile conferences and largely excluded from elite international workshops in number theory (data supporting this fact can be provided upon request). Moreover, there are not many tenured female number theorists at top research universities. This void — at conferences and at key institutions — has profound negative consequences on the recruitment and training of future female mathematicians. This workshop was meant to address these issues. The goals of the workshop were:

1. To train female graduate students and postdocs in number theory and related fields;
2. To generate new research of the highest caliber by female number theorists;
3. To increase the participation of women in research activities in number theory;
4. To build a research network of potential collaborators in number theory.

This workshop was a unique effort to combine strong broad impact with a top level technical research program. In order to help raise the profile of active female researchers in number theory and increase their participation in research activities in the field, this event brought together female senior and junior researchers in the field for collaboration. Emphasis was placed on on-site collaboration on open research problems as well as student training. Collaborative group projects introducing students to areas of active research were a key component of this workshop.

We would like to thank the following organizations for their support of this workshop: BIRS, Clay Institute, Microsoft Research, PIMS, and Number Theory Foundation.

1.2 Outcomes

Participant testimonials, comments from colleagues, and other feedback suggest that significant progress was made towards these goals. In particular, the conference gave greater exposure to the research programs of female researchers in number theory. Through collaborative projects, students participated in new research in the field, and faculty at small colleges were exposed to research topics of current interest. Many new networking and mentorship connections were formed and plans were made for efforts to support the women in number theory community over the next few years.

Most of the group projects led to new research results. The conference organizers are currently submitting a proposal for publication of a conference proceedings volume, containing original research papers from each of the 9 groups as well as some additional survey papers. The organizers expect to publish this volume in 2015 or 2016.

1.3 Participants and Format

The participants were 42 female number theorists – approximately 15 senior and mid-level faculty, 15 junior faculty and postdocs, and 12 graduate students. About half of the participants, mostly faculty, were invited by the conference organizers. The remaining slots were filled through a formal application procedure.

Based on the participants' research interests and expertise, the organizers divided the participants up into 9 research groups of 4-6 members each; usually 2 senior members (group leaders) and 2-4 junior members. Research topics ranged from algebraic, analytic and arithmetic number theory to cryptography. Group leaders chose a project topic for collaborative research during and following the conference. They provided materials and references for background reading ahead of time. The group leaders also gave short talks during first three days of the meeting to introduce all participants to the projects. During the last day of the workshop, junior participants presented the progress made on the group projects.

All the groups made significant research progress during the week. Each group submitted a short written progress report on their project. These reports, along with the project title and the names of the group members, are included below. Collaboration on the research projects is on-going via electronic communication.

1.4 Schedule

Monday

7:00–8:30	Breakfast
8:40–9:00	Introduction and Welcome by BIRS Station Manager, TCPL
9:00-9:30	Projects 3 and 2/4
9:30-10:00	30 second intros
10:00-10:30	Coffee Break, TCPL
10:30-12:00	Group Work
12:00-1:30	Lunch
1:00-2:00	Optional: Guided Tour of The Banff Centre; meet in the 2nd floor lounge, Corbett Hall
1:30-2:00	Optional: Financial info
2:00-2:15	Group Photo; meet in foyer of TCPL (photograph will be taken outdoors).
2:15-2:45	Projects 7 and 10
2:45-3:15	Coffee Break, TCPL
3:15-5:30	Group work
5:30–7:30	Dinner

Tuesday

7:00–9:00	Breakfast
9:00-9:40	Talk - Wei Ho: Asymptotics for ranks of elliptic curves
9:45-10:00	Project 1
10-10:30	Coffee Break, TCPL
10:30-12:00	Group Work
12:00-1:30	Lunch
1:30-2:10	Talk - Ekin Ozman: Twisting Modular Curves
2:15-2:45	Projects 5 and 6
2:45-3:15	Coffee Break, TCPL
3:15-5:30	Group work
5:30–7:30	Dinner

Wednesday

7:00–8:30	Breakfast
8:45-9:25	Talk - Rachel Newton: The transcendental Brauer group of a product of CM elliptic curves
9:30-10:00	Projects 8 and 9
10-10:30	Coffee Break, TCPL
10:30-12:00	Group Work
12:00-1:30	Lunch
1:30-5:30	Free Afternoon
5:30–7:30	Dinner
8:00-9:00	Wine session

Thursday

7:00–9:00	Breakfast
9:00 - 9:40	Talk - Fang-Ting Tu: Automorphic Forms on Shimura Curves of Genus Zero
9:40 - 10:00	Financial info
10-10:30	Coffee Break, TCPL
10:30-12:00	Group Work
12:00-1:30	Lunch
1:30 - 2:00	Talk - Anna Haensch: My summer at NPR
2:15 - 2:45	Group work
2:45-3:15	Coffee Break, TCPL
3:15-5:30	Group work
5:30–7:30	Dinner

Friday

7:00–9:00	Breakfast
9:00 - 10:00	Wrap-up session (3 groups)
10-10:30	Coffee Break, TCPL
10:30-12:00	Group Work
12:00-1:30	Lunch

2 Project Reports

2.1 Automorphic forms and q-expansions

Ana Caraiani, Project Leader (Princeton University)
Ellen Eischen, Project Leader (The University of North Carolina at Chapel Hill)
Jessica Fintzen (Harvard University)
Bonita Graham (Wesleyan University)
Elena Mantovan (California Institute of Technology)
Ila Varma (Princeton University)

Our group studied q-*expansions*, an algebraic analogue of Fourier expansions, of certain functions called *automorphic forms*. Roughly speaking, we aimed to prove that congruences between values of certain automorphic forms can be completely described in terms of properties of their q-expansions.

More precisely, our group focused on a problem concerning a p-adic q-expansion principle. In analogue with the q-expansion principle for modular forms (which describes properties of a modular form, in terms of its q-expansion coefficients), there is a q-expansion principle for Siegel modular forms, as well as a q-expansion principle for automorphic forms on unitary groups. There is also a p-adic q-expansion principle (over the Igusa tower, which parametrizes ordinary elliptic curves, or more generally, ordinary abelian varieties with additional structure). Roughly, this says that a p-adic modular form over the ordinary locus vanishes if its q-expansion coefficients vanish. Our group's goal was to give an analogue of the p-adic q-expansion principle for automorphic forms on unitary groups of signature (n, m).

The p-adic q-expansion principle for modular forms and for Hilbert modular forms has been used to construct p-adic families of modular forms (indexed by weight), which in turn can be used to p-adically interpolate special values of L-functions. (This is an approach taken by N. Katz in the 1970s, for instance [4].) For Siegel modular forms and unitary groups of signature (n, n), a p-adic q-expansion principle (in [3]) has similarly been used to construct p-adic families of automorphic forms (for instance, in [2]).

For unitary groups of signature (n, m), with $n \neq m$, an analogue of the q-expansion principle (using *Serre-Tate deformation coordinates*) has been conjectured to exist, but it is not yet in the literature. The ultimate goal of this project was to state and prove an analogue of the q-expansion principle for unitary groups of signature (n, m).

For unitary groups of signature (n, m), we stated and proved an analogue of the p-adic q-expansion principle, using Serre-Tate coordinates. This builds on work of H. Hida (see, e.g., [3]). We outlined a paper discussing these results, and we are now preparing a paper to submit for publication. For unitary groups of signature (n, n), we also outlined a proof of a p-adic q-expansion principle at cusps (which gives a different expansion from the one using Serre-Tate coordinates). Furthermore, we discussed how we might extend these results to give a p-adic analogue of the algebraic Fourier-Jacobi expansion principle for unitary groups (due to K.-W. Lan [5]); for unitary groups of signature (n, m) with $n \neq m$, this is still in progress, although we expect to continue to make progress on this case in the next few months.

The group generated many related questions for future study. Some of these problems concern the relationships between different approaches to p-adic automorphic forms, as well as how to express our results in the language of perfectoid spaces (a quickly developing area, made popular by Peter Scholze's recent advances in the field). Another problem on the list concerns the action of certain differential operators on p-adic automorphic forms, and in particular how they act on Serre-Tate expansions. These operators are a generalization of certain p-adic differential operators in [1], which generalizes [4]. They also are a generalization to the p-adic case of the C^∞ "Maass-Shimura" differential operators discussed extensively in works of G. Shimura (e.g. [6]).

2.2 Generalized Legendre Families

Aly Deines (University of Washington),
Jenny Fuselier (High Point University),
Ling Long, Project Leader (Louisiana State University and Iowa State University),
Holly Swisher (Oregon State University),
Fang-Ting Tu (National Chiao Tung University, Taiwan)

For the well-understood classical Legendre family of elliptic curves

$$E_\lambda : y^2 = x(1-x)(1-\lambda x),$$

several topics, including the Picard-Fuchs equations, the theory of modular forms and Galois representations, are nicely interlaced. In this project, we are interested in studying the generalized Legendre family of curves

$$C_\lambda^{(N;i,j,k)} : y^N = x^i(1-x)^j(1-\lambda x)^k,$$

where $1 \leq i, j, k \leq N$. The Picard-Fuchs equations for $C_\lambda^{(N;i,j,k)}$ have special solutions that are known as hypergeometric functions (HGF). Due to Schwarz, one can construct so-called Schwarz triangles, which define groups, out of HGFs. A special class of these, known as arithmetic triangle groups, include the classic modular curves which parameterize isomorphism classes of elliptic curves, and Shimura curves, which parameterize 2-dimensional abelian varities admiting quaternionic multiplication. In this project, we are investigating the periods of $C_\lambda^{(N;i,j,k)}$, the Jacobian of $C_\lambda^{(N;i,j,k)}$, automorphic forms (if there are any) for the monodromy groups of HGFs, determining CM values, and values of associated periods.

During WIN3, we began by studying the case when $N = 3$. We obtained a nearly complete analysis of this case, and began to study the cases $N = 4$ and $N = 6$ as well. Since WIN3, we have furthered our understanding of the cases $N = 3, 4, 6$, and have also worked on the $N = 5$ case. We analyze these curves (often of higher genus) based on a number of factors, and then group them into classes based on their attributes. The monodromy groups of suitable periods are triangle groups, which determine a tiling of either the Euclidean plane, the Riemann sphere, or the hyperbolic plane. We have observed different patterns in these cases.

2.3 Shadow Lines in the Arithmetic of Elliptic Curves

Jennifer Balakrishnan, Project Leader (University of Oxford),
Mirela Çiperiani, Project Leader (University of Texas, Austin),
Jaclyn Lang (University of California, Los Angeles),
Bahare Mirza (McGill University),
Rachel Newton (University of Leiden)

We carried out the first computations of *shadow lines*: 1-dimensional vector spaces attached to triples (E, K, p), where E is an elliptic curve defined over $\mathbb{Q}$, K is an imaginary quadratic extension of $\mathbb{Q}$, and p is a prime. Our computations were motivated by questions posed by Mazur and Rubin at the 2002 ICM [10].

Fix an elliptic curve $E/\mathbb{Q}$ of analytic rank 2 and an odd prime p of good ordinary reduction. Assume that the p-primary Tate-Shafarevich group of $E/\mathbb{Q}$ is finite. Let K be a quadratic imaginary field such that the analytic rank of E/K is 3 and the Heegner hypothesis holds for E (that is, all primes dividing the conductor of $E/\mathbb{Q}$ split in K). Assume for simplicity that the p-torsion $E(K)[p]$ is trivial. Fix a choice c of complex conjugation. We are interested in computing a certain subspace of

$$V := E(K) \otimes \mathbb{Q}_p$$

defined by the anticyclotomic universal norms. To define this space, let K_∞ be the anticyclotomic $\mathbb{Z}_p$-extension of K, and let K_n denote the subfield of K_∞ whose Galois group over K is isomorphic to $\mathbb{Z}/p^n\mathbb{Z}$. The module of *universal norms* is defined by

$$\mathcal{U} = \bigcap_{n \geq 0} N_{K_n/K}(E(K_n) \otimes \mathbb{Z}_p),$$

where $N_{K_n/K}$ is the norm map induced by $E(K_n) \to E(K)$ by $P \mapsto \sum_{\sigma \in \mathrm{Gal}(K_n/K)} P^\sigma$.

Consider

$$L_K := \mathcal{U} \otimes \mathbb{Q}_p.$$

Work of Bertolini [8], Cornut [9], and Vatsal [14] implies that L_K is a 1-dimensional $\mathbb{Q}_p$-vector space known as the *shadow line* [11]. The assumption on the finiteness of the p-primary Tate-Shafarevich group of $E/\mathbb{Q}$ implies that L_K is a line in the vector space V.

Our main motivating question is the following question of Mazur and Rubin: As K varies, we presumably get different shadow lines – what are these lines, and how are they distributed?

In order to study this question, we add the assumption that p splits in $K/\mathbb{Q}$ as $(p) = \pi\pi^c$ and figure out how to compute the *anticyclotomic p-adic height pairing* [12, §2.9] on $E(K)$. It is known that $\mathcal{U}$ is contained in the kernel of this pairing [13]. In fact, in our situation, the properties of this pairing together with the fact that the -1-eigenspace of $E(K) \otimes \mathbb{Q}_p$ with respect to the action of c is 1-dimensional implies that $\mathcal{U}$ is equal to the kernel. Thus computing the pairing allows us to determine the shadow line L_K.

Recently, the first two authors together with Stein worked out techniques to compute anticyclotomic Λ-adic regulators of elliptic curves [7], which involves working with universal norms and their cyclotomic p-adic heights. This work provides some crucial input in the computation of the anticyclotomic p-adic height pairing.

Let $\Gamma(K)$ be the Galois group of the maximal $\mathbb{Z}_p$-power extension of K and $I(K) = \Gamma(K) \otimes_{\mathbb{Z}_p} \mathbb{Q}_p$. Mazur, Stein, and Tate gave an explicit description [12, §2.6] of the universal p-adic height pairing

$$(\,,\,) : E(K) \times E(K) \to I(K).$$

One obtains various $\mathbb{Q}_p$-valued height pairings on E by composing this universal pairing with homomorphisms $I(K) \to \mathbb{Q}_p$. Such (non-zero) homomorphisms are in bijection with $\mathbb{Z}_p$-extensions of K. In particular, the anticyclotomic $\mathbb{Z}_p$-extension of K corresponds to a function $\rho : I(K) \to \mathbb{Q}_p$ such that $\rho \circ c = -\rho$. We denote the resulting anticyclotomic p-adic height pairing by $(\,,\,)_\rho$.

At the workshop we came up with an explicit description of ρ using the p-adic logarithm. With this explicit description of ρ, we implemented the following formula of [12] for the anticyclotomic p-adic height of a point $P \in E(K)$:

$$h_\rho(P) = \rho_\pi(\sigma_\pi(P)) - \rho_\pi(\sigma_\pi(P)) + \sum_{w \nmid p} \rho_w(d_w(P)),$$

where ρ_v denotes the composition of ρ with the natural inclusion $K_v^\times \hookrightarrow \mathbb{A}^\times$, σ_π is the π-adic sigma function, and $d_w(P)$ is a local denominator for P at w. An algorithm for computing σ_π was given in [12], and we were able to use an argument in [7] to determine, for a given elliptic curve E, a finite set of places that includes all those w for which $\rho_w(d_w(P))$ is nonzero. Thus we are now able to compute anticyclotomic p-adic heights.

We computed the following example of a shadow line at the workshop. Let $E : y^2 + y = x^3 + x^2 - 2x$. Note that $E/\mathbb{Q}$ has analytic rank 2 and $P_1 = (-1, 1), P_2 = (0, 0) \in E(\mathbb{Q})$ are linearly independent generators of $E(\mathbb{Q})/E(\mathbb{Q})_{tors}$.

Fix $p = 5$ and $K = \mathbb{Q}(\sqrt{-11})$. Note that the class number of K is 1 and E/K had analytic rank 3. In addition, $P_1 = (-1, 1), P_2 = (0, 0) \in E(\mathbb{Q})$ and $Q = \left(\frac{1}{4}, \frac{1}{8}\sqrt{-11} - \frac{1}{2}\right) \in E(K)$ are linearly independent generators of $E(K)/E(K)_{tors}$. Computing the shadow line in this example amounts to finding $a, b \in \mathbb{Q}_5$ for which

$$a(P_1, Q)_\rho + b(P_2, Q)_\rho = 0.$$

We are able to compute $(P_i, Q)_\rho$ by computing $h_\rho(P_i + Q)$. Using this, we found that

$$[a : b] = [2 + 2 \cdot 5 + 4 \cdot 5^3 + 4 \cdot 5^4 + 2 \cdot 5^5 + O(5^6) : 3 + 3 \cdot 5 + 3 \cdot 5^2 + 2 \cdot 5^4 + 4 \cdot 5^5 + O(5^6)].$$

Hence, the shadow line for the triple $(E, K, 5)$ is $(aP_1 + bP_2)\mathbb{Q}_5 \subset E(\mathbb{Q}) \otimes \mathbb{Q}_5$.

2.4 Curves in positive characteristic with many automorphisms

Irene Bouw, Project Leader (Ulm University),
Wei Ho (Columbia University),
Beth Malmskog (Colorado College),
Renate Scheidler (University of Calgary),
Padmavati Srivivasan (Massachuchets Institute of Technology),
Christelle Vincent (Stanford University).

Let q be a power of a prime p. We consider a family of smooth projective curves C_R defined by

$$y^p - y = xR(x),$$

where $R(x) \in \mathbb{F}_q[x]$ is an additive polynomial, i.e., for indeterminates x and y we have $R(x + y) = R(x) + R(y)$. These curves have many interesting properties; for example, they have many rational points and many automorphisms. These properties seem to be closely related. A key to the description of both the $\mathbb{F}_q$-rational points and the automorphism group of C_R is the $\mathbb{F}_q$-vector space

$$W(\mathbb{F}_{q^s}) := \{x \in \mathbb{F}_{q^s} \mid \mathrm{Tr}_{\mathbb{F}_{q^s}/\mathbb{F}_p}(xR(y) + yR(x)) = 0 \quad \forall y \in \mathbb{F}_{q^s}\}.$$

It can be shown that there exists a polynomial $E_R(x) \in \mathbb{F}_q[x]$ such that W is the zero set of E. After replacing $\mathbb{F}_q$ by a finite extension, we may assume that $\mathbb{F}_q$ is the splitting field of E_R.

Van der Geer and Van der Vlugt [15] study the curves C_R in characteristic $p = 2$. In particular, they determine the group of automorphisms that fix the unique point of C_R at infinity. Its Sylow p-subgroup P is an extraspecial group, which is a central extension of W by the Artin–Schreier automorphism $\rho(x, y) = (x, y + 1)$. Using suitable elementary abelian subgroups A of P, Van der Geer and Van der Vlugt show that the Jacobian J_R of C_R is isogenous over $\mathbb{F}_q$ to a product of supersingular elliptic curves E_A, where $E_A = C_R/A$ is the quotient curve. The description of the group P of automorphisms in terms of the vector space W allows them to make this construction completely explicit and determine the zeta function of C_R over $\mathbb{F}_q$.

The goal of the project is to extend the results of Van der Geer and Van der Vlugt to odd characteristic. In particular, we aim to determine the zeta function of C_R over the splitting field $\mathbb{F}_q$ of E_R. Van der Geer and Van der Vlugt sketch the generalization of some of their statements to odd characteristic in Section 13 of [15]. As a first step of the project, we worked out the details of these statements, supplying missing proofs and correcting mistakes.

The description of the group P of automorphisms of C_R is a rather straightforward generalization of that in characteristic 2. This group is also described in [16] without the assumption that R is additive. An important role is played by the maximal elementary abelian subgroups A of P which intersect the center $Z(P) = \langle \rho \rangle$ trivially. A careful analysis of the combinatorics of these subgroups yields a decomposition

$$J_R \sim_{\mathbb{F}_q} \prod J(X_A)$$

of the Jacobian J_R of C_R. Here the product is taken over a suitable collection of subgroups A and $X_A = C_R/A$ is the quotient curve. The key step to compute the zeta function of C_R over $\mathbb{F}_q$ is to determine an $\mathbb{F}_q$-model of the curves X_A. Van der Geer–Van der Vlugt already state an equation of these curves over the algebraic closure.

2.5 π_1-obstructions to Rational Points on Fermat Curves

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Vesna Stojanoska, Project Leader (MIT),
Kirsten Wickelgren, Project Leader (Georgia Tech)

Grothendieck's section conjecture gives a natural map from the rational points $X(k)$ of a k-scheme X to the Galois cohomology pointed set $H^1(G_k, \pi_1(X_{k^s}))$, where G_k is the absolute Galois group $\mathrm{Gal}(k^s/k)$. The Abel-Jacobi map from a pointed curve X to its Jacobian gives rise to a commutative diagram

$$\begin{tikzcd} X(k) \arrow[r] \arrow[d] & \mathrm{Jac}(k) \arrow[d] \\ H^1(G_k, \pi_1(X_{k^s})) \arrow[r] & H^1(G_k, \pi_1(\mathrm{Jac}(X)_{k^s})). \end{tikzcd}$$

It is a consequence of Poincare duality that $\pi_1(\mathrm{Jac}(X)_{k^s})$ is naturally the abelianization of $\pi_1 := \pi_1(X_{k^s})$ at least away from the characteristic of k. Jordan Ellenberg suggested using the lower central series filtration of π_1 to make an obstruction for a rational point p in $\mathrm{Jac}X(k)$ to be in $X(k)$ by obstructing p's image in $H^1(G_k, \pi_1(\mathrm{Jac}(X)_{k^s}))$ from being in the image of the bottom horizontal map. The first of these obstructions goes as follows.

Let $[\pi_1]_2$ denote the closed subgroup of π_1 generated by all the commutators, and let $[\pi_1]_3$ denote the closure of the subgroup generated by elements in $[[\pi_1]_2, \pi_1]$. The short exact sequence

$$1 \longrightarrow [\pi_1]_2/[\pi_1]_3 \longrightarrow \pi_1/[\pi_1]_3 \longrightarrow \pi_1/[\pi_1]_2 = \pi_1(\mathrm{Jac}(X)_{k^s}) \longrightarrow 1$$

gives rise to a map $H^1(G_k, \pi_1(\mathrm{Jac}(X)_{k^s})) \to H^2(G_k, [\pi_1]_2/[\pi_1]_3)$. Any p which is in the image of $X(k)$ must vanish under this map, so having a non-zero image is an obstruction.

The goal of the project is to use Anderson ([17]) and Ihara's ([18]) results about the fundamental group and Jacobians of Fermat curves to compute or partially compute this obstruction when X is a Fermat curve. Let N be odd and let $\overline{U} : x^N + y^N = z^N$, $U : X^N + Y^N = 1$; then $Z = \overline{U} \backslash U = \{[-\zeta_N^i : 1 : 0]\}$. Let $Y \subset U$ be the closed subset $Y = \{(\zeta_N^i, 0), (0, \zeta_N^i)\}$. The genus of the Fermat curve $\overline{U}$ is $\binom{N-1}{2}$ and we have that the following homology groups with coefficients in $\mathbb{Z}/N\mathbb{Z}$ have the listed ranks.

$$\begin{array}{lccccc} & H_1(\overline{U}) & \longleftarrow & H_1(U) & \hookrightarrow & H_1(U, Y) \\ \\ \text{ranks} & 2g = (N-1)(N-2) & & 2g + (N-1) = (N-1)^2 & & N^2. \end{array}$$

Anderson ([17]) largely computes $H_1(U,Y)$ (up to a factor of dlog that we determined) as a $G_{\mathbb{Q}}$-module in the following way. As a $\Lambda_1 = \mathbb{Z}/N\mathbb{Z}[\mu_N \times \mu_N]$-module, $H_1(U,Y)$ is free of rank 1 and is generated by an element β. The action of $\sigma \in G_{\mathbb{Q}}$ on $H_1(U,Y)$ is determined by the action of σ on β

$$\sigma(\beta) = B_{\sigma,N}\beta,$$

where $B_{\sigma,N} \in \Lambda_1^\times$. We are working to explicitly compute $B_{\sigma,N}$ in terms of the classical Kummer map, which we will then use in computing the obstructions described above.

To compute $H_1(\overline{U})$ and $H_1(U)$ as $G_{\mathbb{Q}}$-modules (given $H_1(U,Y)$), we use the exact sequence to find $\ker(\delta)$

$$0 = H_1(Y) \longrightarrow H_1(U) \longrightarrow H_1(U,Y) \xrightarrow{\delta} H_0(Y) \longrightarrow H_0(U) \longrightarrow 0.$$

Further, we find that $H_1(\overline{U}) \simeq \frac{H_1(U)}{\mathrm{Stab}(\epsilon_0\epsilon_1)}$ where $\epsilon_0\epsilon_1$ is a diagonal element in the group ring Λ_1.

A further result of Anderson [loc.cit] is helpful in computing the Galois cohomology groups we need. To explain, define L_f to be the splitting field of $f(x) = 1-(1-x^N)^N$. Let S be the generalized Jacobian of (U,Y), and fix b to be the base point of S given by the difference of the points $(0,1)$ and $(1,0)$ of U. Anderson's theorem is that the field of definition of the coordinates of the set of points $\{P \in S | nP = b\}$ contains L_f; he also shows that these fields are equal if N is prime. When N is prime, $H^1(U,Y)$ (and therefore $H^1(\overline{U})$) is a trivial G_{L_f}-module. For this reason, we need to compute $H^1(\overline{U})$ as a module over the finite Galois group of L_f over $\mathbb{Q}$.

2.6 Computing the Transcendental Brauer Set for a 3-parameter Family of Enriques Surfaces

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Given a smooth, projective, geometrically integral variety X over $\mathbb{Q}$, one may ask whether X has a $\mathbb{Q}$-rational point, i.e. whether $X(\mathbb{Q})$ is nonempty. Since $\mathbb{Q}$ embeds into each of its completions, it is always the case that $X(\mathbb{Q})$ is a subset of the set of adelic points $X(\mathbb{A}_{\mathbb{Q}})$. However, it is possible for $X(\mathbb{Q})$ to be empty even when $X(\mathbb{A}_{\mathbb{Q}})$ is nonempty, and such varieties X are said to fail the Hasse principle.

To explain counterexamples to the Hasse principle, Manin defined an intermediate Brauer set

$$X(\mathbb{Q}) \subset X(\mathbb{A}_{\mathbb{Q}})^{\mathrm{Br}} \subset X(\mathbb{A}_{\mathbb{Q}})$$

and a variety X is said to have the Brauer-Manin obstruction to the Hasse principle when $X(\mathbb{A}_{\mathbb{Q}}) \neq \emptyset$ but $X(\mathbb{A}_{\mathbb{Q}})^{\mathrm{Br}} = \emptyset$. Skorobogatov later refined this by defining the étale Brauer set $X(\mathbb{A}_{\mathbb{Q}})^{\text{et, Br}}$, and provided an example of a surface X such that $X(\mathbb{A}_{\mathbb{Q}})^{\text{et,Br}} = \emptyset$, but $X(\mathbb{A}_{\mathbb{Q}})^{\mathrm{Br}} \neq \emptyset$, thereby showing that the étale-Brauer obstruction is stronger than the Brauer-Manin obstruction. In practice, however, it is often easier to compute the larger algebraic Brauer-Manin set $X(\mathbb{A}_{\mathbb{Q}})^{\mathrm{Br}_1}$, and this can still cause an obstruction to the existence of rational points.

In [19], Várilly-Alvarado and Viray constructed a 3-parameter family of Enriques surfaces $X_{a,b,c}/\mathbb{Q}$ such that

$$\emptyset = X_{a,b,c}(\mathbb{A}_{\mathbb{Q}})^{\text{et,Br}} \subset X_{a,b,c}(\mathbb{A}_{\mathbb{Q}})^{\mathrm{Br}} \subset X_{a,b,c}(\mathbb{A}_{\mathbb{Q}})^{\mathrm{Br}_1} \neq \emptyset$$

thereby showing that the algebraic Brauer-Manin obstruction is insufficient to explain the lack of rational points on Enriques surfaces. The goal of the present project is to determine whether $X_{a,b,c}(\mathbb{A}_{\mathbb{Q}})^{\mathrm{Br}} = \emptyset$.

In general, it is difficult to determine transcendental Brauer classes, i.e. those surviving in $\mathrm{Br}(X)/\mathrm{Br}_1(X)$. However, in [21] Creutz and Viray were able to obtain a presentation of the 2-torsion Brauer classes on double covers of ruled surfaces. In particular, since every Enriques surface (over a separably closed field) is birational to a double cover of a ruled surface whose branch locus has at worst simple singularities, we may employ their method.

We consider the K3 surfaces $Y := Y_{a,b,c}$ defined as the complete intersection of the following three quadrics in $\mathbb{P}^5 = \text{Proj}\ \mathbb{Q}[s,t,u,x,y,z]$:

$$\begin{aligned} xy + 5z^2 &= s^2 \\ (x+y)(x+2y) &= s^2 - 5t^2 \\ ax^2 + by^2 + cz^2 &= u^2 \end{aligned}$$

and the Enriques surface $X = Y/\sigma$, where σ is the fixed point free involution $[s:t:u:x:y:z] \mapsto [-s : -t : -u : x : y : z]$. We focus initially on the case $(a,b,c) = (12, 111, 13)$.

There exist nine pairs of fibrations $Y \to \mathbb{P}^1$ which descend to X. This yields $2 \cdot 2 \cdot \binom{9}{2}$ ways of presenting Y as a double cover of the ruled surface $\mathbb{P}^1 \times \mathbb{P}^1$ branched over a $(4,4)$-curve, B. We explicitly computed these branch loci and, in many cases, determined that B has four singularities and the normalization of B has genus at most 5.

The methods in [21] give conditions to determine which functions in the function field $\mathbf{k}(B)$ give rise to central simple algebras in $\text{Br}(\mathbf{k}(Y))$ that are in fact in the subgroup $\text{Br}(Y)$. This can be described via an exact sequence that relates the Picard group of Y, these candidate functions in $\mathbf{k}(B)$, and $\text{Br}(Y)[2]$. The computations on the K3 surface should allow us to compute an explicit presentation of $\text{Br}(X)[2]$ over some number field. We hope to then descend this to $\mathbb{Q}$ and compute the obstruction. Once this is complete, we would like to compute the obstruction more generally for tuples (a,b,c) satisfying the hypotheses in [19].

2.7 On the hardness of the Ring-LWE problem

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Cryptography is rightfully the most celebrated application of Number Theory, as information security relies on it to preserve data confidentiality, data integrity, authentication, and non-repudiation. Lattice-based cryptography has allowed for efficient cryptographic schemes [26] and applications in fully homomorphic encryption [24, 25]. Both rely on hard problems in lattices. Recently, the *ring learning with errors problem* (Ring-LWE) was introduced, and reductions to hard lattice problems were proved. We define next the RLWE hardness assumption: Given a ring $R = \mathbb{Z}[x]/(f(x))$, and integer $q > 0$, where

- $f(x) \in \mathbb{Z}[x]$ is a monic, irreducible polynomial of degree n,

the *ring-LWE problem* is to distinguish a set of pairs

$$(a_i, b_i = a_i s + e_i) \in R/qR \times R/qR \ \text{ where}$$

- a_i are uniformly random and independent,
- e_i are independent and 'short',
- $s \in R/qR$ is a random secret

from a set of uniformly random pairs. For practical purposes, security estimates in [22, Figure 4] suggest that n and q should be at least 320 and 4093 respectively, with a Gaussian distribution for the error vector of width 8.

On the one hand, Regev [27] showed that the LWE problem is as hard to solve as several worst-case lattice problems. In addition, Lyubashevsky, Peikert, and Regev [23] proved that the hardness of a discrete version of *ring-LWE* follows from the hardness of the original problem for a wide family of appropriate distributions. They also developed efficient algorithms for cryptographic operations over arbitrary cyclotomic fields hence obtaining efficient cryptosystems relying on the hardness assumption for *ring-LWE*. On the other hand, Eisentraeger, Hallgren and Lauter elaborated an attack of *ring-LWE* under some assumptions on f, which distinguishes random pairs with non-negligible probability.

The goal of our project is two-fold; we aim to look at specific number fields that do not satisfy the hardness assumption, and to construct families of number fields for which cryptographic schemes based on the ideal lattice problem *ring-LWE* are efficient.

During our stay at BIRS, we elaborated a probabilistic argument that we hope will extend the attack on *ring-LWE* by Eisentraeger, Hallgren and Lauter for certain ranges of parameters. We also implemented a concrete attack for a certain number field, where the algorithm returned the secret when the given pair was not random. Currently, we are working on relaxing the assumptions in [23] using number-theoretic tools like Mahler measure, monogenic families of Galois extensions, and others.

2.8 Sieve methods in geometry

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Around 200 BC, Eratosthenes developed an ingenious, yet simple method of detecting prime numbers. This is still one of the most effective methods of finding relatively small primes. Around two millennia later, Legendre reformulated the sieve of Eratosthenes in combinatorial terms, giving rise to the simplest method in what is now called sieve theory. It was Brun, at the beginning of the 20th century, who brought in profound new ideas to the sieve concept, his work marking the birth of sieve theory.

Over the following decades and through the new millennium, sieve methods have been vastly refined and expanded: combinatorial and non-combinatorial sieves alike are frequently utilized towards advances in the theory of numbers, with results as astonishing as the current ones on the twin prime conjecture. At WIN 3, our team focused on a better understanding and applications of non-combinatorial sieve methods in geometric contexts. Our work will be described in detail in an upcoming research article.

2.9 Kneser-Hecke-operators for quaternary codes

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Defining $R := \mathbb{Z}/4\mathbb{Z}$ and $S := \mathbb{Z}/2\mathbb{Z}$, a quaternary codes C of length N is a R^N-submodule, where $N \in \mathbb{N}$. Using the standard inner product, the dual of a code C is defined

$$C^{\perp} = \{x \in R^N : (x, c) = 0 \ \forall c \in C\},$$

and we call C self-dual if and only if $C = C^{\perp}$. Define $\mathcal{F} := \{C = C^{\perp} \leq R^N\}$, the set of all self-dual codes of length N. Two codes $C, D \in \mathcal{F}$ are equivalent, denoted $C \simeq D$ if there exists some permutation $\pi \in S_N$ such that $C = \pi(D)$. Let $\mathcal{V}$ denote the $\mathbb{C}$-vector space spanned by the equivalence classes $[C]$ where $C \in \mathcal{F}$. Then $\mathcal{B} := \{[C] : C \in \mathcal{F}\}$ is a $\mathbb{C}$-basis for $\mathcal{V}$.

For any $C \in \mathcal{F}$, if follows from the Krull-Schmidt Theorem that there exist unique integers a and b such that $C \cong R^a \oplus S^b$, as R-modules. In this way, each code has a unique isomorphism type as an R-module, and we define the set of all codes of a certain isomorphism class by

$$\mathcal{F}_{a,b} := \{C = C^{\perp} \leq R^N : C \cong R^a \oplus S^b\} \subseteq \mathcal{F}.$$

For any $C \in \mathcal{F}_{a,b}$, we have $\mid C \mid \cdot \mid C^{\perp} \mid = \mid R \mid^N$, and consequently for a self-dual code of length N we have $2a + b = N$, meaning that the choice of a completely determines the isomorphism type. We note that equivalent codes are always isomorphic as modules, but two codes of the same module type need not be equivalent as codes.

For codes $C, D \in \mathcal{F}$, we call C and D neighbors if and only if

$$C/C \cap D \cong D/C \cap D \cong S.$$

We define a graph Γ by taking the set of equivalence classes in $\mathcal{B}$ as the set of vertices, and placing an edge between two vertices $[C]$ and $[D]$ if there exist $C' \in [C]$ and $D' \in [D]$ such that $C' \sim D'$. Then Γ is a connected graph, as shown by Meyer in [28].

We define a linear operator T on $\mathcal{V}$ by $T([C]) = \sum_{D \sim C}[D]$. Viewed as a matrix, T is just the adjacency matrix for the graph Γ. By arranging the basis elements in $\mathcal{B}$ according to module isomorphism type, we have

$$T = \begin{bmatrix} T_0 & \cdots & & \\ \vdots & T_1 & & \\ & & \ddots & \vdots \\ & & \cdots & T_{\frac{N}{2}} \end{bmatrix},$$

where T_a denotes the adjacency matrix obtained by restricting the vertex set to $\mathcal{F}_{a,b}$. We immediately observe that for any choice of $\mathcal{F}$, $T_0 = [0]$, since there is only one code in $\mathcal{F}$ of isomorphism type S^N.

The eventual goal of this project is to describe the eigenvalues of the T_a and compute the corresponding eigenspaces to obtain a result analogous to that given by Gabi Nebe for binary codes. To understand these eigenspaces we must understand the shape of neighboring codes and their possible overcodes and subcodes. To that end, we have proved the following result: for $C \in \mathcal{F}_{a,b}$, let E be a maximal submodule in C. If $C \cap 2R^N \leq E$ then there exist two neighbors G and F of C, with $G \cong R^a \oplus S^b$ and $F \cong R^{a-1} \oplus S^{b+2}$.

It is known that the maximal eigenvalue of T_a counts the number of neighbors of isomorphism type $R^a \oplus S^b$. It is clear that when C and D are neighbors then $C \cap 2R^N \leq C \cap D$, therefore in view of the result in the preceding paragraph, it is clear that counting neighbors of the same type is equivalent to counting the number of $a-1$ dimensional subspaces of $\mathbb{F}_2^a$, which is precisely $2^a - 1$. Therefore, we have also shown the following: The maximal eigenvalue of T_a is $2^a - 1$.

Finally, knowing the structure of subcodes and overcodes for neighboring codes, we are able to say the following: If $[C] \cong R^a \oplus S^b \cong [D]$ and C and D are in the same connected component, then $C \mod 2 = D \mod 2$. This result is particularly advantageous, since binary codes are very well-studied, and lifting a quaternary code C into this binary setting will allow us to have many more tools at our disposal.

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References

[1] Ellen E. Eischen. p-adic differential operators on automorphic forms on unitary groups. Ann. Inst. Fourier (Grenoble) 62 (2012), no. 1, 177–243.

[2] Ellen E. Eischen. A p-adic Eisenstein measure for unitary groups, Accepted for publication in the Journal für die reine und angewandte Mathematik (Crelles Journal). 32 pages. DOI 10.1515/ crelle-2013-0008.

[3] Haruzo Hida. p-adic automorphic forms on reductive groups, Astérisque (2005), no. 298, 147254, Automorphic forms. I.

[4] Nicholas M. Katz. p-adic L-functions for CM fields, Invent. Math. 49 (1978), no. 3, 199-297.

[5] Kai-Wen Lan. Arithmetic compactifications of PEL-type shimura varieties, London Mathematical Society Monographs, vol. 36, Princeton University Press, 2013.

[6] Goro Shimura. Arithmeticity in the theory of automorphic forms, Mathematical Surveys and Monographs, vol. 82, American Mathematical Society, Providence, RI, 2000.

[7] J. S. Balakrishnan, M. Çiperiani, and W. A. Stein, p-adic heights of Heegner points and anticyclotomic Λ-adic regulators, *Math. Comp.* to appear.

[8] M. Bertolini, Selmer groups and Heegner points in anticyclotomic $\mathbb{Z}_p$-extensions, *Compos. Math.* **99** (1995), 153-182.

[9] C. Cornut, Mazur's conjecture on higher Heegner points, *Invent. Math.* **148(3)** (2002), 495-523.

[10] B. Mazur and K. Rubin, Elliptic curves and class field theory, *Proceedings of the International Congress of Mathematicians* **II**, 185-195, Higher Ed. Press, Beijing, 2002.

[11] B. Mazur and K. Rubin, Studying the growth of Mordell-Weil, *Doc. Math.* (Extra Vol.) (2003), 585-607.

[12] B. Mazur, W. A. Stein, and J. Tate, Computation of p-Adic Heights and Log Convergence, *Doc. Math.* (Extra Vol.) (2006), 577-614.

[13] B. Mazur and J. Tate, Canonical height pairings via biextensions, Arithmetic and Geometry, Progr. Math. 35, Birkhauser, Boston (1983) 195-237.

[14] V. Vatsal, Special values of anticyclotomic L-functions, *Duke Math. J.* **116(2)** (2003), 219-261.

[15] G. van der Geer and M. van der Vlugt, Reed–Muller codes and supersingular curves, *Compos. Math.* **84** (1992), 333–367.

[16] C. Lehr and M. Matignon, Automorphism groups for p-cyclic covers of the affine line, *Compos. Math.* **141** (2005), 1213–1237.

[17] Greg W. Anderson. Torsion points on Jacobians of quotients of Fermat curves and p-adic soliton theory. *Invent. Math.*, 118(3):475–492, 1994.

[18] Yasutaka Ihara. Profinite braid groups, Galois representations and complex multiplications. *Ann. of Math. (2)*, 123(1):43–106, 1986.

[19] A. Varilly-Alvarado and B. Viray, *Failure of the Hasse Principle for Enriques Surfaces*, Adv. Math. **226** (2011), no. 6, 48844901.

[20] W. Barth, K. Hulek, C. Peters, A. Van de Ven, *Compact Complex Surfaces*, 2nd ed., Ergebnisse der Mathematik und ihrer Grenzgebiete. 3. Folge. A Series of Modern Surveys in Mathematics **4**, Springer Verlag, Berlin 2004.

[21] B. Creutz and B. Viray, *On Brauer Groups of Double Covers of Ruled Surfaces*, Preprint, arXiv: 1306.3251.

[22] Richard Lindner, Chris Peikert. Better Key Sizes (and Attacks) for LWE-Based Encryption, CT-RSA 2011.

[23] Lyubashevsky, Peikert, Regev, A Toolkit for Ring-LWE Cryptography. *Advances in Cryptology*, 2013

[24] Gentry, A fully homomorphic encryption scheme. *Ph.D. thesis, Stanford University*, 2009

[25] Gentry, Fully homomorphic encryption using ideal lattices. *In STOC, pages 169178.*, 2009

[26] Micciancio, Generalized compact knapsacks, cyclic lattices, and efficient one-way functions. *Computational Complexity, 16(4):365411, 2007. Preliminary version in FOCS 2002.*

[27] Regev, On lattices, learning with errors, random linear codes, and cryptography. *J. ACM, 56(6):140, 2009. Preliminary version in STOC 2005.*

[28] A. Meyer, Automorphism groups of self-dual codes, PhD thesis, RWTH Aachen University, 2009.

Chapter 16

Recent Advances and Trends in Time Series Analysis: Nonlinear Time Series, High Dimensional Inference and Beyond (14w5157)

April 27 - May 2, 2014

Organizer(s): Yulia Gel (University of Waterloo), Rafał Kulik (University of Ottawa), Hao Yu (University of Western Ontario)

16.1 Overview of the Field and Recent Developments

With the advent of massive and complex data sets and especially phenomenon of high frequency and ultra high frequency observations, the classical paradigms of linear time series and the related Box-Jenkins methodology is not applicable, which leads to a booming interest in developing novel methodology in time series analysis. In particular, it is now well recognized that many financial, biological and environmental observations as well data from complex dynamic computer networks exhibit many similar patterns such as *heavy tails*, *clustering of extremes*, *weak and long range dependence*, and *non-stationary behavior*, which are not well described by the linear models. Those empirical observations led to development of non-linear models such as GARCH (Robert Engle was awarded the Noble Prize in Economics in 2003 for its invention) or stochastic volatility (both in a univariate and multivariate setting), models with local stationarity and/or time varying coefficients, or Poisson shot-noise processes, the latter especially in a context of network traffic modeling. However, while probabilistic structure for some of the models is reasonably well-understood, statistical inference and, especially, its extension to multivariate non-linear time series with the above mentioned characteristics are yet not well developed and constitute a challenging issue both from theoretical and applied point of view.

Moreover, many modern time series methods require transcending traditional boundaries between time series analysis, nonparametric and spatial statistics, applied probability, and discrete mathematics, which leads to fusion of knowledge and ideas across various branches of statistics and mathematics. Such examples include functional data analysis methodology employed to describe time-space phenomena, the recent advances on high dimensional inference of ultra high frequency financial time series and characterizing dynamics of time series as a random network process.

It is also well recognized that theoretical and methodological advances in time series analysis are possible only if the gaps between paradigms of various branches of statistics and applied sciences are bridged together, forging joint interdisciplinary efforts. The workshop aimed to take advantage from the state-of-the-art research from multiple disciplines and builds on the fusion of complementary expertise of leading researchers in time series, nonparametrics, multivariate analysis, functional data analysis, applied probability and computational statistics.

Two main themes of the workshop were **Nonlinear Time Series** and **High Dimensional Inference** applied in the time series context. The list of topics includes

1. High dimensional, multivariate time series;
2. Short memory processes;
3. Long memory processes;
4. Non-stationary models;
5. Non-linear time series;
6. Heavy tailed time series;
7. Change-point and trend detection problems;

The speakers presented variety of methods to deal with non-linear, high dimensional time series, starting with classical methods, and including very recent techniques such as:

- adaptive estimation (wavelets, spectral analysis);
- Bayesian techniques;
- functional data analysis methods;
- bootstrap and resampling techniques;
- empirical likelihood.

16.2 Presentation Highlights

Monday, April 28: The theme for the morning session was *long memory processes*. The conference was opened by talks of **Peter Robinson** and **Liudas Giraitis**. The first speaker focused on more applied aspects of estimation of long memory parameter for panel data, while the second speaker talked about new results on existence of second-order stationary ARCH(∞) processes, that include FIGARCH or IGARCH families. This was a long-standing problem in the area of nonlinear time series with long memory (see [8]).

The second session of the day featured **Ejaz Ahmed** and **Daniel Pena**, who gave talks on statistical aspects of *high dimensional*, possibly *non-stationary time series*. The first speaker presented a new high-dimensional shrinkage estimation strategy ([1]), while the second speaker proposed a new time domain procedure to define dynamic principal components (DPC) that is applicable to non-stationary and relatively short series (([15])).

In the afternoon sessions we continued with statistical aspects of *non-stationary time series*: **Rainer Dahlhaus** discussed local polynomial fitting of time-varying parameter curves ([5]), **Eunice Menezes** presented an overview of wavelets methods, while **David Stoffer** discussed Bayesian methodology ([18]). **Piotr Kokoszka** discussed functional data approach (see [12]) to financial time series, with particular applications to intraday price.

Tuesday, April 29: As on Monday, we started with *long memory processes*. **Murad Taqqu** considered vector-valued multilinear polynomial-form processes with either short or long memory components and discussed possible limiting distributions. **Vladas Pipiras** continued with multivariate long range dependence discussing possible definitions and new parameters modeling the cross spectrum.

In the next session the speakers focused on *dependent random fields*. **Gail Ivanoff** presented a new martingale technique to deal with limit theorems for short range dependent causal linear process, while **Jens-Peter Kreiss** considered more statistical issues of bootstrap for random fields.

The first afternoon session featured **Francois Roueff**, **Mohsen Pourahmadi** and **Nozer Singpurwalla**. The first speaker showed how to use multivariate point processes (more specifically, Hawkes processes) for modeling limit order book of a financial asset. Pourahmadi discussed thresholded generalized principal component regression in the context of multivariate time series ([16]). The session concluded with a more philosophical discussion on connection of quantum physics, probability foundation and statistical inference by Singpurwalla ([13]).

The last session of the day dealt with *heavy tails and point processes*. **Zhengyan Lin** discussed weak convergence of various general functionals of partial sums of dependent random variables statistics to stochastic integrals driven by either Brownian motion or Levy-stable processes. **Bojan Basrak** continued with functional limit theorems for heavy tailed time series, using a non-standard topology (see [3]). Finally, **Robert Lund** showed how to simulate stationary count time series, with a particular focus on a much less investigated phenomenon of negative correlation ([7]).

<u>Wednesday, April 30:</u> The topic of the first session was *high-dimensional autocovariance matrices*. **Thomas Mikosch** presented limit theorems for the largest eigenvalues in a sample covariance matrix for multivariate time series with heavy tails (see [6]). The next speaker, **Timothy McMurry** focused on light-tailed time series and a classical problem of linear prediction, however in a high-dimensional setting.

The second session featured two talks on *change-point problems*. **Herold Dehling** presented his work on robust change-point tests for stationary time series with both short- and long memory, using two-sample U-processes and U-quantile processes, while **Michael Baron** discussed a Bayesian approach to change-point detection in multivariate time series.

The afternoon was free. The participants enjoyed a beautiful visiting Banff and its neighbourhood or Lake Louise.

<u>Thursday, May 1:</u> The first session featured two talks on *time series extremes*. **Holger Drees** presented his new work on estimation of the distribution of a tail chain that appears as a weak limit of a heavy tailed time series, conditionally on one component being large (see [9]). **Gemal Chen** discussed some results obtained in studying finite sample dependent extremes.

The topic of the next session was *limit theorems for weakly dependent time series*. **Zhou Zhou** discussed central and noncentral limit theorems for weighted V-statistics in case of nonstationary nonlinear processes, while **Martin Wendler** considered bootstrap for weakly dependent Hilbert space-valued random variables.

During the third session the speakers presented recent work on different statistical issues for dependent time series data in *spectral domain*. **Dan Nordman** discussed a frequency domain empirical likelihood method for irregularly spaced data ([2]). The main problem that arises is that the lack of the usual orthogonality properties of the discrete Fourier transform for irregularly spaced data. **Piotr Fryźlewicz** also focused on a spectral domain approach to time series, introducing a hierarchically-ordered oscillatory basis of simple piecewise-constant functions that allow for detection of change-points in high frequency data ([10]). Finally, **Sofia Olhede** discussed Whittle likelihood method for nonstationary multivariate processes ([20]).

The last session of the day featured **Lilia Leticia Ramirez Ramirez** and **Slava Lyubchich** who discussed *statistical issues for multivariate time series*. The first speaker presented a method for trend estimation of multivariate time series, without relaying without relying on specific models for the trend and noise components ([17]). The method was applied to the Mexican macroeconomic data. Lyubchich discussed nonparametric methods for nonlinear trend detection and trend synchronism in multiple time series using local factor approach and hybrid bootstrap ([14]).

<u>Friday, May 2:</u> The final morning featured three speakers. **Edit Gombay** discussed change detection for time series following Generalized Linear Models suing likelihood methods. **Rogemar Mamon** used multivariate Ornstein-Uhlenbeck processes to forecasting The workshop concluded with **Reg Kulperger** discussing new theoretical results for estimation in GARCH-in-mean processes.

16.3 Outcome of the Meeting

The main goal of the meeting was to bring researchers working in a very broad field of time series analysis. The participants had an unique opportunity to learn about variety of topics and methods and techniques, as evidenced above. Variety of problems tackles at the meeting is illustrated by the areas of applications considered at the meeting: finance and economics, climate and weather modeling, flood control, brain signal modeling, clinical trials among others.

Participants

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Baron, Michael (University of Texas at Dallas)
Basrak, Bojan (University of Zagreb (Croatia))
Chen, Gemai (University of Calgary)
Dahlhaus, Rainer (Heidelberg University (Germany))
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Drees, Holger (University of Hamburg)
Fry?lewicz, Piotr (London School of Economics (United Kingdom))
Gel, Yulia (University of Waterloo)
Giraitis, Liudas (Queen Mary University of London (United Kingdom))
Gombay, Edit (University of Alberta)
Ivanoff, Gail (University of Ottawa)
Kokoszka, Piotr (Colorado State University)
Kreiss, Jens-Peter (Technical University of Braunschweig (Germany))
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Olhede, Sofia (University College London (United Kingdom))
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Bibliography

[1] E. Ahmed, Penalty, Shrinkage and Pretest Strategies: Variable Selection and Estimation, Springer Briefs in Statistics, 2014.

[2] S. Bandyopadhyay, S. N. Lahiri, D. J. Nordman, A functional limit theorem for dependent sequences with infinite variance stable limits. Preprint, (2014).

[3] B. Basrak, D. Krizmanic, J. Segers, A functional limit theorem for dependent sequences with infinite variance stable limits. Ann. Probab. **40** (2012), 2008–2033.

[4] J. Beran, Y. Feng, S. Ghosh, R. Kulik, Long-memory Processes: Probabilistic Properties and Statistical Methods, Springer Series in Statistics, (2013).

[5] R. Dahlhaus, Locally stationary processes. Handbook of Statistics, 30 (2012).

[6] R. Davis, T. Mikosch, O. Pfaffel, Convergence of the largest eigenvalues of a sample covariance matrix for heavy-tailed multivariate time series. Preprint, (2013).

[7] R. Davis, S. Holan, R.B. Lund, N. Ravishanker, Handbook on Discrete Valued Count Series, (2014+).

[8] R. Douc, F. Roueff, P. Soulier, On the existence of some ARCH(∞) processes. Stochastic Processes and Their Applications **118** (2008), 755–761.

[9] H. Drees and H. Rootzen, Limit theorems for empirical processes of cluster functionals. Ann. Stat. **38** (2010), 2145–2186.

[10] P. Fryźlewicz, A. L. Schroeder, Adaptive trend estimation in nancial time series via multiscale change-point-induced basis recovery. Statistics and Its Interface, **6** (2013), 449–461.

[11] L. Giraitis, H. L. Koul, D. Surgailis, Large Sample Inference for Long Memory Processes. World Scientific Publishing Company Inc., (2012).

[12] L. Horvath, P. Kokoszka, Inference for Functional Data with Applications, Springer Series in Statistics, (2012).

[13] J. Landon, F. X. Lee and N. D. Singpurwalla, A Problem in Particle Physics and Its Bayesian Analysis. Statistical Science **26** (2011), 352–368.

[14] V. Lyubchich, Y. R. Gel, Detecting Trend Synchronism in Multiple Time Series. Preprint, (2014).

[15] D. Peña, V. J. Yohai, Dynamic Principal Components in the Time Domain. Preprint, (2014).

[16] M. Pourahmadi, High-Dimensional Covariance Estimation, Wiley, 2013.

[17] L.L. Ramirez Ramirez, V. Guerrero Guzman, A. Islas Camargo, Trend estimation of multivariate time series with controlled smoothness. Preprint, (2014).

[18] O. Rosen, S. Wood, D. S. Stoffer, AdaptSPEC: Adaptive Spectral Estimation for Nonstationary Time Series. Journal of American Statistical Association **107** (2012), 1575–1589.

[19] P. M. Robinson and C. Velasco, Efficient Inference on Fractionally Integrated Panel Data Models with Fixed Effects. Preprint, (2013).

[20] A.M. Sykulski, S.C. Olhede, J.M. Lilly, J.J. Early, The Whittle Likelihood for Complex-Valued Time Series. Preprint, (2014).

Chapter 17

Dynamics in Geometric Dispersive Equations and the Effects of Trapping, Scattering and Weak Turbulence (14w5080)

May 5 - 9, 2014

Organizer(s): Stephen Gustafson (University of British Columbia), Jeremy Marzuola (University of North Carolina), Daniel Tataru (University of California, Berkeley)

17.1 Overview of the Field

One of the major success stories in analysis over the past couple of decades is the deep and detailed insight into the qualitative properties of solutions to nonlinear dispersive PDE from Mathematical Physics which has been gained through application of techniques from harmonic analysis, spectral theory, the calculus of variations, and dynamical systems. In this way, our understanding of the nonlinear waves which characterize the dynamics of various systems in quantum physics, general relativity, optics, and fluid mechanics (just to name a few) has increased enormously over a remarkably short period.

This understanding extends to questions of local and global well-posedness, low-regularity solutions, singularity formation, asymptotic behaviour, the existence and stability of special solutions (such as solitons, or various threshold solutions), and the role such special solutions play in the general dynamics. Progress has been such that it could be said, very roughly speaking, that our mathematical comprehension of nonlinear dispersive PDE which are (a) posed on Euclidean space, and (b) of a sub-critical (roughly, conserved quantities provide some natural control over the size of solutions), or even (due to groundbreaking advances of the last few years) critical nature, is now rather good.

On the other hand, it is just as reasonable to say that nonlinear wave equations outside of this category are still quite poorly understood, due to inherent new difficulties. For equations posed on compact domains – such as compact manifolds – dispersion takes on a very different character, since waves cannot escape to infinity, and so interact with each other indefinitely. On domains with smooth obstacles or boundary, the effects of trapping or scattering can profoundly impact the behavior of nonlinear waves, whereas in the case of boundaries with edges or corners, the effects of diffraction can also play a role. For equations with non-trivial domain geometry, or target geometry (i.e. for maps into curved spaces), the challenge is to reveal and quantify whatever dispersion inhibiting/enhancing, trapping, or focusing/defocusing effects the geometry introduces. In each of these circumstances, dynamical systems theory has played a major role in studying the underlying Hamiltonian dynamics, analyzing the spectrum of a domain, or characterizing special nonlinear solutions related to underlying symmetries of the operator and the geometry. For super-critical equations, the overriding difficulty is to operate in the absence of useful, natural conserved quantities.

As it happens, numerous PDE of this type arise naturally in applications, in such diverse areas as general relativity, plasma models, magnetics, optics, and water waves. Moreover, some of the key physical examples of super-critical equations, such as the Einstein equations, and the gauge theories of particle physics, are inherently geometric. For all of these reasons, the field seems to be at something of a turning point, with researchers just beginning en masse to explore some of these challenging new directions. In particular, there has been a noticeable recent movement toward problems with a geometric character, leading to remarkable contributions from dynamical systems theory.

17.2 Recent Developments and Open Problems

The workshop was broken up into several themed sessions covering the topics of nonlinear PDE on compact domains; nonlinear/linear wave equations stemming from the study of General Relativity; the equations of Water Waves; and lastly the interaction of statistics and PDE. Below will give an overview of each topic and highlight the advances presented at the workshop.

Deterministic PDE on compact domains

The workshop featured talks by Dave Ambrose, Sebastian Herr, Benoît Grébert and Piotr Bizoń about solutions to nonlinear PDE in various settings where wave interactions take on a very different character on long time scales due to the lack of dispersion.

- In the setting of periodic domains, Ambrose in recent work with J. Doug Wright has a result showing that a dispersive equation of the form

$$u_t = Au + N(u)$$

on a periodic domain can have a measure 0 set of temporally periodic solutions provided that the linear operator, A, is strongly dispersive and the nonlinearity, N, has few enough derivatives in it such that local smoothing estimates can still be employed in a periodic setting on the Duhamel term of the solution,

$$\int_0^t e^{A(t-\tau)} N(u(\tau)) d\tau.$$

Indeed, even a compact manifold like the torus has can have smoothing properties due to averaging. This connects to the works of [45], [37, 15, 16, 85] and can be read about in the pre-print [9]. The techniques are centered around those of small-divisors and Nash-Moser iteration, but connects nicely to the mapping properties of strongly dispersive equations. Right now, the authors can treat several model problems that look somewhat like fifth-order KdV,

$$\partial_t u + \partial_x^5 u - u u_x = 0,$$

among others. The goal will be to push the requirements on the smoothing properties of the operator as low as possible with future refinements to capture more and more interesting models for which people are interested in periodic solutions, such as water wave equations, but also increase the dimension.

- Following the early work of Bourgain [14, 18] and Burq-Gerard-Tzvetkov [22, 23, 24, 25] proving well-posedness properties of nonlinear dispersive equations on compact manifolds, Herr has been working for some time looking at critical nonlinear Schrödinger equations on compact domains and trying to determine the effects of the geometry (and in particular the natural spectrum of the Laplacian) impacts the long time well-posedness properties, see [56, 58, 57]. Recently, in joint work with his student Nils Strunk, Herr has managed to show that on $M = \mathbb{S} \times \mathbb{S}^2$, the energy critical Nonilnear Schrödinger equation,

$$i\partial_t + \Delta_g u = \pm |u|^{p-1} u, u(0, \cdot) = u_0 \in H^1(M),$$

is globally well-posed and that the argument boils down to a trilinear estimate of the form

$$\|P_{N_1} e^{it\Delta}\phi_1 P_{N_2} e^{it\Delta}\phi_2 P_{N_3} e^{it\Delta}\phi_3\|_{L^2(\tau_0 \times M)} \lesssim \left(\frac{\langle N_3 \rangle}{\langle N_1 \rangle} + \frac{\langle 1 \rangle}{\langle N_2 \rangle} \right)^{\delta} \langle N_2 \rangle \langle N_3 \rangle \Pi_{j=1}^{3} \|\phi_j\|_{L^2(M)}$$

for $N_1 \geq N_2 \geq N_3$, some $\delta > 0$. In the case of $M = \mathbb{S} \times \mathbb{S}^2$, the authors are able to reduce the estimate to a statement about exponential sums due to Bourgain, [16]. The result uses the atomic U^p, V^p space machinery that has made great headway in treating critical problems in recent years, following their development in for instance [70, 55, 71]. The spectrum of the Laplacian on compact manifolds is intimately linked to application of the trilinear estimate here, which is why so far it has only been verified in specific cases such as the sphere and the torus (though now including irrational tori thanks to recent work of Strunk [88]. Advances in spectral estimates on more general domains following the work of say, Sogge [86] will be crucial for the advances in understanding nonlinear interactions on compact domains.

- Grébert discussed recent works with Tiphaine Jézéquel and Laurent Thomann, where they study the stability of large homoclinic orbits in periodic Klein-Gordon equations, [49, 50]. In other words, as a nice connection to the results above by Ambrose studying non-existence and the small data results of Herr-Strunk, the authors construct KAM-torus ([48, 89, 10]) like closed solutions for a nonlinear wave equation of the form

$$\partial_t^2 - \Delta_g u - m^2 u + u^{2p+1} = 0$$

for M a volume 1 Riemannian surface without boundary in up to 3 dimensions with $m < \lambda_1$ the second(!) eigenvalue of Δ_g and $p \geq 1$ for $d = 2$, $p = 1$ for $d = 3$. Note that the mass here has an unusual sign for what most would consider for a Klein-Gordon type equation, which allows one to look for stationary solutions using an eigenvalue decomposition

$$u = a_0 e_0 + \sum_{k=1}^{\infty} a_k e_k, \quad \dot{v} = a_0 e_0 + \sum_{k=1}^{\infty} a_k e_k.$$

Decomposing the natural energy of the equation gives an approximate Hamiltonian system for (a_0, b_0), which has elliptic points at $\pm m^{\frac{1}{p}}$ and immediately see that doing an eigenvalue decomposition allows one to show that they are stable under perturbation for at least long time scales. Such KAM-torus like solutions both highlight the difficulties in getting nonlinear equations to disperse in a meaningful sense, as well as give explicit ways to understand the collection or transfer of energy for PDE on compact manifolds. These will play a crucial role in the long-time and large-data understanding of dynamics on compact manifolds.

- The question of so-called weak turbulence for dispersive equations is an important ongoing investigation tied into the underlying statistical mechanics of a Hamiltonian PDE in a compact setting, see [17, 31, 46, 51, 52, 74, 53, 54]. The basic question is whether some form of transfer of energy to high frequency happens over long time scales. Many works have attempted to understand such a phenomenon and Bizoń in joint work with Patryk Mach and Maciej Maliborski presented some recent advances and numerical simulations related to toy models for the Einstein equations. It has been conjectured that there is a mechanism for instability of Anti-De Sitter space through a weakly turbulent transfer of energy to high frequencies, which with collaborators Bizoń has been exploring numerically using semilinear wave equations as leading order toy models. This talk could easily have fit into the machinery of geometric wave equations or statistical mechanics in many ways. However, in the end the strongest results presented showed simulations of numerical solutions to

$$u_{tt} - \Delta u + m^2 u + u^3 = 0$$

on a compact manifold. The goal is to understand the out of equilibrium dynamics for small solutions, which they studied using the power spectrum of the solution in higher Sobolev norms over long times. On the circle for instance, there is a resonant system of ODEs eliminating small divisors such that

$$\pm 2in\dot{a}_n^{\pm} = \varepsilon^2 \sum_{j-k+m=n} a_j^{\pm} \bar{a}_k^{\pm} a_m^{\pm} + 2\varepsilon^2 \left(\sum_k |a_k^{\mp}|^2 \right) a_n^{\pm}.$$

In such a case, an exponential decay appears to arise in the power spectrum preventing a long time motion towards high frequency, which is of course possibly meta-stable. A Yang-Mills wave-map type equation on $\mathbb{S}^3$ exists, which simplify to the form

$$W_{tt} = W_{xx} + \frac{W(1-W^2)}{\sin^2 x}$$

has a similar structure. An equivariant wave map from $\mathbb{R} \times \mathbb{S}^3 \to \mathbb{S}^3$ of the form

$$W_{tt} = W_{xx} + \frac{2\cos x}{\sin x} U_x - \frac{\sin(2U)}{\sin^2 x}$$

looks like it has good unstable behavior but does not have a resonant system. However, a $4d$ wave map from $\mathbb{R}\times$ (some model manifold) $\to$ AdS related to Bianchi Nine Models, which has trully resonant spectrum and can be written

$$W_{tt} = W_{xx} + \frac{3}{\sin x \cos x} U_x - \frac{F(U)}{\sin^2 x}$$

for $F(U) = \frac{4}{3}(e^{-2U} - e^{-8U})$ appears to have preliminary power-law spectrum cascades. This interesting and quite application oriented talk led to a great deal of discussions with people interested in nonlinear wave maps equations and GR throughout the workshop.

Fluids

The workshop featured talks by about various asects of fluids models by Thomas Alazard, Roberto Camassa, Benjamin Harrop-Griffiths, Mihaela Ifrim, Herbert Koch, Jon Wilkening, and Fabio Pusateri.

- The generalized Korteweg-de Vries equation

$$\partial_t u + \partial_x^3 u + \partial_x(|u|^{p-1}u) = 0$$

arises as a long-wave model for water waves ($p = 2, 3$) and in its general form as a model for plasmas for instance. However, for many years it has been mostly an excellent model for studying nonlinear dispersive phenomena because it has such a rich structure. The workshop featured two talks on these types of models, one showing the existence of self-similar blow-up profiles for slightly super-critical KdV problems ($p > 5$) and one showing modified scattering for the mKdV equation ($p = 3$). Both models have effective dynamics driven by in one case a modified elliptic equation solved through careful implicit function theorem techniques and another on the tools of modified scattering. In particular, Harrop-Griffiths observes that the long-time decay properties for mKdV are related to a Painlevé type ODE. See [69] for the blow-up result, with the pre-print by Harrop-Griffiths forthcoming but motivated by recent advances in modified scattering from [62, 63].

- The gravity wave equations have recently seen a great deal of progress as quasilinear techniques have become more readily available and the equations better understood. Through a combination of different menthods, various groups have made progress on the problem recently, especially for gravity-waves in $2d$ on global time scales. Reports on this progress were made by Thomas Alazard, Mihaela Ifrim, Alex Ionescu, and Fabio Pusateri. The gravity-capillary wave equations can be represented as

$$\begin{cases} \partial_t h = |D|\,\psi + \{G(h)\psi - |D|\,\psi\} \\ \partial_t \psi = (\tau\Delta - g)\,h + \left\{ \tau \left(\operatorname{div}\left(\dfrac{\nabla h}{\sqrt{1+|\nabla h|^2}} \right) - \Delta h \right) \right. \\ \qquad\qquad\qquad\qquad \left. -\dfrac{1}{2}|\nabla\psi|^2 + \dfrac{(G(h)\psi + \nabla h \cdot \nabla\psi)^2}{2\left(1+|\nabla h|^2\right)} \right\}. \end{cases}$$

for h the height of the fluid at the interface and ψ a trace of a related velocity field. These equations have a great deal of quaslinear structure, but when $\tau = 0$, breakthroughs have been made in the work of [90, 91, 47, 2, 3, 36]. Recently, our understanding of these equations has improved using a microlocal paradifferential approach in [4, 2, 3], a modified energy method in holomorphic coordinates in [61, 63] and the theory of space-time resonances with weights as in [64]. The directions moving forward include understanding the long-time effects of surface tension (discussed by Pusateri in a model problem), moving to higher dimensions, looking at interactions with internal waves (see the work of Camassa below), etc. There are some benefits to a choice of Eulerian coordinate versus Holomorphic coordinates and vice versa that were also discussed at length in the workshop. The work of Pusateri was motivated by the presentation of Ionescu relating to models for particles in a plasma, where the Euler equations are couple to an electromagnetic field. This Euler-Maxwell system can be treated with a similar modified energy technique and represents joint work with Y. Deng, Y. Guo and B. Pausader.

- Roberto Camassa and Jon Wilkening talked about various numerical and modeling results related to water waves. Wilkening discussed new families of time-periodic and quasi-periodic solutions of the free-surface Euler equations involving standing-traveling waves and collisions of solitary waves of various types. The new solutions are found to be well outside of the KdV and NLS regimes and a Floquet analysis shows that many of the new solutions are linearly stable to harmonic perturbations. Evolving such perturbations (nonlinearly) over tens of thousands of cycles suggests that the solutions remain nearly time-periodic forever. See [5, 6, 7, 8, 92, 93]. Camassa discussed models for internal waves. In particular, he focussed on one of the simplest physical setups supporting internal wave motion, which is that of a stratified incompressible Euler fluid in a channel. He discussed asymptotic models capable of describing large amplitude wave propagation in this environment, and in particular of predicting the occurrence of self-induced shear instability in the waves' dynamics for continuously stratified fluids. See [32, 33, 34]. Many experiments were also compared to the asymptotics and numerics. T. Alazard was submitting a paper about capillary waves around the same week and was able to connect some of their observations to the numerical experiments of Wilkening, [1].

Waves and Geometry

The workshop featured talks by about various aspects of wave equation models by Ben Dodson, Alex Ionescu, Andrew Lawrie, Sun-Jin Oh, Joachim Krieger, Jason Metcalfe, Paul Smith and Jacob Sterbenz.

- A recent asymptotic stability (see [73]) result for equivariant wave maps from $\mathbb{H}^2 \to \mathbb{S}^2$ or $\mathbb{S}^2$ was discussed by Lawrie and Oh as joint work with Sohrab Shashahani. The central equation is

$$\psi_{tt} - \psi_{rr} - \coth r \psi_r + \frac{(g(\psi)g'(\psi)}{\sinh^2 r} = 0$$

  for $g = \sin u$ for target $\mathbb{S}^2$ and $g = \sinh u$ for target $\mathbb{H}^2$. The result brings together many of the ideas from stability theory for wave equations as well as geometric analysis and dispersive equations. A main novelty of the approach addresses the spectrum of the linearized operator about various explicit equivariant wave maps and in particular for a one parameter family of such states. See [75] for a similar asymptotic stability result but in a more restrictive geometry.

- The nonlinear interactions of the wave equation have been a major open area in dispersive PDE for a long time now. At this workshop some new advances were introduced related to long-time behavior of nonlinear waves. In particular, several talks addressed solutions to the problem

$$u_{tt} - \Delta_g u + \mu u^p = 0$$

  in different settings. Metcalfe presented a new result with Chengbo Wang, Hans Lindblad, Chris Sogge and Mihai Tohaneanu proving the Strauss conjecture on black hole-backgrounds, see [77]. In particular, given the Schwarzschild metric or the Kerr metric in $3d$ (any metric that has local energy decay estimates and is asymptotically flat really) the authors prove that for $p > 1 + \sqrt{2}$, or the Strauss exponent, small data smooth solutions exist for all time. In a complimentary talk, Sterbenz talked about recent work he has done with

Daniel Tataru and his student Jesus Oliver showing that local energy decay can be applied to give results in a large variety of geometric settings, in particular, refining Klainerman vector field techniques to treat black hole space times. See for instance [87] for some earlier work with the pre-print forthcoming otherwise. Using concentration compactness tools showing that the energy must push to 0, Dodson in collaboration with A. Lawrie has shown a conditional scattering result for radial initial data for $p = 3$ in $3d$ Euclidean space, see [38]. Namely, if the energy critical norm $\dot{H}^{\frac{1}{2}} \times \dot{H}^{-\frac{1}{2}}$ remains bounded, their result proves that it must scatter to a linear solution. Concentration compactness tools have appeared previously in works such as [65, 66, 67, 68, 39, 40, 41]. This connects back to some numerical work Bizon and collaborators have done in the past as well, see [13]. Finally, Krieger talked about joint work with Wilhelm Schlag on the strongly supercritical wave equation for $p = 7$ in $3d$, see [72]. They are able to prove that a class of large data solutions exist and are stable under certain types of perturbation in the critical space $H^{\frac{7}{6}} \times H^{\frac{1}{6}}$. These solutions are self-similar, but with weak decay due to the supercritical nature of the problem. For a slight shift, Paul Smith discussed work with Baoping Liu on the Chern-Simons-Schrödinger equation in an equivariant setting. This equation is more a nonlinear Schrödinger equation coupled to Magnetic Field, but can be reduced to to a system of the form

$$\begin{aligned}
(i\partial_t + \Delta)\phi &= \frac{2m}{r^2} A_\theta \phi + A_0 \phi + \frac{1}{r^2} A_\theta^2 \phi - g|\phi|^2\phi, \\
\partial_r A_0 &= \frac{1}{r}(m + A_\theta)|\phi|^2, \\
\partial_t A_\theta &= r \mathrm{Im}(\bar{\phi}\partial_r \phi), \\
\partial_r A_\theta &= -\frac{1}{2}|\phi|^2 r, \\
A_r &= 0.
\end{aligned}$$

This is a very nonlocal, nonlinear Schrödinger equation but nonetheless, using again concentration compactness like techniques, they are able to prove global existence and scattering in each equivariant class, which is related to a vortex solution for NLS. See [76].

The Interaction of PDE and Statistical Mechanics

The workshop featured talks by about various aspects of the study of statistics in dispersive PDE by Aynur Bulut, Natasa Pavlovic, Jonathan Mattingly, Andrew Nahmod, Tadahiro Oh, and Nicolas Burq.

- The use of Gibbs Measures in low regular PDE Existence Theory was explored by Burq, Bulut, Nahmod and Oh. In particular, Burq introduced work in progress with Laurent Thomann and Nikolay Tzvetkov defining a modified version of the Gibbs measure approach in dispersive PDE on compact manifolds, which they can possibly introduce for any domain in $\mathbb{R}^2$ with smooth enough boundary, regardless of knowing the spectrum explicitly. This is a major breakthrough in the field and connects strongly to the world of quantum field theory. Nahmod and Bulut both presented low-regularly well-posedness results in specific case of a critical nonlinear wave equation on a domain. For Bulut, it is in joint work with Bourgain on the energy critical wave and Schrödinger equations on the disc. For Nahmod, in joint work with Gigliola Staffilani on the $3d$ quintic nonlinear Schrödinger equation with data below H^1. Oh introduced ongoing work with A. Bényi and O. Pocovnicu to define a Gibbs measure for the nonlinear Schrödinger equation on non-compact spaces. See [11, 20, 21, 26, 27, 28, 29, 30, 79, 80, 81, 82, 83, 84]

- Mattingly presented a large number of examples from the setting of stochastic dynamics where noise assisted in the formation of either cascading energies or preventing a solution from blowing up deterministically. As of yet, his examples include small systems, but if ODE blow-dynamics or cascade dynamics can be found in PDE systems, there are interesting amounts of overlap related to noise-stabilization and cascades in PDE and weak turbulence theory. See [78] for work on the cascades and [59, 60] for noise stabilization.

- Pavlovic discussed recent work with Thomas Chen, Christian Hainzl, and Robert Sieringer on an application of the Quantum de Finetti theorem in the equations in many body quantum mechanics. See [35] for more details, but this is further progress towards being able to apply much of the developments for NLS to large systems of Bosons. As a result, a scattering argument arises for the defocusing Gross-Pitaevskii system under a now understood to be necessary exponential growth bound. De Finetti is a key theorem from probability theory that allows one to write density functionals in relation to a measure over an independent family of solutions. Namely, it says that exchangeable particles (like Bosons) can be written as a combination of independent particles in a measurable way. This also began a collaboration with S. Herr on multilinear estimates in many-body systems related to his studies on the sphere.

17.3 Scientific Progress Made

Many results were presented that made clear previously unknown connections between researchers. As a result, numerous collaborations and discussions took place between people in PDE and probability, numerical analysts and specialists in nonlinear PDE, etc. Also, a number of young people attended and were able to learn a great deal about pioneering areas in the field. Several ongoing collaborations were strengthened at the same time. In the end the meeting was a great success at bringing together many areas of dispersive PDE strongly impacted by geometry and nonlinearity, as well as introducing applications in dire need of such forms of analysis.

Participants

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Haberman, Boaz (University of California - Berkeley)
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Bibliography

[1] Thomas Alazard and Pietro Baldi. Gravity capillary standing water waves.

[2] T. Alazard, N. Burq and C. Zuily, On the Cauchy problem for gravity water waves, Preprint, 2012, http://arxiv.org/abs/1212.0626.

[3] T. Alazard, N. Burq and C. Zuily, On the water waves equations with surface tension, Duke Math. J., 158, no. 3, 2011, 413-499.

[4] T. Alazard, J.M. Delort, Global solutions and asymptotic behavior for two dimensional gravity water waves, Preprint, 2013.

[5] D. M. Ambrose and J. Wilkening, Global paths of time-periodic solutions of the Benjamin- Ono equation connecting pairs of traveling waves, Comm. App. Math. and Comp. Sci. 4 (2009), no. 1, 177-215.

[6] D. M. Ambrose and J. Wilkening, Computation of symmetric, time-periodic solutions of the vortex sheet with surface tension, Proc. Nat. Acad. Sci. 107 (2010), no. 8, 3361-3366.

[7] D. M. Ambrose and J. Wilkening, Computation of time-periodic solutions of the Benjamin-Ono equation, J. Nonlinear Sci. 20 (2010), no. 3, 277-308.

[8] D. M. Ambrose and J. Wilkening, Dependence of time-periodic votex sheets with surface tension on mean vortex sheet strength, Procedia IUTAM 11 (2014), 15-22.

[9] D. M. Ambrose and J. D. Wright. Non-existence of small-amplitude doubly periodic waves for dispersive equations, preprint (2014).

[10] D. Bambusi and B. Grébert. Birkhoff normal form for PDEs with tame modulus. Duke Math. J. 135 (2006), 507567.

[11] A. Bényi, T. Oh and O. Pocovnicu, On the probabilistic Cauchy theory of the cubic nonlinear Schrdinger equation on $\mathbb{R}^d$, $d \geq 3$, preprint (2014).

[12] Piotr Bizoń, Is AdS stable??, preprint (2014).

[13] P. Bizoń and A. Zenginoglu. Universality of global dynamics for the cubic wave equation. Nonlinearity, 22(10):24732485, 2009.

[14] J. Bourgain, Fourier transform restriction phenomena for certain lattice subsets and applications to nonlinear evolution equations. I. Schrödinger equations, Geom. Funct. Anal. 3 (1993), no. 2, 107156.

[15] J. Bourgain. Construction of quasi-periodic solutions for Hamiltonian perturbations of linear equations and applications to nonlinear PDE. Internat. Math. Res. Notices, 1994(11):475 ., approx. 21 pp. (electronic), 1994.

[16] J. Bourgain. Construction of periodic solutions of nonlinear wave equations in higher dimension. Geom. Funct. Anal., 5(4):629-639, 1995.

[17] J. Bourgain. Aspects of long time behaviour of solutions of nonlinear hamiltonian evolution equations. In Geometries in Interaction, pages 105-140. Springer, 1995.

[18] J. Bourgain, On Strichartzs inequalities and the nonlinear Schrödinger equation on irrational tori, Mathematical aspects of nonlinear dispersive equations, Ann. of Math. Stud., vol. 163, Princeton Univ. Press, Princeton, NJ, 2007, pp. 120.

[19] J. Bourgain, Invariant measures for the 2D-defocusing nonlinear Schrodinger equation. Comm. Math. Phys. 176, no. 2, 421- 445, (1996).

[20] J. Bourgain and A. Bulut, Invariant Gibbs measure evolution for the radial nonlinear wave equation on the 3d ball. J. Funct. Anal. 266 (2014), no. 4, 23192340.

[21] N. Burq, Random data Cauchy Theory for Dispersive Partial Differential Equations Proceedings if the International Congress of Mathematicians, Hyderabad, India, 1862-1883, (2010).

[22] N. Burq, P. Gérard, and N. Tzvetkov, Strichartz inequalities and the nonlinear Schrödinger equation on compact manifolds, Amer. J. Math. 126 (2004), no. 3, 569605.

[23] N. Burq, P. Gérard, and N. Tzvetkov, Bilinear eigenfunction estimates and the nonlinear Schrdinger equation on surfaces, Invent. Math. 159 (2005), no. 1, 187223.

[24] N. Burq, P. Gérard, and N. Tzvetkov, Multilinear eigenfunction estimates and global existence for the three dimensional nonlinear Schrödinger equations, Ann. Sci. cole Norm. Sup. (4) 38 (2005), no. 2, 255301.

[25] N. Burq, P. Gérard, and N. Tzvetkov, Global solutions for the nonlinear Schrödinger equation on three-dimensional compact manifolds, Mathematical aspects of nonlinear dispersive equations, Ann. of Math. Stud., vol. 163, Princeton.

[26] Burq, N., Thomann, L. and Tzvetkov, N., Global infinite energy solutions for the cubic wave equation. Preprint, arXiv:1210.2086.

[27] N. Burq, L. Thomann and N. Tzvetkov, Long time dynamics for the one dimensional non linear Schrödinger equation. Preprint, arXiv:1002.4054, (2010).

[28] N. Burq and N. Tzvetkov, Random data Cauchy theory for supercritical wave equations. I. Local theory. Invent. Math. 173, no. 3, 449475, (2008).

[29] N. Burq and N. Tzvetkov, Random data Cauchy theory for supercritical wave equations. II. A global theory. Invent. Math. 173, 477496 (2008).

[30] N. Burq and N. Tzvetkov, Probabilistic well-posedness for the cubic wave equation. J. Eur. Math. Soc. (JEMS) 16 (2014), no. 1, 130.

[31] R. Carles and E. Faou. Energy cascades for NLS on the torus. Discrete and Continuous Dynamical Systems. Series A, 32(6):2063-2077, 2012.

[32] W Choi, R Camassa, Fully nonlinear internal waves in a two-fluid system, Journal of Fluid Mechanics (1999).

[33] R. Camassa and C. Viotti. Transient dynamics by continuous-spectrum perturbations in stratified shear flows, Journal of Fluid Mechanics, (2013).

[34] J. Bona, D. Lannes, J.C. Saut, Asymptotic models for internal waves. (English, French summary) J. Math. Pures Appl. (9) 89 (2008), no. 6, 538566.

[35] T. Chen, C. Hainzl, N. Pavolvic and R. Seiringer, On the well-posedness and scattering for the Gross-Pitaevskii hierarchy via quantum De Finetti, preprint (2014).

[36] D. Coutand, S. Shkoller, Wellposedness of the free-surface incompressible Euler equations with or without surface tension. J. Am. Math. Soc., 20(3), 2007, 829-930.

[37] W. Craig and C.E. Wayne. Newton's method and periodic solutions of nonlinear wave equations. Comm. Pure Appl. Math., 46(11):1409-1498, 1993.

[38] B. Dodson and A. Lawrie, Scattering for the radial $3d$ cubic wave equation, preprint (2014).

[39] T. Duyckaerts, C. Kenig, and F. Merle. Universality of the blow-up profile for small radial type II blow-up solutions of the energy critical wave equation. J. Eur math. Soc. (JEMS), 13(3):533599, 2011.

[40] T. Duyckaerts, C. Kenig, and F. Merle. Profiles of bounded radial solutions of the focusing, energy-critical wave equation. Geom. Funct. Anal., 22(3):639698, 2012.

[41] T. Duyckaerts, C. Kenig, and F. Merle. Universality of the blow-up profile for small type II blow-up solutions of the energy-critical wave equation: the nonradial case. J. Eur. Math. Soc. (JEMS), 14(5):13891454, 2012.

[42] T. Duyckaerts, C. Kenig, and F. Merle. Classification of radial solutions of the focusing, energy critical wave equation. Cambridge Journal of Mathematics, 1(1):75144, 2013.

[43] T. Duyckaerts, C. Kenig, and F. Merle. Scattering for radial, bounded solutions of focusing supercritical wave equations. To appear in I.M.R.N, Preprint, 2012.

[44] L.H. Eliasson and S.B. Kuksin. On reducibility of Schrödinger equations with quasiperiodic in time potentials. Comm. Math. Phys. 286 (2009), no. 1, 125135.

[45] M.B. Erdogan and N. Tzirakis, Global smoothing for the periodic KdV evolution. Int. Math. Res. Not. IMRN 2013, no. 20, 45894614.

[46] E. Faou, P. Germain, and Z. Hani. The weakly nonlinear large box limit of the 2D cubic nonlinear Schrödinger equation. Preprint, arXiv:1308.6267.

[47] P. Germain, N. Masmoudi, J. Shatah, Global solutions for the gravity water waves equation in dimension 3. Ann. of Math. (2) 175 (2012), no. 2, 691754.

[48] B. Grébert and L. Thomann, KAM for the Quantum Harmonic Oscillator. Comm. Math. Phys. 307 (2011), 383427.

[49] B. Grébert, T. Jézéquel and L. Thomann, Stability of large periodic solutions of Klein-Gordon near a homoclinic orbit, preprint (2014).

[50] B. Grébert, T. Jézéquel and L. Thomann, Dynamics of Klein-Gordon on a compact surface near a homoclinic orbit. To appear in DCDS.

[51] Guardia, Marcel; Growth of Sobolev Norms in the Cubic Nonlinear Schrdinger Equation with a Convolution Potential. Comm. Math. Phys. 329 (2014), no. 1, 405434.

[52] M. Guardia and V. Kaloshin. Growth of Sobolev norms in the cubic defocusing nonlinear Schrödinger equation, arXiv preprint arXiv:1205.5188, (2012).

[53] Z. Hani. Long-time instability and unbounded Sobolev orbits for some periodic nonlinear Schrödinger equations. Preprint, arXiv:1210.7509, 2012.

[54] Z. Hani, B. Pausader, N. Tzvetkov, and N. Visciglia. Modified scattering for the cubic Schrödinger equation on product spaces and applications.

[55] M. Hadac, S. Herr, and H. Koch, Well-posedness and scattering for the KP-II equation in a critical space, Ann. Inst. H. Poincaré Anal. Non Linéaire 26 (2009), no. 3, 917941, Erratum: ibid. 27 (3) (2010) 971972.

[56] S. Herr, The quintic nonlinear Schrdinger equation on three-dimensional Zoll manifolds, Amer. J. Math. 135 (2013), no. 5, 12711290.

[57] S. Herr, D. Tataru, and N. Tzvetkov, Global well-posedness of the energy-critical nonlinear Schrdinger equation with small initial data in H1(T3), Duke Math. J. 159 (2011), no. 2, 329349.

[58] S. Herr, D. Tataru, and N. Tzvetkov, Strichartz estimates for partially periodic solutions to Schrödinger equations in 4d and applications, J. reine angew. Math. (to appear), doi:10.1515/crelle-2012-0013.

[59] D. Herzog and J.C. Mattingly, Noise-induced stabilization of planar flows I, preprint (2014).

[60] D. Herzog and J.C. Mattingly, Noise-induced stabilization of planar flows II, preprint (2014).

[61] J. K. Hunter, M. Ifrim, and D. Tataru, Two dimensional water waves in holomorphic coordinates, Preprint, 2014.

[62] M. Ifrim and D. Tataru. Global bounds for the cubic nonlinear Schrödinger equation (NLS) in one space dimension, preprint (2014).

[63] M. Ifrim and D. Tataru. Two dimensional water waves in holomorphic coordinates II: Global solutions, preprint (2014).

[64] A. Ionescu and F. Pusateri, Global solutions for the gravity water waves system in 2d, preprint (2014).

[65] C. Kenig and F. Merle. Global well-posedness, scattering and blow-up for the energy-critical, focusing, nonlinear Schrodinger equation in the radial case. Invent. Math., 166(3):645675, 2006.

[66] C. Kenig and F. Merle. Global well-posedness, scattering and blow-up for the energy-critical focusing nonlinear wave equation. Acta Math., 201(2):147212, 2008.

[67] C. E. Kenig and F. Merle. Scattering for H1/2 bounded solutions to the cubic, defocusing NLS in 3 dimensions. Trans. Amer. Math. Soc., 362(4):19371962, 2010.

[68] C. E. Kenig and F. Merle. Nondispersive radial solutions to energy supercritical non-linear wave equations, with applications. Amer. J. Math., 133(4):10291065, 2011.

[69] H. Koch. Self-similar solutions to super-critical gKdV, preprint (2014).

[70] H. Koch and D. Tataru, Dispersive estimates for principally normal pseudodifferential operators, Comm. Pure Appl. Math. 58 (2005), no. 2, 217 284.

[71] H. Koch, D. Tataru, and M. Visan (eds.), Dispersive Equations and Nonlinear Waves: Generalized Korteweg-de Vries, Nonlinear Schr̈dinger, Wave and Schr̈dinger Maps, Oberwolfach Seminars, vol. 45, Birkhuser, Basel, 2014.

[72] J. Krieger and W. Schlag, Large global solutions for energy supercritical nonlinear wave equations on $\mathbb{R}^3 \times \mathbb{R}$, preprint (2014).

[73] A. Lawrie, S.-J. Oh and S. Shashahani, Stability of stationary equivariant wave maps from the hyperbolic place, preprint (2014).

[74] S. B. Kuksin. Nearly integrable infinite-dimensional Hamiltonian systems. Lecture Notes in Mathematics, 1556. Springer-Verlag, Berlin, 1993.

[75] A. Lawrie and W. Schlag, Scattering for wave maps exterior to a ball. Advances in Mathe- matics, 232(1):5797, 2013.

[76] B. Liu and P. Smith, Global well-posedness of the equivariant Chern-Simons-Schrödinger equation, preprint (2014).

[77] H. Lindblad, J. Metcalfe, C.D. Sogge, M. Tohaneanu and C. Wang, The Strauss conjecture on Kerr black hole backgrounds, preprint (2014).

[78] J.C. Mattingly, T. Suidan, and E. Vanden-Eijnden, Simple Systems with Anomalous Dissipation and Energy Cascade, Comm. Math. Phys. 276 (2007), no. 1, 189220.

[79] A.R. Nahmod and G. Staffilani, Almost sure well-posedness for the periodic $3d$ quintic nonlinear Schrödinger equation below the energy space, preprint (2014).

[80] A.R. Nahmod, N. Pavlovic and G. Staffilani, Almost sure existence of global weak solutions for supercritical Navier-Stokes equations. SIAM J. Math. Anal. 45 (2013), no. 6, 34313452.

[81] A.R. Nahmod, T. Oh, L. Rey-Bellet and G. Staffilani, Invariant weighted Wiener measures and almost sure global well-posedness for the periodic derivative NLS. J. Eur. Math. Soc. (JEMS) 14, no. 4, 1275 - 1330, (2012).

[82] A.R. Nahmod, L. Rey-Bellet, S. Sheffield and G. Staffilani, Absolute continuity of Brownian bridges under certain gauge transformations. Math. Res. Lett. 18, no. 5, 875 - 887 (2011).

[83] T. Oh, Invariant Gibbs measures and a.s. global well-posedness for coupled KdV systems. Differential Integral Equations 22, 637 - 668, (2009).

[84] T. Oh, Invariance of the Gibbs measure for the Schrdinger-Benjamin-Ono system. SIAM J. Math. Anal. 41, no. 6, 2207 - 2225, (2010).

[85] J. Pöschel. Quasi-periodic solutions for a nonlinear wave equation. Comment. Math. Helv. 71 (1996), no. 2, 269296.

[86] C. Sogge, Concerning the Lp norm of spectral clusters for second-order elliptic operators on compact manifolds, J. Funct. Anal. 77 (1988), no. 1, 123138.

[87] J. Sterbenz and D. Tataru, Local energy decay for Maxwell fields Part I: Spherically symmetric black-hole backgrounds, preprint (2013).

[88] N. Strunk, Strichartz estimates for Schrödinger equations on irrational tori in two and three dimensions, ArXiv e-prints (2014).

[89] C.E. Wayne. Periodic and quasi-periodic solutions of nonlinear wave equations via KAM theory. Comm. Math. Phys., 127(3):479-528, 1990.

[90] S. Wu, Well-posedness in Sobolev spaces of the full water wave problem in 2-D, Invent. Math., 130, 1997, 39-72.

[91] S. Wu, Almost global wellposedness of the 2-D full water wave problem, Invent. Math., 177, 2009, 45-135.

[92] J. Wilkening, Relative-Periodic Elastic Collisions of Water Waves, preprint (2014).

[93] J. Wilkening and J. Yu, Overdetermined shooting methods for computing standing water waves with spectral accuracy, Comput. Sci. Disc. 5 (2012), 014017:1-38.

Chapter 18

Mathematical Finance: Arbitrage and Portfolio Optimization (14w5116)

May 11 - 16, 2014

Organizer(s): Constantinos Kardaras (London School of Economics), Walter Schachermayer (University of Vienna), Gordan Žitković (The University of Texas at Austin)

18.1 Overview of the Field

Mathematics of financial markets is one of the most active and exciting areas of contemporary applied mathematics. It provides the mathematical community with a rich source of challenges, which, in turn, enrich the societys understanding of the financial system and help both regulators and the financial industry make better and more informed choices. Its proximity to practice, in addition to its purely mathematical appeal, makes this field especially attractive to young mathematicians. Moreover, it provides for wider employment opportunities both within the academic world and outside of it.

One of the most challenging areas within mathematical finance, namely its foundations, aims to understand the basic structure shared by all financial markets. It uses probabilistic tools, together with a variety of methods from stochastic, functional and convex analysis and partial differential equations, and draws from a host of other mathematical disciplines to accomplish its goals. Prior advances in the foundational issues have not only made a huge impact on the financial practice, but have also inspired a number of breakthroughs in related areas of mathematics traditionally regarded as theoretical.

18.2 Scientific Progress Made

Arbitrage theory. A number of researchers presented results in arbitrage theory. With first conceptual results going back to the work of Harrison, Kreps and Pliska (see [HK79], [HP81] and [Kre81]), a major (mathematical) breakthrough was accomplished by Delbaen and Schachermayer, with their work culminating in the papers [DS94] and [DS98]. The intensity of the research output in the arbitrage theory only increased since, with new contributions being made even today. Indeed, our meeting featured presentations of Beatrice Acciaio, Sara Biagini, Christa Cucchiero, Marco Frittelli, Monique Jeanblanc, Martin Schweizer and Josef Teichmann all of which discussed important new contributions to this rich theory.

Optimal investment. The roots of the optimal-investment (utility maximization) theory can be traced to the seminal work [Mer71] of Robert Merton, or, one may argue, even to Daniel Bernoulli (see [Ber54]). The theory has been adopted by the financial-mathematics community through the work of Karatzas, Kramkov, Lehoczky, Schachermayer, Shreve, Xu (see, e.g., [KLSX91] and [KS99]) and many others, during the 1990-ies. The intensity of mathematical research has not vaned ever since; it is still strong today, as evidenced by a number of interesting talks by Peter Bank, Luciano Campi, Christoph Czichowsky, Paolo Guasoni, Vicky Henderson, Tomoyuki Ichiba, Jan Kallsen, Johannes Muhle Karbe, Steve Shreve, Ronnie Sircar and Peter Tankov, we had the opportunity to hear at the meeting.

Equilibrium Theory and Related Fields. The topic of competitive equilibria - traditionally housed in economics - has found its way to the mainstream of mathematical research in quantitative finance thanks to the versatility and mathematical richness of the stochastic models it supports. With the early research by Duffie, Huang, Karatzas, Lehoczky, Shreve (see [DH85] or [KLS90]) setting the stage, new developments (including the treatment of "incomplete markets") have been appearing regularly to this day. Recent connections with the theory of systems of parabolic PDE and backward SDE have been particularly visible in an array of talks on the subject (and some related fields), byi Michalis Anthropelos, Umut Çetin, Jakša Cvitanić, Christoph Frei, Ioannis Karatzas, Kasper Larsen, Sergio Pulido and Hao Xing.

Other Topics. In addition to the three "classical" domains of research outlined above, financial mathematics casts a broad net over a variety of related mathematical fields and problem areas. One, recent and extremely active area of research is so-called "robust finance" where the dependence on the choice of the underlying probability measure (more precisely, its equivalence class under mutual absolute continuity) is studied and universal (robust) results with respect to this dependence formulated. The talks of Mathias Beiglboeck, Alex Cox, Marco Frittelli, Marcel Nutz and Jan Obloj provide excellent illustration of the scope and depth of this exiting subject.

On the other hand, problems stemming from finance have been providing a steady inflow of interesting problems and inspiration to the areas of optimal stochastic control and games for several decades now. Two talks, one by Bruno Bouchard and the other by Mihai Sîrbu, delivered at this meeting, provide par-excellence examples of such a synergy.

Martin Larson and Johannes Ruf revisited the problem of identifying when a local martingale is a martingale through Novikov's condition, providing a novel treatment that enhances intuition and contributes to the field of stochastic analysis.

A talk on the efficient estimation of the distribution of perpetuities was presented by Scott Robertson, with immediate applications in Actuarial science and Insurance.

Finally, let us mention the talk by Hans Föllmer, which outlined a whole new domain of research at the interface of financial mathematics (risk-measure theory) and statistical mechanics, with envisioned applications in the study of systemic financial risk. Such models are expected to take a leading role in the mathematical support of large-scale financial regulation and the avoidance of and the mitigation of the effects of future catastrophic system-wide financial events.

18.3 Presentation Highlights

Beatrice Acciaio

"*Arbitrage of the first kind and filtration enlargements in semimartingale financial models*"

ABSTRACT. Given a financial market where no arbitrage profits are possible, and an agent with additional information with respect to it, I investigate whether the extra information can generate arbitrage profits. I will first justify why the right concept of arbitrage to consider here is the so-called Arbitrage of the First Kind (or, equivalently, Unbounded Profit with Bounded Risk). Then I will illustrate a simple and general condition ensuring that no arbitrage is available to the informed agent either. The preservation of No-Arbitrage under additional information is shown for a general semimartingale model both when this information is disclosed progressively in time and when

it is fully added at the initial time (which correspond to the initial and to the progressive enlargement of filtration, respectively). In addition, I will provide a characterization of such a stability in a robust context, that is, for all possible semimartingale models. (This is joint work with C. Fontana and C. Kardaras.)

Michalis Anthropelos

"*Equilibrium in risk sharing games*"

ABSTRACT. The paper studies the equilibrium sharing of investment risks among agents whose random endowments are private information. Given that the sharing rules are the ones that optimally allocate the submitted endowments, we propose a Nash game where agents' strategic sets consist of the endowments are going to submit for sharing. First, it is proved that the best response problem admits a unique solution, which shall be called best endowment response and differs from the true agent's risk exposure. The Nash equilibrium risk sharing admits a finite dimensional characterization and it is proved to be unique in the case of two agents. The game benefits the low risk averse agents since their expected utilities are higher at the Nash risk sharing equilibrium than the optimal risk sharing one. (This is joint work with C. Kardaras.)

Peter Bank

"*Optimal investment with price impact*"

ABSTRACT. We present a price impact model where bid and ask prices are specified by a system of coupled diffusions driven both by a common noise and the buy and sell orders of an investor. The coupling causes the spread to decline after a transaction. The resulting nonlinear wealth dynamics are shown to be separable in a profit and loss part given, as in a linear model, by a stochastic integral and a separate cost term which only depends on the large investor's transactions and the resulting spread. Absence of arbitrage is easily derived from the corresponding liquid model. For the illiquid optimal investment problem we obtain existence of optimal investment policies for utility from terminal wealth. In the special case of arithmetic Brownian motion and exponential utility, the singular optimal control problem turns out to have a deterministic solution which can be computed explicitly. (This is joint work with Moritz Voss)

Mathias Beiglboeck

"*An optimal principle from mass transport and applications to model-independence.*"

ABSTRACT. Model-independent pricing has grown into an independent field in Mathematical Finance during the last 15 years. A driving inspiration in this area has been the fruitful connection to the Skorokhod embedding problem. We discuss a more recent approach to model-independent pricing, based on a link to Monge-Kantorovich optimal transport. Based on a similar technique in optimal transport we derive a "variational principle" that is applicable to model-independent pricing. This transport-viewpoint also sheds new light on Skorokhod's classical problem.

Sara Biagini

"*Robust Fundamental Theorem for Continuous Processes*"

ABSTRACT. We study a continuous-time financial market with continuous price processes under model uncertainty; more precisely, under a family $\mathcal{P}$ of possible physical measures. A robust notion $\mathrm{NA}_1(\mathcal{P})$ of no-arbitrage

of the first kind is introduced; it postulates that a nonnegative, nonvanishing claim cannot be superhedged for free by using simple trading strategies. Our first main result is a version of the fundamental theorem of asset pricing: $\mathrm{NA}_1(\mathcal{P})$ holds if and only if every $P \in \mathcal{P}$ admits a measure Q that is an equivalent martingale measure before a certain lifetime. The second main result provides the existence of optimal superhedging strategies for general contingent claims and a representation of the superhedging price in terms of martingale measures.

Bruno Bouchard

"*Stochastic target games via regularized viscosity solutions: application to super-hedging under coefficients' uncertainty*"

ABSTRACT. We study a class of stochastic target games where one player tries to find a strategy such that the state process almost-surely reaches a given target, no matter which action is chosen by the opponent. Our main result is a geometric dynamic programming principle which allows us to characterize the value function as the viscosity solution of a non-linear partial differential equation. Because abstract measurable selection arguments cannot be used in this context, the main obstacle is the construction of measurable almost-optimal strategies. We propose a novel approach where smooth supersolutions are used to define almost-optimal strategies of Markovian type, similarly as in verification arguments for classical solutions of Hamilton-Jacobi-Bellman equations. The smooth supersolutions are constructed by an extension of Krylov's method of shaken coefficients. We apply our results to a problem of option pricing under model uncertainty with different interest rates for borrowing and lending.

Luciano Campi

"*Utility indifference pricing for non-smooth payoffs in a model with non-tradable assets*"

ABSTRACT. We consider the problem of exponential utility indifference valuation under the simplified framework where traded and nontraded assets are uncorrelated but where the claim to be priced possibly depends on both. Traded asset prices follow a multivariate Black and Scholes model, while nontraded asset prices evolve as generalized Ornstein-Uhlenbeck processes. We provide a BSDE characterization of the utility indifference price (UIP) for a large class of non-smooth, possibly unbounded, payoffs depending simultaneously on both classes of assets. Focusing then on European claims and using the Gaussian structure of the model allows us to employ some BSDE techniques (in particular, a Malliavin-type representation theorem due to Ma and Zhang (2002)) to prove the regularity of Z and to characterize the UIP for possibly discontinuous European payoffs as a viscosity solution of a suitable PDE with continuous space derivatives. The optimal hedging strategy is also identified essentially as the delta hedging strategy corresponding to the UIP. Since there are no closed-form formulas in general, we also obtain asymptotic expansions for prices and hedging strategies when the risk aversion parameter is small.

Umut Çetin

"*Equilibrium with risk averse market makers and related inverse problems*"

ABSTRACT. We analyse the existence of a continuous-time Nash equilibrium in a financial market with risk averse market makers and an informed trader with a private information. When the insiders signal is static, the optimal strategies of the agents turn out to be solutions of a forward-backward system of partial and stochastic differential

equations. If the private signal of the insider varies in time, existence of equilibrium depends on the solution of a linear inverse problem, which is equivalent to a backward parabolic PDE with an initial condition.

Alex Cox

"*An optimal stopping approach to the n-marginal Root problem, and applications to variance options*"

ABSTRACT. Recently, the problem of finding robust bounds on option prices which incorporate information from vanilla options has generated renewed interest in solutions to the classical Skorokhod Embedding Problem (SEP). It is natural to consider generalisations of the problem where the prices of the vanilla options are known both at the maturity of the option, and also at intermediate times. In this talk, we consider a generalisation of Root's solution to the SEP where we look for an ordered sequence of stopping times, each of which embeds a given distribution. In particular, we are able to identify these stopping times as the exit times from certain domains, and we are able to characterise these domains naturally as the stopping regions of a suitable multiple stopping problem. Moreover, we are able to show optimality for these stopping times, and hence derive sub-hedging strategies which enforce the price bounds in any suitable model. (Joint work with Jan Obloj and Nizar Touzi.)

Christa Cuchiero

"*A convergence result for the emery topology and a variant of the proof of the fundamental theorem of asset pricing*"

ABSTRACT. We work in the general setting of admissible portfolio wealth processes as introduced by Y. Kabanov. We show that in this setting the (NUPBR) condition (No unbounded profit with bounded risk) implies the so called P-UT property, a boundedness property in the Emery topology which has been introduced by C. Stricker. Combining this with results from Memin-Slominski and a maximality assumption leads to convergence in the Emery topology and thus to a short variant of the proof of the fundamental theorem of asset pricing initially proved by Delbaen and Schachermayer. (The talk is based on joint work with Josef Teichmann.)

Jakša Cvitanić

"*Moral Hazard in Dynamic Risk Management*"

ABSTRACT. We consider a contracting problem in which a principal hires an agent to manage a risky project. When the agent chooses volatility components of the output process and the principal observes the output continuously, the principal can compute the quadratic variation of the output, but not the individual components. This leads to moral hazard with respect to the risk choices of the agent. Using a recent theory of singular changes of measures for Ito processes, we formulate a principal-agent problem in this context, and solve it in the case of CARA preferences. In that case, the optimal contract is linear in these factors: the contractible sources of risk, including the output, the quadratic variation of the output and the cross-variations between the output and the contractible risk sources. Thus, path-dependent contracts naturally arise when there is moral hazard with respect to risk management. We also provide comparative statics via numerical examples, showing that the optimal contract is sensitive to the values of risk premia and the initial values of the risk exposures. (Joint with N. Touzi and D. Possamai)

Christoph Czichowsky

"*Strong Supermartingales and Portfolio Optimisation under Transaction Costs*"

ABSTRACT. In this talk, I will sketch how to develop a duality theory for portfolio optimisation under transaction costs and some of the new phenomena arising in this context. This talk is based on joint work with Walter Schachermayer.

Hans Föllmer

"*Spatial risk measures: local specification and phase transition*"

ABSTRACT. In the spatial setting of a large network, the local specification of convex risk measures can be seen as a non-linear extension of the local specification of equilibrium states in Statistical Mechanics. We discuss the corresponding aggregation problem of passing from local to global risk measures and the appearance of phase transitions. This will involve a non-linear extension of backwards martingale convergence, arguments from preference theory, and a spatial version of Dynkin's construction of entrance boundaries for Markov processes.

Christoph Frei

"*Finding local equilbria by splitting multidimensional BSDEs*"

ABSTRACT. We consider a model of a financial market where investors take not only their own absolute performance, but also the relative performance compared to their peers into account. The goal is to find equilibria where every investor has an individually optimal strategy. This problem is related to the study of multidimensional backward stochastic differential equations (BSDEs). We introduce a new notion of local solution by splitting multidimensional BSDEs over time. This allows us to show that the BSDE from our financial problem is locally but not globally solvable. From this, we deduce that there exist local but no global equilibria in our model of a financial market. By considering the relative performance, investors may ruin each other so that equilibria exist only over a short time.

Marco Frittelli

"*Robust Arbitrage under Uncertainty*"

ABSTRACT. In a model independent financial market, we introduce a topological notion of Robust Arbitrage, without fixing an a-priori set of reference probability measures. This notion relies only on the market structure and can be dually represented in terms of weakly open sets of probability measures. We then show that the absence of Robust Arbitrages with respect to an opportune filtration enlargement, guarantees the existence of full support martingale measures.

Paolo Guasoni

"*The Limits of Leverage*"

ABSTRACT. When trading incurs proportional costs, leverage can scale an asset's 1eturn only up to a maximum multiple, which is sensitive to the asset's volatility and liquidity. In a continuous-time model with one safe and one risky asset with constant investment opportunities and proportional transaction costs, we find the efficient portfolios that maximize long term expected returns for given average volatility. As leverage and volatility increase, rising rebalancing costs imply a declining Sharpe ratio. Beyond a critical level, even the expected return declines. For funds that seek to replicate multiples of index returns, such as leveraged ETFs, our efficient portfolios optimally trade off alpha against tracking error. (Joint work with Eberhard Mayerhofer)

Vicky Henderson

"*The Value of Being Lucky: Option Backdating and Non-diversifiable risk*"

ABSTRACT. The practice of executives influencing their option compensation by setting a grant date retrospectively is known as backdating. Since these options are usually granted at-the-money, selecting an advantageous grant date will be valuable to the executive. There is substantial evidence that backdating took place in the US, particularly prior to the tightening of SEC reporting requirements. In this talk, we develop and solve a utility-indifference model to quantify the value of the opportunity to backdate options. We show that the magnitude of ex ante gains from backdating is significant. Our model can be used to explain why backdating was more prevalent at firms with highly volatile stock prices. Explanations hinge on the executive's inability to perfectly hedge and desire to exercise options early. Joint work with Jia Sun (China Credit Ratings) and Elizabeth Whalley (Warwick Business School)

Tomoyuki Ichiba

"*Some Aspects of Universal Portfolios*"

ABSTRACT. We discuss Cover's universal portfolios in the context of Stochastic Portfolio Theory. By enlarging the class of portfolio generating functions, we see universal portfolios are generated by functions, given excess growth rates of constant rebalanced portfolios. These generating functions and resulting universal portfolios can be represented as integrations with respect to tilted version of maximal entropy measure. In this way we may answer one of the open questions posed by Fernholz & Karatzas (2009). With analyses of concentration of measures we evaluate performance of universal portfolios. Finally, we discuss universal portfolios under large equity market models.

Monique Jeanblanc

"*Arbitrages in progressive enlargement of filtrations*"

ABSTRACT. We study a financial market in which some assets, with prices adapted w.r.t. a reference filtration $\mathbb{F}$ are traded. One then assumes that an agent has some extra information, and may use strategies adapted to a larger filtration $\mathbb{G}$. This extra information is modeled by the knowledge of some random time τ, when this time occurs.

We restrict our study to progressive enlargement setting, and we pay a particular attention to honest times. Our goal is to detect if the knowledge of τ allows for some arbitrage (classical arbitrages and arbitrages of the first kind), i.e., if using $\mathbb{G}$-adapted strategies, one can make profit.

The results presented here are based on two joint papers with Aksamit, Choulli, Deng, in which the authors study No Unbounded Profit with Bounded Risk (NUPBR) in a general filtration $\mathbb{F}$ and the case of classical arbitrages in the case of honest times, density framework and immersion setting. We shall also study the information drift and the growth optimal portfolio resulting from that model. (Based on joint work with A. Aksamit, T. Choulli, J. Deng, T. Schmidt.)

Jan Kallsen

"*On portfolio optimization and indifference pricing with small transaction costs: rigorous proofs based on duality*"

ABSTRACT. Portfolio optimization problems with frictions as e.g. transaction costs are hard to solve explicitly. In the limit of small friction, solutions are often of much simpler structure. In the last twenty years, considerable progress has been made both in order to derive formal asymptotics as well as rigorous proofs. However, the latter usually rely on rather strong regularity conditions, which are hard to verify in concrete models. Some effort is still needed to make the results really applicable in practice. This talk is about a step in this direction. More specifically, we discuss portfolio optimization for exponential utility under small proportional transaction costs. As an example, we reconsider the Whalley-Willmott results of utility-based pricing and hedging in the Black-Scholes model. We relax the conditions required by Bichuch who gave a rigorous proof for smooth payoffs under sufficiently small risk aversion.

Ioannis Karatzas

"*The Inflationary Bias of Real Uncertainty and a Harmonic Fisher-Equation*"

ABSTRACT. We argue that real uncertainty by itself causes long-run nominal inflation. We start with an infinite-horizon, cash-in-advance economy with a representative agent, and with real uncertainty modelled by independent, identically distributed endowments. Suppose the central bank fixes the nominal rate of interest. We show that the equilibrium long-run rate of inflation is strictly higher, on almost every path of endowment realizations, than it would be if these endowments were constant. Indeed, we present an explicit formula for the long-run rate of inflation, based on the famous Fisher equation. This posits that, in the absence of real uncertainty, the rate of inflation should depend on the monetary rate of interest and on the time-preference of the agents in the economy, and on nothing else. The long-run Fisher equation for our stochastic economy turns out to be similar, but with the rate of inflation replaced by the harmonic mean of the growth rate of money.

We also show that these features are also present, albeit with less explicit results, when one considers an economy with fiat money and a continuum of agents, one non-durable commodity, countably many time periods, and a central bank. (This is joint work with John Geanakoplos, Martin Shubik and William D. Sudderth.)

Kasper Larsen

"*Taylor approximation of incomplete Radner equilibrium models*"

ABSTRACT. In the setting of exponential investors and uncertainty governed by Brownian motions we first prove the existence of an incomplete equilibrium for a general class of models. We then introduce a tractable class of exponential-quadratic models and prove that the corresponding incomplete equilibrium is characterized by a coupled set of Riccati equations. Finally, we prove that these exponential-quadratic models can be used to approximate the incomplete models we studied in the first part. (Joint work with Jin Hyuk Choi.)

Martin Larsson

"*Novikov-type conditions for processes with jumps*"

ABSTRACT. We provide a novel proof for the sufficiency of Novikov-Kazamaki type conditions for the martingale property of nonnegative local martingales with jumps. The proof is based on explosion criteria for related processes under a possibly non-equivalent measure. (Joint work with Johannes Ruf.)

Johannes Muhle-Karbe

"*Trading with small price impact*"

ABSTRACT. An investor trades a safe and several risky assets with linear price impact to maximize expected utility from terminal wealth. In the limit for small impact costs, we explicitly determine the optimal policy and welfare, in a general Markovian setting allowing for stochastic market, cost, and preference parameters. These results shed light on the general structure of the problem at hand, and also unveil close connections to optimal execution problems and to other market frictions such as proportional and fixed transaction costs. (Joint work with Ludovic Moreau and H. Mete Soner)

Marcel Nutz

"*Nonlinear Lévy Processes and their Characteristics*"

ABSTRACT. We develop a general construction for nonlinear Lévy processes with given characteristics. More precisely, given a set Θ of Lévy triplets, we construct a sublinear expectation on Skorohod space under which the canonical process has stationary independent increments and a nonlinear generator corresponding to the supremum of all generators of classical Lévy processes with triplets in Θ. The nonlinear Lévy process yields a tractable model for Knightian uncertainty about the distribution of jumps for which expectations of Markovian functionals can be calculated by means of a partial integro-differential equation. (Joint work with Ariel Neufeld.)

Jan Obłój

"*Robust hedging of barrier options with beliefs on implied Volatility*"

ABSTRACT. We develop an abstract robust modelling framework accommodating as inputs market priced of options and modelling beliefs formulated in terms of pathspace restrictions. This naturally allows us to talk about robust market models. As an example we consider pricing and hedging of barrier options with beliefs about future levels of implied volatilities. We construct local volatility models which satisfy such constraints and use them to combine static and robust hedging methods. We discuss asymptotic convergence when beliefs become stronger (model specific) or weaker (model independent). (Joint work with Sergey Nadtochiy)

Sergio Pulido

"*Existence and uniqueness results for multi-dimensional quadratic BSDEs arising from a price impact model with exponential utility*"

ABSTRACT. In this work we study multi-dimensional systems of quadratic BSDEs arising from a price impact model where an influential investor trades illiquid assets with a representative market maker with exponential preferences. The impact of the strategy of the investor on the prices of the illiquid assets is derived endogenously through an equilibrium mechanism. We show that a relationship exists between this equilibrium mechanism and a multi-dimensional system of quadratic BSDEs. We also specify conditions on the parameters of the model that guarantee that the system of BSDEs has a unique solution, which corresponds to a family of unique equilibrium prices for the illiquid assets. The proof relies on estimates that exploit the structure of the equilibrium problem. Finally, we provide examples of parameters for which the corresponding system of BSDEs in not well-posed. (This is joint work with Dmitry Kramkov.)

Scott Robertson

"*Continuous Time Perpetuities and the Time Reversal of Diffusions*"

ABSTRACT. In this talk we consider the problem of obtaining the distribution of a continuous time perpetuity, where the non-discounted cash flow rate is determined by an ergodic diffusion. Using results regarding the time reversal of diffusions, we identify the distribution of the perpetuity with the invariant measure associated to a certain (different) ergodic diffusion. This enables efficient estimation of the distribution via simulation and, in certain instances, an explicit formula for the distribution. Time permitting, we will talk about how Large Deviations Principles and results concerning Couplings of diffusions can be used to estimate rates of convergence, thus providing upper bounds for how long simulations must be run when obtaining the distribution.

Johannes Ruf

"*Convergence of local supermartingales*"

ABSTRACT. We characterize the event of convergence of a local supermartingale. Conditions are given in terms

of its predictable characteristics and jump measure. Furthermore, it is shown that L^1-boundedness of a related process is necessary and sufficient for convergence. The notion of extended local integrability plays a key role. (Joint work with Martin Larsson.)

Martin Schweizer

"*Some ideas on bubbly markets*"

ABSTRACT. We introduce a notion of bubbly markets. This is an economically motivated and formulated concept which captures the idea that a given financial markets contains "bubbles". We give dual characterisations of bubbly markets in terms of numeraires and martingale measures, and we show in particular that in any "reasonable" bubbly market, discounted prices must be strict local martingales, for any numeraire and any martingale measure associated to that numeraire. This can be viewed as a "robust" notion of a market containing a bubble. We show by examples how different concepts in our setting are related, discuss related literature, and explain how existing work fits into our framework. If time permits, we also discuss the issue of valuation principles for financial products in markets with bubbles. (The talk is based on ongoing joint work with Martin Herdegen, ETH Zürich).

Steve Shreve

"*Should banks escrow traders' bonuses?*"

ABSTRACT. We consider the principle agent problem of a bank deciding whether it is advantageous to escrow traders' bonuses. The escrow model is the following. Each year a trader manages a portfolio for a bank. At the end of the year, based on the trader's performance, the bank pays a bonus into an escrow account. If he has not had a disastrous year, the trader can consume from the bonus paid the previous year. Within each year the trader has a continuous-time optimal control problem, and the problem across years is set up as infinite-horizon discounted dynamic programming. It is shown that is sometimes to the bank's advantage to escrow the bonus, and sometimes it is not. (This is work in progress with Jing Wang.)

Mihai Sîrbu

"*A new look at zero-sum stochastic differential games*"

ABSTRACT. We revisit the well studied problem of zero-sum stochastic differential games. We consider a symmetric formulation over (path-dependent) feed-back strategies, carefully restricted to produce strong solutions of the state equations. Using a stochastic modification of Perron's method we show that the lower and upper values are solutions to the corresponding Hamilton-Jacobi-Bellman-Isaacs equations. If the Isaacs condition hods, the game has a value over such pure feed-back strategies. If the Isaacs condition does not hold, then generalized/mixed strategies need to be considered to obtain a value.

Ronnie Sircar

"*Optimal Investment with Transaction Costs and Stochastic Volatility*"

ABSTRACT. Two major financial market frictions are transaction costs and uncertain volatility, and we analyze their joint impact on the problem of portfolio optimization. When volatility is constant, the transaction costs optimal investment problem has a long history, especially in the use of asymptotic approximations when the cost is small. Under stochastic volatility, but with no transaction costs, the Merton problem under general utility functions can also be analyzed with asymptotic methods. Here, we look at the long-run growth rate problem when both frictions are present, using separation of time scales approximations. This leads to perturbation analysis of an eigenvalue problem. We also describe some related infinite horizon problems where these methods can be effective.

Peter Tankov

"*Optimal discrete-time hedging with directional views, or how to make some money while hedging your option*"

ABSTRACT. We consider the hedging error due to discrete-time rebalancing of a given hedging strategy, in the presence of drift of the underlying asset price. The problem is to choose the optimal rebalancing times. Under the mean-variance criterion, the choice of rebalancing times is reduced to a non-degenerate Linear-Quadratic optimal control. A modified version of the Sharpe ratio is also considered and we obtain explicit expressions for the optimal rebalancing times. These results are obtained under an asymptotic framework. (Joint with J. Cai, M. Fukasawa and M. Rosenbaum.)

Josef Teichmann

"*FTAP for large financial markets*"

ABSTRACT. For a sequence of (small) markets defined on a single stochastic basis we can characterize the existence of an equivalent separating measure by a condition reminiscent to NFLVR. In particular no weak star closures are needed to state this condition. (Joint work with Christa Cuchiero and Irene Klein.)

Hao Xing

"*Existence of close to Pareto optimal incomplete Radner equilibrium*"

ABSTRACT. We consider an equilibrium model between exponential investors whose random endowments cannot be spanned by the traded asset. We first characterize the set of endowments which induce Pareto optimal equilibrium. For endowments close to this set, we establish three existence results of equilibria which are not Pareto optimal. In a non-Markovian setting, the first existence result is established by analysing a system of coupling quadratic BSDEs, via the techniques introduced by Tevzadze (2008). Then the first result is improved by a BMO-norm estimate in the second result. In a Markovian setting, equilibrium is established using partial regularity results for system of parabolic PDEs with quadratic nonlinearity in gradient. (This is work in progress with Constantinos Kardaras and Gordan Žitković.)

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Bibliography

[Ber54] Daniel Bernoulli, Exposition of a new theory on the measurement of risk, Econometrica **22** (1954), no. 1, 23–36, Translation from the Latin by Dr. Louise Sommer of work first published 1738.

[DH85] Darrell Duffie and C. F. Huang, Implementing Arrow-Debreu equilibria by continuous trading of few long-lived securities, Econometrica **53** (1985), no. 6, 1337–1356.

[DS94] Freddy Delbaen and Walter Schachermayer, A general version of the fundamental theorem of asset pricing, Math. Ann. **300** (1994), no. 3, 463–520.

[DS98] F. Delbaen and W. Schachermayer, The fundamental theorem of asset pricing for unbounded stochastic processes, Math. Ann. **312** (1998), no. 2, 215–250.

[HK79] J. Michael Harrison and David M. Kreps, Martingales and arbitrage in multiperiod securities markets, J. Econom. Theory **20** (1979), no. 3, 381–408.

[HP81] J. Michael Harrison and Stanley R. Pliska, Martingales and stochastic integrals in the theory of continuous trading, Stochastic Process. Appl. **11** (1981), no. 3, 215–260.

[KLS90] Ioannis Karatzas, John P. Lehoczky, and Steven E. Shreve, Existence and uniqueness of multi-agent equilibrium in a stochastic, dynamic consumption/investment model, Math. Oper. Res. **15** (1990), no. 1, 80–128.

[KLSX91] I. Karatzas, J. P. Lehoczky, S. E. Shreve, and G. L. Xu, Martingale and duality methods for utility maximization in an incomplete market, SIAM Journal of Control and Optimisation **29(3)** (1991), 702–730.

[Kre81] David M. Kreps, Arbitrage and equilibrium in economies with infinitely many commodities, J. Math. Econom. **8** (1981), no. 1, 15–35.

[KS99] D. Kramkov and W. Schachermayer, The asymptotic elasticity of utility functions and optimal investment in incomplete markets, Ann. Appl. Probab. **9** (1999), no. 3, 904–950.

[Mer71] R. C. Merton, Optimum consumption and portfolio rules in a conitinuous-time model, J. Economic Theory **3** (1971), 373–413.

Chapter 19

Imaging and Modeling in Electron Microscopy - Recent Advances (14w5048)

May 18 - 23, 2014

Organizer(s): Peter Binev (University of South Carolina), Nigel Browning (Pacific Northwest National Lab), Wolfgang Dahmen (RWTH Aachen), Ronald DeVore (Texas A & M University), Thomas Vogt (University of South Carolina), Paul Voyles (University of Wisconsin, Madison)

The idea of this workshop is to bring together mathematicians and specialists in electron microscopy to discuss the future developments of the methods and approaches in assessing and understanding the data from materials at the nanoscale. There are several research areas in mathematics that can produce results beneficial for electron microscopy. While trying to establish connections between mathematicians working in these areas with scientists employing electron microscopy in their research, the goal is to go further than that and start fruitful collaborations that will provide new challenging mathematical problems, solutions of which will enhance the understanding of the materials in the nanoscale.

19.1 Overview of the Field

The field of Mathematical Electron Microscopy is to be developed and this workshop is one of the steps towards forming the general research area and identifying the research directions. The goal is to go outside the standard data and image processing research and address the challenging problems arising with the constantly developing nanoimaging instruments. It is about combining an accurate mathematical modeling of the processes that produces the data with successfully solving the mathematical problems needed for its faithful interpretation.

Previous small workshops at the University of South Carolina provided a first assessment of how new mathematical tools and theories could advance data analysis in modern electron microscopy and, in particular, in such areas as cryo-electron microscopy of biological matter and aberration-corrected scanning transmission electron microscopy. Based on these initial workshops a recently published book [56] entitled “Modeling Nanoscale Imaging in Electron Microscopy” (Springer, March 2012) summarized relevant methodologies such as super-resolution techniques, special de-noising and alignment methods, the application of mathematical and statistical learning theory, as well as a detailed introduction to compressed sensing and its possible influence on electron microscopy. The community is also very interested in implementing new measurement techniques based on ideas related to the single pixel camera and compressed sensing which could significantly reduce the measurement times and open up whole new fields of soft and/or hybrid materials to STEM imaging and tomography. Our goal to continue to push the boundaries of the electron imaging by enhancing data acquisition and state-of-the-art image analysis was also partially supported by a highly competitive seed grant from the National Academies Keck Futures Initiative.

The proposal for a BIRS workshop was an attempt to involve more members of the scientific community in the realization of this goal.

19.2 Recent Developments and Open Problems

The scope of the conference was purposefully allowed to be broad and talks bridged interests from quantum physics (Simulating core-loss scattering in the STEM by Christian Dwyer [8]) to biological applications (Chandrajit Bajaj [2], Yoel Shkolnisky [45], Amit Singer [46]). A series of talks on mathematical themes such as greedy algorithms (Deanna Needell [35]), compressed sensing approaches (Gitta Kutyniok [25]), de-noising techniques (Bin Han [17], Niklas Mevenkamp [32]) and image registration techniques (Benjamin Berkels [4]) was interspersed with talks on experimental approaches to imaging (Mark Davenport [7], Kevin Kelly [21], Thomas Vogt [55], Joachim Mayer [31], Sarah Haigh [14], Jarzy Sadowski [37], and Zineb Saghi [38]). Intriguing future directions were presented in presentations by Nigel Browning and Bryan Reed [36] on dynamic transmission electron microscopy (DTEM) which highlighted the need for better tool to correct and align terra-bytes of data in the near future. Dirk Van Dyck's talk ("Addressing Feynmans Challenge The 3D shape of nano-crystals from single projections at atomic resolution" [53]) reminded us that many new imaging tools were developed to establish structure-property relationships in nanomaterials and how much progress we have made in the past two decades.

Lively discussions after the talks and in the scheduled discussion sessions centered on broad ("How can Mathematics help Electron Microscopy?"[6]) as well as more focused issues ("Elemental quantification using energy dispersive x-ray spectrometry in the STEM"[16] and "Improving Precision and Signal to Noise Ratio in Electron Micrographs"[57]).

While the usual meaning of "imaging" is "visual representation of the information received from the data", it is often the case that it is perceived as a much broader process that includes the extraction of this information. To some extend this is the case in choosing the title of this workshop. One of the main points from this workshop is that the extraction of the information is better done with methods that are not image processing per se. There are several open questions in this field that remain to be answered. A number of them were posed in some of the talks and during the discussions. They are often problem specific but in general can be summarized in two main theme questions: **(i)** How to better extract relevant information from the data received by the existing data gathering procedures? and **(ii)** How to change these procedures to allow more reliable and efficient information extraction?

19.3 Presentation Highlights

The workshop featured 31 talks and three discussions. Due to the interdisciplinary nature of the workshop, the diversity of the subjects was significant and we had to go a bit against the guidelines suggesting fewer talks. In the summary below the talks are formally separated into six groups. This separation is for the purposes of the presentation and it should be clear that many of the talks could have been put in other group(s). The first two groups (Subsections 19.3.1 and 19.3.2) contain talks which are either mathematical in their nature or realize a new mathematical concept through processing experimental data. While in the first group (Subsection 19.3.1) the emphasis is on improving the acquisition process and formulating new theoretical results that could be relevant as a mathematical background for developing new methods in this direction, the second group (Subsection 19.3.2) features mathematical and algorithmic advances in processing the data. The quest of improving the instrumentation and creating new ways of collecting data is presented in the third group of talks (Subsection 19.3.3). The fourth group (Subsection 19.3.4) is rather small and includes only the talks in which modeling and simulation were the primary topics. Nevertheless, these topics were presented as part of the research in several other talks. The final two groups (Subsections 19.3.5 and 19.3.6) are devoted to receiving the 3D information of the observed object. Electron tomography is the primary subject of the talks from Subsections 19.3.5 while Subsections 19.3.6 features results for cryo-electron microscopy and research for biological applications.

19.3.1 Mathematics of Data Assimilation

The talk of B. Berkels [4] first considered the problem of averaging a series of noisy scanning transmission electron microscopy (STEM) images producing an improved image that surpasses the quality attainable by single shot STEM images. The main task in tackling this problem is the task of transform- ing two or more images into a common coordinate system, from the perspective of electron microscopy. The classical registration approach for image pairs is extended to handle the registration of hundreds of consecutive images to a single image with a special emphasis on input data with a low signal-to-noise ratio and periodic structures. One of the key ingredients is the use of a non-rigid transformation model that is able to cope with the frame-to-frame distortions resulting from the serial pixel-wise acquisition of STEM images. In the second part, it was discussed how to find global minimizers of a class of variational models that have a convex regularization term like total variation. This is achieved by constructing a convex minimization problem with a pointwise constraint in a higher dimension whose minimizers fulfill a thresholding theorem: The 0.5-level set of a minimizer of the convex problem is the subgraph of a minimizer of the original problem. Unlike the functional in the existing convexification models, the target functional in the proposed reformulation is strongly convex. Two immediate advantages of the strong convexity are that the reformulation has a unique solution and that more efficient minimization algorithms can be used.

The practical use of the above ideas was presented in the talk of A. Yankovich [60]. He considered atomic-resolution by scanning transmission electron microscopy (STEM) and the question "how precisely can the positions of the atoms be measured?". Precision smaller than the resolution is routinely attainable, but in STEM it is limited by practical problems, such as image distortions caused by instabilities of the electron probe and the sample, before reaching the fundamental signal-to-noise ratio (SNR) precision limit. A non-rigid registration of a series of STEM images [5] is used to undo the effect of instabilities and enable averaging to improve the SNR and thus the precision. Non-rigit registration and averaging results in reproducible sub-pm precision [61], 5-7 times better than what is attainable with rigid registration and the best ever reported in electron microscopy. We have applied this high precision STEM method to measuring the surface atom distortions on a Pt nanocatalyst, for which the catalytic activity of the nanoparticles is determined by their atomic surface structure. Another important problem is determining three dimensional atomic structures of materials from the acquired two dimensional images. NR registration of STEM images enables extraction of 3D atomic structure information using the standardless atom counting method with the best-reported uncertainties. Previous results using the same method reported a few atom uncertainty and were limited by image Poisson noise. The extremely high SNR images resulting from NR registration allows for standardless atom counting with < 1 atom uncertainty for a majority of the atomic columns in the Pt nanocatalyst, with no limitation from Poisson noise.

The problem of recovering a sparse image from a small number of noisy measurements was considered in M. Davenport's talk [7]. In the case where the measurements are acquired in a nonadaptive fashion as in the standard compressive sensing framework, lower bounds on the minimax mean-squared error of the recovered vector very nearly match the performance of ℓ_1-minimization techniques, and hence in certain regimes these techniques are essentially optimal. Surprisingly, in the case where the measurements are acquired sequentially in an adaptive manner, the speaker showed that in certain worst-case regimes, adaptivity does not allow for substantial improvement over standard nonadaptive techniques in terms of the minimax mean-square error. Nonetheless, there are important regimes where the benefits of adaptive sensing are clear and overwhelming, and can be achieved via relatively simple algorithms.

The talk of K. Kelly [21] was giving insides about how to translate the mathematical breakthroughs of compressive sensing into actual imaging systems. A particular example are optical systems that acquire portions of the spectrum from ultraviolet to infrared. These cameras rely on making many multiplexed measurements over time summed into a single or a few detectors. In the case of video, the motion in the scene during acquisition disrupts the scene reconstruction. To overcome this, they designed and developed various algorithms to successfully reconstruct both the background and foreground. A few comments were made on how to exploit this in the design of compressive optical microscopy instrumentation for sum-frequency generation imaging of molecular vibrations and darkfield imaging of plasmon resonances.

The talk of A. Stevens [48] considered techniques in machine learning and compressive sensing with applications in electron microscopy. The contribution of compressive sensing is twofold- - it can be used to reduce dose (spatial compression) and increase acquisition speed (time compression). In the case of spatial compressive sensing, Bayesian dictionary learning was used. This method infers the underlying basis space and a sparse representation from the compressed measurements. For temporal compressive sensing the Gaussian mixture model is used. Both of the approaches are relatively recent developments from statistical machine learning. Computational experiments in spatial and temporal compressive sensing will be presented.

D. Needell addressed in her talk [35] the problem of identifying a high resolution image from a subsampled, or lower resolution image. This is usually referred to as super-resolution. The problem can me modeled as a sparse recovery problem when the measurement operator has a pre-defined specific structure. The talk contained some new work on greedy algorithms which can handle the structure in the measurement operator for super-resolution. Experimental results as well as theoretical guarantees were presented.

In her talk R. Ward [58] presented a general framework which aims to address the question: for which sets of points, using what randomized linear maps, and to what extent is dimensionality reduction in ℓ_1 possible? Through the Johnson-Lindenstrauss Lemma and related results, it is known that a small set of points in a high-dimensional space can be linearly embedded into a space of much lower dimension in such a way that Euclidean distances between the points are nearly preserved, and that a random projection can be used for such embeddings. At the same time, it is known that a result of this kind is not possible if we replace Euclidean distance by the ℓ_1 norm, at least not for arbitrary sets of points. Certain sets, such as sparse vectors, can be linearly embedded in low dimension with respect to the ℓ_1 norm, and sparse random matrices work well for such embeddings.

19.3.2 Mathematics of Data Processing

G. Kutyniok considered in her talk [25] the important question about how to extract the individual components from imaging data composed of several geometrically distinct constituents. She utilized the novel methodology of Compressed Sensing to show that this geometric separation problem can indeed be solved both numerically and theoretically. For the separation of point- and curvelike objects, the solution of choice is to deliberately overcomplete a representation system made of wavelets (suited to pointlike structures) and shearlets (suited to curvelike structures). The decomposition principle is to minimize the ℓ_1-norm of the representation coefficients or to perform iterative thresholding. The theoretical results, which are based on microlocal analysis considerations, show that at all sufficiently fine scales, nearly-perfect separation is indeed achieved.

In his talk O. Scherzer [42] introduced variational motion estimation and decomposition for images that are defined on an evolving surface. While optical flow is traditionally computed from a sequence of flat images and used for motion estimation, the concept of optical flow is extended to a dynamic non-Euclidean setting to provide a concept for decomposition of flows. An application to biological imaging was presented.

The talk of Z. Shen [44] provided some insides about the wavelet frame-based image and video restorations. It started with some of main ideas and various examples including image and video inpainting, denoising, decomposition, image deblurring and blind deblurring, segmentation, CT image reconstruction, 3D reconstruction in electron microscopy, and etc. In all of these applications, spline wavelet frames derived from the unitary extension principle are used. This allows to establish connections between wavelet frame based method and various PDE based methods, that include the total variation model, nonlinear diffusion PDE based methods, and model of Mumford-Shah. A convergence analysis in terms of objective functionals and their approximate minimizers was discussed.

A new image processing tool that can find applications in different fields and in electron microscopy, in particular, was discussed in the talk of B. Han [17]. He introduced directional separable complex tight framelets and showed that directionality can be greatly improved by using separable complex tight framelets. While keeping the efficient tensor product structure, this approach has the advantages of much better improved directionality and the use of finitely supported complex tight framelets. For the image denoising problem, we show that separable complex tight framelets have significant performance gains (typically, 0.5db to 1db improvement) compared with several state-of-the-art image denoising methods such as undecimated wavelet transform, dual tree complex wavelet transform, shearlets, curvelets, total variation based method, and etc.

In his talk F. Krahmer [23] presented a recently introduced algorithm, called PhaseLift, for phase recovery that is computationally tractable, numerically stable, and comes with rigorous performance guarantees. PhaseLift is optimal in the sense that the number of amplitude measurements required for phase reconstruction scales linearly with the dimension of the signal. However, it specifically demands Gaussian random measurement vectors – a limitation that restricts practical utility and obscures the specific properties of measurement ensembles that enable phase retrieval. Two partial derandomizations of PhaseLift were presented. First one is a construction that only requires sampling from certain polynomial size vector configurations, called t-designs. Such configurations have been studied in algebraic combinatorics, coding theory, and quantum information. Reconstruction guarantees are given for a number of measurements that depends on the degree t of the design. If the degree is allowed to grow logarithmically with the dimension, the bounds become tight up to polylog-factors. Second one uses Fourier measurements with random masks as they are encountered in x-ray crystallography. Here the number of measurements is optimal up to a single logarithmic factor.

In his talk N. Mevenkamp [32] proposed modifications of the classical non-local means algorithm (NLM) to certain characteristics typical for Scanning Transmission Electron Microscopy (STEM) imaging. The focus was on three aspects: periodic recurrence of patterns, local horizontal distortions, and the noise type. The periodic distribution of the objects within the image is exploited to formulate an efficient strategy to search for similar patches. A periodic search grid is approximated from the images Fourier transform. The local horizontal distortions inherent to STEM images cause difficulties to recognize self similarities with the classical patch similarity measure. The proposition is to counter these horizontal distortions by allowing line shifts that improve patch regularity. The most dominant source of noise in STEM imaging is typically Poisson distributed. However, the NLM algorithm was originally designed to remove additive Gaussian noise. The proposed modifications have been shown to increase the denoising performance on STEM images, especially in high intensity regions. Finally, it was discussed a method to correct the horizontal distortions in STEM images based on the NLM weights.

19.3.3 Experimental Approaches to Nano Imaging and Data Processing

B. Reed introduced in his talk [36] a new data acquisition procedure Movie-Mode Dynamic Transmission Electron Microscopy (MM-DTEM) that can benefit greatly from recent developments in applied mathematics. The idea of doing experiments inside the microscope, of actually capturing the crucial during moments instead of merely before and after, is now one of the biggest growth areas in TEM. An essential difficulty with this is time resolution, the importance of which derives from general physical scaling laws. Simply put, small things tend to move fast. The nanometer- and micrometer-scale processes most relevant to materials science typically happen on nanosecond to microsecond scales, far faster than the multi-millisecond scales of conventional TEM. This need inspired the development of MM-DTEM, exemplified by the prototype instrument at Lawrence Livermore National Laboratory which is capable of capturing nine TEM images or diffraction patterns in the span of less than one microsecond. MM-DTEM enables direct visualization of details of phase transformations, microstructural evolution, and propagating chemical reactions at the actual time, length, and temperature scales of the real-world applications. MM-DTEM works by coupling a unique arbitrary-waveform laser, a photoemission-based TEM, and a high-speed fully programmable electrostatic deflector system. The development of such an instrument raises both challenges and opportunities. DTEM experiments must make maximal use of the information provided by every single precious electron, for any wasted beam current implies performance degradation because of finite brightness, space charge, and stochastic blur effects.

The focus S. Haigh's talk was on applications that have demanded the development of novel experimental approaches:

1) Two dimensional materials like graphene are widely studied using plan-view TEM/STEM imaging. However, this approach cannot be applied after the various individual atomic layers are used encapsulated so as to fabricate a complex heterostructured device. She demonstrated how a side-view approach to imaging these materials has facilitated new insights into electrical device performance including the use of elemental mapping to locate atomic layers [15, 12].

2) The vast majority of STEM imaging is in vacuum. In-situ liquid cell experiments are increasingly popular but these have not generally been considered compatible with elemental analysis due to the cell geometry. She reported on the first use of a redesigned liquid cell that has allowed them to perform the first elemental mapping of nanostructures submerged in liquid with nanometer spatial resolution [62].

3) She also reported on recent results using tomography to obtain full elemental distributions in three dimensions with nanometer spatial resolution for different nanoparticle compositions. This has allowed them to overcome the limitations of interpretation associated with two dimensional projections [47] providing a much clearer under-

standing of catalytic performance.

In his talk J. Mayer [31] reported about some initial results with the currently most advanced electron microscopy instrument, FEI Titan 60-300 PICO. PICO is a fourth-generation transmission electron microscope capable of obtaining high-resolution transmission electron microscopy images approaching 50 pm resolution in the CC- and CS-corrected mode at 300 keV. It is currently one of only two microscopes in the world capable of chromatic aberration correction [K]. In the PICO instrument, HRTEM images can be obtained with simultaneous correction of the spherical and the chromatic aberration. Furthermore, a spherical aberration corrector also exists in the illumination system for Cs-corrected STEM imaging. The benefits of chromatic aberration corrected imaging are particularly large for HRTEM imaging at low accelerating voltages and for energy filtered (EFTEM) imaging with large energy window width [51]. The recent results focusing on these two applications were reported.

The talk of S. Findlay [11] was dedicated to some of the challenges for scanning transmission electron microscopy (STEM) discussing the steadily improving high-angle annular dark-field (HAADF) mode acquisitions, as well as some recent developments such as annular bright field imaging. He reviewed some limitations of na¨ve interpretation of STEM images, in particular that an image with atomic scale features cannot automatically be interpreted as allowing perfect column-by-column analysis. Select recent advances in analysis which account for the detailed scattering of the probe were presented. One is the ability to put experimental HAADF images on an absolute scale, which through comparison with simulations allows the number of atoms in a column to be counted, and in some cases the depth of individual dopant atoms to be determined. Another is an approach for removing the effects of elastic and thermal probe scattering from a spectrum image, disentangling the fine structure signals from adjacent columns to allow a more direct and meaningful comparison with standard first-principles simulations of energy loss fine structure. However, both approaches require the basic structure of the specimen to be known. The outstanding challenge is whether the same quantitative rigor can be achieved on samples when the structure is not known in advance. Finally, some ideas were given as to how this might be achieved as the potential for simultaneous collection of multiple imaging modes is increasingly being realized.

In his talk J. Sadowski [37] introduced the direct imaging photoelectron emission microscope (PEEM) and low-energy electron microscope (LEEM) combined with an imaging analyzer and a tunable high-brilliance synchrotron radiation source (XPEEM mode). He presented examples of application of the LEEM/XPEEM technique to the in situ, real-time investigations of the 2D layered materials, including few-layer graphene on transition metals and dichalcogenides. LEEM is a powerful technique for studying the dynamic and static properties of surfaces and thin films including growth and decay, phase transitions, reactions, surface structure and morphology. It utilizes low energy electrons to image surfaces with <5nm lateral resolution and atomic layer depth resolution (see, [3] and [2]). In the LEEM/XPEEM setup, when using the electron irradiation, the elastically and inelastically backscattered electrons, Auger and secondary electrons may be used, while photoelectrons, Auger and secondary electrons are utilized for imaging when sample is irradiated with photons. The choice of the imaging, diffraction or spectroscopy mode depends upon the information to be obtained: structural, chemical, magnetic or electronic, from the topmost or rather deeper layers. The strength of the technique lies in the combination of the real-time structural and spectroscopic measurements in a single analytical system.

In his talk T. Vogt [55] discussed the use of scanning transmission electron microscopy data and images in materials science, He made the case to better integrate STEM with other analysis techniques and warned about the dangers of 'cartoon science' and the use of 'selective imaging' that could dominate the use of STEM in the near future.

19.3.4 Modeling and Simulation

One of the major challenges in simulating inelastic scattering in the TEM/STEM is the large number of inelastic channels that must be included, even for a specific energy loss. In his talk C. Dwyer [8] considered this problem from a formal perspective, combining ideas from symmetry (group) theory and information theory. These ideas enable a formal analysis, and thereby optimization, of the efficiency of inelastic scattering simulations (and quantum mechanical calculations in general). Applied to simulations of core-loss scattering in the TEM/STEM, these ideas provide up to a 10-fold improvement in efficiency compared to current methods.

The talk of I. Lobato [29] presented a new parameterization of the electron scattering factor using five analytic non-relativistic hydrogen electron scattering factors as a basis functions. This new parameterization for the elastic electron scattering factors and its derived quantities such as the X-ray scattering factor, the electron charge density distribution and the atomic potential obey all the correct physical constraint conditions, have the correct asymptotic behavior and can be calculated analytically. The talk also presented an investigation of the accuracy of the main parameterized electron scattering factors for large variety of diffraction experiments including reflection that lies on the Zero Laue zones and Higher order Laue zones. The comparison of all these results allows to draw reliable conclusions about the range of applicability of the different parameterizations.

19.3.5 Electron Tomography

Electron tomography (ET) has become an important technique for the 3D characterization of nanomaterials [33]. Recently, significant advances in transmission electron microscopy have allowed spatial, temporal and spectroscopic imaging at unprecedented resolution. Extending these innovative techniques to 3D is of great interest for many nanotechnology applications. It necessitates, however, the development of powerful tomography algorithms that are capable of producing reliable reconstructions from datasets that are often limited due to constraints about e.g., sample geometry, total electron dose, total acquisition time and beam damage [34, 39].

In her talk Z. Saghi [38] presented some recent algorithmic developments with emphasis on compressed sensing ET (CS-ET) [Sa, 27]. By using the prior knowledge that the signal is sparse or compressible in a chosen transform domain (e.g. pixel or gradient domains), CS-ET employs a non-linear optimization algorithm to recover the sparsest solution consistent with the acquired projections. Based on simulations and experimental data, they compare CS-ET with traditionally employed algorithms and show that artifacts related to the limited number and angular range of available projections can be greatly reduced, making the segmentation and subsequent quantitative analysis much more reliable. Applied to innovative imaging modes, it is expected CS-ET to have a significant impact in the field of nanotechnology with unprecedented ability to follow changes in space and time, generate chemically-sensitive 3D reconstructions, and provide high quality 3D data that can be used as reliable starting point for detailed nanometrology and further simulations of the properties and behavior of nanodevices. There is a great potential in the 3D study of beam-sensitive materials, and in atomic scale ET using aberration-corrected microscopes and a small number of well-oriented projections.

In her talk I. Arslan [1] discussed the problems and specificity of electron tomography in the scanning transmission electron microscope (STEM) for recovering the 3D structure of nanoparticles with intricate shapes. considered advanced reconstruction algorithms for electron tomography. The standard 3-D reconstruction techniques of weighted back projection and simultaneous iterative reconstruction technique (SIRT) applied to the small number of projections available for beam sensitive materials typically leave elongation artifacts due to the missing wedge and no longer provide the necessary resolution. The suggested solution is to use a combination of a regularization using total variation (TV) minimization with the discrete algebraic reconstruction technique (DART). The presented examples of layered materials and small metal particles in supports are paving the road for future investigations towards in-situ/ex-situ 3-D imaging.

The mathematical part of this research was presented by T. Sanders [41]. He presented the issues arising in the combination of TV-minimization with the additional restriction by DART that the class of solutions should contain only piecewise constants with their values restricted to a few discrete levels. A critical one is the determination of these discrete levels based on a parameter selection. In the standard DART method even a semi-automated procedure for this selection is nontrivial. The suggested solutions are based on thorough analysis of all the steps in the 3D reconstruction from the original data to the final result and, in addition for the new method to select the discrete levels, make adjustments to the alignment and preprocessing of the tilt series.

The problem of limited angle in (STEM) electron tomography, also referred as the <u>missing wedge</u>, was considered in the talk of P. Lamby [26]. Motivated by the advances in the theory of sparse recovery, several algorithms have been recently developed that regularize the reconstruction problem using range constraints, the ℓ_1-norm and (possibly anisotropic) versions of the total variation semi-norm as priors. To solve the resulting typically underdetermined constrained optimization problems one needs iterative solvers which however converge only slowly because the data matrix A is badly conditioned. For example, with the regularized ART algorithm from [18] one can often observe notable improvements of the reconstruction appearing even after thousands of iterations which is computationally unacceptable for 3D reconstructions. Many algorithms developed for compressed sensing, like the Augmented Lagrangian Method [28] or Bregman iterations [30] accentuate the problem since they require iterative solution of the normal equation involving the matrix $A^{\mathrm{T}}A$ which is even worse behaved. These algorithms typically work well only in cases that the full range of angles is present. The idea presented in the talk is to combine the above mentioned algorithms with multigrid techniques, similar to the ones that have been proposed in [22] for overdetermined problems. Multigrid naturally acts as preconditioning of the system and one can hope for accelerated convergence. However, because of the structure of the system matrix, the standard multigrid theory is not applicable. The theoretical challenges for this approach were discussed and some experimental results with synthetical and real data were presented.

In his talk D. Van Dyck [53] referred to Richard Feynman who pointed out [10] in the fifties that, "It would be very easy to make an analysis of any complicated chemical substance; all one would have to do would be to look at it and see where the atoms are." since all structure-property relations are encoded in the 3D atom positions for a given set of elements. Nowadays, resolution and sensitivity of the latest generation aberration-corrected Transmission Electron Microscopes (TEM) suffice to detect even single light atoms from the Periodic Table of Elements [13, 24, 49, 19] and to pinpoint their position with a lateral precision that reaches the 2pm wavelength of the imaging electrons at 300kV of acceleration voltage [59] but the depth (z) information remains less certain. In the past, only a few favorable cases allowed for an extraction of atom positions in beam (z) direction with high precision. They included the study of a graphene double layer [54] and the study of nanocrystals of which the surfaces were protected by embedding in a sacrificial matrix [52]. Also, the combination of projections from different viewing directions yields remarkable results [43] as long as linear models for the interaction between the electron beam with the object apply and beam-induced sample alterations are ignored. However for the study of nanoparticles such as for catalysts there is a need for a tomographic method that allows a fast characterization of the shape of pristine particles at atomic resolution. The talk presented a new approach to atomic resolution tomography that meets these demands.

19.3.6 Cryo-Electron Microscopy and Biological Applications

In cryo-electron microscopy (cryo-EM), a microscope generates a top view of a sample of randomly-oriented copies of a molecule. The cryo-EM problem is to use the resulting set of noisy 2D projection images taken at unknown directions to reconstruct the 3D structure of the molecule.

The talk of Y. Shkolnisky [45] considered the recovery of the structure of large proteins (3D density maps) from their 2D cryo-EM images. A central stage in the method is to determine a three-dimensional model of the protein given many of its 2D projection images. The direction from which each image was taken is unknown, and the images are small and extremely noisy. The goal is to determine the direction from which each image was taken, and then to combine the images into a three-dimensional model of the molecule. The presented algorithm determines the viewing directions of all cryo-EM images at once, which is robust to extreme levels of noise. It is based on formulating a synchronization problem, that is, to estimate the relative spatial configuration of pairs of images, and then to estimate a global assignment of orientations that satisfies all pairwise relations. Information about the spatial relation of pairs of images is extracted from common lines between triplets of images. These noisy pairwise relations are combined into a single consistent orientations assignment, by constructing a matrix whose entries encode the pairwise relations. This matrix is shown to have rank 3, and its non-trivial eigenspace is shown to reveal the projection orientation of each image. In particular, it is shown that the non-trivial eigenvectors encode the rotation matrix that corresponds to each image.

The talk of A. Singer [46] considered tone of the fundamental challenges in cryo-EM, in which the molecule under examination exhibits structural variability. The heterogeneity problem is the task of mapping the space of conformational states of a molecule. It has been previously shown that the leading eigenvectors of the covariance matrix of the 3D molecules can be used to solve this problem. Estimating the covariance matrix is however challenging, since only projections of the molecules are observed, but not the molecules themselves. In the talk this problem was viewed as a noisy matrix completion problem, and an estimator for the covariance matrix was derived as a solution to a certain linear system. While it was proven that the resulting estimator for the covariance matrix is consistent in the classical limit as the number of projection images grow indefinitely, an interesting open question regarding the sample complexity of the problem remains. Namely, how many images are required in order to resolve heterogeneous structures as a function of the volume size and the signal to noise ratio? Solving this question requires to extend the analysis of the spike model in principal component analysis (PCA) in high dimensions, as one encounters limiting distributions that differ from the classical Marcenko-Pastur distribution.

In his talk T. Zhang [63] proposed a semidefinite programming approach to determine the 3D structure of small macromolecules by extending Kam's theory for single particle reconstruction in cryo-EM. The 3D reconstruction requires us to solve for U and V in the equation $Z = XU + YV$, where X, Y, Z are matrices of size $n \times d$, and U, V are d by d orthogonal matrices. We relax this to a semidefinite program, and show that when $n > d$, we can recover U and V exactly. A phase transition is observed at $n = d$. Based on this, a new method is proposed that would potentially enhance the capabilities of three-dimensional electron microscopy techniques by being able to answer biological questions related to small protein structures that have so far remained unresolved. The method is tested by numerical experiments on the simulated data of the Kv1.2 potassium channel complex.

In his talk C. Bajaj [2] highlighted the current progress on several co-mingled computational mathematics algorithms for refinement of 3D Electron Microscopy map and models of macromolecular assemblies. The attempt is to recover the three-dimensional structure of an individual molecule, a protein or a macromolecular assembly at the finest possible resolution and in its natural environment. Despite the advances in X-ray imaging and Electron Microscopy (EM), it has been difficult to simultaneously achieve the goals of recovering shape and conformation at finer resolution, and the larger scale of protein/nucleic acid assemblies. The proposed algorithms are based on new improved solutions to low discrepancy sampling of rotational product spaces SO(3)n, and non-equispaced SO(3) Fourier transforms for fast multidimensional rotational correlations.

The talk of J. Evans [9] considered time-resolved imaging of biological or nanomaterial structural dynamics, a highly data intensive task. In it the attempt is not only to collect enough data to solve the three-dimensional structure of an object, but also to collect that same data at multiple time points during a reaction cycle to see how the object changes over time. Handling the data, which for a single dataset can be on the order of terabytes in size, is a barrier unto itself but analyzing the data and identifying slight changes from one image to the next can be even more daunting - especially when the timing offset or magnitude of changes is unknown a priori. The talk described some of the challenges identified from current ultrafast x-ray diffraction experiments and simulated Dynamic TEM datasets to highlight areas where the development of automated algorithms could dramatically improve throughput and reliability of interpretation.

19.4 Scientific Progress Made

Several recent scientific achievements of the participants in the workshop and their research groups were presented at the workshop and reflected upon in the highlights above.

19.5 Outcome of the Meeting

This workshop provided various newly formed collaborations the opportunity to present new results and join a growing community of mathematicians and experimentalists which has formed over the past 5 years with the goal to apply modern mathematical tools to data with unprecedented quality and complexity

The subject of advanced electron imaging is growing and starting to have impacts as evidenced by recent publications from the participants in this initiative [5, 61]. We anticipate that the growing use of aberration-corrected electron microscopes at universities and the emergence of new electron and x-ray sources such as DTEM and free electron lasers at national laboratories will entice more materials scientists and structural biologists to tackle grand challenges such as protein folding and ultra-fast imaging of chemical reactions. These will create an enormous need in new data management, automated mining and analysis approaches that calls for continuing collaborations of imaging experimentalists and mathematicians. We hope that we can continue and expand this collaboration within the next few years and look forward to other BIRS events.

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Bibliography

[1] Ilke Arslan, Advanced reconstruction algorithms for electron tomography in the physical sciences, talk at BIRS workshop **14w5048** (2014).

[2] Chandrajit Bajaj, Macro-molecular Map and Model Refinement Techniques for Electron Microscopy, talk at BIRS workshop **14w5048** (2014).

[3] E. Bauer, Low energy electron microscopy, Rep. Prog. Phys. **57** (1994), 895-938.

[4] Benjamin Berkels, Image registration techniques for electron microscopy, talk at BIRS workshop **14w5048** (2014).

[5] B. Berkels, P. Binev, D.A. Blom, W. Dahmen, R.C. Sharpley, T. Vogt, Optimized imaging using non-rigid registration, Ultramicroscopy **138** (2014), 46-56.

[6] Nigel Browning and Peter Binev, How can Mathematics help Electron Microscopy?, moderated discussion at BIRS workshop **14w5048** (2014).

[7] Mark Davenport, Adaptive sensing for compressive imaging, talk at BIRS workshop **14w5048** (2014).

[8] Christian Dwyer, Simulating core-loss scattering in the STEM, talk at BIRS workshop **14w5048** (2014).

[9] James Evans, Data analysis challenges for observing protein dynamics with fast electrons and x-rays, talk at BIRS workshop **14w5048** (2014).

[10] R.P. Feynman, There's Plenty of Room at the Bottom, Engineering and Science **23** (1960), 22-36.

[11] Scott Findlay, Quantitative interpretation of atomic resolution scanning transmission electron microscopy images in the presence of multiple scattering: progress and challenges, talk at BIRS workshop **14w5048** (2014).

[12] T. Georgiou et al., Vertical field-effect transistor based on graphene–WS2 heterostructures for flexible and transparent electronics, Nature Nanotech. **8** (2013), 100103.

[13] Ç.Ö. Girit, J.C. Meyer, R. Erni, M.D. Rossell, C. Kisielowski, L. Yang, C.-H. Park, M.F. Crommie, M.L. Cohen, S.G. Louie, A. Zettl, Graphene at the Edge: Stability and Dynamics, Science **323** (2009), 1705-1708.

[14] Sarah Haigh, Exploring the limitations of energy dispersive X-ray mapping of nanomaterials with the Titan ChemiSTEM, talk at BIRS workshop **14w5048** (2014).

[15] S. J. Haigh et al., Cross-sectional imaging of individual layers and buried interfaces of graphene-based heterostructures and superlattices, Nature Materials **11** (2012), 764-767.

[16] Sarah Haigh and Zineb Saghi, Elemental quantification using energy dispersive x-ray spectrometry in the STEM, moderated discussion at BIRS workshop **14w5048** (2014).

[17] Bin Han, Image denoising using directional separable complex tight framelets, talk at BIRS workshop **14w5048** (2014).

[18] G. T. Herman and R. Davidi, Image reconstruction from a small number of projections, Inverse Problems **24** (2008), 45011-45028.

[19] P.Y. Huang, S. Kurasch, J.S. Alden, A. Shekhawat, A.A. Alemi, P.L. McEuen, J.P. Sethna, U. Kaiser, and D.A. Muller, Imaging Atomic Rearrangements in Two-Dimensional Silica Glass: Watching Silicas Dance, Science **342** (2013), 224-227.

[20] B. Kabius, P. Hartel, M. Haider, H. Müller, S. Uhlemann, U. Loebau, J. Zach, and H. Rose, First application of Cc-corrected imaging for high-resolution and energy-filtered TEM, J. Electron Microscopy **58** (2009), 147-155.

[21] Kevin Kelly, Multidimensional Compressive Imaging with a Two-Dimensional Modulator, talk at BIRS workshop **14w5048** (2014).

[22] H. Köstler, C. Popa, M. Prümmer, and U. Rüde, Towards an algebraic multi-grid method for tomographic image reconstruction improving convergence of ART. In European Conference in Computational Fluid Dynamics ECCOMAS CFD, P. Wesseling, E. Onate, and J. Periaux, eds.), TU Delft, The Netherlands, 2006.

[23] Felix Krahmer, A partial derandomization of phase retrieval via PhaseLift, talk at BIRS workshop **14w5048** (2014).

[24] O.L. Krivanek, M.F. Chisholm, V. Nicolosi, T.J. Pennycook, G.J. Corbin, N. Dellby, M.F. Murfitt, S.S. Own, Z.S. Szilagyi, M.P. Oxley, S.T. Pantelides, S.J. Pennycook, Nature **464** (2010), 571-574.

[25] Gitta Kutyniok, A Compressed Sensing Approach to Component Separation in Imaging, talk at BIRS workshop **14w5048** (2014).

[26] Philipp Lamby, Solving the Regularized Reconstruction Problems Arising in Limited-Angle Tomography, talk at BIRS workshop **14w5048** (2014).

[27] R. Leary, Z. Saghi, P.A. Midgley, D.J. Holland, Compressed Sensing Electron Tomography, Ultramicroscopy **131** (2013), 70-91.

[28] Chengbo Li, An efficient algorithm for total variation regularization with application to the single pixel camera and compressive sensing, Masters thesis, Rice University, Houston, Texas, 2009.

[29] Ivan Lobato, On accurate modeling of electron scattering factors for TEM, STEM and diffraction, talk at BIRS workshop **14w5048** (2014).

[30] Y. Mao, B.P. Fahimian, S.J. Osher, and J. Miao, Development of optimization of regularized tomographic reconstruction algorithms utilizing equally-sloped tomography, IEEE Transactions on Image Processing **19(5)** (2010), 1259-1268.

[31] Joachim Mayer, PICO - Chromatic Aberration Correction in TEM and its impact on new experiments and signals, talk at BIRS workshop **14w5048** (2014).

[32] Niklas Mevenkamp, Non-local Means based Denoising and Reconstruction of STEM Images, talk at BIRS workshop **14w5048** (2014).

[33] P.A. Midgley et al, Nanotomography in the chemical, biological and materials sciences, Chemical Society Reviews **36** (2007), 1477-1494.

[34] P.A. Midgley and R.E. Dunin-Borkowski, Electron tomography and holography in materials science, Nature Materials **8** (2009), 271-280.

[35] Deanna Needell, Greedy algorithms in super-resolution, talk at BIRS workshop **14w5048** (2014).

[36] Bryan Reed, Movie Mode DTEM, talk at BIRS workshop **14w5048** (2014).

[37] Jerzy Sadowski, Spectro-microscopy of 2D materials: challenges and perspectives, talk at BIRS workshop **14w5048** (2014).

[38] Zineb Saghi, Compressed sensing approaches for novel 3D imaging modes in the TEM , talk at BIRS workshop **14w5048** (2014).

[39] Z. Saghi and P.A. Midgley, Electron Tomography in the (S)TEM: From Nanoscale Morphological Analysis to 3D Atomic Imaging, Annual Review of Materials Research **42** (2012), 59-79.

[40] Z. Saghi et al, 3D Morphology of Iron Oxide Nanoparticles with Reactive Concave Surfaces – a Compressed Sensing - Electron Tomography (CS-ET) Approach, Nano Letters **11** (2011), 4666-4673.

[41] Toby Sanders, Practical 3-D Reconstruction Techniques for Electron Tomography, talk at BIRS workshop **14w5048** (2014).

[42] Otmar Scherzer, Optical Flow Decomposition on Evolving Surfaces, talk at BIRS workshop **14w5048** (2014).

[43] M.C. Scott, C.-C. Chen, M. Mecklenburg, C. Zhu, R. Xu, P. Ercius, U. Dahmen, B. C. Regan, and J. Miao, Electron tomography at 2.4-ångström resolution, Nature **483** (2012), 444-447.

[44] Zuowei Shen, Image Restoration: Wavelet Frame Approach, Total Variation and Beyond, talk at BIRS workshop **14w5048** (2014).

[45] Yoel Shkolnisky, Viewing Direction Estimation in cryo-EM Using Synchronization, talk at BIRS workshop **14w5048** (2014).

[46] Amit Singer, Covariance Matrix Estimation for the Cryo-EM Heterogeneity Problem, talk at BIRS workshop **14w5048** (2014).

[47] T.J.A. Slater, A. Macedo, S.L.M. Schroeder, et al., Nano Letters **14** (2014), 1921-1926.

[48] Andrew Stevens, Machine Learning and Compressive Sensing for Electron Microscopy, talk at BIRS workshop **14w5048** (2014).

[49] K. Suenaga, Y. Sato, Z. Liu, H. Kataura, T. Okazaki, K. Kimoto, H. Sawada, T. Sasaki, K. Omoto, T. Tomita, T. Kaneyama, Y Kondo, Visualizing and identifying single atoms using electron energy-loss spectroscopy with low accelerating voltage, Nature Chemistry **1** (2009), 415-418.

[50] R.M. Tromp, Low energy electron microscopy, IBM J. Res. Develop. **44** (2000), 503-516.

[51] K.W. Urban, J. Mayer, J.R. Jinschek, M.J. Neish, N.R. Lugg, and L.J. Allen, Achromatic Elemental Mapping Beyond the Nanoscale in the Transmission Electron Microscope, Phys. Rev. Lett. **110** (2013), 185507.

[52] S. Van Aert, K.J. Batenburg, M.D. Rossell, R. Erni, and G. Van Tendeloo, Three-dimensional atomic imaging of crystalline nanoparticles, Nature **470** (2011), 374-377.

[53] Dirk Van Dyck, Addressing Feynman's Challenge - The 3D Shape of NanoCrystals from Single Projections at Atomic Resolution, talk at BIRS workshop **14w5048** (2014).

[54] D. Van Dyck, J.R. Jinschek, F.R. Chen, Big Bang tomography as a new route to atomic-resolution electron tomography, Nature **486** (2012), 243-246.

[55] Thomas Vogt, From Picture to Data - the iconoclastic struggle in materials science, talk at BIRS workshop **14w5048** (2014).

[56] T. Vogt, W. Dahmen, and P. Binev, eds., Modeling Nanoscale Imaging in Electron Microscopy, Nanostructure Science and Technology, Springer, New York, 2012.

[57] Paul Voyles and Wolfgang Dahmen, Improving Precision and Signal to Noise Ratio in Electron Micrographs, moderated discussion at BIRS workshop **14w5048** (2014).

[58] Rachel Ward, Linear dimension reduction in the L_1 norm: When and how is it possible?, talk at BIRS workshop **14w5048** (2014).

[59] X. Xu, S.P. Beckman, P. Specht, E.R. Weber, D.C. Chrzan, R.P. Erni, I. Arslan, N. Browning, A. Bleloch, C. Kisielowski,Distortion and Segregation in a Dislocation Core Region at Atomic Resolution, Phisical Review Letters **95** (2005), 145501.

[60] Andrew Yankovich, Applications of NR registration for enhanced signal to noise ratio, spatial precision, and standardless atom counting in STEM images, talk at BIRS workshop **14w5048** (2014).

[61] A.B. Yankovich, B. Berkels, W. Dahmen, P. Binev, S.I. Sanchez, S.A. Bradley, Ao Li, I. Szlufarska, and P.M. Voyles, Picometre-precision analysis of scanning transmission electron microscopy images of platinum nanocatalysts, Nature Communications **5** (2014), Article number: 4155.

[62] X-ray Energy-Dispersive Spectrometry During In Situ Liquid Cell Studies Using an Analytical Electron Microscope, Microscopy and Microanalysis **20** (2014), 323-329.

[63] Teng Zhang, A Semidefinite Programming Approach to 3D Reconstruction of Macromolecules, talk at BIRS workshop **14w5048** (2014).

Chapter 20

Programming with Chemical Reaction Networks: Mathematical Foundations (14w5167)

June 8 - 13, 2014

Organizer(s): Anne Condon, (U. British Columbia), Chris Thachuk, (U. Oxford), David Doty, (Caltech)

20.1 Overview

Here we report on the "Programming with Chemical Reaction Networks: Mathematical Foundations" workshop, held at BIRS in July 2014. Our workshop brought together mathematicians, computer scientists, physicists, and chemists who may not normally cross paths, to answer foundational questions on the capabilities of programs that are described abstractly as chemical reaction networks. What can such programs compute? How energy efficient can they be? How would we verify that such programs are correct?

We'll first give a short overview of chemical reaction networks, the motivation for studying them, and how the workshop was structured for this purpose. In the next section we'll describe the research questions that were the focus of the workshop, and progress on some of these questions.

20.1.1 What are CRNs?

Stochastic chemical reactions networks (CRNs) describe how certain species of molecules within a solution, such as DNA strands, can react to produce new species.

CRNs are specified as a set of reactions along with initial counts of molecular species. An example is a CRN with three reactions

$$\begin{aligned} X + Y &\overset{k_1}{\rightleftharpoons} B + B \\ X + B &\overset{k_2}{\rightleftharpoons} X + X \\ Y + B &\overset{k_3}{\rightleftharpoons} Y + Y, \end{aligned}$$

with initial counts of being $\#X = 10$, $\#Y = 5$ and $\#B = 0$. The likelihood of a given reaction depends on the relative counts of its species and on the number of reactants, and the reaction rate constants [17].

Traditionally used to describe extant chemical systems, CRN's are increasingly being used for molecular programming. Molecular programming is the process of designing molecules that store information and execute instructions in purposeful ways. Nucleic acids—DNA and RNA molecules—are interesting to program because of their digital sequences and dynamic structural properties, and because they extend the reach of computational devices by naturally interacting with "wet" biological systems.

20.1.2 Motivation for the study of CRNs

Because of their simplicity, CRNs are natural language for specifying and reasoning about molecular programs—systems of interacting molecules. Much recent progress in molecular programming has been aided by the use of CRNs, without getting bogged down in low-level details.

CRNs can in principle be "compiled" to produce physical embodiments in the form of so-called DNA strand displacement systems (DSDs). DSDs have been experimentally demonstrated to simulate arbitrary logic circuits [17], compute the square root of a number [15], or implement a tiny neural network [16].

Chemical reaction networks provide a means of exploring intriguing new research directions at the intersection of computer science and biochemistry, such as how to compute in an energy efficient manner in the sense envisioned by Bennett [3], and how to store information at unprecedented scales in a medium that can persist for centuries.

CRNs can also describe programs that execute in biological processes. For example, it has been shown that the cell of eukaryotic organisms computes an approximate majority algorithm to determine when to begin the process of mitosis [4]—partitioning into two daughter cells. In fact, the CRN with three reactions described in section 20.1.1 computes approximate majority.

Longer term, molecular programs show promise for the development of biosensors capable of "point-of-care" diagnostics (*e.g.,* malaria testing). Molecular programs inserted into cells might act as smart drugs, comprised of logic circuitry that can detect the disease state of a cell and respond with the appropriate treatment, sparing healthy cells from unnecessary dosage.

20.1.3 Interdisciplinary nature of the topic

Some of the challenges faced when designing CRNs are akin to those in distributed computing, and research on CRNs draws naturally from the theory of population protocols. As CRNs are by nature probabilistic and may be applied to problems in human health, verifying their correctness is of paramount concern and builds on formal verification and model checking techniques. Understanding the potential for energy-efficient computation requires the expertise of mathematicians, physicists and complexity theorists.

Although theoretical in nature, this line of research is informed directly by experimental endeavors in programming the behavior of matter at the molecular level, using DNA, enzymes, and other biochemical molecules as engineering tools repurposed from their biological function to serve as computational primitives. To ensure that theoretical models remain grounded in reality, research on this topic benefits from the perspectives of leading experimental scientists.

20.1.4 Structure and outcomes of the workshop

The workshop was structured to provide ample opportunity for those present to learn from those with complementary expertise. Early in the workshop there was a strong focus on identifying important research questions, drawing on the broad perspectives of those present, and facilited by a wiki page. The workshop then included a mix of informal problem-solving sessions and expository talks, with progress reports on the last day.

The workshop was highly interactive, with strong communication among all attendees, particularly between students and more senior researchers. Furthermore, the informal nature of the discussions allowed younger researchers to witness research in its earliest stages, before concrete problems have even been formulated, teaching them by example the creative process of research. This unique environment permitted early stage researchers to learn the main results, techniques, and perspectives of programming chemical reaction networks, to identify unifying conceptual principles underlying the different projects, and to generate novel research directions for the future based on this interdisciplinary interaction.

There have already been some publications as an outgrowth of the workshop, and more to follow. One open problem discussed at the workshop, concerning a fundamental distributed computing problem known as "leader election" that has been found to be of importance in chemical reaction networks, was resolved by two of the workshop participants, David Doty and David Soloveichik, both of whom were postdocs. Their paper, entitled "Stable leader election in population protocols requires linear time", appeared at the 29th International Symposium on Distributed Computing. Seung Woo Shin, a graudate student funded by the grant, presented his masters thesis research on verifying chemical reaction networks at the workshop. This work was later published at the "2014 Verification of Engineered Molecular Devices and Programs" workshop.

20.2 Research Themes and Open Problems

Here we describe several topics and open problems contributed by workshop participants. For some of the topics, we also describe progress that was made by participants during the workshop; for other topics, progress was largely a better understanding and sharpening of the problem.

20.2.1 Leader election

Overview. Biological organisms are exemplars of self-organisation. Mathematical approaches like reaction-diffusion systems attempt to capture geometrical self-organization — how complex patterns can arise from uniform initial conditions. Analogously we ask how well-mixed chemical systems can transform uniform initial conditions to controlled amounts of desired species. Having certain species present in precise counts (eg a species LL with exactly 1 molecule) is a prerequisite for a number of sophisticated CRNs in the literature. For example, constructions for polynomial-time Turing machine simulation requires a "leader": a species with initial count 1, which is used to coordinate interaction among the other species in a controlled way [1].

If a CRN starts with uniform initial conditions where all initially-present species have count proportional to the total volume, then it is possible to "elect" a leader through two reactions:

$$\begin{array}{lcl} X & \to & L \\ L + L & \to & L \end{array}$$

However, this takes expected time $O(n)$, which is slow compared with other basic forms of CRN computation. For example, for example, the reaction $X \to Y + Y$ "quickly" computes multiplication by 2 in the sense that it takes expected time $O(\log(n)$ to convert n copies of X into $2n$ copies of Y.

Algorithms for leader election have been extensively studied in the distributed computing literature. The possibility of fast leader election is a long standing open problem in "population protocols," a model which is formally equivalent to a subclass of CRNs. Angluin et al. [2], developed an algorithm which appears to elect a leader in sublinear time with high probability based on extensive numerical simulation. Although the complexity of the population protocol has so far hindered efforts to prove correctness, it informs our understanding of what may or may not be possible, and suggests new techniques for a positive result. Proving either a positive or negative result would be an important development outside of the CRN literature and would engage the larger CS theory community.

Research questions and challenges. A central question is: Is there a CRN with an initial state with count n of a species X in volume n and count 0 of everything else, that in expected time $\log^k(n)$ for some constant k reaches a state $\bar{c}$ with 1 copy of L (and arbitrary counts of everything else), such that every state reachable from $\bar{c}$also has count 1 of L? There are also many interesting variants of the problem:

- Deterministic versus small probability of error uniform initial state (n copies of X in volume n) versus the CRN must handle all initial configurations with n molecules (the latter proved to be impossible to handle) population protocols (2-reactants, 2-products) versus allowing any reactions (the latter can be done by cheating with the reaction $2X \to 3X$)

- How to count the expected time until done: Is it the last time the leader changes (from a copy count of 0 or 2 to 1)? The time at which the CRN enters a state from which it is impossible to change the count of L (which may happen much later than the last time L changes)? Or the first time at which the leader gets count 1?
- Is there only 1 leader species, or do we allow a set $\mathcal{L} = \{L_1, \ldots, L_k\}$ of leader species, so long as eventually exactly one L_i is present?

In each variant, one option makes the leader election problem easier to solve, so that is the option to choose if trying to show leader election is possible, and the other option should be chosen if the goal is to show leader election is impossible. The following observations are good to keep in mind:

- Leader election is not speed fault-free [9].
- If stabilization must happen simultaneously with the last time the leader count changes, that reaction must take $\Omega(n)$ time (assuming there is exactly one leader species; this does not apply if we allow a set $\mathcal{L}$ of several leader species). The lesson is that to prove leader election is impossible, one should focus not on the last reaction to change L, but instead on the reaction that stabilizes $\#L$ (or focus on something else).
- It seems leader election can be done if one allows the number of species to grow with n ($O(\log n)$ species seem to suffice).
- Leader election can be done in expected time $\approx O(\sqrt{n})$ with a non-uniform initial state with nF_1 and $\sqrt{n}/n^{1/4}\ F_2$. This violates the hypothesis of a uniform initial state, but it served as a counter-example to several ideas for how to prove leader election is impossible, since those ideas if correct would work on this CRN as well.

20.2.2 CRN Equivalences

Overview. Researchers are attempting to use DNA strand displacement cascades to implement a wide variety of chemical reaction networks with interesting algorithmic behaviors. This raises the general question of when we can say such an implementation is correct.

In this context there is a 'formal' CRN, the one being implemented, together with an 'implementation' CRN. The implementation CRN often contains many more chemical species in addition to species corresponding to those in the formal CRN. We call these additional species intermediate species and call those corresponding to species in the formal CRN formal species. Although every reaction that we are trying to implement is a one-step reaction involving only formal species, in the implementation CRN they are often implemented via a multi-step pathway which goes through states containing intermediate species.

There are a number of concepts of equivalence between the formal and implementation CRN, which seek to make precise the notion that the implementation is correct. The first notion is widespread, the second was known in the state-transition system literature but introduced into CRN theory by Qing Dong in 2012, and the third was introduced by Seung Woo Shin in 2011:

- Reachability equivalence. A necessary condition for an implementation to be correct is to require that given any two states containing only formal species, the second is reachable from the first in the formal CRN if and only if it is reachable in the implementation CRN.
- Bisimulation equivalence. A stronger notion is bisimulation equivalence. This is based on the idea of interpreting any intermediate species as a combination of formal species. Bisimulation equivalence requires that the implementation CRN, under such an interpretation, contains exactly the same reactions as the formal CRN. In particular, this ensures that any reaction pathway that exists in one CRN has a corresponding pathway in the other.
- Pathway decomposition equivalence. Pathway decomposition equivalence is a stronger notion than reachability equivalence, but neither implying nor implied by bisimulation equivalence. The main observation that gives rise to this notion is that most pathways of the implementation CRN can be formed by composing

smaller pathways. We call those pathways that cannot be thus decomposed "prime pathways". The implementation CRN is pathway decomposition equivalent to the formal CRN if they have the same set of prime pathways.

Research questions and challenges. How do these notions compare to those that naturally arise in category theory? The key observation, due to Jose Meseguer, Ugo Montanari and Vladimiro Sassone in the early 1990s, is that any Petri net gives rise to a "symmetric monoidal category": a category where there is a way of adding objects and adding morphisms. However, the formalism of Petri nets is just another language for talking about chemical reaction networks, so any chemical reaction network also gives a symmetric monoidal category. The objects are the formal linear combinations of species, e.g. $A + B + 2C$ where A, B, and $C$are chemical species. Addition of these is defined in the obvious way. The morphisms are the reaction pathways, built from the basic reactions in the CRN by composition and addition.

There are various kinds of maps and equivalences between symmetric monoidal categories:

- Symmetric monoidal functor - this is the simplest kind of map between symmetric monoidal categories; it sends objects to objects and morphisms to morphisms in a way that preserves composition and addition.
- Symmetric monoidal equivalence - this is a symmetric monoidal functor $F : C \to D$ equipped with a symmetric monoidal functor G:DCG:DC that serves as an inverse. Two symmetric monoidal categories that have an equivalence of this sort between them are the same for all practical purposes.
- Symmetric monoidal adjunction - this concept is intermediate between the previous two. This is a symmetric monoidal functor $F : C \to D$ equipped with a symmetric monoidal functor $G : D \to C$ that obeys conditions weaker than those of an inverse. In category theory adjunctions are considered very important and much more interesting than equivalences.

It is natural to ask how these concepts relate to the concepts of equivalence for CRNs. Suppose C and D are two symmetric monoidal categories coming from CRNs: C coming from the formal CRN and D coming from the implementation CRN. The existence of a symmetric monoidal functor $F : CD$ implies that given formal states S and S', if S' is reachable from S in the formal CRN then it is reachable in the implementation CRN. However, the converse may not hold. Thus, reachability equivalence may not hold.

If there is a symmetric monoidal equivalence $F : C \to D$, then reachability equivalence holds, as well as bisimulation equivalence. However, symmetric monoidal equivalence is too strong to hold in most examples found in practice. We successfully applied the more flexible notion of symmetric monoidal adjunction to one realistic example, but we proved that bisimulation equivalence does not imply the existence of a symmetric monoidal adjunction. An important open question is thus to find additional conditions on a symmetric monoidal adjunction that imply bisimulation equivalence.

20.2.3 Robust CRNs: An experimentally motivated questions about CRN-to-DNA technologies

Overview. One can write down formal CRNs which are interesting in many ways, such as: exhibiting complex temporal dynamics under the mass action model (oscillations, chaos, ...) or performing computation with counts under the stochastic model. Can we implement any interesting CRN we can write down in a real test tube with real molecules?

David Soloveichik et al. showed that, in theory, it is possible to use DNA strand displacement to approximate the dynamics of any arbitrary formal CRN, with arbitrary accuracy, up to scaling rate constants (and in certain concentration regimes.) Luca Cardelli proposed another CRN to DNA compilation scheme using DNA strand displacement with nicked double stranded DNA complexes.

This inspired many researchers to work on actually engineering complex chemical reaction networks in the wet-lab - in order to understand the kinds of real world problems or issues we would need to solve to really get this technology to work, and these efforts are leading to significant breakthroughs. Following are some questions about CRNs and CRN-to-DNA technologies that are directly experimentally motivated based on experimental experience over the last few years.

Research questions and challenges. How can we design or program robust or fault tolerant CRNs? Experimentally, we find that not all our molecules are perfect - some may have synthesis errors - and therefore our implementations are not perfect. So, if we set out to implement the reaction $X \rightarrow Y$, it is possible that we really are implementing $X \rightarrow (1\delta)Y$, for some δ that depends on the extent of synthesis errors. Alternatively this could be viewed as "every so often, we consume the reactant(s) without releasing the product(s)". Could we build CRNs that are somehow robust to errors of this kind?

Strand displacement rate can be controlled over 5 to 6 orders of magnitude based on toehold strength, but blunt end or zero toehold strand displacement still happens at a non-zero rate. This means, from an experimental standpoint, that there are no pure implementations of any reactions. In particular, if one wants to implement a bimolecular reaction $A + B \rightarrow C$ with rate constant k_1, one is really implementing that reaction *and* another, which looks like $B \rightarrow C$ with rate constant k_2. Ideally, $k_2 << k_1$, but getting this to work in practice can be tricky. Can we build CRNs robust to this kind of more difficult error?

20.2.4 CRNs with limited geometry

Overview. Chemical reaction networks are known to be Turing-universal with probability $1 - \varepsilon$ (for any $\varepsilon > 0$. CRNs augmented with a constant number of stacks are Turing-universal. This was demonstrated using a DNA strand displacement system construction that exploited the fact that DNA can easily form polymers. The stacks in that construction behave as one would expect: a molecule can be added to the top of the stack, can be removed from the top of the stack, and molecules not on the top are not accessible to other reactions. A stack of type i initiates from a special subunit molecule called $\perp_i$. Simplifying details, this leads to CRN reactions of the form:

$$\begin{array}{lll} \perp_i \ldots X] + Y & \rightarrow & [\perp_i \ldots XY] \\ [\perp_i \ldots XY] + \mathrm{Pop}_i & \rightarrow & [\perp_i \ldots X] + Y \end{array}$$

As with many results that demonstrate CRNs capable of complex computation the stack machine construction assumes that certain molecular species are present in exact initial quantities, in particular there is exactly one copy of each stack.

Research questions and challenges. What is the power of CRNs augmented with stacks, without the initial context assumption (i.e., that the concentrations of stack subunit species, $\perp_i$, are given as part of the input)? The inspiration of this question can be found in the ability for DNA strand displacement systems to form polymers—-complexes consisting of multiple DNA strands bound via hybridization of complementary domains. While polymers can simulate stacks, they are more general and open up new possibilities for programming CRNs. Interesting thought experiments in this model may include:

- Beginning from a population of input X, can stacks be used to output $\log(|X|)$ copies of an output species Y?
- Could consensus of two input species X and Y be computed exactly, and efficiently, with the use of a constant number of stack types?
- What additional computational power, if any, arises when the model is broadened to included: (i) double ended stacks / queues, (ii) stacks/queues/polymers that can be efficiently concatenated with another, at their ends, (iii) polymers that can be efficiently "merged" with another, at multiple locations along the polymer?

20.2.5 CRNs and circuit complexity

Overview. Consider CRNs in which we give input using the binary convention: to specify the ith bit is 1, have count 1 of X_i in the initial state; otherwise have count 0.

Research questions and challenges. What is the relationship between resource bounds (e.g., number of species/reactions) for CRNs and resource bounds (e.g., number of gates, depth) for Boolean circuits?

Precise question (one example): Let $n \in \mathbb{N}$ and let $\phi : \{0,1\}^n \to \{0,1\}$ be a Boolean function with n inputs. What is the relationship between the Boolean circuit size $size_{BC}(\phi)$ of ϕ (the minimum number of wires in a Boolean circuit with AND, OR, and NOT gates that computes ϕ) and the "CRN size complexity" $size_{CRN}(\phi)$ of ϕ (the minimum number of species/reactions in any CRN that stably computes ϕ)?

Here, "the CRN stably computes ϕ" is formally defined in several papers, e.g., [4]. Briefly, it means that there are species Y ("yes") and N ("no"), and starting from the initial state $\bar{x}$ for any state $\bar{c}$ reachable fro $\bar{x}$, there is a stat $\bar{o}$ reachable from $\bar{c}$ with the following property: If $\phi(\bar{x}) = 1$ then Y is present in $\bar{o}$ and N is absent, and if $\phi(\bar{x}) = 0$ then N is present in $\bar{o}$ and Y is absent, and this remains true in any state reachable from $\bar{o}$.

It is clear that $size_{CRN}(\phi) = O(size_{BC}(\phi))$. The reverse direction is not clear.

Some preliminary work suggests perhaps $size_{CRN}(\phi)$ could be characterized in terms of the depth of Boolean circuits that compute ϕ.

20.2.6 Families of CRNs

Overview. Models of computation are often presented either as (i) a single device that works for all inputs (e.g. a Turing machine, a Python program), or (ii) a family of devices where we have one device for each input length (e.g. a family of Boolean circuits with exactly one circuit cncn for each input string length nn). The relationship between standard models and CRNs where in both models we have (i) one device for all inputs is beginning to be well-understood (but still has interesting questions), a number of the questions above are best formalized in the (ii) family of devices setting. The purpose of this section is to describe how the latter setup might look.

Families of devices can be uniform or nonuniform: we say that a family of devices is uniform if there is an algorithm that describes the entire family. For example, we say that a language L is accepted by a uniform Boolean circuit family $\mathcal{C}$ if there exists a computable function $f : 1 \to \mathcal{C}$ such that

$$\mathcal{C} = \{c_n \forall n \in \mathbb{N}, f(1^n) = c_n \text{ is a circuit that accepts} \{0,1\}^n \cap L\}.$$

The distinction between single-machine versus families of devices has appeared in work on CRNs. For example, here are two example ways for a CRN to compute a function of its input.

The input could be the initial count of some single species X. Then any natural number nn can be represented, or equivalently one could represent a binary string xx by using natural number nn as input, if x is the nth binary string in lexicographic order. The input could be a binary string x of length n represented by nn different input species $X_1, \ldots X_n$. The presence or absence of each of these species is then able to represent any bit string of length nn. Indeed, for each $n \in \mathbb{N}$ there is exactly one CRN, and we call the entire infinite set of CRNs a family.

Research questions and challenges. What is the relationship between uniform families of CRNs and uniform families of Boolean circuits, asynchronous Boolean circuits, or other "standard" models? One can also ask about CRN size, time, restricted forms of input and output, and many other questions in this setting). In order not to trivialize the theory, when we have an infinite set of devices computing some function or deciding a language, it is important to set up clear input and output conventions, and to define how powerful the individual devices can be. We propose the following definition of language acceptance by a uniform family of CRNs

Let $\mathcal{R}$ be a set, called a family, of CRNs. We say that a language L is accepted by a uniform family of CRNs $\mathcal{R}$ if there exist two functions: (1) $f : 1 \to \mathcal{R}$ and (2) e (called the input encoder) with domain $0, 1$ and range the set of all multisets over the (input) species of the CRNs, and $\mathcal{R} = \{r_n \forall n \in \mathbb{N}, f(1^n) = r_n$ is a CRN that accepts the input $e(x)$ for all $x \in \{0,1\}^n \cap L\}$.

Usually, we require that f and e are very simple (e.g. logspace computable) in a complexity theoretic sense, as we want the CRN to do the work and not (say) the input encoder e. As an example, $e(x)$ could be the indicator species for the string x; but we want to consider other input formats, including counts. One could have a similar definition of uniform families of CRNs that compute functions. If there are no (computability) restrictions on ee and ff we say the family is nonuniform; this incredibly powerful model finds most use in proving lower bounds.

20.2.7 Relating space-bounded, logically reversible Turing machines with CRNs

Overview. The overarching problem here is to understand how reversible CRNs relate to other reversible computing models, particularly space bounded reversible Turing machines (TMs).

There is a rich history of research on reversible space bounded Turing machines. Following his seminal results on time-bounded, logically reversible TMs, Bennett (1973) asked whether TM-SPACE(s) = reversible-TM-SPACE(s). Fifteen years later he made some progress towards this, showing that TM-SPACE(s) $\subseteq$ reversible-TM-SPACE(s^2). Many others worked to improve Bennett's result; finally Lange, McKenzie and Tapp (2000) answered Bennett's 1973 question in the affirmative. More recently, Thachuk et al. described what it means for a DNA strand displacement system (DSD) to use space (or equivalently volume) efficiently. Roughly, just as memory-efficient TMs reuse memory, space-efficient DSDs "recycle" strands by running reactions in both the forward and reverse directions. They also introduced restricted CRN models that can be compiled into DSDs in a space-preserving way.

While these CRN models have plausible physical realizations as DSD's, it is not clear that logically reversible, space-bounded reversible TMs have such physical realizations that preserve space. Roughly, the problem is that such TMs may "run" all of their transitions in the "forward" direction (rather than in both the forward and backwards directions, as do our recycling CRNs and DSDs), and so when one tries a straightforward approach to "compile" these space-bounded TMs into DSDs, the space blows up exponentially. Can this exponential space blow-up be avoided?

Reearch questions and challenges. One concrete first step to tackling this would be to study Bennett's 1989 construction. The description is at a fairly high level; it has an elegant and simple recursive structure that should be easily amenable to analysis. Is there a lower-level description, or "implementation" at the TM transition level, in which it is clear that transitions run alternately in the forwards and backwards direction? Progress on this should provide a nice strengthening of traditional complexity-theoretic results on space-bounded logically reversible computation and link this traditional work with current work on CRNs.

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Bibliography

[1] D. Angluin, J. Aspnes, and D. Eisenstat. Stably computable predicates are semilinear. In PODC, pages 292–299, 2006.

[2] D. Angluin, J. Aspnes, and D. Eisenstat. Fast Computation by Population Protocols With a Leader. In 20th International Symposium on Distributed Computing, pp61-75, 2006.

[3] C.H. Bennett. Logical reversibility of computation. IBM journal of Research and Development, 17(6):525–532, 1973.

[4] L. Cardelli and A. Csikász-Nagy. The cell cycle switch computes approximate majority. Scientific Reports, 2, 2012.

[5] E. Cardoza, R. Lipton, A.R. Meyer. Exponential space complete problems for Petri nets and commutative semigroups (Preliminary Report) Proceedings of the eighth annual ACM symposium on Theory of computing, pages 50–54, 1976.

[6] H.L. Chen, D. Doty, and D. Soloveichik. Deterministic function computation with chemical reaction networks. DNA Computing and Molecular Programming, pages 25–42, 2012.

[7] A. Condon, A.J. Hu, J. Maňuch, and C. Thachuk. Less haste, less waste: on recycling and its limits in strand displacement systems. Journal of the Royal Society: Interface Focus, 2(4):512–521, 2012.

[8] Q. Dong. A bisimulation approach to verification of molecular implementations of formal chemical reaction network. Master's thesis. SUNY Stony Brook, 2012.

[9] H-L. Chen, R. Cummings, D. Doty and D. Soloveichik, Speed faults in computation by chemical reaction networks, Distributed Computing, 1–18, 2015.

[10] D. Doty and M. Hajiaghayi. Leaderless deterministic chemical reaction networks. In Proceedings of the 19th International Meeting on DNA Computing and Molecular Programming, 2013.

[11] M.R. Lakin, D. Parker, L. Cardelli, M. Kwiatkowska, and A. Phillips. Design and analysis of DNA strand displacement devices using probabilistic model checking. Journal of The Royal Society Interface, 2012.

[12] M.R. Lakin, D. Stefanovic and A. Phillips. Modular Verification of Two-domain DNA Strand Displacement Networks via Serializability Analysis. In Proceedings of the 19th Annual conference on DNA computing, 2013.

[13] R. Landauer. Irreversibility and heat generation in the computing process. IBM Journal of research and development, 5(3):183–191, 1961.

[14] L. Qian, D. Soloveichik, and E. Winfree. Efficient Turing-universal computation with DNA polymers (extended abstract). In Proceedings of the 16th Annual conference on DNA computing, pages 123–140, 2010.

[15] L. Qian and E. Winfree. Scaling up digital circuit computation with DNA strand displacement cascades. Science, 332(6034):1196–1201, 2011.

[16] L. Qian, E. Winfree, and J. Bruck. Neural network computation with DNA strand displacement cascades. Nature, 475(7356):368–372, 2011.

[17] G. Seelig, D. Soloveichik, D.Y. Zhang, and E. Winfree. Enzyme-free nucleic acid logic circuits. Science, 314(5805):1585–1588, 2006.

[18] S. W. Shin. Compiling and verifying DNA-based chemical reaction network implementations. Master's thesis. California Insitute of Technology, 2011.

[19] D. Soloveichik, M. Cook, E. Winfree, and J. Bruck. Computation with finite stochastic chemical reaction networks. Natural Computing, 7(4):615–633, 2008.

[20] C. Thachuk. Space and energy efficient molecular programming. PhD thesis, University of British Columbia, 2012.

[21] C. Thachuk and A. Condon. Space and energy efficient computation with DNA strand displacement systems. In Proceedings of the 18th Annual International Conference on DNA computing and Molecular Programming, 2012.

[22] G. Zavattaro and L. Cardelli. Termination Problems in Chemical Kinetics. In Proceedings of the 2008 Conference on Concurrency Theory, pages 477-491, 2008.

Chapter 21

Entropy Methods, PDEs, Functional Inequalities, and Applications (14w5109)

June 29 - July 4, 2014

Organizer(s): E. Carlen (Rutgers University), J. Dolbeault (CNRS and Université Paris-Dauphine), D. Matthes (Technische Universität München), D. Slepčev (Carnegie Mellon University)

Entropy methods are one of the fundamental tools for the analysis of nonlinear PDEs, the proof of functional inequalities, and for capturing concentration phenomena in probability theory. This workshop has shown that entropy methods and related theories have clearly acquired maturity, and are of great importance for theoretical considerations and in applications. The scientific community behind the entropy method is very active and has a wide spectrum of interests, ranging from mathematical biology to differential geometry, and from discrete stochastic models and scientific computing, with very diverse motivations at least as far as applications are concerned. The involved researchers share a common knowledge and understand each other well. Workshops at Banff are perfect for extended interactions under such circumstances.

21.1 Recent Developments, Presentation Highlights and Open Problems

21.1.1 Advances in the theory

Novel variational approaches

Gradient flows in space of probability measures have provided a powerful tool for establishing well-posedness of a class of dissipative equations, as detailed in the book of Ambrosio, Gigli and Savaré [4]. This meeting has shown that a remarkably broad progress has been made during the last four years on problems and techniques that go beyond the reach of the previously studied setting.

LIERO and SAVARE discussed a new metric on the space of probability measures: the Hellinger-Kantorovich distance. An essential motivation for introducing this metric was to overcome a conceptual limitation of the Wasserstein distance, namely that any two measures of different total mass are infinitely far apart from each other. Instead, the Hellinger-Kantorovich distance allows to compare non-negative measures of arbitrary finite mass. The basic idea is to minimize over "paths" connecting the two measures which involve not only transport, but also annihilation and creation of mass. A key observation about the Hellinger-Kantorovich distance is the following: If measures of compact support are spatially close to each other, then the geodesic between the two is essentially defined by the usual Wasserstein mass transport, only that mass can decrease or grow along the path. If instead the measures are sufficiently far apart in space, then the geodesic path almost exclusively works by teleportation, i.e., annihilation of mass at the source and creation of mass at the target location.

Even though the definition of this metric is very recent, a lot of interesting properties have been proven already, some of them with an intriguing geometric interpretation. Despite the theory being so young and still under strong development, it seems very likely that in the near future, it might play a role in the analysis of reaction–diffusion equations that is comparable to the role that the Wasserstein distance nowadays plays in the context of non-linear diffusion and non-local aggregation equations.

STEFANELLI discussed a general framework for obtaining various nonlinear evolution equations through a convex minimization [2, 25, 27]. The WIDE (Weighted Inertia-Dissipation-Energy) Principle provides a scheme that works well in a significant number of existence problems corresponding to classical evolution equations. A reinterpretion evolution equations in the language of thermodynamics was discussed by ZIMMER. He addressed the question of deriving macroscopic evolutions driven by entropy or free energy from particle models. A dynamic scale-bridging approach based on particle evolutions with noise and the large deviation principle [1, 21] has been developed and applied to a number of problems. In particular it allows to consider the Vlasov-Fokker-Planck equation as GENERIC (General Equation for Non-Equilibrium Reversible-Irreversible Coupling) equation. This is a promising avenue to formulating such equations and for giving them a structure that merits further exploration. LEONARD discussed the entropy approach to special solutions to the Navier-Stokes equation with fixed initial and final data. This comes as an significant extension of Arnold's approach of the Euler equation. The current task is to understand what is the special status of these solutions among all other ones. KIM [3] talked about approximating solutions of solutions to (nonlinear) parabolic equations on bounded domain with oblique boundary conditions by solutions of equations on the whole space where a drift term has been added outside the original domain. TUDORASCU presented a global existence result for one-dimensional pressureless Euler/Euler-Poisson systems with or without viscosity [28]. It is obtained by employing the sticky particles model. Stability and uniqueness of solutions were obtained via a contraction principle in the Wasserstein metric. WU discussed the gradient flow approach to nonlocal-interaction equations in heterogeneous environments [32]. The fact that mobility varies in space endows the physical space with a manifold structure. Wu studied gradient flows of nonlocal interaction energy on manifolds with boundary including the case of non-convex sets [13].

21.1.2 Functional inequalities and asymptotic behavior

Entropy methods provide a direct connection between functional inequalities and quantitative estimates of asymptotic behavior of solutions of evolution equations. In typical settings, such as for Fokker-Planck or porous medium equations the functional inequalities provide a quantitative measure of the convexity of the entropy (or free energy) near the equilibrium, which in turn implies rates of convergence of solutions towards the equilibrium. The advances presented go beyond this framework and include equations where uniform convexity of the entropy near the equilibrium does not hold, estimates on asymptotics of discrete approximations, duality based approaches, symmetry breaking and systems of equations.

When participants were asked about their favorite talks by the organizers, several mentioned the presentation of ARNOLD, and said that it gave them an interesting new perspective on one of the oldest topics in entropy methods, namely to estimate the exponential rate of convergence to equilibrium for linear Fokker-Planck equations. The new ingredients for the old problem are hypocoercivity (degeneracy of the diffusion matrix) and non-symmetry (allowing drift terms that are not in gradient form). Both new effects need to be combined in the appropriate way in order to end up with a system whose solutions converge exponentially fast towards a stationary state that is non-degenerate in the sense that it possesses a density function. The talk was restricted to the situation where the drift force is a linear function on space, and it will require significant work to extend the results further. In this linear setting, however, a quite complete characterization of possible combinations of hypercoercive diffusion operators and non-symmetric drifts was given. Old results by Hörmander and more recent results by Villani were combined with genuinely new ideas. In the end, the calculation of the optimal exponential rate of equilibration was reduced to solving surprisingly simple problems in linear algebra.

A quite beautiful geometric approach to functional inequalities was presented by STURM. In his talk, he discussed the role of the auxiliary dimension N in the curvature-dimension condition $CD(K, N)$ for metric measure spaces [5, 14]. In fact, most of the results in the literature on logarithmic Sobolev and transportation inequalities or on the contractivity of the heat flow are concerned with the case in which the dimension parameter is irrelevant, that is $N = \infty$. However, if it is known that a manifold satisfies $CD(K, N)$ with some finite N, then these characteristic inequalities and contraction estimates can be improved both qualitatively and quantitatively. After giving a geometric interpretation of the refined curvature dimension condition, two approaches to the derivation of the improved inequalities were presented: the first is based on a refined analysis of mass transportation on manifolds, the second approach uses the Γ-calculus from the Bakry-Emery method.

FILBET explained that when writing discrete functional inequalities corresponding to a discretization of the continuous problem, the geometry of the mesh enters in the value of the optimal constants. Consequently, numerical rates of convergence towards equilibrium may be faster than expected. Relating best constants in the functional inequalities with discretized evolution equations is a challenging open question.

CAÑIZO discussed the entropy – entropy production inequalities for the linear Boltzman equation [9]. HUANG discussed an application of entropy methods to asymptotic behavior of the porous medium equations with fractional pressure in one dimension. Connection to Bakry-Emery method and transport inequalities was also included. JANKOWIAK discussed the flow which paves the way to further studies mixing gradient flows and duality notions [19]. NAZARET discussed symmetry breaking issues in weighted functional inequalities, which are a severe obstruction for understanding the optimality cases and the asymptotic regimes in the corresponding evolution equations. Moreover, weights raise a number of conceptual difficulties that should be treated with powerful tools like the $CD(\rho, N)$ condition, which turns out to be difficult to implement in practical cases. STAŃCZY talked about a model of gravitating particles [20, 31] that takes the form of a nonlocal parabolic equation. He focused on existence of stationary solutions and showed that for a fixed mass there can exist more than one stationary solution.

21.1.3 Applications

The range of applicability of the entropy method has been constantly widened in the last decade. In the beginning, applications were centered around the classical topics from mathematical physics, like nonlinear diffusion, or lubrication theory. Then, in the context of the very successful analysis of the Keller-Segel model by entropy methods, applications to systems in biology became very popular, a trend that peaked around the time of the previous entropy workshop at Banff about four years ago. Clearly, macroscopic equations for swarming, herding etc. are an extremely active field of research for the entropy community. The current meeting gave the organizers the impression that reaction-diffusion systems from chemistry might play the pivotal role for applications of the entropy methods in the near future.

This development reflects the successful extension of entropy related concepts to more and more complex equations. First results were concerned with scalar drift-diffusion equations — first linear, then non-linear, possibly degenerate. Later, the entropy structure in fourth (and higher) order non-linear diffusion equations was understood. The biological applications emerged when the theoretical results were extended to equations with non-local interaction terms. In that context, the entropy method was also applied to special systems of two coupled non-linear equations. Current developments aim at gaining a sound understanding of entropy dissipation in much more general systems of coupled diffusion equations. The main difficulty in this most recent step is the complete loss of comparison principles, which poses a more significant problem than it did, e.g., for fourth order diffusion equations.

Reaction-diffusion equations

Mainly due to the absence of comparison principles, reaction-diffusion systems are out of the reach of the standard parabolic theory. The difficulties are not just a short-coming of the techniques: there are rather harmless-looking systems with very few species which admit solutions that blow up in finite time. The talks focussed on systems to which the duality method can be applied, and which consequently do not blow up.

DESVILLETTES and FELLNER discussed progresses made in the theory of systems of reaction-diffusion equations [11], which allows to consider, for instance, networks of linear reversible equations. Purely algebraic computations provide Lyapunov functionals. Lyapunov estimates and duality methods respectively give compactness and prevent concentration. For systems, so far, no Maximum Principle approach can be expected to work. Hence the approach based on the combination of Lyapunov and duality methods is at the moment the only one that provides some hope for a general theory, which is still to be done. GENTIL discussed an interesting result under very special conditions on the coefficients of the system, [23]. The participants were intrigued by the possibility to combine the approach with the techniques discussed by other speakers (Desvillettes and Fellner).

A different point of view on the mathematical modeling of chemical reactions was presented by MAAS. Quite general reactions between K different species were considered, and a time-dependent stochastic model was written down for the number of particles from each of the species. The stochastic dynamics for the corresponding probability densities on $\mathbb{N}^K$ can be formulated as a gradient flow for the relative entropy functional in a suitable transportation metric on the discrete space. Such gradient flows on discrete spaces have recently been advanced by Maas and collaborators [26, 22] The thermodynamic limit (volume going to infinity, keeping the particle densities fixed, so that accordingly $\mathbb{N}^K$ approaches $\mathbb{R}_+^K$) was then rigorously analyzed in the framework of Γ-convergence. The limiting dynamics is governed by a non-linear second order diffusion equation for probability densities $\mathbb{R}_+^K$ (not on physical space), which still has the form of a gradient flow. Clearly, it would be nice to eventually connect these spatially homogeneous dynamics with a clear variational structure to the dynamics for space-dependent concentrations discussed before.

In this context, we further mention again the talks of LIERO and SAVARE, which highlighted a significant advance in the representation of systems with reactions (annihilation and creation of mass) as gradient flows. Currently, this approach is restricted to scalar equations. We expect that the connection between the entropy/duality approach for genuine systems and the novel gradient flow structure will become a key topic for future research.

Biological systems

The thorough analysis of the Keller-Segel system from chemotaxis modelling in the past years is probably one of the greatest success stories for the entropy method. In this workshop, we have had a variety of talks that were concerned with further extensions both of the related analytical tools and of the biological model underlying the equations.

BLANCHET presented a conceptually novel proof for global well-posedness of the parabolic-parabolic Keller-Segel system in the regime of sub-critical mass. The proof is obtained by further development of techniques from an earlier work on the parabolic-elliptic system. The key idea is to write the coupled equations as a gradient flow — in a joint Wasserstein-L^2-metric — of one functional, and to use the dissipation of another Lyapunov functional to derive additional estimates. The general concept of representing systems of evolution equations as gradient flow of <u>one</u> functional in a <u>combined</u> metric for the components seems promising for a variety of further applications. In fact, novel estimates on the large-time behavior of solutions seem within reach.

The topic of CHEN's talk was the behavior of solutions to (parabolic-elliptic) Keller-Segel systems with non-linear diffusion of power type for the bacterial density [15]. These chemotaxis equations were considered in arbitrary space dimension, and two dimension-dependent critical exponents for the diffusion were defined: the larger one is such that the equations are invariant under mass rescaling, the smaller one is such that the associated entropy functional is conformally invariant. The main result concerns the range of exponents strictly between the critical numbers. Similarly as for the "standard" Keller-Segel system in two dimensions, there is a sharp threshold for an L^p-norm of the initial datum below which the corresponding solution exists globally, and above which it blows up in finite time. The proof combines the standard entropy approach (involving the log-HLS inequality) with suitabel interpolation estimates, and is yet another nice example for the strength of the entropy method.

A different approach to the mathematical modeling of the underlying biological system was discussed by STEVENS. Instead of describing the motion of bacteria by means of a drift towards higher concentrations of the signaling substance which diffuses on a very short time scale, it seems (at least for certain populations of microorganisms) more reasonable to model the motion in terms of reinforced random walks. The resulting "macroscopic" equations have some resemblance to the established Keller-Segel system, but the elliptic equation for the concentration of the signaling substance is replaced by an ordinary differential equation in time. A variety of analytical results has been proven recently about the (non-)existence of global solutions to this kind of systems. The picture is not yet as complete as (and quite different from) the one for the classical Keller-Segel equations, but it seems that the behavior is at least as rich: for all the physically relevant dimensions, parameter regimes for global existence, finite-time blow-up and infinite-time blow-up of solutions have been identified. So far, these results have been obtained mainly by PDE techniques. It will be a challenge for the community to try to recover and hopefully improve them with entropy methods.

A new ansatz for mathematical modeling of a biological system was also the topic SCHMEISER's presentation. Here, the subject was not related to chemotaxis, but to cell motion by flat protrusions (lamellipodia) [29, 30]. The talk visualized the entire route from the very first microscopic modeling ansatz, motivated by observations of biologists in recent experiments, to the analysis of the macroscopic equations by means of the entropy method. It was quite impressive to see how a model developed on a basis of very few (biologically well-supported) assumptions leads to equations with an interesting mathematical structure, and how closely the results on numerical experiments are to the experimental observations. This is a part of long term program of Schmeiser's group on theoretical and numerical approaches for the modeling of the cytoskeleton (actin filaments), a program that will probably provide a number of further structurally interesting equations.

Many-agent systems: patterns and new models

Schools of fish, flocks of birds, and swarms of locust provide widely known examples of organization in many-agent systems. It is believed that the agents in such systems are governed by simple rules which includes the influence of the environment and the interactions with other agents. The nonlocal-interaction equations provide one of the simplest models of such interactions. In addition to them the participants talked about more refined models with an additional function which describes the (emotional) state of the agent, and systems in which agents are "rational" and have well defined goals.

BERTOZZI talked about an agent-based model of emotional contagion coupled with motion in one dimension, [8]. The model involves movement with a speed proportional to a fear variable that undergoes a temporal consensus averaging based on distance to other agents. They studied the Riemann initial data for this problem, leading to shock dynamics that is studied both within the agent-based model as well as in a continuum limit.

CARRILLO and LAURENT talked about patterns arising in models of collective behavior of autonomous agents, more precisely about (local) minimizers of nonlocal-interaction energies. Despite of their simplicity, these exhibit a broad variety of patterns. Laurent presented conditions on the regularity of the interaction potential at the origin that provide estimates on the dimensionality of the support of minimizers [6]. Carrillo presented conditions (sharp in some cases) on the potential that guarantee existence of global minimizers. He also connected the optimality conditions with nonlocal obstacle problems [10, 12] .

DEGOND presented intriguing ideas on reconciling approaches to collective behavior of rational agents (game theory) and agents subject to dynamical effects as can be modeled by kinetic theory [18, 17]. A striking feature of the model is that kinetic stationary and Nash equilibria coincide. This builds a bridge between the so-called econophysics and more classical approaches of economic theory. In terms of modeling at least it seems that there is a considerable potential for future developments, in a spirit similar to the approach of mean-field games.

Hydrodynamics

LAURENÇOT presented a thorough analysis of the thin-film approximation of the Muskat problem for two immiscible fluids placed on top of each other [24]. In leading order, one obtains a system of two diffusion equations of porous medium type, each of the equations governing one of the layers. Again, the mathematical difficulty is to deal with a coupled system of equations. The structural property that facilitates the analysis is that the system can be written as a gradient flow for one energy functional in a metric that combines both components, and there is one additional Lyapunov functional whose dissipation provides useful estimates. The general situation is thus almost identical to the one discussed in Blanchet's talk, and existence follows by similar methods.

The most impressive result of the talk was the richness found in the asymptotic behavior of solutions. Similarly as for the scalar porous medium equation, solutions become self-similar in the long-time limit. However, there exists a whole family of qualitatively different self-similar profiles, with different non-trivial topologies. For instance, the lower fluid might lose connectedness of its support, having the upper fluid penetrate down to the bottom. Obtaining estimates on the rate of convergence is currently an open problem.

In her talk, CHUGUNOVA picks up a classical story from lubrication theory. The thin film approximation for a droplet hanging from a stationary cylinder is considered, which leads to the well-known fourth order thin film equation, plus an additional gravity term. For the lubrication of a flat surface, the entropy and energy estimates derived by Bernis and Friedman [7] give a quite precise estimate on the rate of relaxation to a flat horizontal film. The results presented in this talk went into the opposite direction: general solutions approach the shape of a hanging droplet (in H^1) not faster than on algebraic time scale. This seemingly counter-intuitive result was proven by a clever "inversion" of the classical estimates.

YAO talked about the α-patch problem which is a modification of the surface quasi-geostrophic equation. She presented results on finite-time singularity formation.

21.1.4 Discretizations and numerical methods

One of the intended focal points of the meeting was to discuss the role of the entropy method for finite-dimensional systems, in particular for difference equations arising in discretizations of PDEs with a known entropy structure. The main motivation for this is the design of structure preserving numerical schemes that inherit a discretized version of the entropy structure of the original evolution equation. Tthe number of speakers addressing this topic turned out to be smaller than expected. Still, several conceptually very interesting approaches have been presented.

WOLFRAM presented a fully Lagrangian discretization of non-local aggregation and drift equations. Thanks to its Lagrangian nature, the scheme automatically preserves the solution's non-negativity and total mass, and the deformation of the initial mesh provides a nice intuitive picture of the transport underlying the evolution of the density. Moreover, the scheme is "automatically adaptive" in the sense that the mesh is finer in regions where the mass density is high. Thus, the neighborhood of blow-up points are well resolved by the scheme. In practice, the key difficulty is the initialization of the scheme, which requires the solution of a Monge-Ampere equation. The originally rather easy idea turned into a long-term project with manifold unexpected technical difficulties. There are many possibilities for further extensions and for rigorous numerical analysis.

CRAIG talked about a numerical scheme for nonlocal-interaction equations which is inspired by the established blob method from computational fluid dynamics [16]. The method is based on the approximate calculation of particle trajectories, where the force exerted on a given particle is not simply the superposition of the forces generated by all of the other particles as point sources, but rather an averaged quantity. Roughly speaking, the point sources are replaced by spatially extended (but still narrowly supported) "blobs". Thanks to this weak averaging, the is method convergent of arbitrary order, provided the initial datum is sufficiently regular.

Finite-volume discretizations for several classes of non-linear drift-diffusion equations were discussed by FILBET. Choosing the discrete fluxes in a suitable way, it can be shown that the approximations produced by the fully discrete scheme inherit the entropy dissipation properties of the original solutions, at least qualitatively. Indeed, the respective entropy decays exponentially fast to its minimum in numerical experiments, and this is justified analytically by proving discrete versions of the entropy-entropy dissipation estimates. Currently, the results remain qualitative in the sense that the provable rate of dissipation for the entropy in the discrete setting is typically different from the known optimal rate of decay of the original equation. This is due to the non-trivial geometry of the mesh, which makes it extremely hard to obtain sharp constants in the discrete functional inequalities.

Finally, it should be mentioned that structure preserving discretization of gradient flows also played a major role in the talk of MAAS, [26, 22], which has been reviewed above in the context of applications to reaction-diffusion equations. A consistent framework has been developed to give sense to, e.g., transportation distances between probability measures on graphs, the curvature of discrete manifolds, and the modulus of convexity for functionals on discrete spaces. The approach is very intuitive, and the calculus that has been developed in this framework has various interesting applications. For instance, it allows to prove functional inequalities for functions on graphs, like discretized versions of the log-Sobolev or Talagrand inequalities. The resulting discrete inequalities are very similar to the ones presented by Filbet, but the relation between the seemingly disjoint approaches still needs to be clarified.

21.2 Progress Made and Outcome of the Meeting

There has been a remarkable progress in the field over the past four years, since the previous BIRS workshop on a similar topic. Mathematical developments led to a large number of publications, many of them authored by young researchers. There has also been a significant broadening of the field and a shift of focus. While previously the focus has been on single equations, gradient flows in Wasserstein spaces and on specific applications, like the Keller-Segel system, now there is a variety of systems being studied by a broader range of techniques, as clear already from the talks described above. The entropy methods have found their way to discrete descriptions of the systems and remarkable structures have been discovered. The spectrum of applications and relevant models that have some shared mathematical structure has also increased.

The workshop was a great opportunity for researchers to learn about these developments and share their insights and perspective. One of the challenges is be keep a scientific community of people with such a large array of interests united, particularly as far as applications are concerned. We feel that the workshop has accomplished a lot towards that goal.

The workshop has also been an opportunity for many participants to continue existing collaboration on various projects and to initiate some new ones. The organizers did not hear that some spectacular conjecture had been solved during the meeting, but this is also something not so common in the area. However, we have good hope that the meeting will provide a serious boost to the various research directions including ones that have not been mentioned above.

The variety of open problems and emerging mathematical questions should be a clear signal for attracting new PhD students and young researchers in the area of entropy methods and related methods. In the next years, a special effort in that direction is expected from senior participants, in order to promote the topic.

Participants

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Bibliography

[1] S. Adams, N. Dirr, M. Peletier, and J. Zimmer. Large deviations and gradient flows. Philos. Trans. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci., 371(2005):20120341, 17, 2013.

[2] G. Akagi and U. Stefanelli. Doubly Nonlinear Equations as Convex Minimization. SIAM J. Math. Anal., 46(3):1922–1945, 2014.

[3] D. Alexander and I. Kim. A Fokker-Planck type approximation of parabolic PDEs with oblique boundary data. To appear in Transactions AMS, 2014.

[4] L. Ambrosio, N. Gigli, and G. Savaré. Gradient flows in metric spaces and in the space of probability measures. Lectures in Mathematics ETH Zürich. Birkhäuser Verlag, Basel, second edition, 2008.

[5] K. Bacher and K.-T. Sturm. Localization and tensorization properties of the curvature-dimension condition for metric measure spaces. J. Funct. Anal., 259(1):28–56, 2010.

[6] D. Balagué, J. A. Carrillo, T. Laurent, and G. Raoul. Dimensionality of local minimizers of the interaction energy. Arch. Ration. Mech. Anal., 209(3):1055–1088, 2013.

[7] F. Bernis and A. Friedman. Higher order nonlinear degenerate parabolic equations. J. Differential Equations, 83(1):179–206, 1990.

[8] A. Bertozzi, J. Rosado, M. Short, and L. Wang. Contagion shocks in one dimension. J. Stat. Phys., 2014. online first.

[9] M. Bisi, J. A. Cañizo, and B. Lods. Entropy dissipation estimates for the linear Boltzmann operator. Preprint arXiv:1405.0366, 2014.

[10] J. Cañizo, J. Carrillo, and F. Patacchini. Existence of compactly supported global minimizers for the interaction energy. Preprint, 2014.

[11] J. A. Cañizo, L. Desvillettes, and K. Fellner. Improved duality estimates and applications to reaction-diffusion equations. Comm. Partial Differential Equations, 39(6):1185–1204, 2014.

[12] J. Carrillo, M. Delgadino, and A. Mellet. Regularity of local minimizers of the interaction energy via obstacle problems. Preprint, 2014.

[13] J. Carrillo, D. Slepčev, and L. Wu. Nonlocal-interaction equations on uniformly prox-regular sets. Preprint, 2014.

[14] F. Cavalletti and K.-T. Sturm. Local curvature-dimension condition implies measure-contraction property. J. Funct. Anal., 262(12):5110–5127, 2012.

[15] L. Chen and J. Wang. Exact criterion for global existence and blow up to a degenerate Keller-Segel system. Doc. Math., 19:103–120, 2014.

[16] K. Craig and A. Bertozzi. A blob method for the aggregation equation. Preprint, 2014.

[17] P. Degond, J.-G. Liu, and C. Ringhofer. Evolution of the distribution of wealth in an economic environment driven by local Nash equilibria. J. Stat. Phys., 154(3):751–780, 2014.

[18] P. Degond, J.-G. Liu, and C. Ringhofer. Large-scale dynamics of mean-field games driven by local Nash equilibria. J. Nonlinear Sci., 24(1):93–115, 2014.

[19] J. Dolbeault and G. Jankowiak. Sobolev and Hardy–Littlewood–Sobolev inequalities. J. Differential Equations, 257(6):1689–1720, 2014.

[20] J. Dolbeault and R. Stańczy. Bifurcation diagrams for fermidirac particles. To appear in Disc. and Cont. Dynamical Systems A, 2014.

[21] M. H. Duong, M. A. Peletier, and J. Zimmer. GENERIC formalism of a Vlasov-Fokker-Planck equation and connection to large-deviation principles. Nonlinearity, 26(11):2951–2971, 2013.

[22] M. Erbar and J. Maas. Gradient flow structures for discrete porous medium equations. Discrete Contin. Dyn. Syst., 34(4):1355–1374, 2014.

[23] P. Fougères, I. Gentil, and B. Zegarlinski. Solution of a class of reaction-diffusion systems via logarithmic Sobolev inequality. Preprint, 2014.

[24] P. Laurençot and B.-V. Matioc. A gradient flow approach to a thin film approximation of the Muskat problem. Calc. Var. Partial Differential Equations, 47(1-2):319–341, 2013.

[25] M. Liero and U. Stefanelli. Weighted inertia-dissipation-energy functionals for semilinear equations. Boll. Unione Mat. Ital. (9), 6(1):1–27, 2013.

[26] J. Maas. Gradient flows of the entropy for finite Markov chains. J. Funct. Anal., 261(8):2250–2292, 2011.

[27] A. Mielke and U. Stefanelli. Weighted energy-dissipation functionals for gradient flows. ESAIM Control Optim. Calc. Var., 17(1):52–85, 2011.

[28] T. Nguyen and A. Tudorascu. One-dimensional pressureless gas systems with/without viscosity. Preprint, 2014.

[29] D. Oelz and C. Schmeiser. Derivation of a model for symmetric lamellipodia with instantaneous cross-link turnover. Archive for Rational Mechanics and Analysis, 198(3):963–980, 2010.

[30] D. Oelz and C. Schmeiser. Simulation of lamellipodial fragments. J. Math. Biol., 64(3):513–528, 2012.

[31] R. Stańczy. On an evolution system describing self-gravitating particles in microcanonical setting. Monatsh. Math., 162(2):197–224, 2011.

[32] L. Wu and D. Slepčev. Nonlocal interaction equations in environments with heterogeneities and boundaries. Preprint, 2013.

Chapter 22

Spin Glasses and Related Topics (14w5082)

July 20 - 25, 2014

Organizer(s): Michael Cranston (University of California, Irvine), Erwin Bolthausen (University of Zurich), Dmitry Panchenko (Texas A&M University)

22.1 Overview of the conference

Spin glasses has been an active area of research in theoretical physics since about mid-seventies. On the mathematics side, it has been increasingly more active over the last two decades, and over the last ten years or so it has become a tradition to organize a conference on the mathematics of spin glasses once every one or two years. This year the conference took place at the Banff International Research Station, which allowed us to bring together many of the mathematicians and physicists working in the area of spin glass models and various related areas, and gave us all a chance to share recent results and ideas, as well as to have many wonderful discussions in a great collaborative environment that BIRS provides. As the organizers, we tried to ensure the success of the conference by careful planning.

First of all, we attempted to increase the diversity in a number of ways. First of all, although the main focus of the conference was on the mathematics of spin glasses and related areas, out of 35 participants we had 5 theoretical physicists as participants and speakers. The diversity of topics represented was also an important factor in making the conference successful. Among invited participants, we had experts working on various models of spin glasses, random matrices, various extremal processes, Brownian motion, optimization and algorithms, random combinatorial optimization problems, biological applications of spin glass models, and genealogy in populations dynamics. Furthermore, there were 5 female researchers (unfortunately, one of them could not make it at the very last moment due to lost passport). Finally, we also had a significant number of young researchers – 5 postdocs and 4 current Ph.D. students – with all of them giving a talk (except one beginning Ph.D. student).

In addition, we were encouraged by the BIRS recommendations to create a schedule that leaves plenty of time for discussions and collaboration, and we tried to do that. We had a relaxing schedule of only 28 talks that ended at 4 p.m. every day, and many participants worked in groups after that both before and after dinner. Moreover, we left Friday morning completely open, which resulted in a wonderful three-hour discussion session led by Giorgio Parisi.

This was a second spin glass meeting at BIRS in the last 6 years. We consider the meeting to have been a great success and we hope to be back in the future.

22.2 Overview of the field

Few materials in the history of solid state physics have been as intriguing and perplexing as certain alloys of ferromagnets and conductors, such as $AuFe$ or $CuMg$, known as *spin glasses*. The attempts to study these magnetic alloys theoretically gave rise to a class of *disordered spin models*, whose analysis by both physicists and mathematicians has grown into one of the most fascinating fields of statistical mechanics over the last 35 years. Probably, the two most famous models are the Edwards-Anderson model and its mean-field analogue, the Sherringon-Kirkpatrick (SK) model. Even the simpler SK model has proven to possess a very rich structure that was very hard to discover and took a long time to confirm mathematically. Theoretical physicists, starting with the groundbreaking work of Giorgio Parisi, have created a general theory of this model, mostly within the framework of the celebrated replica method, with the physical properties of the system described by such famous features as the "replica symmetry breaking"and "ultrametricity". After more than two decades, the predictions of the physicists in the SK model have been now mostly confirmed mathematically in recent years, but many interesting problems remain.

Furthermore, the ideas developed by theoretical physicists in the setting of the SK model have found striking applications in unexpected areas, for example, in the models arising from optimization—such as the satisfiability of Boolean formulas, the in depend set problem, the matching problem, the traveling salesman problem, the assignment problem, the graph partitioning problem—as well as in the models arising in biology, such as the Hopfield model of neural networks. In many of these models, the physicists came up with detailed predictions about the structure of the Gibbs measure, which relates to the structure of the solution space, so mathematicians have their hands full for many years to come.

Encouraging progress in various directions has been happening for a while now, and a number of interesting recent results were presented at this conference.

22.3 Presentation Highlights

Louis-Pierre Arguin (Université de Montreal) spoke on "Fluctuation bounds for interface free energies in spin glasses." The quantitative dependence of free energy fluctuations on the quenched disorder is a fundamental thermodynamic property of all disordered systems. Bounds on such fluctuations have been used to prove uniqueness of the Gibbs state in a class of two-dimensional disordered systems, including the two-dimensional random field Ising model. Moreover, it has been noted by several authors that determining quantitative bounds on the interface free energy variance with respect to the couplings would allow a resolution of a long-standing open problem at the heart of the statistical mechanics of short-range spin glasses in finite dimensions: how many pure states (or at zero temperature, ground states) are present in the spin glass phase?Thus, one way to understand the structure of the Gibbs states of disordered systems is to get good bounds on the fluctuations of the free energy difference between two states. This approach has led to the proof of the absence of phase transition in the 2D Random Field Ising Model (RFIM) by Aizenman and Wehr. This talk explained a method to obtain lower bounds for the variance of the free energy difference of the Edwards-Anderson (EA) spin glass model on $\mathbb{Z}^d$ between certain incongruent states (if they exist...). Unlike the RFIM, there is no dominance of the $(+)$ and $(-)$ states in the EA model. One interesting point of the method is to overcome this lack of monotonicity. The lower bound is also used to rule out particular structures of the Gibbs states in $d = 2$. This is joint work with C. Newman, D. Stein and J. Wehr.

Antonio Auffinger and Wei-Kuo Chen (both are postdocs at the University of Chicago) gave two talks about their joint work on Parisi measures and bipartite spherical spin glass models. Chen's talk focused on various important properties of Parisi measures, heuristically and numerically observed by physicists, and recently proved by the two of them mathematically. The most important one (this was quite a high impact result) is that the Parisi functional order parameter in the Sherrington-Kirkpatrick model (which determines all other parameters of the model) is unique. They proved this by showing that the Parisi functional is strictly convex. For this purpose they developed and applied techniques from stochastic control theory. Auffinger's talk focused on their recent results about bipartite models. In particular, they proved a formula for the free energy based on the Crisanti-Sommers representation of the mixed spherical model and showed that the mean number of local minima at low levels of energy is exponentially large in the size of the system.

David Belius (Université de Montreal) spoke on ”The subleading order of two dimensional cover times.” The cover time is the time it takes for a Markov process on a finite or compact state space to visit the whole state space. This time can be studied by considering the extrema of a correlated random field, namely the field of occupation times, placing it in a similar category to many spin glass problems. In this talk Belius presented a recent result on the cover time of the two dimensional torus by Brownian motion, where the field of occupation times turns out to be log-correlated. He used techniques inspired by those for Branching Brownian Motion (BBM) to establish the exact subleading correction for the expectation of the cover time, which corresponds to the well-known $3/2$-correction for BBM. The leading order had been established by Dembo, Peres, Rosen and Zeitouni [Ann. of Math., 160 (2004)]. This involves a multiscale analysis of the field of occupation times, and the identification of an approximate hierarchical structure. This work establishes deep connections with the asymptotics of BBM proved in the groundbreaking work of Maury Bramson which was motivated by a model for the propagation of genes in a population, and its relations with traveling waves for the KPP equation. This is joint work with Nicola Kistler.

Nathanael Berestycki (University of Cambridge) Spoje on ”Liouville Brownian Motion.” A subject of considerable interest in recent years has been to develop a notion of random surface, understand its geometry and relate it to the theory developed by physicists in the context of Liouville quantum gravity. In particular conformal invariance properties are expected and the so-called KPZ relation is believed to hold. Consider a uniform random triangulation of a random surface with a large but finite number of faces, represented so that every triangle is equilateral. Such a triangulation can also be represented in the plane via the circle packing theorem. Either way, after rescaling, it is strongly conjectured that the density of vertices converges, to a measure with density with respect to Lebesgue measure given by the exponential of a constant times a Gaussian Free Field. Even defining this limiting measure ? is nontrivial and was one of the main results in in these two landmark papers (Duplantier-Sheffield, Rhodes-Vargas). In his talk, the speaker introduced and discussed a canonical notion of Brownian motion in the random geometry of Liouville quantum gravity, called Liouville Brownian motion which is supposed to be the scaling limit of a random walk on a random triangulation. He discussed some of its basic properties, for instance related to the time spent in the thick points of the Gaussian Free Field. He also discussed the construction of this process in the supercritical phase of Liouville quantum gravity and showed a certain duality with the subcritical phase.

Anton Bovier (Rheinische Friedrich-Wilhelms-Universitat Bonn) spoke on” Extremal processes of Gaussian processes indexed by trees.” Gaussian processes indexed by trees form an interesting class of correlated random fields where the structure of extremal processes can be studied. One popular example is Branching Brownian motion, which has received a lot of attention over the last decades, not the least reason being its connection to the KPP equation. The KPP equation was derived to model the spread of a gene in a population and has a long history. Analysis of this equation involves branching Brownian motion an approach initiated by McKean with a fundamental contribution by Bramson. More recent developments in the field are by Lalley and Sellke. In his talk Bovier reviewed the construction of the extremal process of BBM in the time to ∞ limit (with Arguin and Kistler) which has an interesting description as a decorated Poisson-Dirichlet point process. He also presented more recent results on variable speed BBM, obtained recently with Lisa Hartung.

Amir Dembo (Stanford University) spoke on ”Spin glasses on locally tree like graphs'” a collaboration with Gerschenfeld and Montanari. This is work motivated by earlier results of Bray ad Viana, 1985. Many problems of interest in computer science and information theory can be phrased in terms of a probability distribution over discrete variables associated to the vertices of a large (but finite) sparse graph. In recent years, considerable progress has been achieved by viewing these distributions as Gibbs measures and applying to their study heuristic tools from statistical physics. The model is a Gibbs measure on a finite sparse graph with n vertices. The Hamiltonian of the Gibbs measure involves only a coupling between adjacent vertices and an external field term. As n tends to infinity, the graph is assumed to locally converge to a tree. The main result is an existence of the free energy in the $n \to \infty$ limit for high temperatures.

Silvio Franz (Université de Paris-Sud 11) spoke on ”Glassy critical points and the Random Field Ising Model.” Research in recent years has emphasized the importance of fluctuations in understanding glassy phenomena in supercooled liquids. The present comprehension of long lived dynamical heterogeneities in these systems compares the growth of their typical size to the appearance of long range correlations at second order phase transition points. Unfortunately, in supercooled liquids, the theoretical study of these correlations beyond the mean field is just at an embryonic level. One of the difficulties lies in the fact that -with good physical reasons- the critical point corresponds to an unstable field theory. It turns out that one can cure the instability introducing appropriate physical constraints. In that case true critical points appear and they can be analyzed theoretically through the replica method. In usual phase transition often there is a line of first order transitions that ends at a second order terminal critical point. The most popular case are ferromagnets: at low temperatures there is a first order transition when the magnetic field crosses zero (the magnetization has a discontinuity) and this transition line ends at the usual critical point. The same phenomenon happen for the gas liquid transition: it is a first order transition at low temperatures that ends in a second order transition at the critical point. A similar situation can occur for liquids undergoing a glass transition, where lines of discontinuous glass transitions can terminate in critical points. In this talk the focus was on these terminal points, where the glass transition becomes continuous and activation does not play a major role in establishing equilibrium. The speaker presented the field theory of these critical points and showed that the universality class of the Random Field Ising Model appears.

Yan Fyodorov (Queen Mary College, London) spoke on ”High-dimensional random landscapes and random matrices.” In this talk, Fyodorov discussed a picture of the “topology trivialization transition” (in the sense of an abrupt reduction of the number of stationary points and minima of the underlying energy landscape) which takes place at zero temperature in p-spin spherical model of spin glasses with increasing random magnetic field, as well as in related high-dimensional models not restricted to the sphere. After developing the general formalism based on the high-dimensional Kac-Rice formulae it is combined with the Random Matrix Theory (RMT) techniques to perform analysis of the random energy landscape of p-spin spherical spin glasses and a related glass model, both displaying a zero-temperature one-step replica symmetry breaking glass transition as a function of control parameters (e.g. a magnetic field or curvature of the confining potential). In particular, the emphasis was on the role of the “edge scaling” and the Tracy-Widom distribution of the largest eigenvalues of random matrices for providing some universal features of the above transition. For the simplest case $p = 2$, he discussed the large deviation function for the minimal energy extracted via a variant of the replica formalism. He also discussed how random matrix methods can be used to get insights into topology of random real algebraic varieties. The talk was based on the paper arXiv:1307.2379 as well as on joint works with Pierre Le Doussal.

David Gamarnik (Massachusetts Institute of Technology) talked about his joint work with Maghu Sudan related to the problem of constructing algorithms for solving randomly generated constraint satisfaction problems, such random K-SAT problem, and, more precisely, about the limitations of local algorithms. This is a very interesting work, because they establish a fundamental barrier on the power of local algorithms to solve such problems, despite the conjectures put forward in the past. In particular, they refute a conjecture regarding the power of so-called i.i.d factors to find nearly largest independent sets in random regular graphs. They also showed that a broad class of local algorithms, including the so-called Belief Propagation and Survey Propagation algorithms, cannot find satisfying assignments in the random NAE-K-SAT problem above a certain asymptotic threshold, below which even simple algorithms succeed with high probability. Their negative results are based on the analysis of the geometry of feasible solutions of random constraint satisfaction problems, which was first predicted by physicists heuristically and confirmed by rigorous methods. According to this picture, the solution space exhibits a clustering property whereby the feasible solutions tend to cluster according to the underlying Hamming distance. Their main idea was to show that success of local algorithms would imply violation of such a clustering property.

Véronique Gayrard (Aix-Marseille Universit?e and CNRS) spoke on ”Aging in mean-field spin-glasses.”

She presented recent results on the activated aging dynamics of mean-field spin glasses (REM, p-spin SK model, GREM-like trap model.) The key result is a very general criterion for the convergence of clock processes in random dynamics in random environments that is applicable in cases when correlations are not negligible: An important ingredient is based on a general criterion for convergence of sums of dependent random variables due to Durrett and Resnick [Ann. Probab. 6 (1978) 829-846]. The power of this criterion is demonstrated by applying it to the case of random hopping time dynamics of the p-spin SK model. It is proved that on a wide range of time scales, the clock process converges to a stable subordinator almost surely with respect to the environment. Also, the time-time correlation function converges to the arcsine law for this subordinator, almost surely. Another application of the general criterion is for the aging behavior of a truncated version of the Random Energy Model evolving under Metropolis dynamics. There, it is proved that the natural time-time correlation function defined through the overlap function converges to an arcsine law distribution function, almost surely in the random environment and in the full range of time scales and temperatures for which such a result can be expected to hold. This establishes that the dynamics ages in the same way as Bouchaud's REM-like trap model, thus extending the universality class of the latter model.

Giuseppe Genovese spoke on "SK-spherical spin glass approximation for the Hopfield model with Gaussian patterns." By means of a mapping into an appropriate bipartite spin glass, it is possible to decompose the free energy of the Hopfield model with Gaussian patterns into the free energies of a SK model and a spherical one. We will discuss some results in this direction obtained in collaboration with A. Barra, F. Guerra and D. Tantari. In our paper we investigate the high storage regime of a neural network with Gaussian patterns. Through an exact mapping between its partition function and one of a bipartite spin glass (whose parties consist of Ising and Gaussian spins respectively), we give a complete control of the whole annealed region. The strategy explored is based on an interpolation between the bipartite system and two independent spin glasses built respectively by dichotomic and Gaussian spins: Critical line, behavior of the principal thermodynamic observables and their fluctuations as well as overlap fluctuations are obtained and discussed. Then, we move further, extending such an equivalence beyond the critical line, to explore the broken ergodicity phase under the assumption of replica symmetry and we show that the quenched free energy of this (analogical) Hopfield model can be described as a linear combination of the two quenched spin-glass free energies even in the replica symmetric framework.

Cristian Giardina (University of Modena and Reggio Emilia) spoke on "Central limit theorems for Ising models on random graphs." A classical result of Newman established the central limit theorem for the magnetization over large blocks for the Ising model using the fact that the spins are associated random variables under the Gibbs measure in the ferromagnetic case. For various classes of random graphs with N vertices, we prove that the total spin of the Ising model defined on them satisfies a central limit theorem, provided it is centered by the total magnetization and rescaled by the square root of N. We consider both quenched and annealed measures in the one-phase region. We conjecture that when the vertex degrees do not fluctuate, the variance of the limiting Gaussian law is the same in the two settings. We substantiate this claim with the analysis of some configuration models. Joint work with C. Giberti, R. van der Hofstad, M.L. Prioriello.

Friedrich Götze (University of Bielefeld) gave a talk about "Asymptotic approximations for spectra of random matrices". From the fundamental contribution by E. Wigner [Annals of Math. Vol 67, 325-328] it is known that Hermitian $n \times n$ random matrices with independent entries have a $n \to \infty$ limit distribution of the eigenvalue statistics given by the so-called semi-circle distribution. If one drops the Hermitian assumptions, the situation becomes much more complicated, and eigenvalue statistics with an elliptic shape appear in the limit. It however turns out, as recently proved by Götze, together with Naumov and Tikhomirov, that products of such matrices in nearly all natural cases have a limit distribution of the density of states which is circular. Friedrich Götze gave an overview on the recent progresses in this field, as well as on very precise new results concerning finite n error bounds.

Aukosh Jagannath (a Ph.D. student of Gèrard Ben Arous at New York University) gave a talk about his recent work on the approximate ultrametricity of Gibbs measures in spin glass models. The main idea of his work was the following. In a number of spin glass models, the famous Parisi ultrametric ansatz was proved rigorously in the work of Panchenko (one of the organizers of the conference). This is a statement about the geometry of the Gibbs measure in the thermodynamic limit when the size of the system goes to infinity. Jagannath's work was to show that this picture also holds in an approximate sense for systems of finite but large size. His idea was to use the information about the geometry of the sample from the Gibbs measure to carefully reconstruct the nested sequence of clusters in a controlled way which showed that they satisfy the Parisi ansatz approximately.

Kay Kirkpatrick talked about "Non-normal asymptotics of the mean-field Heisenberg model". This work is about spin models of magnets and superconductors which are of XY-type, i.e. spin states given by the circle, or of Heisenberg type where the spin state is a d-dimension sphere, $d \geq 2$. These models have interesting phase transitions. Together with Elizabeth Meckes, there are recent results on a non-Gaussian scaling limit of the mean-field models exactly at critical temperature. This is an extension of work done by Ellis-Newman [J. of Stat. Physics, Vol. 19, 149–161 (1978)] for the Curie-Weiss model.

Emanuele Mingione (a Ph.D. student of Pierluigi Contucci at the University of Bologna) talked about his work (with collaborators) on a multi-species version of the Sherrington-Kirkpatrick model. They introduced a new model where the spins of the system are divided into several groups (called species) and interactions between spins depend on the species they come from. Under a certain assumption (which essentially means that the interactions within species are stronger than inter-species interactions) they suggested an analogue of the Parisi formula for the free energy and showed, using Guerra's interpolation method, that it actually gives an upper bound on the free energy. The formula they suggested was very interesting because it suggested that, when comparing likely realizations of such a system, the inner-species similarity between these two populations will be synchronized in all the species. This was later proved in the work of Panchenko, completing the proof of the free energy formula in this model.

Charles Newman (New York University) spoke on "Statistical mechanics and the Riemann hypothesis." In this talk Newman reviewed a number of old results concerning certain statistical mechanics models and their possible connections to the Riemann Hypothesis. A standard reformulation of the Riemann Hypothesis (RH) is: The (two-sided) Laplace transform of a certain specific function Ψ on the real line is automatically an entire function on the complex plane; the RH is equivalent to this transform having only pure imaginary zeros. Also Ψ is a positive integrable function, so (modulo a multiplicative constant C) is a probability density function. A (finite) Ising model is a specific type of probability measure $\mathbb{P}$ on the points $S = (S_1, \ldots, S_N)$ with each $S_j = \pm 1$. The Lee-Yang theorem implies that for non-negative $a_1, \ldots, a_N$, the Laplace transform of the induced probability distribution of $a_1 S_1 + \cdots + a_N S_N$ has only pure imaginary zeros. The big question here is whether it's possible to find a sequence of Ising models so that the limit as N tends to ∞ of such distributions has density exactly $C\Psi$?. He discussed some hints as to how one might try to do this.

Dmitry Panchenko (professor at the University of Toronto, and one of the organizers) talked about his recent work on diluted spin glass models. The main motivation for his work was the conjectured Mézard-Parisi formula for the free energy in the diluted spin glass models, such as the random K-sat model, or diluted p-spin models. One possible approach to proving this formula is to show that the structure of Gibbs measure in these models is described by the Mézard-Parisi ansatz, and Panchenko proved recently that this ansatz holds in all cases when the distance between two spin configurations drawn from the Gibbs measure takes finitely many values in the thermodynamic limit (the called finite-replica symmetry breaking case). The general case remains an open problem.

Giorgio Parisi (professor at the University of Rome La Sapienza) talked about his work (with collaborators) on fractal free energy landscapes in structural glasses. Realistic models for glasses seem intractable, so he described a model which is a simplification, but its solution and behaviour are still very complicated. Using theory and numerical simulation, they showed that the landscape is much rougher than is classically assumed, and they determined analytically critical exponents for the basin width, the weak force distribution and the spatial spread of quasi-contacts near jamming. Their value was found to be compatible with numerical observations.

Nicholas Read (professor at Yale University) talked about the the famous Edwards-Anderson short range spin glass model and, in particular, about the metastate interpretation of replica symmetry breaking in these models. The main idea of his talk was to show how the replica symmetry breaking scheme of Parisi can be described in terms of a non-trivial metastate picture proposed by Newman and Stein.

Jason Schweinsberg talked about "The genealogy of a population undergoing selection". Consider a population of constant size N in which each individual dies at rate 1 and during lifetime each experiences muations at rate r. Mutations are assumed to be beneficial, so that the fitness of an individual increases (linearly) in the number of mutations. When an individual dies, a replacemnt is chosen at random from the population with probability proportional to the individual's fitness. It is shown that the genealogy of this population is given by the Bolthausen-Sznitman coalescent, confirming non-rigorous predictions of Neher and Halltschek and Desai, Walczak, and Fisher. The Bolthausen-Sznitman coalescent arises in connection with spin glass models as an alternative description of Ruelle's probability cascades, and was recently also shown to describe the genealogy of branching Brownian motion with absorption.

Allan Sly (professor at the University of California, Berkeley) talked about his joint work with Jian Ding and Nike Sun (another participant) about the maximum independent sets in random d-regular graphs. In a very impressive work, they found explicit formulas for the leading order and logarithmic correction terms in the case when d is large enough and showed that the remaining fluctuations are of order one. This confirmed the so called one-step replica symmetry breaking predictions of the physicists.

Shannon Starr (University of Alabama, Birmingham) spoke "About eigenvectors for random matrices." In analogy with the random overlap structure for spin glasses, it seems useful to know the distribution of the eigenvector inner-products for models of random matrices, especially non-Hermitian models such as GinibreÕs ensemble. Starr described an attempt to determine these, and to find reported values in the literature.

Daniel Stein (New York University) spoke on "Predictability in non equilibrium discrete spin dynamics." In this talk, he considered a dynamical many-body system with a random initial state subsequently evolving through stochastic dynamics. The question addressed is what is the relative importance of the initial state (ÒnatureÓ) vs. the realization of the stochastic dynamics (ÒnurtureÓ) in predicting the final state? We discuss this question and present both old and new results for low-dimensional homogeneous and disordered Ising spin systems.

Nike Sun (a Ph.D. student of Amir Dembo at Stanford University) described her work (with collaborators) on the Potts and independent set models on d-regular graphs. They proved that the replica symmetric (Bethe) prediction applies for all parameter values in the ferromagnetic Potts model on typical d-regular graphs, and the independent set model on typical bipartite d-regular graphs. Interestingly, these results are in contrast with the anti-ferromagnetic Potts model and the independent set model at high fugacity on non-bipartite graphs, where the replica symmetric prediction is known to fail.

Daniele Tantari (University of Rome La Sapienza) spoke on "Parallel retrieval in multitasking associative networks." Recently multitasking associative networks have been introduced in the statistical mechanics community to mimic the parallel processing capabilities of the immune system, the latter being thought of as a network of interacting B and T lymphocytes. In this talk, after a streamlined introduction to fundamentals of theoretical immunology, Tantari introduced these models (mainly bipartite spin glasses embedded on a finite connectivity topology) and spoke about their phase diagrams, and applied replica tricks and/or cavity techniques, in order to distinguish between a ferromagnetic region -where the system performs extensive parallel retrieval- and a spin glass one, where the amount of interferences among the patterns increases: Tantari gave a proof that this clonal cross-talk diminishes the multitasking features of these networks. Further, she showed that a second order phase transition occurs when varying the level of load (number of memo- rized patterns), networkÕs dilution and fast noise: from low to high load, from fully connected to finite connectivity regimes.

Olivier Zindy (Université Pierre et Marie Curie, Paris) talked about "Poisson-Dirichlet statistics for the extremes of log-correlated Gaussian fields". Gaussian fields with logarithmically decaying correlations, such as branching Brownian motion, the two-dimensional Gaussian free field, the occupation field of two-dimensional random walks, and many others, are conjectured to form a new universality class of extreme value statitics (notably in works by Carpentier and Ledoussal, and Fyodorov and Bouchaud). This class is the borderline case between the class of i.i.d. random variables, and models where correlations start to affect the statistics, the latter being the case for the low-temperature SK-model. In his talk, Zindy describes a general approach based on rigorous works in spin glass theory to describe features of the Gibbs measure of these Gaussian fields. It is shown that at low temperature, the normalized covariance of two points sampled from the Gibbs measure is either 0 or 1. This is used to prove that the joint distribution of the Gibbs weigths converges in a suitable sens to that of a Poisson-Dirichlet variable. (Joint work with Louis-Pierre Arguin).

Participants

Arguin, Louis-Pierre (University of Montreal)
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Ben Arous, Gerard (New York University)
Berestycki, Nathanael (University of Cambridge)
Bolthausen, Erwin (UniversitŁt Zrich)
Bovier, Anton (Rheinische Friedrich-Wilhelms-UniversitŁt Bonn)
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Dembo, Amir (Stanford University)
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Gayrard, Vronique (Aix-Marseille Universit and CNRS)
Genovese, Giuseppe (UniversitŁt Zrich)
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Kirkpatrick, Kay (University of Illinois)
Mingione, Emanuele (University of Bologna)
Newman, Charles (New York University)
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Parisi, Giorgio (University of Roma La sapienza)
Read, Nicholas (Yale University)
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Starr, Shannon (University of Alabama, Birmingham)
Stein, Daniel (New York University)
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Tantari, Daniele (La Sapienza Universit di Roma)
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Chapter 23

Statistics and Nonlinear Dynamics in Biology and Medicine (14w5079)

July 27 - August 1, 2014

Organizer(s): Giles Hooker (Cornell University), Jiguo Cao (Simon Fraser University), David Earn (McMaster University), Edward Ionides (University of Michigan), Darren Wilkinson (University of Newcastle)

23.1 Overview of the Field and Recent Developments

This workshop brought together researchers from several different disciplines to work on the problem of performing statistical inference with mechanistic models of real-world systems in biology and medicine. This involved

- Statisticians, whose work is traditionally associated with estimating parameters from data, assessing uncertainty in those estimates and developing methods to perform inference about data and the processes that generate it.
- Applied Mathematicians and Probabilists whose work is focussed on understanding mechanistic models and describing their behavior. This is particularly the case for stochastic models that evolve probabilistically over time.
- Subject area experts who wish to use mechanistic models and statistics to answer substantive questions about their fields of interest. In this meeting we had representatives from fields in Systems Biology, Immunology, Epidemiology and Ecology.

Historically, there has been little communication between these fields: statisticians generally have not worked with the type of mechanistic modeling that applied mathematicians tend to employ and applied mathematicians have rarely been interested in data or in formal statistical questions beyond "the proposed model exhibits the type of behavior we appear to see in the real world".

This has resulted in little attention being given to the problems of conducting statistical inference in these models – estimating parameters, establishing methods to test for goodness of fit, inferential tests about relevant parameter values or properties of the system. Moreover, development of methods to address these problems has frequently been carried out within application disciplines and there has been little cross-talk between the communities carrying out this research.

This workshop was designed to address these problems. The last decade has seen the development of a small community of statisticians, applied mathematicians and probabilists with research interests specifically addressed towards these issues and who also have established collaborations with researchers in relevant application areas. This workshop provided a venue for all these communities to come together, share ideas, perspectives and establish new collaborative links. Informal feedback from workshop participants has been very positive with many new ideas emerging and the common refrain that the participants had all learned a great deal.

Mathematically, the field is concerned with the problem of fitting models of systems dynamics to data. That is, we posit a Markovian model for the evolution of the state vector x of a system over time:

$$P(x(t+\delta)|x(t),\theta) = g(x(t),\theta)$$

in which x is a vector of values describing the state of the system and θ a vector of unknown parameters and the model describes the (probabilistic) evolution of $x(t)$ from from times t to $t+\delta$. This framework encompasses a very general class of models including finite population models, based on the Gillespie algorithm [20], diffusion processes:

$$dx = f(x,\theta)dt + \Sigma(x,\theta)dW$$

and should be taken to be broad enough to include ordinary differential equations (ODEs)

$$\dot{x} = f(x,\theta).$$

Ordinary differential equation models make the evolution of a system's state explicitly deterministic. However, these models have been extensively studied with the applied mathematics literature and produce important challenges for statistical inference. A significant portion of the existing statistical methodological development focusses on these models and they are therefore also included here.

In addition to a model of system evolution, a model is also proposed for the process that generates observations, these can be as simple as the addition of Gaussian noise to the value of the state at a given time

$$y_i = x(t_i) + \varepsilon_i, \varepsilon_i \sim N(0,\Sigma)$$

but may be more complex. Frequently, not all components of the state vector x can be directly observed, or observed at all, and often only some transformation of x is observable. In general we write

$$P(y_i|x(t_i),\theta) = h(x(t_i),\theta)$$

and assume that observations between observation times are independent. This provides the framework of a <u>partially observed Markov process</u> (pomp) under which framework much of the existing methodology is based.

Given this set-up of mechanistically-inspired mathematical models of the evolution of a process that is itself imperfectly observed, key statistical challenges include:

1. Estimating θ from the data $y_1,\dots,y_n$ and quantifying uncertainty about that estimate, including whether it is identifiable from data at all.

2. Testing hypotheses about θ directly, or about the long-term behavior of the system.

3. Designing systems that improve the estimate of parameters.

4. Assessing the fit of these systems and whether the data contains evidence that the model is insufficient to characterize system properties.

Each of these tasks is computationally and methodologically challenging. While the first of these has received most attention – including at this workshop – none of these can be said to be well understood.

The indirect nature of observations, in this case, makes statistical inference relatively difficult and several approaches have been developed to render it tractable. Broadly, these can be classified into two approaches:

Direct Methods explicitly optimize fit to the data. In the case of ordinary differential equations, this translates to minimizing the squared error between the data and a solution of the ODE. This task is possibly the best studied of problems addressed in this workshop, but represents a particularly challenging optimization problem because the squared error surface that results from nonlinear dynamic models can exhibit many local modes and ridges; a problem that can be exacerbated by numerical solution methods for ODE models. For this reason, many purpose-driven optimization methods have been produced since the late 1970's; for instance in [55, 3, 6, 5, 2, 23, 37, 12, 45] as well as stochastic search methods such as simulated annealing [34, 13]. In this context, Bayesian MCMC methods can also be employed, [32] or using specialized annealing methods [8] or proposals that make use of local geometry [7, 53].

For models of stochastic dynamics, parameters are obtained by maximizing a log likelihood

$$l(\theta) = \log P(y_1, \ldots, y_n|\theta).$$

This likelihood has no closed-form solutions, making estimation challenging. See, for example, expressions in [1, 24]. To counter this, most estimation methods employ particle filters [14, 9] have generally been employed either to maximize the likelihood via stochastic optimization – an important version of this is in the iterated filtering of [33]; similar developments in Bayesian analysis can be found in [22, 42]. Alternatively, approximations can be sometimes used [36, 41]. Applications can be found in [15, 10, 26, 21, 30, 27, 16, 28].

Indirect Methods seek to transform the data so as to produce a simpler numerical problem, although this may entail a reduction in statistical precision. There are a large number of way in which this has been proposed, particularly:

- Fitting numerically estimated derivatives in ODE models. In particular, the following two-stage estimate has received substantial attention in the statistics literature:

  1. Produce a non-parametric estimates $\hat{x}(t)$ and $\hat{\dot{x}}(t)$ of the state vector and its derivative as it evolves over time.
  2. Choose parameters to minimize the deviation between $D\hat{x}(t)$ and $f(\hat{x}(t), \theta)$.

  This method, called either "two-stage least squares" or "gradient matching" has the advantage of avoiding the need to numerically solve the ODE at multiple values of θ, and implicitly avoids the estimation of initial conditions, but requires that enough data be recorded on each state variable to produce reliable non-parametric estimators in the first step. See for example [39, 3, 55, 44, 18, 43, 38, 57]. An alternative form is provided by matching the integrals of the data; see [29, 50, 58, 54, 19], an approach which Itai Dattner updated at this workshop. While a substantial literature on its asymptotic properties exists under the assumption of data generated from an ODE model, little literature exists on its performance in stochastic models.

- More general approaches focus on fitting a set of summary statistics of the data. These are inspired as approximations to sufficient statistics, but can be very general in nature. They may represent qualitative features such as the duration and amplitude of cycles [51], if these are observed, or may be more indirect and given in terms of estimated parameters from time-series models or power spectra as in [49, 4].

  Once calculated, the model (including the data-generating model) is then simulated many times at any given parameter value and the statistics are recalculated for every statistic. Parameters are then selected based on the correspondence of their simulated statistics with those calculated from the observed data.

In Approximate Bayesian Computation (ABC), a posterior is built up of parameters generated from the prior for which simulations were close to those observed; see [47, 46, 52] for examples. Synthetic likelihood assumes an approximately normal distribution for the statistics and optimizes a Gaussian log likelihood [56].

Many of these schemes are computationally intensive methods requiring multiple simulations of stochastic systems. Thus, a great deal of research focusses on improving the computational efficiency of these methods to allow both higher dimensional systems. This entails methods to approximate stochastic models of system behavior by simplified models which can be more efficiently simulated. These approximations take the form of reductions in the dimension of the state vector as well as simplifications of dynamic processes, and generic means to achieve these reductions remains an important open problem.

A final aspect of these set of problems is the roadblocks that exist in the practical implementation of these methods by practitioners. Mechanistic models require more substantial input from the user in specifying the model than the linear regression models more commonly used in Statistics. Moreover, the form in which the model must be put often changes depending on the estimation/inference methodology. This means that developing useful software interfaces to methods is a vitally important task and considerable effort has been made by a number of groups to make these methods accessible; vis [40, 31, 35, 48, 11].

23.2 Presentation Highlights

23.2.1 Monday, July 28

The starting session of the workshop featured three plenary talks from Hulin Wu, Simon Wood, and Suzanne Ditlevsen. These researchers have had long involvement in statistics for Ordinary Differential Equations, Stochastic Models especially in Ecology and in the mathematical analysis of these models respectively. They were all exceptionally well-placed to provide an overview of these areas and create a context for the workshop.

Hulin Wu discussed the extension of parameter estimation in Ordinary Differential Equation models to large scale systems biology data. Modern biological techniques allow high-throughput data to be generated on many thousands of genes as well as proteins, RNA and multiple additional components of biological system. The scale of these data pose both modeling and computational challenges. In particular, with thousands or tens of thousands of measured elements of a system acting at several different scales, it is not possible to derive equations for system dynamics from first principles. We must thus employ some form of model selection to choose the structure of these models automatically. Hulin presented methods based on combining the gradient matching ideas described above with LASSO type penalties to both circumvent the computational cost associated with solving ODEs many times and to allow a natural integration of modern model selection methods. These allow the problem of estimating parameters to scale up to 1000's of protein species. These ideas were demonstrated on data describing immune responses to the influenza virus.

Simon Wood provided a description of indirect methods for stochastic systems and their advantages. In particular, he described extensions to the synthetic likelihood methods developed in [56]. These methods create summary statistics of the data and choose parameters so that the distribution of simulations of these summary statistics fit the observed summaries as well as possible. The purpose of this data reduction is to improve the conditioning of the resulting optimization problem. Especially when the observation error is low, directly maximizing a likelihood can be high numerically challenging in chaotic systems where likelihood surfaces exhibit multiple local optima. Further, a judicious choice of summary statistics will produce parameter estimates with close to the same precision as those obtained by maximum likelihood. A key challenge in this is that a normal sampling distribution is assumed for a high dimensional set of summary statistics; some solutions to this were later described by Matteo Fasiolo.

Suzanne Ditlevsen presented an analysis of the modeling choices that statisticians must make in choosing the level of detail that they include in a system under study. In many cases, a simplified description of a system will be more effective at eliciting scientifically-relevant information from data than a more complete, but less-well-determined model. As an example, she presented an example of determining firing times in a noisy neuron model. While it is possible to simulate systems such as a Hogkin-Huxley model of action potentials, these models contain much more detail than can be observed from data consisting of a sequence of inter-spike intervals. Rather, by reducing the model to a simplified oscillation with a suitably-characterized Brownian drift, it is still possible to estimate noise intensity and firing thresholds from such data. This is an important example of the role that applied mathematical analysis plays in the interface between statistics and nonlinear dynamics.

The Monday afternoon session was comprised of short, four-minute talks from all participants as a means of sparking informal discussion and presenting perspectives on these problems. Problems such as data-driven determination of the type of stochastic disturbances to a model, parameter identifiability and the scaling of inference were all touched on by various members and resulted in lively discussion over the succeeding days.

23.2.2 Tuesday, July 29

Tuesday Morning was devoted to statistical problems involving Ordinary Differential Equations. These models are mathematically relatively easy to work with, but pose numerical problems, both in approximating solutions to these equations and optimizing the choice of parameters for them. For this reason, most of the talks in the session focussed on indirect methods for estimating parameters, although Oksana Chkrebtii presented very novel work on viewing numerical error in estimating differential equations as a further source of uncertainty that can be accounted for under a Bayesian framework.

Tuesday afternoon was focussed on models arising in epidemiology and modeling infectious diseases and in this context talks were all based around statistical methods to uncover additional structure in complex disease models, incorporating climactic variability, spatial distribution and indirect observational processes.

Eberhard Voit discussed the identification of metabolic pathway models. He emphasized that the metabolic pathway systems have strong constraint on the parameters and some intrinsic features. He then discussed the difficulty of estimating suitable parameter values from time series data. He pointed out that there are many instances where the common criterion of the sum of squared residual errors may not be sufficient to evaluate the fit of the model. The even greater challenge is that the most popular functional forms are not known whether to be able to describe biological processes. So it is important to consider the structural uncertainty when modeling metabolic pathway systems.

Jens Timmer gave a wide-ranging talk on sources of uncertainty in parameter estimation in differential equation modeling. These include uncertainty about the performance of numerical optimizers as well as statistical uncertainty in both parameters and model predictions resulting that is inherited from noisy measurements as well as uncertainty about model structure. He advocated the use of local optimizers based on relaxation methods as well as profile likelihood as a tool for expressing uncertainty both about parameters and about predictions. Finally he presented a new observability criterion that allows the investigation of what measurements would most improve parameter identifiability and the precision of parameter estimates.

Itai Dattner focused the statistical inference for ordinary differential equations linear in the parameters. He proposed a new estimation method to address this problem. This method is based on matching the integral of the right hand side function to the observations at each time. The method requires a smooth, but avoids numerical integration and derivative estimation, and can be used in both fully or partially observed systems. He then showed his theoretical and numerical results of this method in the talk.

Giles Hooker discussed gradient matching for mis-specified ODE models. Two-stage methods are often motivated by the computational cost of repeatedly solving ordinary differential equations. This talk took a different view that these methods can also be motivated as providing robustness towards model mis-specification. In particular, it proposed a model in which an ODE is forced by a smooth, stationary stochastic process. The autocovariance of this process can be estimated by the discrepancy between $\hat{\dot{x}}(t)$ and $f(\hat{x}(t), \hat{\theta})$ and this can then be used to correct confidence intervals for $\hat{\theta}$. Speculatively, it may be possible to employ similar techniques to produce confidence intervals for parameters resulting from other methods that do not insist on an exact solution of the ODE such as the profiling methods in [45].

Oksana Chkrebtii considered the problem of exact Bayesian inference for the solution of intractable differential equation models. In the case where exact solutions are not available in closed form, many existing inferential tools rely on approximations based on time discretisation. Oksana showed that ignoring discretisation error can lead to biased parameter estimates, even for apparently simple ODE models. She went on to introduce a new formalism for the modelling and propagation of solution uncertainty via a Bayesian inferential framework, making extensive use of Gaussian process representations of uncertain functions, allowing exact inference and uncertainty quantification for discretised differential equation models. She illustrated the methods on some challenging chaotic ODE and PDE systems.

Aaron King demonstrated practical issues involved in fitting partially observed stochastic dynamic models to disease transmission data. He showed how time series data can inform key transmission parameters, and then moved on to the topic of how such models can and should be used for making forecasts. Studying cholera in Bangladesh, he showed how rainfall and global climate measures such as El Niño can be used to improve predictive properties of model-based forecasts. Fitting models using appropriate statistical criteria also enables quantification of the associated forecast uncertainty.

Vanja Dukic described a problem in epidemic modeling across spatially distributed locations. The model requires the inclusion of travel structure patterns between US states and incorporates data from Google's Flu Trends. This leads to computational problems in both developing a tractable expression of likelihood and in fitting a system that involves 204 state variables. Vanja presented a Bayesian proposal mechanism to allow tractable inference.

Jooh Ha Park presented a new statistical approach to inference for nonlinear dynamic systems of high dimension, which is a current computational challenge in applications such as the study of space-time systems. Joon Ha's motivating example was joint estimation of disease epidemics in multiple cities, for which full likelihood-based methods have previously been considered intractable. He proposed a variation of Sequential Monte Carlo (SMC) method for estimating latent states which can provide a computationally feasible solution to the joint estimation of dynamic trajectories of interacting systems. This method was shown to reduce the computational cost by a huge amount in a toy, linear-Gaussian example where the sub-systems are weakly interacting, while achieving the desired property that the sampled latent states form a proper sample from its true distribution according to the underlying model. The approach was then applied to the measles epidemic in the UK from 1950 to 1953. Preliminary results, fitting the five largest cities, showed that the proposed methods yield a reasonable estimate of epidemic history with relatively low computational cost. The conventional SMC method applied on the same set of data could not generate any result. Joon Ha also showed how to estimate key epidemic parameters using his space-time filter in conjunction with the Iterated Filtering method of Ionides et. al, 2011, recovering the known result that the transmission rate of measles is substantially different between during school term and during school holidays.

Jiguo Cao talked about selecting ordinary differential equation (ODE) models among competing candidates. He and his collaborators proposed a method for ODE model selection when the competing ODE models are special cases of a full model. Their model selection method has two steps: in the first step, the parameters in the full ODE model are estimated from noisy data; in the second step, the least squares approximation and the adaptive LASSO methods are combined to identify parameters in the full ODE model which are zero. He then talked about their theoretical and numerical results of this method.

23.2.3 Wednesday, July 30

The Wednesday half day was devoted to the presentation of mathematical analysis and approximation in support of statistical methodology. This takes the form both of supporting the development of computational tools via appropriate analysis and approximation methods, as presented by Matteo Fasiolo and Darren Wilkinson as well as tools for understanding the behavior of dynamic systems and hence aiding (or warning against) the reduction of them to simpler more-tractable models (Junling Ma and Lea Popovic). It was felt that this was a useful prelude to an afternoon left free for discussion and relaxation.

Junling Ma presented a mathematical analysis of epidemic models on structured graphs. In particular, when the contact network of the model is fixed, the basic reproduction numbers of the epidemics changes. Fixed network structure implies that a node cannot reinfect its neighbors before its neighbors recover. This means that the basic reproductive number differs between SIR and SIS models. In turn, this means that the basic reproduction number cannot be readily imputed by examining the the exponential growth rate of the epidemic. For large average degree networks this effect reduces but the result has important implications for forecasting epidemic models in small world networks.

Matteo Fasiolo discussed extensions of the pseudo-likelihood methods described by Simon Wood on Monday. In these methods, simulated data are generated from a stochastic process at a candidate set of parameters and summary statistics are generated from these data. The simulation is repeated enough times to estimate a mean and covariance of the summary statistics and this is used to construct a pseudo-likelihood for the observed test statistics based on a multivariate normal distribution. Parameters are then chosen to maximize this pseudo-likelihood. The methodology avoids many of the computational challenges associated with direct likelihood estimation of partially observed Markov processes and allows for measurements to be made at different scales than the models. For example, ecological models of forest growth simulate forests at the level of individual trees, but data are obtained from remote sensing measurements for which this level of resolution is not very relevant.

Matteo presented a relaxation of the normal assumptions employed for the summary statistics based around saddle point approximations. He demonstrated that the use of these approximations can substantially improve the performance of these estimators especially in cases where the simulation distribution of summaries can be expected to be skewed. Moreover, saddle point approximations can be obtained at much less computational cost than a fully non-parametric approach which would have to overcome the curse of dimensionality.

Lea Popovic considered biochemical mechanisms for which molecular-level stochasticity is critical to biological function. Cellular functions in biological organisms comprise of complex interactions of different proteins, DNA, mRNA molecules, and others. Sources of stochasticity in cells are multiple: some are due to inherent randomness of biochemical reactions between the species, while others are due to variations in cellular composition, cellular division mechanisms, etc. Biochemical reactions may be understood by writing down systems of differential equations or by writing down Markov chain models that explicitly represent these sources of stochasticity. Lea discussed examples where deterministic differential equations are insufficient to understand the biological processes, such as stochastic switching, diffusion moderated sensitivity, and sharpening of spatial patterns. Lea discussed and demonstrated mathematical tools which help to understand how these behaviors can be understood as appropriate limits of stochastic systems.

Darren Wilkinson gave an overview of computationally intensive Bayesian inference for partially observed

Markov processes. Markov process models are often intractable in the sense that the discrete time transition density of the process cannot be directly evaluated, and so algorithms that are "likelihood-free" (in the sense that they do not require evaluation of the likelihood of the Markov process) are particularly valuable. Fortunately, it turns out to be possible to develop likelihood-free inferential algorithms that target the exact posterior distribution, provided that one is able to simulate exact forward realisations from the model. The particle MCMC algorithm known as particle marginal Metropolis Hastings (PMMH) turns out to be especially effective in this context. Darren provided an explanation of the PMMH algorithm and its application to intractable Markov processes, and illustrated it in the context of inference for the rate constants of stochastic kinetic biochemical network models using time course data. Such models are used extensively in system biology for mechanistic modeling of gene expression.

23.2.4 Thursday, July 31

Thursday morning sessions were devoted to tools specifically aimed at fitting stochastic dynamic models – ie, those in which the system evolves probabilistically. Presentations on particle filtering and Sequential Monte Carlo by Ed Ionides and Alexandre Bouchard-Coté covered new advances in sequential simulation methods, while Simon Preston examined a localized form of Approximate Bayesian Computation, based instead on simulating entire systems. Michael Dowd provided an introduction to larger scale problems in biological Oceanography in which PDE systems for fluid dynamics interract with stochastic models of Ocean Biology.

The afternoon session was devoted to ecological applications and examined models of animal movement, integral projection models for plant growth that move from individual-level rules to population observations, host-parasite dynamics and software.

Edward Ionides presented a new iterated filtering algorithm. Iterated filtering algorithms recursively combine parameter perturbations with latent variable reconstruction, providing stochastic optimization procedures for latent variable models. Previously, theoretical support for these algorithms was based on using conditional moments of the perturbed parameters to approximate derivatives of the log likelihood function. A new theoretical approach was presented based on the convergence of an iterated Bayes map. A new algorithm supported by this theory was shown to give substantial numerical improvements on a toy example and a computational challenge, inferring parameters of a partially observed Markov process model for cholera transmission.

Michael Dowd presented a survey of statistical methods in Oceanography. In particular, this task mus combine partial differential models of fluid dynamics with ecological, often stochastic, models for ocean biology. Data for these models are obtained by remote sensing as well as by tracts taken from marine gliders. Assimilating models with these data require complex computational tools involving ensembles of multiple models, approximate smoothing methods to impute states and Bayesian state space models to treat both model identification and sampling design.

Alexandre Bouchard-Coté described a Divide-and-Conquer Sequential Monte Carlo (SMC) method for statistical inference on a collection of auxiliary distributions organized into a tree. Compared with standard SMC method, their Divide-and-Conquer SMC exploits multiple populations of weighted particles while still being an exact approximate method. He then showed the application of this method for infer a phylogenetic tree.

Simon Preston described piecewise approximate Bayesian computation (PW-ABC), an approach to inference for discretely but perfectly observed Markov process models, based on dividing the dataset into subsets and using ABC within each subset. The approach is easy to parallelise, and naturally reduces the dataset used for ABC. This reduced dimension obviates the need for summary statistics and large tolerances, making the procedure simple to implement and accurate. Simon explained that the main challenge is the combination of ABC samples in order to form the full posterior density. He discussed two strategies — one involving Gaussian approximations and the other based on kernel density estimates. He discussed the behaviour of the two approaches in the large ABC sample limit, in addition to presenting some numerical results which illustrated the performance of the method in practice. Finally, Simon explored the use of such methods in the context of deterministic models, and the relationship to multiple shooting methods.

Greg Dwyer presented a field ecologists viewpoint on the topic of population dynamics models with a particular application in modeling Gypsy moth outbreaks. These insects undergo outbreaks in which population densities increase by orders of magintude and then crash because of epizootics of fatal, directly transmitted diseases known as baculoviruses. There is severe, density-dependent mortality caused by baculoviruses that suggests they help to drive the long-period, large-amplitude cycles observed in Gypsy moths. Greg pointed out that an important component of fitting these models is auxiliary experiments in which relevant parameters can be estimated directly rather than resorting to methods in partially observed Markov processes. In particular, it is possible conduct field experiments in which transmission rates can be directly observed by isolating small populations. This then allows parameters to be estimated before being applied to larger-scale observation processes to be assessed for model validity. In the case of Gypsy moth outbreaks, individual host variability in infection risk was evident in small scale experiments and also provided a better fit tp long-term data.

Perry de Valpine focussed on the development of software tools to enable the use of complex dynamic models within statistical estimation routines. A particularly difficult aspect of developing software to implement generally-usable statistical methods with such models is the need to allow a very flexible set of model structures, along with the fact that different statistical methods are generally optimized for models expressed in different ways. Perry introduced a new software package called `NIMBLE` that is aimed at allowing a flexible interface between models and statistical methods. It instantiates models with a `BUGS`-like syntax that then allows an interface to methods in `R`. These models can be compiled into `C++` to allow for fast simulation. The framework is very recently developed and provides a promising interface for ecological modelers.

Steve Ellner focussed on challenges in developing statistical methods for estimating integral projection models – a recently developed set of tools in mathematical ecology [17]. These models provide a means of generating population-level observables from individual-level rules for a discrete-time Markov chain through integrodifference equations. Such models have the capacity to answer questions such as whether having a good environment very early on is important to reproductive success, or is total lifetime environment the most relevant quantity. Statistical problems for these models are largely unexamined, such as selecting covariates, indentification of key events, and combining stochastic and deterministic processes.

Scott McKinley presented an analysis of models of animal movement patterns. Many classical movement models assume a scale-free distribution of movement in animal displacement as a first approximation to modeling movement trajectories. Scott advocated for a multi-scale approach involving differing behaviors at local scales from long-range movement. A mathematical analysis of this multi-scale framework demonstrates important consequences for population processes in terms of encounter rates and the functional response of predators.

23.2.5 Friday, August 1

The final session of the morning was left aside for a discussion of modeling strategies. This was moderated by Edward Ionides and featured Priscilla Greenwood and James Ramsay as discussants: two of the most distinguished researchers associated with the field. A debate was suggested on the provocative proposition that "No one should fit an ODE to data who knows how to fit an SDE to data." A lively discussion ensued regarding the role of random effects in modeling and particularly the use of random processes a means of "hiding" or "accounting for" (depending on one's viewpoint) poor model fit. Both discussants presented provocative and thought-provoking arguments, Jim Ramsay particularly delighting the attendees with his presentation of the naive Albertan's view of statistical models.

The meeting concluded with the general agreement that it had been highly stimulating and effective in cross-fertilizing ideas between participants from different subject areas and a plan that further workshops would be useful and should be planned.

23.3 Scientific Progress Made

Much of the purpose of the meeting was to make connections between disparate disciplines and to establish cross-disciplinary links rather than to specifically develop new mathematics. However, some important new developments were announced as part of the program of talks. These all point towards making the practical use of methods for data from dynamical systems easier, more broadly applicable, and more computationally efficient.

Particularly important developments are

- A new iterative filtering method that significantly reduces the computational challenges of performing stochastic maximum likelihood with particle filters. Edward Ionides proposed a much simpler means of updating parameters in an older method [33] that makes implementation of these methods significantly simpler and their description much easier.
- Methods to account for smooth stochastic disturbances to ordinary differential equation models when conducting statistical inference (Giles Hooker) present the potential to significantly broaden the scope of models to which two-stage methods can be applied. This helps to bridge the gap between deterministic and stochastic dynamical models – the breadth of models to which these methods can be validly applied remains under investigation.
- The introduction of saddle point approximations for synthetic likelihood (Matteo Fasiolo) serves to significantly broaden the range of models and summary statistics for which synthetic likelihood methods can be validly used. They also represent a modern revival of a rather classical set of tools that have new use in computationally-intensive statistics.
- The use of model selection methods within ordinary differential equations (Hulin Wu and Jiguo Cao) represent important new developments for high-dimensional state-space models. These are particularly valuable in the era of high throughput experiments, particularly in systems biology, when we have only a partial understanding of the processes involved. They allow us to discover a mechanistic model rather than to construct one from scratch.
- The new software platform `NIMBLE` (Perry de Valpine) represents an important new means of implementing statistical methodology for complex dynamical models. Developing general-use software that can be applied across a range of models and methods and that also does not incur unreasonable set-up costs for users is a significant challenge and this additional resource can be expected to make collaboration and methods development significantly easier.

23.4 Outcome of the Meeting

The goal of the meeting was to generate cross-disciplinary collaboration and understanding in the shared problem of statistical methodology with nonlinear dynamical systems models. In this the meeting was clearly successful; the most common sentiment being that "I learned a great deal." Indeed, there was a considerable amount of cross-disciplinary conversation. There was also general agreement that holding meetings on this topic on a regular basis will be very beneficial for the subject area.

In addition, some concrete projects emerged. The `NIMBLE` software project presented by Perry de Valpine is expected to grow and attract collaboration from attendees. Further, James Ramsay and Giles Hooker are currently writing a book, to be the first statistical treatment of the problem. The meeting furnished much by the way of material for this project, both in terms of updates to methodology and reminders about further subjects to be treated. A manuscript is expected by the end of 2015.

All participants heartily thanked BIRS and its staff for providing truly exceptional facilities and organization to support the meeting.

Participants

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Bibliography

[1] Ait-Sahalia, Y. (2008). Closed-form likelihood expansions for multivariate diffusions. Annals of Statistics 36(2), 906–937.

[2] Baake, E., M. Baake, H. G. Bock, and K. M. Briggs (1992). Fitting ordinary differential equations to chaotic data. Physical Review A 45, 5524–5529.

[3] Bellman, R. and R. S. Roth (1971). The use of splines with unknown end points in the identification of systems. Journal of Mathematical Analysis and Applications 34, 26–33.

[4] Benton, T. G. (2006). Revealing the ghost in the machine : Using spectral analysis to understand the influence of noise on population dynamics. Proceedings of the National Academies of Sciences 103(49), 18387–18388.

[5] Biegler, L., J. J. Damiano, and G. E. Blau (1986). Nonlinear parameter estimation: a case study comparison. AIChE Journal 32(1), 29–45.

[6] Bock, H. G. (1983). Recent advances in parameter identification techniques for ODE. In P. Deuflhard and E. Harrier (Eds.), Numerical Treatment of Inverse Problems in Differential and Integral Equations, pp. 95–121. Basel: Birkhäuser.

[7] Calderhead, B. and M. Girolami (2011). Statistical analysis of nonlinear dynamical systems using differential geometric sampling methods. Interface Focus.

[8] Campbell, D. and R. Steele (2012). Smooth functional tempering with application to nonlinear differential equation models. Statistical Computing 22, 429–443.

[9] Carvalho, C. M., M. S. Johannes, H. F. Lopes, N. G. Polson, M. Johannes, and F. M. Associate (2010). Particle Learning and Smoothing. Statistical Science 25(1), 88–106.

[10] Cauchemez, S. and N. M. Ferguson (2007). Likelihood-based estimation of continuous-time epidemic models from time-series data: Application to measles transmission in london. Journal of the Royal Society Interface 5, 885–897.

[11] CBIM (2014). DEDiscover: Differential Equation Modeling Solution.

[12] Chen, J. and H. Wu (2008). Efficient local estimation for time-varying coefficients in deterministic dynamic models with applications to hiv-1 dynamics. Journal of the American Statistical Association 103, 369–384.

[13] Colijn, C. and M. C. Mackey (2005). A mathematical model of hematopoiesis I . Periodic chronic myelogenous leukemia. Journal of Theoretical Biology 237(2), 117–132.

[14] Doucet, A., S. Godsill, and C. Andrieu (2000). On sequetial Monte Carlo sampling methods for Bayesian filtering. Statistics and Computing 10, 197–208.

[15] Earn, D. J. D. (2009). Mathematical epidemiology of infectious diseases. In M. A. Lewis, M. A. J. Chaplain, J. P. Keener, and P. K. Maini (Eds.), Mathematical Biology, Volume 14 of IAS/ Park City Mathematics Series, pp. 151–186. American Mathematical Society.

[16] Earn, D. J. D., D. He, M. B. Loeb, K. Fonseca, B. E. Lee, and J. Dushoff (2012). Effects of school closure on incidence of pandemic influenza in Alberta, Canada. Annals of Internal Medicine 156(3), 173–181.

[17] Easterling, M. R., S. P. Ellner, and P. M. Dixon (2000). Size-specific sensitivity: applying a new structured population model. Ecology 81(3), 694–708.

[18] Ellner, S. P., Y. Seifu, and R. H. Smith (2002). Fitting Population Dynamic Models to Time-Series Data by Gradient Matching. Ecology 83(8), 2256–2270.

[19] Font, J. and A. Fabregat (1997). Testing a predictor-corrector integral method for estimating parameters in complex kinetic systems described by ordinary differential equations. Computers and Chemical Engineering 21(7), 719–731.

[20] Gillespie, D. T. (1976). A general method for numerically simulating the stochastic time evolution of coupled chemical reactions. Journal of Computational Physics 22, 403–434.

[21] Goldstein, E., J. Dushoff, J. Ma, J. Plotkin, D. J. D. Earn, and M. Lipsitch (2009). Reconstructing influenza incidence by deconvolution of daily mortality times series. PNAS 106, 21825–21829.

[22] Golightly, A. and D. J. Wilkinson (2011). Bayesian parameter inference for stochastic biochemical network models using particle Markov chain Monte Carlo. Interface focus 1(6), 1–14.

[23] Graepel, T. (2003). Solving Noisy Linear Operator Equations by Gaussian Processes: Application to Ordinary and Partial Differential Equations. In Twentieth International Conference on Machine Learning.

[24] Greenwood, P. and W. Wefelmeyer (1998). Cox's factoring of regression model likelihoods for continuous-time processes. Bernoulli.

[25] He, D., J. Dushoff, R. Eftimie, and D. J. D. Earn (2013). Patterns of spread of influenza A in Canada. Proceedings of the Royal Society B-Biological Sciences 280(1770), 20131174.

[26] He, D., E. L. Ionides, and A. a. King (2010). Plug-and-play inference for disease dynamics: measles in large and small populations as a case study. Journal of the Royal Society Interface 7(43), 271–283.

[27] He, D. H., J. Dushoff, T. Day, J. L. Ma, and D. J. D. Earn (2011). Mechanistic modelling of the three waves of the 1918 influenza pandemic. Theoretical Ecology 4(2), 283–288.

[28] He, D. H., J. Dushoff, T. Day, J. L. Ma, and D. J. D. Earn (2013). Inferring the causes of the three waves of the 1918 influenza pandemic in England and Wales. Proceedings of the Royal Society B-Biological Sciences 280(1766).

[29] Himmelblau, D., C. Jones, and K. Bischoff (1967). DETERMINATION OF RATE CONSTANTS FQR COMPLEX KINETICS MODELS. IEC Fundamentals 6(4), 539–543.

[30] Hooker, G., S. P. Ellner, L. D. V. Roditi, and D. Earn (2011). Parameterizing state-space models for infectious disease dynamics by generalized profiling: Measles in ontario. Journal of the Royal Society Interface 8, 961–975.

[31] Hooker, G., L. Xiao, and J. Ramsay (2014). CollocInfer: Collocation Inference for Dynamic Systems. R package version 1.0.0.

[32] Huang, Y., D. Liu, and H. Wu (2006). Hierarchical bayesian methods for estimation of parameters in a longitudinal hiv dynamic system. Biometrics 62(2), 413-423.

[33] Ionides, E. L., C. Bretó, and A. A. King (2006). Inference for nonlinear dynamical systems. Proceedings of the National Academy of Sciences.

[34] Jaeger, J., M. Blagov, D. Kosman, K. Kolsov, Manu, E. Myasnikova, S. Surkova, C. Vanario-Alonso, M. Samsonova, D. Sharp, and J. Reinitz (2004). Dynamical analysis of regulatory interactions in the gap gene system of drosophila melanogaster. Genetics 167, 1721–1737.

[35] King, A. A., E. L. Ionides, C. M. Bretó, S. P. Ellner, M. J. Ferrari, B. E. Kendall, M. Lavine, D. Nguyen, D. C. Reuman, H. Wearing, and S. N. Wood (2014). pomp: Statistical inference for partially observed Markov processes (R package).

[36] Koyama, S., L. C. Perez-Bolde, C. R. Shalizi, and R. E. Kass (2010). Approximate methods for state-space methods. Journal of the American Statistical Association, 170–180.

[37] Li, Z., M. Osborne, and T. Prvan (2005). Parameter estimation in ordinary differential equations. IMA Journal of Numerical Analysis 25, 264–285.

[38] Lu, T., H. Liang, H. Li, and H. Wu (2011). High Dimensional ODEs Coupled with Mixed-Effects Modeling Techniques for Dynamic Gene Regulatory Network Identification. Journal of the American Statistical Association 106(496), 1242–1258.

[39] Nevers, N. D. E. (1966). Rate Data and Derivatives. A.I.Ch.E. Jornal 12(6), 1110–1115.

[40] NIMBLE Development Team (2014). NIMBLE Users Manual, Version 0.1.

[41] Overgaard, R. V., N. Jonsson, C. W. Tornø e, and H. Madsen (2005). Non-linear mixed-effects models with stochastic differential equations: implementation of an estimation algorithm. Journal of Pharmacokinetics and Pharmacodynamics 32(1), 85–107.

[42] Picchini, U. and S. Ditlevsen (2011). Practical estimation of high dimensional stochastic differential mixed-effects models. Computational Statistics & Data Analysis 2(3).

[43] Poyton, A. A., M. S. Varziri, K. B. McAuley, P. J. McLellan, and J. O. Ramsay (2006). Parameter estimation in continuous dynamic models using principal differential analysis. Computational Chemical Engineering 30, 698–708.

[44] Ramsay, J. (1996). Principal Differential Analysis: Data Reduction by Differential Operators. Journal of the Royal Statistical Society. Series B(Methodological) 58(3), 495–508.

[45] Ramsay, J. O., G. Hooker, D. Campbell, and J. Cao (2007). Parameter estimation in differential equations: A generalized smoothing approach. Journal of the Royal Statistical Society, Series B 16, 741–796.

[46] Ratmann, O., C. Andrieu, C. Wiuf, and S. Richardson (2009). Model criticism based on likelihood-free inference , with an application to protein network evolution. Proceedings of the National Academies of Sciences 106(26), 10576–10581.

[47] Ratmann, O., O. Jø rgensen, T. Hinkley, M. Stumpf, S. Richardson, and C. Wiuf (2007). Using Likelihood-Free Inference to Compare Evolutionary Dynamics of the Protein Networks of H . pylori and P . falciparum. PloS Computational Biology 3(11), 2266–2278.

[48] Raue, A., M. Schilling, J. Bachmann, A. Matteson, M. Schelke, D. Kaschek, S. Hug, C. Kreutz, B. D. Harms, F. J. Theis, U. Klingmller, and J. Timmer (2013). Lessons learned from quantitative dynamical modeling in systems biology. PLoS ONE 8(9), e74335.

[49] Reuman, D. C., R. A. Desharnais, R. F. Costantino, O. S. Ahmad, and J. E. Cohen (2006). Power spectra reveal the influence of stochasticity on nonlinear population dynamics. Proceedings of the National Academies of Sciences 103(49), 18660–18665.

[50] Tang, Y. (1971). On the Estimation of Rate Constants for Complex Kinetic Models. Ind. Eng. Chem. Fundam. 10(2), 321–322.

[51] ien, J. H. and J. Guckenheimer (2008). Parameter estimation for bursting neural models. Journal of Computational Neuroscience 24(3), 358–373.

[52] Toni, T., D. Welch, N. Strelkowa, A. Ipsen, and M. P. H. Stumpf (2009). Approximate Bayesian computation scheme for parameter inference and model selection in dynamical systems. Journal of the Royal Society Interface 6, 187–202.

[53] Transtrum, M. K., B. B. Machta, and J. P. Sethna (2011, Mar). Geometry of nonlinear least squares with applications to sloppy models and optimization. Phys. Rev. E 83, 036701.

[54] Vajda, S., P. Valko, and A. Yermakova (1986). A Direct-indirect Procedure for estimation of Kinetic Parameters. Computers and Chemical Engineering 10(1), 49–58.

[55] Varah, J. M. (1982). A spline least squares method for numerical parameter estimation in differential equations. SIAM Journal on Scientific Computing 3, 28–46.

[56] Wood, S. N. (2010). Statistical inference for noisy nonlinear ecological dynamic systems. Nature 466(August).

[57] Wu, H., H. Xue, and A. Kumar (2012). Numerical discretization-based estimation methods for ordinary differential equation models via penalized spline smoothing with applications in biomedical research. Biometrics 68(2), 344–52.

[58] Yermakova, A., S. Vajda, and P. Valko (1982). Direct integral method via spline-approximation for estimating rate constants. Applied Catalysis 2, 139–154.

Chapter 24

Approximation algorithms and the hardness of approximation (14w5051)

August 3 - 8, 2014

Organizer(s): Chandra Chekuri, (University of Illinois at Urbana-Champaign), Joseph Cheriyan, (University of Waterloo), Ryan O'Donnell, (Carnegie Mellon University), Mohammad R. Salavatipour, (University of Alberta), David P. Williamson, (Cornell University)

24.1 Overview of the Field

Most of the many discrete optimization problems arising in the sciences, engineering, and mathematics are NP-hard, that is, there exist no efficient algorithms to solve them to optimality, assuming the P$\neq$NP conjecture.[1] The area of approximation algorithms focuses on the design and analysis of efficient algorithms that find solutions that are within a guaranteed factor of the optimal one. Loosely speaking, in the context of studying algorithmic problems, an approximation guarantee captures the "goodness" of an algorithm – for every possible set of input data for the problem, the algorithm finds a solution whose cost is within this factor of the optimal cost. A hardness threshold indicates the "badness" of the algorithmic problem – no efficient algorithm can achieve an approximation guarantee better than the hardness threshold assuming that P$\neq$NP (or a similar complexity assumption). Over the last two decades, there have been major advances on the design and analysis of approximation algorithms, and on the complementary topic of the hardness of approximation, see [45], [46].

The long-term agenda of our area (approximation algorithms and hardness results) is to classify all of the fundamental NP-hard problems according to their approximability and hardness thresholds. This agenda may seem far-fetched, but remarkable progress has been made over the last two decades. Approximation guarantees and hardness thresholds that "match" each other have been established for key problems in topics such as:

- covering and partitioning (the set covering problem [17]),
- algebra (overdetermined system of equations [21])
- graphs (clique, colouring [47]),

[1] This workshop is a sequel to our workshop 11w5117 on the same topic; some of the introductory/filler text is the same for both reports, but the actual contents are different.

- combinatorial optimization (maximum cut [18],[26]),
- constraint satisfaction (maximum satisfiability problems [18],[21]), etc.

24.2 Objectives of the Workshop Proposal

The goals of the workshop are as follows:

1. To bring together researchers in the fields of approximation algorithms (who work on finding algorithms with good approximation guarantees) and complexity theory (who work on finding hardness thresholds), and to stimulate the exchange of ideas and techniques between the two groups.
2. To focus on a few key topics that could lead to deep new results in the areas of approximation algorithms, combinatorial optimization, hardness of approximation, and proof complexity. We describe a few ambitious topics below.

   (a) The most famous problem in all of discrete optimization is the Traveling Salesman Problem (TSP). Yet despite the attention paid to this problem, its approximability remains poorly understood. The best known approximation algorithm for the symmetric case is a 3/2-approximation algorithm due to Christofides from 1976. On the other hand, the known hardness-of-approximation results are weak, and there is a substantial gap between upper bounds and lower bounds.

   Recently, there has been remarkable progress on some special cases of the TSP and on some variants of the TSP, but, as of now, there has been no improvement on the approximation guarantee of 3/2 for the TSP. Some of the recent advances were covered in the 2011 BIRS workshop, and a whole day was devoted to talks on the TSP and related problems. Many of these advances are based on new and beautiful connections with probability theory, coupled with technically difficult exploitation of methods and structures that are studied in combinatorial optimization. For example, Oveis Gharan, Saberi, and Singh [38] used properties of strongly Rayleigh measures coupled with an elaborate analysis of the structure of near-minimum cuts to obtain the first improvement on the 3/2-approximation guarantee for a key special case called the graphic TSP; also, see Asadpour et al. [7]. The most recent result on this special case is a 7/5-approximation algorithm of Sebő and Vygen [43] that hinges on a probabilistic lemma of Momke and Svensson [34] coupled with an in-depth and novel analysis of structures that are well known in combinatorial optimization. An, Kleinberg, and Shmoys [1] improved on a 20-year old 5/3-approximation guarantee of Hoogeveen [23] for the s-t path TSP, which is a variant of TSP; they use a randomized rounding algorithm, and their improvement uses probabilistic methods coupled with an analysis of near-minimum cuts. Very recently, Sebő [42] has improved on this result to obtain an 8/5-approximation guarantee, by using further probabilistic insights.

   It has long been conjectured that there is a 4/3-approximation algorithm for the TSP, and a 3/2-approximation algorithm for the s-t path TSP. By re-focusing attention on these conjectures, our goal is to continue the momentum from the 2011 BIRS workshop on the TSP.

   (b) Another focus topic will be approximation algorithms for disjoint paths and related routing problems. These problems are intimately related to fundamental topics on structural graph theory as well as to multicommodity flows. At the 2011 BIRS workshop, Chuzhoy [15] presented a plenary talk on her breakthrough work that obtained the first poly-logarithmic approximation algorithm with constant congestion for the maximum edge-disjoint paths problem (MEDP). This built on a long line of work and numerous tools. There has been subsequent exciting progress including the work of Chuzhoy and Li [16] who improved the congestion bound from 14 to 2.

   Despite this progress, the approximability of the maximum disjoint paths problem is wide open if the congestion bound is kept at one. Let n denote the number of nodes of the input graph. The known upper bound is $O(\sqrt{n})$ while the lower bound is only sub-logarithmic in n (namely, $\Omega(\log^{\frac{1}{2}-\varepsilon} n)$), see

Andrews et al. [3]. The approximability threshold is poorly understood even for restricted instances such as planar graphs and graphs of bounded treewidth. The impetus from the recent results and tools promises to lead to exciting new advances on algorithms for routing problems. The results of Chuzhoy [15] have been extended to the maximum node-disjoint paths problem with constant congestion by Chekuri and Ene [14]. In addition, there are strong connections to structural aspects of graph theory. The recent progress on disjoint path problems is based on proving the existence of routing structures whose size is proportional to the treewidth of the graph, see [14]. This points to further connections between the above algorithmic results and the theory of Graph Minors developed by Robertson and Seymour, [41].

Our aim is to start systematic explorations of this connection. On the one hand, this could lead to the design of powerful new algorithmic tools for some of the routing problems that arise in many applied areas, and on the other hand, it could provide new techniques for attacking some of the significant conjectures within the theory of Graph Minors.

(c) A key component of the workshop will focus on the notorious Unique Games Conjecture (UGC) and surrounding issues in the complexity of optimization problems. Since its proposal in 2002 by Khot [25], the UGC has led to major new (conditional) inapproximability results for constraint satisfaction problems (CSPs). This culminated in Raghavendra's 2009 work [40] giving a polynomial-time algorithm for optimally approximating each CSP, assuming the UGC.

The workshop will explore two directions that are at the vanguard of UGC research: improving optimization algorithms via Lasserre / sum-of-squares (SOS) proofs methodology, and going beyond the UGC in complexity results.

(<u>Lasserre / SOS algorithms.</u>) In 2011, it was shown that the powerful Lasserre SDP hierarchy of algorithms (see [29], and also see [44], [33]) could be used to obtain a subexponential-time algorithm for Unique Games (UG) (as in Arora et al. [4]) and some related problems, see Barak et al. [11] and Guruswami et al. [19]. (The 2011 BIRS workshop included two talks on these topics, by Georgiou and Steurer.) These results are motivating further advances in optimization using Lasserre algorithms.

A very recent, important work of Barak et al. [8] emphasized and applied the connection between Lasserre algorithms and Sum-of-Squares (SOS) proof complexity; they showed that the known "hard instances" of the UG problem can be analyzed by constant-degree SOS proofs, and hence solved by a polynomial-time algorithm. Subsequent research furthered the connection to proof complexity, see O'Donnell et al. [37]. The organizers are eager to bring together researchers working on optimization algorithms and on proof complexity, with the belief that these newly developed connections may lead to dramatic breakthroughs in efficient approximation algorithms.

(<u>Beyond the UGC.</u>) One emerging stream of current research is concerned with going beyond the UGC. In one direction, going beyond the UGC has involved "upgrading" known UG-hardness results to full-fledged NP-hardness results. New techniques in this area, such as "smooth Label Cover" (see Guruswami et al. [20] and Hastad [22]) and "PCPs robust against low-degree polynomials" (see Chan [12] and Khot et al. [28]), are giving hope that many optimization tasks known to be "UG-hard" can be proved to be NP-hard without needing to resolve the UGC.

In the other direction, going beyond the UGC involves introducing alternative conjectures which can lead to inapproximability results not provable via UGC; one example is the Projection Games Conjecture introduced at the 2011 BIRS workshop by Moshkovitz [35].

3. To include many younger researchers, and foster a relaxed interaction with established researchers. Our goal is to have a third of the workshop participants from this group. We expect a good number of female participants, similar to the workshop 11w5117. (There were five female participants.)

4. To allow groups of Canadian researchers working in this area to meet, and either initiate or renew collaborations.

24.3 Recent Developments and Open Problems

The study of approximation algorithms and the hardness of approximation is one of the most exciting areas among researchers in theoretical computer science; every major conference in the field has several papers on these topics. Significant progress is being made. We give a few examples of recent, dramatic innovations:

Arora, Barak and Steurer [4] recently presented a sub-exponential-time algorithm for Unique Games. This is a landmark result on one of the most perplexing questions in the area, namely the Unique Games Conjecture (UGC). While this result does not disprove the UGC, it gives strong indications that the UGC may not be true. The implication is that some of the remarkable tight approximation thresholds proved assuming the UGC need to be revisited; one possibility is that substantially deeper methods may be needed to prove the tightness of these approximation thresholds assuming the P$\neq$NP conjecture.

Chuzhoy and Li [16] (FOCS 2012) recently presented an approximation algorithm for maximizing the number of edge disjoint paths with congestion two that achieves a poly-logarithmic approximation guarantee with respect to a standard LP relaxation. This is a remarkable achievement, because their LP relaxation has an integrality ratio that is much higher (than poly-logarithmic) for congestion one, meaning that poly-logarithmic approximation guarantees for congestion one are not possible (based on their LP relaxation); moreover, qualitatively speaking, the approximation guarantee for congestion two is best possible, due to lower bounds from the area of hardness of approximation.

Chekuri and Chuzhoy [13] (STOC 2014) very recently made substantial progress on an important graph theoretic problem. This was inspired by techniques from the recent work of Chuzhoy [15], Chuzhoy and Li [16] and Chekuri and Ene [14] on approximating the maximum disjoint paths problem. They showed that any graph G with treewidth at least $k^{98-o(1)}$ has a grid minor of size k. This establishes the first polynomial relationship between treewidth and the size of the largest grid-minor in a graph; previous bounds from the seminal work of Robertson and Seymour on graph minors and subsequent improvements required the treewidth of G to be an exponential function of k to ensure that G has a grid-minor of size k. This work is an example of the rich interplay between structural and algorithmic results.

24.4 Presentation Highlights

24.4.1 LP-Based Algorithms for Capacitated Facility Location

The first plenary talk was given by Hyung-Chan An (EPFL, Lausanne), on some recent advances obtained jointly with Mohit Singh and Ola Svensson, [2].

Linear programming has played a key role in the study of algorithms for combinatorial optimization problems. In the field of approximation algorithms, this is well illustrated by the uncapacitated facility location problem. A variety of algorithmic methodologies, such as LP-rounding and the primal-dual method have been applied to and evolved from algorithms for this problem. Unfortunately, this collection of powerful algorithmic techniques had not yet been applicable to the more general capacitated facility location problem. In fact, all of the known algorithms with good performance guarantees were based on a single technique, local search, and moreover, no linear programming relaxation was known to efficiently approximate the problem.

In their new paper, they present a linear programming relaxation with constant integrality gap for capacitated facility location. An et al. demonstrate that fundamental concepts from matching theory, including alternating paths and residual networks, provide key insights that lead to the strong relaxation. Their algorithmic proof of the integrality gap is obtained by finally accessing the rich toolbox of LP-based methodologies: they present a constant factor approximation algorithm based on LP-rounding. Their results resolve one of the ten open problems selected by the textbook on approximation algorithms of Williamson and Shmoys [46].

24.4.2 Open Questions in Parallel Repetition of Games and PCPs

Irit Dinur (Weizmann Institute) presented a plenary talk on a collection of questions that addresses parallel repetition and PCPs.

1. Parallel repetition of k player games ($k = 3$ or more): while we know a lot about the value of a repeated two player game, much less is known for k player games.
2. Direct sum of games: if parallel repetition is the direct product of games, then the direct sum operation is easy to define for XOR games. Some interesting things are known here, but no version of the XOR lemma has been proved, as of now.
3. Derandomized parallel repetition: What results can we expect to get if we disallow randomization? Is there a PCP theorem with polynomially small error?

24.4.3 On the Power of Symmetric LP/SDP Relaxations

Prasad Raghavendra (UC Berkeley) presented a plenary talk on two recent results obtained jointly with James Lee, David Steurer, and Ning Tan [31].

1. They show that for $k < n/4$, the k-rounds sum-of-squares or Lasserre SDP relaxation achieves the best possible approximation guarantee for Max-CSPs among all symmetric SDP relaxations of size at most $\binom{n}{k}$.
2. They show how to construct linear programs for TSP that are instance-optimal among all symmetric linear programs.

24.4.4 Sum-of-Squares Method, Tensor Decomposition, and Dictionary Learning

The final plenary talk was given by David Steurer (Cornell), and it presented recent results obtained jointly with Boaz Barak and Jonathan Kelner [10].

The sum-of-squares method is a widely-studied, conceptually simple meta-algorithm that, for a broad range of problems, captures the best known algorithms and potentially achieves better and plausibly optimal guarantees for these problems. Barak et al. introduce a general approach for proving guarantees of efficient approximation algorithms based on the sum-of-squares method by exploiting connections to proof complexity. Following this approach, they give efficient algorithms with significantly improved guarantees for several problems arising in machine learning and optimization, in particular, robust tensor decomposition and dictionary learning.

24.5 Scientific Progress Made and Outcome of the Meeting

The schedule of the workshop provided ample free time for participants to work on joint research projects. A number of new research projects were initiated during the workshop, while some other researchers used the opportunity to continue to work on projects started earlier. The research talks and the plenary talks were very well received.

Poloczek, Schnitger, Williamson, and van Zuylen gave a randomized greedy algorithm that obtains an expected 3/4-approximation for the maximum satisfiability problem. It remained open whether there is a deterministic algorithm that achieves the same approximation guarantee without using linear programming. After Poloczek's talk at the workshop, Svensson pointed out that such an algorithm can be obtained by derandomizing the fractional greedy algorithm of Buchbinder, Feldman, Naor, and Schwartz [9] using the method of conditional expectation. In the meantime, this algorithm was analyzed exactly and shown to run in linear time. Moreover, the algorithmic idea has been extended to further combinatorial optimization problems.

As a result of some discussions started during the workshop, Ene, Nguyen, and Vondrak can show that there is a $(k-1)$-approximation for the problem of partitioning a ground set into k pieces while minimizing a separation cost measured by a (possibly non-monotone, asymmetric) submodular function, plus additive assignment costs for element/label pairs. They can also show a Δ-approximation for this problem when the submodular function is given explicitly as a sum of predicates depending on Δ elements each. Both results match the hardness result that Vondrak presented in the workshop for Hypergraph Labeling, which is a special case of this problem.

Anupam Gupta, inspired by questions after his talk on greedy algorithms for the Steiner Forest problem, developed a cleaner presentation of the algorithm, with an improved analysis. He also started new collaborations with Chandra Chekuri on a generalization of the multi-way cut problem, and with Bruce Shepherd on the edge-disjoint-paths problem.

Participants James Lee, Prasad Raghavendra, and David Steurer used the workshop to restart their collaboration on characterizing the power of semidefinite programs (SDPs). Since then, they have introduced a method for proving lower bounds on the efficacy of SDP relaxations for combinatorial problems. In particular, they show that the cut, TSP, and stable set polytopes on n-vertex graphs are not the linear image of the feasible region of any SDP (i.e., any spectrahedron) of dimension less than 2^{n^c} for some constant $c > 0$. Their result yields the first super-polynomial lower bounds on the semidefinite extension complexity of any explicit family of polytopes.

Irit Dinur, David Steurer, and Prasad Raghavendra submitted a new joint grant application partly based on discussions started at the Banff workshop.

The above are only a few examples of the research progress made during or after the workshop, and there are other ongoing projects that started at the workshop.

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Bibliography

[1] H.-C. An, R. Kleinberg, and D.B. Shmoys, Improving Christofides' algorithm for the s-t path TSP. Proceedings of the ACM Symposium on the Theory of Computing: 875-886 (2012)

[2] H.-C. An, M. Singh, O. Svensson, LP-Based Algorithms for Capacitated Facility Location. CoRR abs/1407.3263 (2014)

[3] M. Andrews, J. Chuzhoy, V. Guruswami, S. Khanna, K. Talwar, and L. Zhang, Inapproximability of Edge-Disjoint Paths and low congestion routing on undirected graphs. Combinatorica 30(5): 485-520 (2010)

[4] S. Arora, B. Barak, and D. Steurer, Subexponential algorithms for Unique Games and related problems. Proceedings of the IEEE Symposium on the Foundations of Computer Science: 563-572 (2010)

[5] S. Arora, J.R. Lee, and A. Naor, Fre'chet embeddings of negative type metrics. Discrete & Computational Geometry 38(4): 726-739 (2007)

[6] S. Arora, S. Rao, and U.V. Vazirani, Expander flows, geometric embeddings and graph partitioning. J.ACM: 56(2) (2009)

[7] A. Asadpour, M. Goemans, A. Madry, S. Oveis Gharan, and A. Saberi, An $O(\log\ n/\log\log\ n)$-approximation algorithm for the asymmetric Traveling Salesman Problem. Proceedings of the ACM-SIAM Symposium on Discrete Algorithms: 379-389 (2010)

[8] B. Barak, F. Brandao, A. Harrow, J. Kelner, D. Steurer, and Y. Zhou, Hypercontractivity, sum-of-squares proofs, and their applications. Proceedings of the ACM Symposium on the Theory of Computing: 307-326 (2012)

[9] N. Buchbinder, M. Feldnan, J. Naor, and R. Schwartz. A tight linear time (1/2)-approximation for unconstrained submodular maximization. Proceedings of the IEEE Symposium on the Foundations of Computer Science: 649-658 (2012)

[10] B. Barak, J. A. Kelner, and D. Steurer, Dictionary Learning and Tensor Decomposition via the Sum-of-Squares Method. Proceedings of the IEEE Symposium on the Foundations of Computer Science (2014). CoRR abs/1407.1543 (2014)

[11] B. Barak, P. Raghavendra, and D. Steurer, Rounding semidefinite programming hierarchies via global correlation. Proceedings of the IEEE Symposium on the Foundations of Computer Science: 472-481 (2011)

[12] Siu On Chan, Approximation resistance from pairwise independent subgroups. Technical Report TR12-110, ECCC (2012)

[13] C. Chekuri and J. Chuzhoy. Polynomial bounds for the Grid-Minor Theorem. Proceedings of the 46th ACM Symposium on Theory of Computing, 2014: 60–69.

[14] C. Chekuri, and A. Ene, Poly-logarithmic Approximation for Maximum Node Disjoint Paths with Constant Congestion. Proceedings of the ACM-SIAM Symposium on Discrete Algorithms 2013: 326-341

[15] J. Chuzhoy, Routing in undirected graphs with constant congestion. Proceedings of the ACM Symposium on the Theory of Computing: 855-874 (2012)

[16] J. Chuzhoy, and S. Li, A Polylogarithmic Approximation Algorithm for Edge-Disjoint Paths with Congestion 2. Proceedings of the IEEE Symposium on the Foundations of Computer Science: 233-242 (2012). Arxiv version: CoRR abs/1208.1272 (2012)

[17] U. Feige, A threshold of $\ln n$ for approximating Set Cover. J. ACM 45(4): 634-652 (1998)

[18] M. X. Goemans, and D. P. Williamson, Improved approximation algorithms for Maximum Cut and Satisfiability problems using semidefinite programming. J. ACM 42(6): 1115-1145 (1995)

[19] V. Guruswami, A. K. Sinop, Lasserre hierarchy, higher eigenvalues, and approximation schemes for quadratic integer programming with PSD objectives. Proceedings of the IEEE Symposium on the Foundations of Computer Science: 482-491 (2011)

[20] V. Guruswami, P. Raghavendra, R. Saket, and Y. Wu, Bypassing UGC from some optimal geometric inapproximability results. Proceedings of the ACM-SIAM Symposium on Discrete Algorithms: 699-717 (2012)

[21] J. Hastad, Some optimal inapproximability results. J.ACM 48(4): 798-859 (2001)

[22] J. Hastad, On the NP-hardness of Max-Not-2. Approx-Random: 170-181 (2012)

[23] J. A. Hoogeveen, Analysis of Christofides' heuristic: Some paths are more difficult than cycles. Operations Research Letters 10: 291-295 (1991)

[24] K. Jain, A factor 2 approximation algorithm for the generalized Steiner network problem. Combinatorica 21(1): 39-60 (2001)

[25] S. Khot, On the power of unique 2-prover 1-round games. Proceedings of the ACM Symposium on the Theory of Computing: 767-775 (2002)

[26] S. Khot, G. Kindler, E. Mossel, and R. O'Donnell, Optimal inapproximability results for MAX-CUT and other 2-variable CSPs? SIAM J. Comput. 37(1): 319-357 (2007)

[27] S. Khot, and O. Regev, Vertex cover might be hard to approximate to within $2 - \varepsilon$. J. Comput. Syst. Sci. 74(3): 335-349 (2008)

[28] S. Khot, M. Safra, and M. Tulsiani, Towards an optimal query efficient PCP? Technical Report TR12-109, ECCC (2012)

[29] J. B. Lasserre, An explicit exact SDP relaxation for nonlinear 0-1 programs. IPCO (Integer Programming and Combinatorial Optimization): 293-303 (2001)

[30] L. Lau, R. Ravi, and M. Singh, Iterative Methods in Combinatorial Optimization. Cambridge University Press, Cambridge, U.K., 2011.

[31] J. R. Lee, P. Raghavendra, D. Steurer, N. Tan, On the Power of Symmetric LP and SDP Relaxations. IEEE Conference on Computational Complexity 2014: 13-21

[32] N. Linial, E. London, and Y. Rabinovich, The geometry of graphs and some of its algorithmic applications. Combinatorica 15(2): 215-245 (1995)

[33] L. Lovasz, and A. Schrijver, Cones of matrices and set functions, and 0-1 optimization. SIAM Journal on Optimization 1: 166–190 (1991)

[34] T. Momke, and O. Svensson, Approximating graphic TSP by matchings. Proceedings of the IEEE Symposium on the Foundations of Computer Science: 560-569 (2011)

[35] D. Moshkovitz, The Projection Games Conjecture and the NP-hardness of $\ln n$-approximating Set-Cover. Approx-Random: 276-287, 2012.

[36] E. Mossel, R. O'Donnell, and K. Oleszkiewicz, Noise stability of functions with low influences: invariance and optimality. Proceedings of the IEEE Symposium on the Foundations of Computer Science: 21-30 (2005)

[37] R. O'Donnell, and Y. Zhou, Approximability and proof complexity. Proceedings of the ACM-SIAM Symposium on Discrete Algorithms 2013: 1537-1556

[38] S. Oveis Gharan, A. Saberi, and M. Singh, A randomized rounding approach to the Traveling Salesman Problem. Proceedings of the IEEE Symposium on the Foundations of Computer Science: 550-559 (2011)

[39] P. Raghavendra, Optimal algorithms and inapproximability results for every CSP? Proceedings of the ACM Symposium on the Theory of Computing: 245-254 (2008)

[40] P. Raghavendra, Approximating NP-hard problems: efficient algorithms and their limits. Ph.D. thesis, University of Washington, 2009.

[41] N. Robertson, and P. D. Seymour, Graph Minors I. J.Comb. Theory, Ser.B 35(1): 39-61 (1983), to Graph Minors XXIII. J.Comb. Theory, Ser.B 100(2): 181-205 (2010)

[42] A. Sebő, Eight-Fifth Approximation for the Path TSP. IPCO 2013: 362-374. Arxiv version: CoRR abs/1209.3523 (2012)

[43] A. Sebő, and J. Vygen, Shorter tours by nicer ears: 7/5-approximation for graphic TSP, 3/2 for the path version, and 4/3 for two-edge-connected subgraphs. Combinatorica (2014). Arxiv version: CoRR, abs/1201.1870v2 (2012)

[44] H. D. Sherali, and W. P. Adams, A hierarchy of relaxations between the continuous and convex hull representations for zero-one programming problems. SIAM Journal on Discrete Mathematics 3 (3):411–430 (1990)

[45] V. V. Vazirani, Approximation Algorithms. Springer-Verlag, Berlin, (2001)

[46] D. P. Williamson, and D. B. Shmoys. The Design of Approximation Algorithms. Cambridge University Press, Cambridge, U.K., 2011.

[47] D. Zuckerman, Linear degree extractors and the inapproximability of Max Clique and Chromatic Number, Theory of Computing 3(6): 103-128 (2007)

Chapter 25

Mathematical Modelling of Particles in Fluid Flow (14w5122)

August 18 - 22, 2014

Organizer(s): Bruce R. Sutherland (University of Alberta), Stuart Dalziel (University of Cambridge), Eckart Meiburg (University of California, Santa Barbara)

This report presents a review of the material covered at the workshop "Mathematical Modelling of Particles in Fluid Flow". The scope of the workshop was very broad both in terms of the range of problems covered (e.g. aerosol drug inhalation, cementing in oil and gas wells, avalanches, volcanic eruptions, sand dune evolution, etc) and the tools employed to understand the phenomena (e.g. theory guided by in situ observations and laboratory experiments, and various numerical modelling techniques including "level-set methods" and "smoothed particle hydrodynamics"). As well as lectures, group and individual discussions were actively encouraged. In particular, participants were asked to write perhaps more provocative questions on pieces of paper, which were then read and posed to the participants by a moderator on Monday and Wednesday afternoon. At the end of the meeting, the participants were asked to answer several questions on a Google poll. The content of the talks, the discussions, direct feedback and poll results are used to compose the details of this report.

25.1 Overview of the Field

Although the resuspension, transport and sedimentation of particles in a fluid is important in wide-ranging disciplines, a mathematical understanding of these processes remains elusive in all but the simplest circumstances.

Consider, for example, the process of sedimentation in which particles fall under gravity and accumulate at the ground. In the mid-nineteenth century, Stokes formulated the settling rate of a single sphere in relatively high-viscosity fluid. The model proved accurate in predicting the settling of highly dilute solutions (less than 1% by volume), but it under-predicted the settling rate of more dense solutions because the return flow of fluid around a particle hindered the settling of its neighbour. The effect of the return flow could be heuristically accounted for. But this still yielded incorrect predictions for the settling rate observed in experiments of moderately dilute suspensions.

Only 40 years ago was this relatively simple problem resolved [1]. Most issues, however, remain under active investigation. What is the influence of the domain size and geometry upon settling? What is the correct mathematical treatment of the thickening sediment layer at the bottom of the domain? At what point should this sediment layer be treated as particles in a fluid and at what point as fluid in a porous material? Under what circumstances can the particle-fluid matrix be described as a continuous, though non-Newtonian, fluid? How should one treat the behaviour of non-spherical and non-electrically neutral particles such as clay? How is sedimentation, coagulation and dispersal affected by turbulence? How is turbulence affected by the presence of particles (particularly colloidal molecules which have recently been used as drag reduction agents in pipelines)?

An indication of the active research in mathematically modelling settling particles in fluids flow is evident through several review articles in the well-cited Annual Review of Fluid Mechanics [2, 4, 5, 3].

More challenging still is the problem of sediment resuspension by a fluid moving over a bed of particles. In the simplest scenario, due to A. Shields (1936), particles are transported along the bed and possibly resuspended into the body of the fluid if the stress of the fluid acting on the bottom is sufficiently large to overcome the reduced weight of the immersed particle. In ongoing research, this criterion has been modified through various empirical formulae to account for turbulent flow and multiple particle sizes. But such approaches do not account for transient effects, such as wave-breaking on beaches, nor do they consider the possibility of resuspension from stagnation points in the flow where the stress is zero but the strain is large. The boundary conditions on the flow itself are modified by the presence of the particle layer (even if it is not yet moving) in ways that are not yet properly understood.

Understanding particle sedimentation, resuspension and transport has important consequences in environmental, industrial and medical sectors. Specifically, industrial applications include the management of waste water, dredging in river deltas, settling in tailing ponds and the determination of offshore oil drilling sites. Fisheries are concerned with nutrient transport in the benthic boundary layer. Aerosols such as dust and ash not only affect air quality, but dust raised by storms over the African desert act as a seed for the formation of hurricanes in the Atlantic Ocean. In medicine there is a need to understand drug transport through inhalation.

Historically, research into particle settling has been dominated by chemical engineers and environmental scientists. Their training gives them a valuable intuition for the dynamics of particles in fluids. But they do not bring to bear upon the problem the range of tools available to a mathematician.

Perhaps the greatest fundamental advances in the understanding of particle transport by fluid flows has been accomplished through the development of numerical simulations. Historically the first numerical approaches were based on averaged forms of the Navier-Stokes equations complemented with closure relations that mimicked the classical approaches for turbulence modelling [6]. However, these closure relations were derived from heuristic arguments, and suffer the same limitations as the numerous turbulence models available at present. Their major drawback is the lack of universality: the models contain a set of parameters that can be flow-dependent or hard to determine experimentally. Therefore the performance of the averaged models is unreliable and the results can be flow-dependent. In addition, the well-posedness and stability of the various averaged models are not intensively studied. To our knowledge, there are no successful attempts for the development of a homogenization theory similar to the one developed for porous media flows.

To help overcome these difficulties, more than a decade ago methods were developed to solve efficiently the full Navier-Stokes and particle equations for problems with a large number of particles [7], [8]. Unlike direct simulations of turbulence, the simulation of particulate flows requires additional relations to account for particle interactions. The spatial scale of such interactions can vary from zero (elastic collisions) to the lubrication scale (interactions in very viscous fluids). These cannot be realistically resolved by any numerical discretization. Approximations, such as the penalty method, fictitious domain method and immersed boundary method, necessarily sacrifice accuracy for efficiency in order to reduce the complexity of the overall problem and make it solvable. With the advance of powerful parallel computer clusters, the direct simulation approach has the potential to become a tool for modelling certain particulate flows of practical interest.

All this said, the most realistic prospect for a breakthrough in the description of particulate flows will likely involve a combination of mathematics guided by experiments, observations and and simulations that combine the direct approach with the solution of the averaged equations, similarly to the numerical upscaling developed for porous media flows [9].

The workshop brought together applied mathematicians with researchers actively engaged in numerical modelling and laboratory experiments of particle resuspension, transport and sedimentation. The common objective was to advance mathematical and computational models used in industry, the environment and in medical science.

Interdisciplinary interactions were established through the cross-pollination of ideas between mathematicians and practitioners as well as the exchange of ideas between researchers with medical, engineering and geophysics backgrounds.

25.2 Recent Developments and Open Problems

The exponential growth in speed and memory of computers has greatly advanced the study of particles in fluid flow. But much more progress needs to be made to understanding how to mathematical model the physics governing interactions between individual particles and complex fluid flows.

Our workshop identified the following as some of the most significant open problems:

1. When particles have a diameter comparable to the dissipative (Kolmogorov) scale in a turbulent flow, no one knows what are the expression of forces acting on those particles. The interplay of particles with turbulence is poorly understood: does the presence of particles enhance or damp turbulence?
2. If a particle is deformable (eg a bubble, a water droplet, a fiber, a capsule), how does the surrounding fluid affect the particle and how does the particle deformation affect the fluid? Does the deformation act as an additional reservoir of energy?
3. The growth of water droplets in a cloud provides a particular challenge. The microscopic ($\sim 1\mu$m) growth phase is understood from thermodynamics. The rapid growth of large droplets ($\sim 250\mu$m) has been modelled through the engulfment of smaller drops as the large droplet falls through them. But it is not well understood how the combined physics and chemistry of condensation, surface tension, etc affect the growth of moderately large droplets.

A far greater challenge involves understanding systems having a high concentration of particles. In addition to the problems above, particle-particle interactions with a fluid greatly complicates the problem. Our workshop identified the following open questions:

1. It remains a challenge to capture erosion of a bed of particles by an overlying fluid flow. Though heuristics exist to model erosion by steady flows, the understanding of particle resuspension and transport by transient bursts in turbulent flows and about points of flow separation (as at the top of sand dunes) remains poorly understood. When erosion does begin to take place, large particles can eject small particles from the particle bed through the process of "saltation", adding to the complexity of modelling such flows.
2. The settling of a dilute suspension of spherical particles is well-understood, and progress has been made in understanding the settling of anisotropic particles and moderately dense suspensions. Poorly understood are the complex dynamics of flocculation, which occurs when the particles (such as clay) are attracted to one another through electostatic forces. Individual flocs are fractal-like structures whose settling rates in fluid are poorly understood as is the effect of hydrodynamics forces upon the structure of the settling particles.
3. Although avalanches and turbidity currents (submarine avalanches) have been investigated for many decades, the dynamics of a mobile suspension of particles and their eventually run-out remains poorly understood. The modelling of each phenomenon is fundamentally different because particles provide most of the momentum in snow and rock avalanches, whereas the momentum of the interstitial fluid plays an important role in avalanches of rock, sand and clay down the continental shelves of the ocean. In systems with a wide range of particle sizes, the run-out is much larger than predicted by present mathematical models. This is because small particles can gain substantial momentum through collisions with larger particles and the effective rheology of the fluid as 'seen' by the large particles is altered by the presence of small particles.

4. In very dense particle suspensions (pastes, slurries, cements), the macroscopic properties of the flow are non-Newtonian, meaning that the strain on the medium is not proportional to the applied stress. It remains poorly understood how the rheology of such media (which characterize the stress-strain relationship) depends upon the range of particle shapes and sizes, their concentration in the fluid medium, and possibly other factors. (For example, in foam, deformability and surface tension also play a role.)

As well as these challenges in mathematical and physical modelling of fluid-particle systems there remain outstanding problems in experimental and numerical modelling:

1. Despite advances in multigrid methods, mesh refinement and parallel computing, numerical models that resolve individual particles in fluids at this time can capture on the order of 10^4 particles interacting over time scales of seconds. It remains a challenge to bridge the gap between such simulations and physical systems with billions of particles in time scales of hours or longer. To do so requires the determination of appropriate scaling laws that allow us to upscale our findings from small-scale DNS simulations and laboratory experiments to larger-scale phenomena.
2. Likewise there remains a gap between numerical models of industrial processes in the energy and chemical industries in which the flows are confined within complex containment systems involving mixers and sieves.
3. On a more fundamental level, in some circumstances there is a disconnect between laboratory experiments and numerical simulations. In order to provide validation of numerical models, experiments should be performed of very simple configurations to collect data that can be used for direct comparison with simulations.

Finally, an ongoing challenge is the recruitment and training of next generation of graduate students. The study of particles in fluid flow requires solid foundation in mathematics and physics. And so it is unfortunate that most physics departments have shifted their focus away from fluid dynamics research. Numerical modelling thrives in mathematics and engineering departments. But there remains a need for more laboratory experimentalists researching fundamental, rather than focused industrial, processes.

25.3 Presentation Highlights

Talks were given by seven plenary speakers whose research spanned the range of physical, industrial and environmental problems as well as experimental, observational and numerical investigation methods. Collectively they summarized the advances and outstanding research problems facing the community of scientists examining particles in fluid flow. Synopses of these talks are given below.

1. Stuart Dalziel: The impact of a droplet on a bed of particles

   This talk focused on dropping things. Dr Dalziel discussed experiments and their physical interpretation for a number of novel configurations with work spanning nearly twenty years. He began with a brief discussion of the role of the hydrodynamic wake behind a rigid body falling onto a bed of particles and how this vortex-ring-like wake could be more important for resuspending particles than the classical ballistic mechanism. From this he moved on to looking at how a vortex ring by itself could resuspend material in an otherwise quiescent flow. This work, which can be viewed as a prototype for resuspension due to turbulence, demonstrated the role of deposition of secondary vorticity, through viscosity, leading to boundary lager separation as a resuspension mechanism. He demonstrated the approximate self-similarity of the craters produced by the vortex rings and the energetic relationships in the system.

   Dr Dalziel then returned to a variant of his initial problem to consider a falling droplet rather than a rigid sphere. Looking from afar, the droplet produces a 'splash' that is superficially similar to that of a solid particle, but that raises somewhat more material than might have been expected. Dr Dalziel also talked briefly about the additional dynamics if the droplet if the fluid is enclosed in a membrane that ruptures on impact, instantaneously removing the restoring force for waves in the system and resulting in a previously unseen Richtmyer-Meshkov growth mechanism.

The final configuration considered was Richtmyer-Meshkov instability of a granular layer subject to an impulsive vertical acceleration. As with the classical instability, surface features are inverted and amplified by an acceleration directed towards the lighter phase (air). Elements while the overall mechanism can be identified as Richtmyer-Meshkov, there are features that can be understood as the triggering of avalanches.

2. Rama Govindarajan: Droplets: sinking/rising under gravity; clustering; imparting buoyancy

   Dr. Govindarajan's talk was in two parts. The first part was about three-dimensional simulations of an initially spherical single drop of fluid rising under gravity through another fluid. A comprehensive phase diagram of symmetry-breaking and bubble-breaking were discussed and the connection made to dynamics. She also asked how a rising bubble is fundamentally different from a sinking drop. The second part was about dynamics of droplets in the vicinity of vortices, when the droplets were allowed to grow and shrink. Inertia and thermodynamics are important in the resulting clustering and dynamics. She showed that particles can cluster in unexpected regions, and that buoyancy due to phase change can modify the dynamics a lot. The relevance of this work to clouds were discussed.

3. Andrew Hogg: The flow of fluidised particles

   The 2010 eruption of Eyjafjallajokull, Iceland posed many problems for the operational forecasting of the atmospheric dispersion of volcanic ash and the assessment of the risk for air travel; European airspace was closed for several weeks . Mathematical models of the ash dispersion encompassed advection by the atmospheric winds, diffusion by atmospheric turbulence and settling under gravity. But The models neglected the sustained perturbation to the atmospheric stratification caused by the intrusion of the ash plume.

   In this study we investigate how ash intrusions may be driven by buoyancy processes associated with the disruption of the atmospheric stratification and we show that these effects may be dominant within the first few hundred to thousand kilometers from the volcano. This suggests that current operational models of such motions are flawed due to their omission of these effects and that the risk to aircraft due to airborne ash may not be fully assessed.

4. Jim McElwaine: Particle sedimentation and resuspension in geophysical flows

   Avalanches, turbidity currents, debris flows and pyroclastic flows are all gravity currents driven by the weight of solid particles. How these particles move vertically within the flow, including their entrainment and deposition, critically effects the flow dynamics. For example a debris flow where the solid particles are fully suspended is much more mobile than one where granular friction is dominant. In other flows a two layer structure often occurs with a dilute particle cloud above a shallow dense layer. Dr. McElwaine formulated a simple model that can reproduce this behaviour and showed the results of direct numerical simulations. He gave a comparison with lab experiments and field data and showed how these effects can be incorporated in shallow water models.

5. Eckart Meiburg: Double-diffusive sedimentation

   When particles settle through thermal and/or compositional density gradients, double-diffusion may fundamentally alter their dynamics. The example of sedimentation from buoyant, freshwater river plumes into the saline ocean below serves to explain the fundamental physical principles. In typical estuaries the density contribution of the sediment is less than that of the salinity, so that the overall stratification is stable. Within this overall stable density profile, however, the sediment itself is unstably stratified. Its available potential energy can be released in the form of double-diffusive fingering, which drastically alters the effective settling velocity of the sediment. This effect has been demonstrated in laboratory flow visualization experiments. For the purpose of modeling the global sediment cycle, it is essential to have accurate estimates of the sediment flux from river plumes, as rivers represent the main vehicle responsible for the transport of sediment from land into the coastal oceans. In spite of its importance, however, a generally accepted comprehensive description of the double-diffusive sediment flux from river plumes is still elusive, and scaling laws and/or reliable quantitative measurements of this sediment flux as a function of the governing flow parameters are as of yet unavailable. Traditionally, this flux has been estimated based on the Stokes settling velocity of the individual sediment grains, without accounting for double-diffusive effects.

Dr Meiburg explored the nonlinear regime of such processes by means of two- and three-dimensional direct numerical simulations (DNS). The initial instability growth in the DNS is seen to be consistent with the dominant modes predicted by linear stability analysis. The subsequent vigorous growth of individual fingers gives rise to a secondary instability, and eventually to the formation of intense plumes that become detached from the interfacial region. The simulations show that the presence of particles with a Stokes settling velocity modifies the traditional double-diffusive fingering by creating an unstable 'nose region' in the horizontally averaged profiles, located between the upward moving salinity and the downward moving sediment interface. The effective thickness l_s (l_c) of the salinity (sediment) interface grows diffusively, as does the height H of the nose region. The ratio H/l_s initially grows and then plateaus, at a value that is determined by the balance between the flux of sediment into the rose region from above, the double-diffusive/Rayleigh-Taylor flux out of the nose region below, and the rate of sediment accumulation within the nose region. For small values of $H/l_s \leq O(0.1)$, double-diffusive fingering dominates, while for larger values $H/l_s \geq O(0.1)$ the sediment and salinity interfaces become increasingly separated in space and the dominant instability mode becomes Rayleigh-Taylor-like. A scaling analysis based on the results of a parametric study indicates that H/l_s is a linear function of a single dimensionless grouping that can be interpreted as the ratio of in- and outflow of sediment into the nose region. The simulation results furthermore indicate that double-diffusive and Rayleigh-Taylor instability mechanisms cause the effective settling velocity of the sediment to scale with the overall buoyancy velocity of the system, which can be orders of magnitude larger than the Stokes settling velocity.

While the power spectra of double-diffusive and Rayleigh-Taylor dominated flows are qualitatively similar, the difference between flows dominated by fingering and leaking is clearly seen when analyzing the spectral phase shift. For leaking-dominated flows a phase-locking mechanism is observed, which intensifies with time. Hence the leaking mode can be interpreted as a fingering mode which has become phase-locked due to large scale overturning events in the nose region, as a result of a Rayleigh-Taylor instability.

6. Joseph Monaghan: How to simulate several liquids and species of particles using SPH

   SPH (smoothed particle hydrodynamics) is a particle method that replaces a fluid by a set of particles that interact according to the equations of fluid dynamics. In his talk Dr Monaghan described how SPH can be used for problems involving liquids containing particulate matter which he referred to as dust. The dust particles were considered sufficiently numerous to allow them to be treated collectively as a fluid which was represented by a set of SPH particles which interact with the fluid SPH particles by drag terms. He showed how solid bodies (stirrers) can also be handled by replacing them by SPH particles in a straightforward way.

7. Anne-Virginie Salsac: Fluid structure interaction of a microcapsule in flow

   A capsule consists of an internal medium enclosed by a semi-permeable membrane that controls exchanges between the environment and the internal contents and has a protection role. Natural capsules are cells, bacteria or eggs. Artificial capsules are widely used in industry (pharmaceutical, cosmetic, food industry, etc) for the protection of active substances, aromas or flavours and the control of their release. They are also used in bioengineering applications, such as drug targeting and artificial organ fabrication.

   In most situations, capsules are suspended into another liquid and are thus subjected to hydrodynamic forces when the suspension is flowing. The motion of the suspending and internal liquids creates viscous stresses on the membrane, which lead to its deformation and possible breakup. The three-dimensional fluid-structure interactions may be modelled coupling a boundary integral method (for the internal and external fluid motion) with a finite element method (for the membrane deformation). This Dr Salsac showed to be a stable and accurate coupling strategy. She concentrated on the case of ellipsoidal capsules and explored their motion and deformation when subjected to a simple shear flow.

   When designing artificial capsules, it is also necessary to control and tune the capsule deformation, so that it has the desired behaviour. Dr Salsac showed how the mechanical properties of microcapsules can be obtained from a microfluidic experiment.

25.4 Scientific Progress Made

As intended, the significant progress was made through the cross-fertilization of ideas stemming from different disciplines. Feedback provided by the Workshop participants after the meeting expressed great excitement at the breadth of topics covered. Many participants were inspired by seeing numerical and experimental techniques used in other disciplines.

Laboratory experimentalists were inspired by the new techniques (discussed by David Rival) to measure flow through porous media. Many researchers were excited to see the range of numerical methods used to model particulate flow.

As an example for cross-fertilization among different fields, double-diffusive particle dynamics (discussed by Eckart Meiburg) were understood to be important in a broad range of applications. Important examples can be found in the fields of environmental multiphase fluid dynamics (the global sediment cycle, sedimentation from buoyant freshwater river plumes, the formation of giant submarine fans with volumes of millions of km^3 such as the Bengal/Ganges fan off the coast of India), climate change (the dynamics of rain droplets in clouds, the removal of CO_2 from the surface of the ocean by marine snow, deep-sea CO_2 sequestration), energy (the formation of deep-sea oil and gas deposits by submarine turbidity currents), water supply and sustainable development (loss of storage in water reservoirs as a result of sedimentation).

Some who had not heard of smooth-particle hydrodynamics (discussed by Joseph Monaghan), a technique championed in astrophysics, were inspired to learn and adapt this method to their own research. New interpolation methods in the context of immersed boundaries will be employed by the broader numerical community to enhance the accuracy of simulations of particle-particle and particle-boundary interactions.

The different numerical modelling approaches all have their strengths and weaknesses. The Workshop made progress in identifying schemes that can provide the most insight for a given problem at reasonable computational cost.

The multiphase problems in geophysical fluid dynamics have lots of similarities with processes occurring in chemical process industries. Generally, there is a need for tacking problems that occur in nature with all its coupling of multi-physics. Some researchers appreciated scaling techniques and empirical methods used to start with a "toy problem" and build it up to a complicated scenario. Conversely, some researcher benefited by seeing asymptotic techniques used to simplify complex scenarios.

Computational strategies for fully resolved particulate flows have moved on considerably - and perhaps now reliably reproduce physical flows and effects That said, many of the numerical models developed are looking for applications. And many of the laboratory experiments presented would benefit from accurate numerical models that could give more microscopic insight into the observed macroscopic dynamics. The dialogue afforded by the meeting has brought these groups together. Experimentalists have been given guidance to design and analyze their studies in a way that can be modelled numerically with direct comparison of results. The close collaboration between computational and experimental researchers is crucial, as both sides can contribute in areas that are not easily accessible to the other group.

25.5 Outcome of the Meeting

As evident from feedback following the meeting, immediate benefits of the Workshop include the wide-ranging new collaborations that have been created and past collaborations that have been reinvigorated by topic raised.

New links have been forged between numerical modellers who have been developed different simulation methods but see the potential for advancement through technology exchange. This includes application of particle-resolving simulations, smoothed-particle hydrodynamics and lattice-Boltzmann methods to the chemical process industry. Research into fibers in fluid flow have provided a new challenge for some of the numerical modellers that will now be pursued.

New experimental results into turbidity currents and avalanches have inspired some modellers to apply their codes to these circumstance. This research has also inspired an experimentalist working on fibers to advance his research to the study of particle-laden flows and it has given new insight to a sedimentologist to reinterpret his observations of submarine channels.

New test cases have been developed to combine different numerical technologies and laboratory experiments. The novel use of hydrogel to study flow through porous media will be adopted by several of the experimentalist participants. New research is planned to use this technique to examine pore-pressure-driven flows.

Finally, new interdisciplinary collaborative partnerships were formed between researchers focusing on fundamental fluid dynamics and applied mathematics on one hand, and researchers interested in bio-, aerodynamical and environmental applications on the other.

Participants

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Bibliography

[1] G. K. Batchelor, Sedimentation in a dilute dispersion of spheres, J. Fluid Mech. **52** (1972), 245–268.

[2] R. H. Davis and A. Acrivos, Sedimentation of noncolloidal particles at low Reynolds numbers, Annu. Rev. Fluid Mech. **17** (1985), 91–118.

[3] E. Guazzelli and J. Hinch, Fluctuations and instability in sedimentation, Annu. Rev. Fluid Mech. **43** (2011), 97–116.

[4] A. Guha, Transport and deposition of particles in turbulent and laminar flow, Annu. Rev. Fluid Mech. **40** (2008), 311–341.

[5] C. Kleinstreuer and Z. Zhang, Airflow and particle transport in the human respiratory system, Annu. Rev. Fluid Mech. **42** (2010), 301–334.

[6] F. Toschi and E. Bodenschatz, Lagrangian properties of particles in turbulence, Annu. Rev. Fluid Mech. **41** (2009), 375–404.

[7] R. Glowinski, T. Pan, T. Hesla, D. Joseph, and J. Periaux, A fictitious domain approach to the direct numerical simulation of incompressible viscous flow past moving rigid bodies: application to particulate flow, J. Comput. Phys. **169** (2001), 363–385.

[8] N. Sharma and N. Patankar, A fast computation technique for the direct numerical simulation of rigid particulate flows, J. Comp. Phys. **205** (2005), 439–450.

[9] Y. Efendiev, T. Hou, and X.-H. Wu, Convergence of a nonconforming multi scale finite element method, SIAM J. Numer. Anal. **37** (2000), 888–910.

Chapter 26

Mathematics of the Cell: Integrating Genes, Biochemistry and Mechanics (14w5075)

September 7 - 12, 2014

Organizer(s): Alex Mogilner (New York University), Eric Cytrynbaum (University of British Columbia), Adriana Dawes (Ohio State University), David Sept (University of Michigan)

26.1 Overview of the Field

26.1.1 Introduction

Biology is being touted by many as THE science of the 21st century, much as physics was at the forefront of science in the 20th century. Over the last two decades, mathematical modeling, analysis and computation have played an important in this transition. Mathematical biology is barely one hundred years old, and for a long time its focus was the deep mathematical analysis of equations inspired by biology, much like the landmark 1952 paper of Alan Turing that proposed a biologically abstract model for pattern formation during tissue development. Coincidentally, in the same year, Hodgkin and Huxley developed a biologically concrete model to understand the electrical activity in nerve cells. In the last two decades, the number of mathematically deep and biologically realistic studies has undergone explosive growth. The impact of mathematics on biology, physiology and medicine is increasing, while biologically-relevant mathematics is becoming more diverse and sophisticated.

Scientific and technological changes are accelerating, and it is important to foresee paradigmatic shifts in science and prepare in advance. Many scientists have started to realize that individual biological processes can no longer be studied in isolation but need to be considered as integrated events. Thus, the next shift is the rise of *Integrative Biology*, loosely defined as multidisciplinary research across all levels of biological organization, from molecules to the biosphere. We focus on the cell level of biological organization because cells are the smallest autonomous units of life and occupy the midpoint between the molecular and macroscopic scales. In order to understand how living systems are built and function, we need to understand the mathematical principles that underlie cellular organization and function. It is in the cell where we will first understand the basic processes of life at the molecular level in a physiological context. The cell provides the natural coordinate system in space and time onto which we have to map and integrate genomic, biochemical and mechanical information about the molecular networks that make up living systems.

Mathematical cell biology will be an integrative hub of much of modern quantitative biological research. Mathematics will provide the structure, abstraction and language to integrate across scales. Thus, future Mathematical cell biology will require bringing together scientists and mathematicians with different areas of expertise able to use a diversity of techniques and work at the interfaces of disciplines. It is essential to make mathematicians a part of the process of biological discovery and to make biologists understand and appreciate the power of mathematics and to be able to actively participate in model development.

26.1.2 Mathematical Cell Biology

The exact tools that have been used previously in physical and chemical sciences may simply not be directly applicable to cell biology. This has nothing to do with vitalism, but simply with the fact that cell biology occurs on multiple and radically different scales, both in terms of time, space, and complexity. Understanding how cellular-scale behaviors arise from molecular actions is fundamentally difficult due to the large number of many different kinds of molecules all interacting in complex networks. Another difficulty is that cell biological systems consist of thousands of molecules and so are not microscopic, but they are not macroscopic either; often, fluctuations of chemical or physical quantities in the cell are comparable in magnitude to the average values of these quantities. The main difference between modeling in biology and physics stems from the inherent redundancy and heterogeneity of evolved molecular machines that have to be elucidated. This makes cell modeling very difficult but also unavoidable as new technologies produce staggering amounts of data about the spatiotemporal behavior of molecular assemblies. With increasing frequency, these data are quantitative – correlation functions, statistical regressions, and other similarly sophisticated forms – that cannot be reduced to simple qualitative statements, so mere qualitative cartoon drawing in the discussion section of a paper is not sufficient. Rather, to integrate and make sense of these data, quantitative modeling is needed as hypotheses generating machine and a natural endpoint for the experimental efforts.

26.2 Recent Developments and Open Problems

There are a few specific areas of cell biology where mathematical modeling is especially useful.

Cytoskeletal dynamics

All cells with a nucleus have dynamic polymers collectively referred to as the cytoskeleton. Two out of three primary filament types are actin filaments and microtubules. The cytoskeleton is involved in a wide range of cellular functions including cell division and cell migration. Further, the cytoskeleton provides a structural framework within the cell, allowing it to both exert and respond to extracellular stimuli. Microtubules are the most rigid structures in the cell, typically emanating from the microtubule organizing center (centrosome) next to the nucleus. Actin filaments can assume a variety of different conformations including bundles, where the filaments are arranged in a parallel or antiparallel fashion, or branched networks. These branched networks typically found at the edge of migrating cells, form a broad thin structure called a lamellipod. The cytoskeleton is involved in determining cell shape and movement. It should not be surprising that actin filaments and microtubules do not act alone. Rather, their function is regulated by a multitude of associated proteins. Some of these associated proteins help to polymerize or depolymerize the filaments, crosslink filaments into networks or bundles. Motor proteins exert forces between filaments, organelles, cell membrane and extracellular matrix. Biochemistry and cell biology have given us a wealth of data about the components and parts of this system, but many details are still missing. More than that, how the system is organized to work coherently in space and time is still an elusive question. Given the inherent complexity of this system, mathematical and physical models are playing an increasingly important role in elucidating the underlying behavior of the cytoskeleton and its role in many cellular functions. Open problems include, but are not limited to: how are cytoskeletal elements self-organize into contractile or expanding structures, what are the mechanisms behind history-dependent mechanochamical behavior of the cytoskeleton, what are the differences in prokaryotic and eukaryotic cytoskeletal dynamics,

Cell polarity

When the cells move directionally, or even when they are stationary but functioning in a group of other cells or preparing for division, they polarize their morphology and distributions of key molecular players inside the cells become asymmetric. This symmetry break poses a challenging problem that is a right up the alley of mathematicians: how is a combination of spatial-temporal positive and negative feedbacks coupled to achieve the polarization? How does this process work in the presence of huge fluctuations? Ever since the fundamental Turings discovery, reaction-diffusion models of interacting chemicals were investigated and applied to explain various polarization events. However, recently, mechanical pathways were also discovered to be able to break symmetry, even in the absence of the underlying biochemistry. However, more often than not, mechanical and biochemical pathways are coupled to achieve faithful and rapid polarization. The details, and more importantly, the design principles of these couplings are not clear.

Cell signaling

Cell signaling is part of a complex system of communication that governs basic cellular activities and coordinates cell actions. The ability of cells to perceive and correctly respond to their microenvironment is the basis of development, tissue repair, and immunity as well as normal tissue homeostasis. Errors in cellular information processing are responsible for diseases such as cancer, autoimmunity, and diabetes. By understanding cell signaling, diseases may be treated effectively. Cell is constantly bombarded by tens of environmental stimuli and stresses. Meanwhile, there is a very finite number of 'hubs in signaling relays inside the cell. How does the cell convert the multitude of outer signals into another multitude of behaviors using a very finite signal processing toolbox? This is a great problem for a mathematician.

Traditional work in biology has focused on studying individual parts of cell signaling pathways. Mathematical biology research helps us to understand the underlying structure of cell signaling networks and how changes in these networks may affect the transmission and flow of information. Such networks are complex systems in their organization and may exhibit a number of emergent properties including bistability and ultrasensitivity. Analysis of cell signaling networks requires a combination of experimental and theoretical approaches including the development and analysis of simulations and modeling.

Role of aqueous medium in cell processes

Cells are filled, besides cytoskeleton, with fluid cytoplasm. The cytoplasm is a very strong electrolyte. Recently, it became clear that cells can move and generate forces by converting cytoskeletal contractions into squeezing the fluid and generating hydrostatic pressure. This pressure delaminates cell membrane from underlying actin producing bubbles. The same pressure can move nucleus as a piston inside the cell. Besides hydrostatic pressure, the osmotic pressure is a big part of the picture because ion concentrations inside and outside the cell vary a lot. Osmotic and hydrostatic pressures create flows that transport molecular cargo and help cell movements. Understanding this biofluid dynamics is impossible without solving complex problems of fluid mechanics coupled with statistical physics of polyelectrolytes.

Cell motility

Cells crawl by, first, pushing out the front, then it assembles tight adhesions to the surface at the leading edge and weakens such adhesions at the rear, and finally the cell develops contractions that pull up the weakly adherent rear toward the strongly adherent front, completing the motility cycle. This process is an important part of wound healing, morphogenesis and cancer, among many other biological and medical phenomena but it is the elegance of the seemingly simple, yet underlined by layers of complexity, motile cycle that inspired thousands research papers in the last four decades. The devil, of course, is in the details, and it is these increasingly meticulous and numerical molecular details of the motile machinery that require mathematical modeling. First, we have to understand the actin treadmill how dynamic network of filaments translocates in space by assembly/disassembly. Then, we have to figure out how myosin and actin self-organize to contract the cell body. Finally, we have to elucidate mathematically how tens of adhesion proteins first assemble at the leading edge gluing it to the substrate and then disassemble at the cell rear letting it go.

From individual cell to tissues

Developmental biology is the study of the process by which multiple cells form tissues and by which organs grow and develop. Modern developmental biology studies the genetic control of cell growth, differentiation and morphogenesis. In recent years, mathematical modelling of developmental processes has earned new respect. Not only have mathematical models been used to validate hypotheses made from experimental data, but designing and testing these models has led to testable experimental predictions. There are now impressive cases in which mathematical models have provided fresh insight into biological systems, by suggesting, for example, how connections between local interactions among system components relate to their wider biological effects.

26.2.1 Objectives of the workshop

One of the most effective ways to achieve goals of collaboration and integration of theoretical and experimental approaches is to organize a small meeting at which mathematicians and biologists discuss in depth recent advances, new paradigms and trends, and plan future collaborations. The format of BIRS 5-day workshop was ideal for such a meeting. We started to pursue the goals described above 7 years ago, with the first meeting focused on Mathematical Biology of the Cell, and devoted to defining this discipline. The meeting was a big success, and was followed by the second in 2011. In the second meeting we concentrated on the narrower area of mathematics of cytoskeleton and cell motility and division, which has attracted a large number of modeling efforts. One of the best signs of its success is that a great number of collaborations were started at that meeting.

We want to emphasize that this area is not settling down into a comfortable routine. In fact, the emerging challenge we are facing is that we have to go past successful mathematical modeling of certain aspects (i.e. biochemical or mechanical) of cell behavior, and start integrating genetic, biochemical and mechanical models into multi-scale mathematical platforms that will allow for prediction of cell behavior in physiological circumstances. This poses a set of mathematical, computational and biological problems that we hoped to discuss, define and start planning to solve in 2014. And so, we continued in 2014 with having unprecedented level of interaction between experimentalists and modelers and transitioning into the systems level of modeling cell biological phenomena.

26.3 Presentation Highlights

A number of talks were devoted to discussions of actin dynamics and relevant self-organization phenomena. David Sept explained that highly unusual characteristics of parasites actin result from isodesmic polymerization rather than the nucleation-elongation kinetics of conventional eukaryotic actins. These findings expand the repertoire of how actin functions in cell motility and offer clues about the evolution of self-assembling, stabilized protein polymers. Thomas Pollard showed that in yeast cell division punctate protein structures arise in separate locations in the cortex and join each other around the equator of the cell by a diffuse and capture mechanism to form "nodes", the precursors of the cytokinetic contractile ring During mitosis nodes grow actin filaments and a search, capture, pull and release mechanism organizes the nodes into the contractile ring. Alexander Bershadsky discussed the processes of actin cytoskeleton self-organization driven by actin assembly and cross-linking and myosin II contractility. He showed how computational modeling demonstrates the evolution of the radial pattern of stress fibers into the chiral pattern and how self-organization of the actin cytoskeleton provides built-in mechanism of establishing left-right asymmetry. This mechanism may play a key role in a variety of morphogenetic processes. W. Bement brought to our attention a fascinating discovery that anaphase onset in frog and echinoderm embryos is associated with cortical excitability, manifested as waves of Rho activity and F-actin that traverse the underside of the plasma membrane. Remarkably, the excitability entails F-actin mediated Rho inhibition. He proposed that chaotic phase is explained by the development of cortical excitability which is normally restricted to a discrete portion of the cell cycle Cdk1 and that excitability provides the cell with the means to balance the conflicting needs of speed, precision and flexibility during cell fission.

Other talks addressed how actin and myosin generate force. Anders Carlsson investigates mechanisms by which polymerized actin can exert forces with the required orientation and magnitude. He showed three possible mechanisms leading to endocytic invagination: a) lateral segregation of nucleation-promoting factors into an inner core and an outer ring creates curvature-generating forces via differences in polymerization rates, b) spontaneous curvature of a coat-protein layer bends the membrane, and c) motor activity creates a contractile ring that buckles the coat protein layer. He proved that mechanism a) by itself can produce invagination, but mechanisms b) and c) cannot. However, either mechanisms b) or c) can reduce the requirements for mechanism a). Ben Fogelson asked how an individual stress fiber behaves and, in particular, how much force it generates. By using data from cells grown on micropatterns, he was able to construct a simple 1-D model of actomyosin force production to explain a puzzling peak in force production at intermediate stress fiber lengths. Cecile Sykes talked about reconstitution of the actin cortex of cells inside liposomes, and using it as a simplified system to study endocytosis. She showed how these cortices contract in the presence of myosin motors, and how such experiments shed light of the mechanisms of cell shape changes.

A group of talks were devoted to modeling various aspects of cell movement. K. Keren posed the problem of how actin network translocates forward and illustrated that the complex reaction-diffusion problem for the polymeric and monomeric actin produces solutions that compare well with experimental measurements, and thus diffusion is able to move the monomers effectively forward. In a related talk, Garegin Papoian reported development of detailed physico-chemical, stochastic models of lamellipodia and filopodia, which are projected by eukaryotic cells during cell migration, and contain dynamically remodeling actin meshes and bundles. His simulations showed that some processes, such as binding and unbinding of capping proteins, may be dominated by rare events, where stochastic treatment of filament growth dynamics is obligatory. The talk shed light on how actin transport due to diffusion and facilitated transport such as advective flow and active transport, tunes the growth dynamics of the branched actin network. Wolfgang Loosert described how simple physical measurements of shape dynamics and motion reveal an underlying wave-like process of the cellular scaffolding that drives persistent migration and how wave-like dynamics of the scaffolding contributes to the ability of cells to recognize and follow surface nano-topography, and allows cells to couple to each other when moving in groups. A couple of talks addressed a very important problem of cells moving in 1D and 3D. David J. Odde explored the behavior of the motor-clutch model, and assessed which model parameters control the stiffness at which sensing is optimal. Using a Master Equation approach, he developed an analytical description of the model, and obtained a dimensionless number that defines the optimal substrate stiffness. He speculated that the motor-clutch model may be useful for in silico identification of combination drug targets for brain cancers, and is generally applicable to animal cell adhesion and migration in 1D, 2D, and 3D environments. Damir Khismatullin reported development of a fully three-dimensional computational model of amoeboid chemotaxis by incorporating the intracellular force field due to actin polymerization into our algorithm for passive cell deformation and adhesion, known as VECAM. The resulting model (VECAM-Active) takes into account passive mechanical properties of the cell, extracellular diffusion of chemoattractant molecules, intracellular release and diffusion of signaling molecules, intracellular active force generation, cell adhesion and physiological shear flow conditions. Using VECAM-Active, Damir has investigated the amoeboid movement of leukocytes and cancer cells in a rectangular microchannel. His simulation data indicated that the model captured a number of deformation patterns of motile cells: from a finger-like projection, which is a feature of cells migrating through the endothelial layer or into a chemoattractant-filled micropipette, to a lamellipodium-like projection that is observed for many cells actively migrating on a flat substrate.

Another group of talks focused on cell signaling. Sasha Jilkine introduced adipogenesis, the differentiation process of adipocyte (fat cell) formation from precursor cells contributing to increase of fat tissue in obesity. Previous work has found that some of these proteins increase and then decrease significantly during differentiation. She showed that three coupled network motifs found in adipocytes can explain these observations. Andre Levchenko asked how cells exposed to a diverse range of molecular cues are informed about the appropriate direction of migration. These cues can change in space and in time, and co-exist in a consistent or contradictory fashion. How live cells interpret these cues and compute the appropriate program of polarization and directional migration is not well understood. He discussed recent findings and modeling suggesting how integration of such cues can take place through a relatively simple set of molecular circuits. Orion Weiner focussed on recent advances in optogenetics, which enable us to interrogate signaling cascades in a manner that has been difficult or impossible with previous tools. Alba Diz-Muoz started by saying that far from being a passive participant, the plasma membrane is now known to physically, as well as biochemically, influence cell processes ranging from vesicle trafficking to actin assembly. In particular, changes in plasma membrane tension regulate cell shape and movement. She recently found that membrane tension (the force a cell has to overcome to protrude the plasma membrane) is necessary and sufficient to determine leading edge size and number. Research in recent years has shed light on the role of forces in cytoskeletal organization, but how changes in membrane tension are translated into changes in cell signaling is unknown. She reported how to use a combination of atomic force microscopy and fluorescence imaging of intracellular signals to uncover how neutrophils sense tension.

Many talks tackled the problem of cell polarity. Stan Maree discussed a fascinating similarity between animal and plant cells with respect to the organization of cytoskeletal elements in the regions of active protrusive growth and cell wall extension. He showed a multiscale model of a motile keratocyte, describing how the molecular players cause cell polarity and deformation. He then contrast this to the cell shape changes that occur in the pavement cells in the leaves of plants that form jigsaw-like patterns. He posed, by mathematically and computationally exploring the system, that similar modular principles play a role in animal and plant cells. Adriana Dawes turned her attention to highly conserved molecular players in polarization, including Par proteins, Rho proteins and actomyosin. Using a combination of modeling and experiments, she demonstrated the likely interactions between these key players responsible for initiation and maintenance of polarization in early embryos of the nematode worm C. elegans. Vernica A. Grieneisen addressed how computational and mathematical approaches combined with molecular studies and in vivo microscopy can help us understand polarity on three different levels: on the scale of the tissue, the cellular and subcellular tissue level.

A few talks discussed microtubules and molecular machines that use them. Dan Fletcher described recent work investigating the effect of volumetric confinement on the assembly of mitotic spindles in Xenopus egg extract, in particular, a limiting component model that addresses the effect of volumetric confinement on cytoskeletal assembly. This talk contributed to the growing view that cytoskeletal structures in cells are defined not only by their molecular components but also by the boundary conditions imposed on them. Melissa Gardner discussed length control of the metaphase mitotic spindle that is thought to be achieved through a mechanism in which spindle pole separation forces from plus-end directed motors are balanced by forces from minus-end directed motors that pull spindle poles together. Paradoxically, she describe that in contrast to this notion, metaphase mitotic spindles with inactive Kinesin motors often have shorter spindle lengths, along with poorly aligned spindle microtubules. A mechanistic explanation for this paradox is unknown. She showed that results of computational modeling, in vitro reconstitution, live-cell fluorescence microscopy, and electron microscopy suggest that the yeast Kinesin motor can efficiently align spindle microtubules along the spindle axis. Holly Goodson started by saying that the concept of critical concentration is a central idea in the understanding of biological polymers such as actin and microtubules. Classically, the critical concentration is accepted to be a single discrete value with several equivalent definitions. However, the mathematical underpinnings of this understanding are based on analysis of equilibrium polymers, which is problematic because these cytoskeletal filaments are instead steady-state polymers. This incongruity raises questions about whether present understanding of critical concentration as it applies cytoskeletal filaments is complete or even approximately correct. She has used computational models of systems of dynamic microtubules to investigate this issue.

Two fascinating talks were about the role of water in cells. Yoichiro Mori formulated a prototypical mathematical model that couples membrane mechanics with chemical diffusion and osmotic water flow. He then presented a numerical scheme for this problem, and demonstrated some computational examples. Sean Sun mathematically analyzed cellular pressure and volume control by considering both cytoskeletal dynamics and active regulation of cellular osmotic content. He showed that water permeation across the cell membrane is a major contribution to the slow phase of cellular mechanical response. He further demonstrated that water permeation alone can drive cell motility in confined environments. The last finding is significant for cancer cell motility in some situations.

26.4 Scientific Progress Made

There are a number of new understandings that emerged from the meeting. First, the concept of a motile cell as a free boundary object emerged, in which local boundary movements are governed by distributed spatial-temporal mechanochemical process inside the cell. Second, a few signaling pathways coupled to mechanical forces found their first mathematical representation. Third, a number of people realized how to make 3D, rather than 2D, modeling of cells practical and found a few open problems that need mathematical investigation. Forth, actomyosin cortical flow creating friction with the extracellular environment was realized to be a universal mechanism of coupling cell deformations to the substrate. Fifth, a number of design principles of multi-scale self-organization of cytoskeletal systems was classified. In general, we started to see general design principles of cell dynamics from mathematical point of view.

26.5 Outcome of the Meeting

The main result of the meeting is new collaborations that resulted from it. K. Keren started to collaborate with A. Mogilner on modeling collective migration of fish keratocytes they already had a working model of individual cells as free boundary objects, and now they started to use microscopy, biochemical perturbations and partial differential equations to understand how cells keep collective polarity and coherent movements. G. Papoian is planning to apply his 3D modeling methods to simulating D. Fletchers in vitro 3D actin assay with the goal to predict the hysteresis effects. A. Carlsson and W. Loosert are combining their experimental and theoretical efforts to elucidate actin waving behavior and its role in cell locomotory behavior. A. Levchenko and L. Edelstein-Keshet conceived a new idea on how complex stochastic Rac/Rho pathway leads to cell polarization. S. Sun is helping E. Paluch to simulate blebs in complex environments. J. Allard and A. Upadhyaya collaborate on developing very detailed models of cell-cell interactions. A few groups of people started to write grant proposals after finding ways to enhance each other research. Generally speaking, there is a growing sense of mathematical cell biology as a vibrant subdiscipline with an above average degree of cohesion of theory and experiment that is the most important outcome of this meeting.

26.6 What Lays Ahead

Cell biology is transitioning into a quantitative science characterized by increasing integration of modeling into experiment. In this transition, we have to proceed with numerous, often arbitrary, assumptions about the nature of processes and parameter values governing cell systems. One great future challenge is to improve quantitative experimental methods with an eye toward synchronizing modeling and experiments. Then, frequent back-and-forth between theory and experiment using models of varying scope and level of realism will allow us to overcome the arbitrariness and uncertainty. Another significant challenge is to make switching from one type of model to another a more standard, less ad hoc procedure, to ease modeling use and integration between theory and experiment. Models along this course will be impermanent and should be judged by how useful they are and what we can learn from them, not by how close we are to the elusive whole-cell model.

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Chapter 27

Probability on Trees and Planar Graphs (14w5159)

September 14 - 19, 2014

Organizer(s): Louigi Addario-Berry (McGill University), Omer Angel (University of British Columbia), Christina Goldschmidt (University of Oxford, United Kingdom), Asaf Nachmias (University of British Columbia and Tel Aviv University, Israel), Steffen Rohde (University of Washington, USA)

27.1 Overview of the subject

STATISTICAL PHYSICS IN TWO DIMENSIONS

Statistical physics in two dimensions has been one of the hottest areas of probability in recent years. The introduction of Schramm's SLE and further developments by Lawler, Schramm and Werner on the one hand, and the application of discrete complex analysis, as pioneered by Smirnov, on the other, have led to several breakthroughs and to the resolution of a number of long-standing conjectures. These include the conformally invariant scaling limits of critical percolation and Ising models, and the determination of non-intersection and other critical exponents and dimensions of sets associated with planar Brownian motion (such as the frontier and the set of cut points). It is manifest that much progress will follow, possibly including the treatment of self-avoiding walks, the $O(n)$ loop model and the Potts model. While the bulk of this body of work applies to specific lattices, there are many fascinating problems in extending results to more general planar graphs.

One natural next step is to study the classical models of statistical physics in the context of random planar maps. There are deep conjectured connections between the behaviour of the models in the random setting versus the Euclidean setting, most significantly the KPZ formula of Knizhnik, Polyakov and Zamolodchikov from conformal field theory. This formula relates the dimensions of certain sets in Euclidean geometry to the dimensions of corresponding sets in the random geometry. Establishing this connection rigorously may provide a systematic way to analyze models on the two dimensional Euclidean lattice: first study the model in the random geometry setting, where the Markovian properties of the underlying space make the model tractable; then use the KPZ formula to translate the critical exponents from the random setting to the Euclidean one. Several models, notably the self avoiding walk and the $O(n)$ model are much easier to analyze in the setting of random geometry. As mentioned before, much of this picture is conjectural. However, with our rapidly growing understanding of the structure of random planar maps and discrete complex analysis, there is hope of making progress in this direction.

Random maps

Random planar maps is a widely studied topic at the intersection of probability, combinatorics and statistical physics. There are many natural classes of finite planar maps from which one can draw a random element: triangulations or p-angulations, maps of more general face size, maps of higher genus, and even the set of all planar graphs on n vertices. As in the case of random walks, where the large scale behaviour is invariant to the microscopic properties of the walk (it converges to Brownian motion), it is expected that random planar maps exhibit a similar universality (with the exception of random trees, which lie in a different universality class: see the last section of this proposal).

Let us consider a concrete example. Fix $p \geq 3$, and let T_n be a random p-angulation of the sphere $\mathbb{S}^2$, chosen uniformly among such all p-angulations with n vertices (considered up to orientation-preserving homeomorphism). In the recent culmination of a series of papers, Le Gall and (independently) Miermont show that when $p = 3$ or when $p \geq 4$ is even, the random graph metric of T_n scaled by $n^{-1/4}$ converges (in the Gromov–Hausdorff sense) to a random compact metric space homeomorphic to the sphere. This limiting metric has been termed the Brownian Map.

A second approach to the investigation of random maps is to study the unscaled or "infinite volume" limit of random maps. One such limit, known as the uniform infinite planar triangulation (UIPT), was shown to exist by Angel and Schramm, and is obtained by taking the local limit of uniform random finite triangulations; other models of maps possess similar limits. The research in this area is focused on almost sure geometric properties of the limiting object: it is an invariant, planar, recurrent, and polynomially growing graph (the volume growth exponent is 4), with a very fractal geometry. In particular, the random walk on it exhibits anomalous diffusion. Many questions about the UIPT and its (unfortunately named) counterpart, the stochastic hyperbolic infinite triangulation, remain open; for example, the speed of the random walk on the UIPT is conjectured to be $n^{1/4}$.

All the research described above is concerned with the graph distance of random maps. However, planar maps can also be viewed as manifolds and, as such, are endowed with a conformal structure. For example a triangulation gives rise to a Riemann surface by making each triangle equilateral. In particular, there are natural embeddings of these maps in the sphere or the plane, given by the Riemann uniformization of the conformal structure.

There are also discrete analogues of this embedding based on tools from discrete conformal geometry, and we can find embeddings using circle packings (see next section), rubber bands or square tilings. Understanding how these embeddings behave can shed light on many models of statistical physics on random planar maps. For instance, a concrete conjecture states that the empirical mass measure of the circle packing of a random triangulation on n vertices (that is, the measure giving each circle mass $1/n$) converges to Liouville quantum gravity, a continuous model of random surfaces developed by Duplantier and Sheffield. Proving this conjecture will advance us considerably towards the goals presented in the previous section.

Circle packing and random walks on planar graphs

An important tool in the study of planar maps is the theory of circle packing, which provides a canonical and conformally natural way to embed a planar graph into the plane. A circle packing is a collection of circles in the plane with disjoint interiors. The tangency graph of a circle packing is a planar graph in which the vertex set is the set of circles and two circles are neighbours if they are tangent in the packing. It is clear that the tangency graph is planar. Conversely, the celebrated Koebe–Andreev–Thurston Circle Packing Theorem states that any finite planar graph can be realized as a tangency graph of a circle packing. Many extensions and generalizations of this theorem are known.

This beautiful theory has a wide range of applications, in combinatorics, computer science, differential geometry, geometric analysis, and complex analysis as well as discrete probability. In particular, circle packings have been indispensable for the analysis of random walks on planar graphs.

An example that highlights the connection to probability is a seminal theorem of He and Schramm which states that a bounded degree infinite triangulation is transient if and only if it can be circle packed in a bounded domain. This bounded circle packing gives rise to a natural definition of a geometric "boundary" of a transient planar graph. A natural problem is to understand the relation between this and other notions of boundary, such as the Poisson and Martin boundaries. A deep result in this area is that the Poisson boundary contains the geometric boundary. In the context of (continuous) manifolds, these questions have been central in geometric analysis, since the work of Yau, and are very difficult. The additional assumption of planarity provides us with a rich set of ideas and tools.

RANDOM TREES AND CRITICAL PERCOLATION

Random trees have a long and illustrious history in the combinatorics literature. However, work on their scaling limits is a much more recent development which was initiated in a sequence of seminal papers by Aldous. The prototypical result is that the random graph metric obtained from drawing a random uniform tree from the set of n^{n-1} rooted trees on n labelled vertices converges (again, in the Gromov–Hausdorff sense), when rescaled by $n^{-1/2}$, to a random compact metric space. This is the so-called Brownian continuum random tree (BCRT).

This topic is more mature than the topic of random planar maps and the universality phenomenon for random trees is much better understood. In particular, the BCRT is known to be the limit for a large class of random trees: critical Galton–Watson trees whose offspring distributions have finite variance, unordered binary trees, uniform unordered trees, critical multitype Galton–Watson trees and many others. Moreover, the techniques used to prove convergence to the BCRT have also been adapted to give new limits each having its own domain of attraction: the stable trees (the scaling limits of critical Galton–Watson trees whose offspring distribution are in the domain of attraction of a stable law of index in $(1, 2)$), Lévy trees, fragmentation trees (which are the scaling limits of the so-called Markov branching trees) and the minimum spanning tree of the complete graph.

The BCRT is now recognized as central to the scaling limits of many discrete and highly varied objects. For example, the scaling limit of critical Erdős–Rényi random graphs, has been shown by Addario-Berry, Broutin and Goldschmidt to be composed of a number of rescaled BCRT's glued together. Excitingly, there is evidence that this limiting object is a universal limit for a wide variety of models including random graphs with a fixed degree sequence, percolation on random regular graphs, critical percolation on high-dimensional tori and on the hypercube, the critical vacant set left by random walk on a random regular graph, and the SIR epidemic model. The Brownian map discussed above is also defined as a certain quotient of the BCRT. This fruitful and expanding area of study should yield interesting developments for many years to come.

27.2 Overview of the workshop

During the week of the workshop we heard many superb lectures on the topics above, we also had two spontaneous simulation sessions (where participants demonstrated some computer simulations) and a comprehensive problem session. All this stimulated much work and many discussions. What follows is a summary of some of the substantial open problems that were presented during the workshop. Feedback from participants was enthusiastic. For example, Yuval Peres wrote:

> This was a superb and very timely workshop. Great progress is being made in this area, where several strands of thought (Mathematical Models of quantum gravity, circle packings, planar maps and random walks) are showing deeper connections than ever before. The excitement was tangible during many of the talks.
>
> This will certainly have a long term effect on my research, and I am sure this holds for most of the participants.

27.3 Overview of some of the open problems arising from or presented at the workshop.

As noted, a large number of open problems were presented, sparking discussions among participants.

MACROSCOPIC CIRCLES IN THE CIRCLE PACKING OF THE UIPT?
Ori Gurel-Gurevich

Consider the circle packing of the UIPT. It is a circle packing covering the plane without accumulation points (since the UIPT is one-ended almost surely). Normalize so that the circle of the origin ρ of the UIPT is centred at the origin and of radius 1. A circle in this packing is called **macroscopic** if its radius is comparable to its distance from the origin.

Question 27.3.1 *Is it true that almost surely there are only finitely many macroscopic circles?*

A positive answer would enable us to gain much progress towards further rigorous understanding of the KPZ correspondence and other various properties of the SRW on the UIPT (in particular, this would imply that the distance exponent is $1/4$).

BOUNDARY OF THE UIHPT
Nicolas Curien

Consider the uniform infinite half-planar triangulation (with root-edge in the boundary). Consider the uniformization of the map (i.e. view it as a Riemann surface by putting the metric of an equilateral triangle inside each face) with the root-edge mapped to the interval $[0, 1]$. Now focus on the boundary, and rescale it in such a way that the first n edges counted to the right of 0 are mapped onto $[0, 1]$. Put mass $1/n$ at every vertex in the boundary. This yields a random measure μ_n on $\mathbb{R}$ such that $\mu_n((0, 1]) = 1$. It is conjectured that, in the limit, $\mu_n \to \mu$, where μ is the exponential of a GFF plus a log-singularity (see Sheffield (2010)).

Independently of μ, sample an SLE$_6$ process $(\gamma_t)_{t\geq 0}$ in the upper half-plane and let $T = \{t \in \mathbb{R}_+ : \gamma_t \in \mathbb{R}\}$. Consider $(t; \gamma_t; \mu([0, \gamma_t]))_{t\in T}$, up to time-reparametrization (taking as a convention that $\mu([0, -2]) = -\mu([-2, 0])$). Under the $(\star)$ assumption of Curien (2014), any subsequential limit μ will satisfy

$$(t; \mu([0, \gamma_t]))_{t\in T} \overset{\text{(d)}}{=} \left(t; \begin{cases} S_t^+ & \text{if } t \in \tau^+ \\ -S_t^- & \text{if } t \in \tau^- \end{cases} \right)_{t\in\tau^+\cup\tau^-} \tag{27.3.1}$$

(up to time-reparametrization), where S^+ and S^- are independent $(3/2)$-stable processes with only negative jumps, τ^+ is the set of record times of new minima for S^+ and τ^- is the set of record times of new minima for S^-.

Question 27.3.2 *Does the law of the LHS of (27.3.1) characterize the law of μ?*

This is of interest because, by results of Duplantier, Miller and Sheffield (2014), it is known that if instead of μ we take a GFF with the correct log-singularity, its law is indeed characterized by the corresponding quantity. If the answer to the question is in the affirmative, and the (currently unproven) $(\star)$ condition holds, then this would prove the conjecture that μ is the exponential of a GFF plus the log-singularity.

A similar conjecture exists in the upper half-plane.

A somewhat weaker version for SLE specialists: suppose you are given a random variable X (of unknown law) and, independently, sample an SLE_6 in a box of height 1 and width X, started from the top-left-hand corner. Let N_X be the number of crossings of the SLE between the top and bottom of the box.

Question 27.3.3 *Given the law of N_X, can one recover the law of X?*

k-DEPENDENT COLOURINGS
Omer Angel

Recently Holroyd and Liggett resolved a problem that fascinated many people for some years, by showing that there is a stationary, proper 4-colouring of $\mathcal{Z}$, which is 1-dependent (i.e. for any two sets $S, T \subset \mathcal{Z}$ with $d(S,T) > 1$, the colours in S are independent of the colours in T. Holroyd and Liggett also find 2-dependent 3-colouring of $\mathcal{Z}$, and 1-dependent q-colouring of $\mathcal{Z}^d$ for some q. In particular, these constructions provide new and more natural examples of processes which are k-dependent but not a block factor of i.i.d. variables. Many questions remain open around these strange colourings.

Question 27.3.4 *What is the minimal number q of colours so that a k-dependent q-colouring of $\mathcal{Z}^d$ exists?*

Question 27.3.5 *Is there a q-dependent k-colouring of the d-regular tree, for some q, k?*

THE GINIBRE ENSEMBLE AND THE GFF
Nathanaël Berestycki

Consider the Ginibre ensemble, that is an $n \times n$ random matrix in which all entries are independent complex Gaussians of mean zero and variance $1/n$. Let p_n be the characteristic polynomial and let $h_n(z) = \log|p_n(z)| - \mathbb{E}[\log|p_n(z)|]$. A theorem of Rider and Virág (2007) states that $h_n \to h$ weakly as $n \to \infty$, where h is a planar Gaussian free field conditioned to be harmonic outside the unit disk.

Question 27.3.6 *Is it true that a rescaled version of $|p_n(z)|$, viewed as a measure, converges to e^h, a Liouville quantum gravity measure? Is this related or not to the enumeration of planar maps via matrix integrals?*

LIOUVILLE BROWNIAN MOTION
Nathanaël Berestycki

Take $(B_t, t \geq 0)$ a Brownian motion in a domain $D \subseteq \mathbb{R}^2$, h an independent Gaussian free field on D and h_ε a suitably mollified version thereof. Let $\gamma > 0$ and consider the limit time change

$$\phi(t) = \lim_{\varepsilon \to 0} \varepsilon^{\gamma^2/2} \int_0^t e^{\gamma h_\varepsilon(B_s)} \mathrm{d}s.$$

Consider the Liouville Brownian motion, $Z_t = B_{\phi^{-1}(t)}$ and its first exit time from the ball of radius 1 around the origin,

$$\tau = \inf\{t : Z_t \notin B(0,1)\}.$$

Question 27.3.7 *What is the behaviour of $\mathbb{P}(\tau > t)$ as $t \to \infty$ (in the annealed setting, so that we average over the GFF as well as the law of the Brownian motion)?*

It is known that $\mathbb{E}[\tau^q] < \infty$ if and only if $q < 4/\gamma^2$; we would like to be able to say that

$$\mathbb{P}(\tau > t) \sim Ct^{-\frac{4}{\gamma^2}} \text{ as } t \to \infty.$$

Observe that if $\tau_{\text{BM}} = \inf\{t : B_t \notin B(0,1)\}$ then

$$\tau = \lim_{\varepsilon \to 0} \varepsilon^{\gamma^2/2} \int_0^{\tau_{\text{BM}}} e^{\gamma h_\varepsilon(B_s)} \mathrm{d}s.$$

Question 27.3.8 *If μ_γ is the Liouville quantum gravity measure, is τ comparable to $\mu_\gamma(B(0,1))$?*

A fact due to Barral and Jin is that $\mathbb{P}(\mu_\gamma(B(0,1)) > t) \sim Ct^{-\frac{4}{\gamma^2}}$, but their ingenious proof does not seem easily replicable.

EDGE-FLIPS IN A TRIANGULATION
Ken Stephenson

The edge flip dynamics on triangulations of size n chooses each edge at rate 1, and (if possible) removes it and adds the other diagonal of the resulting quadrangle. Little is known about this Markov chain.

Question 27.3.9 *What is the mixing time of this Markov chain as a function of n?*

The speaker demonstrated using his CirclePack software and issued a general invitation to study edge-flips in triangulations.

SURPRISE PROBABILITIES IN LAZY SRW ON FINITE GRAPHS
Yuval Peres

Consider a lazy simple random walk on a finite graph on n vertices and let τ_y be the hitting time of a vertex y. What is the best possible upper bound for the "surprise probabilities" $P_x(\tau_y = t)$ in terms of n and t? It can be shown that in any Markov chain

$$P_x(\tau_y = t) \leq \frac{n}{t}.$$

Norris, Peres and Zhai proved that for the lazy random walk one has

$$P_x(\tau_y = t) \leq \frac{4e \log n}{t}.$$

Question 27.3.10 *Can one prove $P_x(\tau_y = t) \leq \frac{C\sqrt{\log n}}{t}$ for general MArkov chains?*

There is a construction where this is sharp.

In a similar spirit, let $p^*(x,y) = \max_t p^t(x,y)$ for the lazy SRW on a graph. It is known (Norris, Peres and Zhai) that

$$\sum_y p^*(x,y) \leq C \log n.$$

This is sharp as seen by taking the path of length n. Is following strengthening true:

Question 27.3.11 *Is it true that for any Markov chain*

$$\sum_y \sum_t |p^{t+1}(x,y) - p^t(x,y)| \leq C \log n\,?$$

POSITIVE SPEED IN UNIMODULAR NON-AMENABLE GRAPHS?
Tom Hutchcroft

It is well known that on any non-amenable graph with bounded degrees the speed of the simple random walk is positive (with respect to the graph distance). This statement fails without the requirement of bounded degree: take the graph of $\mathbb{N}$, add 2^n edges between vertices n and $n+1$ and a single edge between n and $2n$. In this example the SRW after T steps will be roughly at vertex T, but the graph distance from the origin is of order $\log T$.

Question 27.3.12 *Let (G, ρ) be a unimodular or a stationary random graph that is a.s. non-amenable, does the simple random walk have positive speed?*

Another related question was asked during this presentation by Yuval Peres:

Question 27.3.13 *If (G, ρ) is a unimodular (or a stationary) random graph that is almost surely recurrent, is it true that two independent random walkers collide infinitely often? That is, the number of n's such that $X_n = Y_n$ is infinite.*

There are examples of recurrent graphs where this does not hold, but they are very far from stationary (e.g. the 2 dimensional comb graph, see Peres and Krishnapur).

SQUARINGS OF A SQUARE
Louigi Addario-Berry

A squaring of a rectangle is a tiling of a rectangle by squares: in other words, the squares have disjoint interiors and their union is the entire rectangle. For concreteness, consider rectangles of height 1 whose lower-left corner is at the origin in $\mathbb{R}^2$. Write s_n for the number of squarings using exactly n squares. How does s_n grow as n becomes large? This basic enumerative question remains unanswered and, perhaps surprisingly, almost unstudied.

Say that a squaring of a rectangle is perfect if it contains no non-trivial sub-squaring of a rectangle (each single square is a trivial sub-squaring). Write r_n for the number of perfect squarings with n squares. Tutte (1963) conjectures that

$$r_n = (1 + o(1)) \frac{4^n}{243\pi^{1/2} n^{5/2}};$$

establishing this would likely be a useful step towards finding asymptotics for s_n, and would be interesting in its own right. The conjecture for the growth of p_n is based on a classic construction of Brooks, Smith, Stone and Tutte (1940), which builds perfect squarings of rectangles from 3-connected planar graphs. The construction is neither invertible nor size-preserving, but if it is "almost invertible" and "almost always size-preserving" then the number of planar maps and the number of perfect squarings should be asymptotically equal.

The construction mentioned above works as follows. Let G be a 3-connected planar graph, and fix an oriented edge st of G. View G as an electrical network in which each edge is a unit resistor. Remove edge st, put potential 1 at s and ground at t. The squaring corresponding to G is constructed by creating a square s_e for each edge e of G; the side length of s_e is precisely the current flowing through e in the electrical network. The horizontal and vertical positions of the squares are determined (uniquely) by using Kirchoff's laws: the vertical position of the top s_e is given by the higher-potential endpoint of e. Horizontal positions are determined similarly, using the planar dual G^* of G.

In the above construction, a square s_e may degenerate to a point if no current flows along edge e in the network. This is the reason that the construction is not bijective and is not always size-preserving (there may be fewer squares in the squaring than there are edges in $G - st$). As a step towards solving the above enumerative questions, one might therefore study the following. Let (G, st) be a uniformly random 3-connected planar graph with n edges, together with an oriented edge of G. Viewed as an electrical network, what the probability p_n that some edge of G has zero current? In particular, does $p_n \to 0$ as $n \to \infty$?

GREEN FUNCTION OF RWS WITH MEMORY
Remco van der Hofstad

Let $p_n(x)$ denote the number of n-step SRW on Z^d from the origin to x and let $G_z(x) = \sum_{n\geq 0} z^n p_n(x)$. The critical point is $z_c = 1/(2d)$. Let $b_n(x)$ denote the number of n-step non-backtracking walks from the origin to $x \in \mathcal{Z}^d$ and denote the Green function $B_z(x) = \sum_{n\geq 0} z^n b_n(x)$. The critical point is $z_c = 1/(2d-1)$. These two functions satisfy an interesting relation:

$$B_z(x) = \frac{1-z^2}{1+(2d-1)z^2} G_{\frac{z}{1+(2d-1)z^2}}(x)\,.$$

Now consider walks of memory 2 (i.e., they are not allowed to close a square) and let $m_n(x)$ be the number of such walks of length n and $M_z(x) = \sum_{n\geq 0} z^n m_n(x)$.

Question 27.3.14 *What is the critical point of M_z? Is there a nice formula relating M_z, B_z and G_z?*

REMOVING SYMMETRY ASSUMPTION IN PERCOLATION
Vincent Tassion

Many methods in the study of percolation depend on symmetries of the underlying graph, even where the result should hold for more general graphs. We would like to ave methods to study percolation that are less reliant on such symmetries.

As an example, consider percolation on $\mathcal{Z} \times \mathbb{N}$, for some parameter p, and consider the events A_+, A_- that $(0, n)$ is connected respectively to the right and left halves of the boundary. By symmetry, $\mathbb{P}(A_+) = \mathbb{P}(A_-)$.

If we add a generator $(1, 1)$, then the graph becomes the triangular lattice. There is a simple argument to show that $\mathbb{P}(A_-) \geq \mathbb{P}(A_+)$, and this is based on symmetry of the triangular lattice.

Question 27.3.15 *Is it true that $\mathbb{P}(A_+) \leq \mathbb{P}(A_-)$ if we take the generator set $(1, 0), (0, 1)$ and some additional (x_i, y_i) with $x_i, y_i \geq 0$?*

Intuitively, adding such diagonal edges helps connectivity in the corresponding direction.

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Chapter 28

Multiscale Models of Crystal Defects (14w5069)

September 21 - 26, 2014

Organizer(s): Mitchell Luskin (Minnesota), Christoph Ortner (Warwick), Florian Theil (Warwick)

28.1 Overview of the Field

The mathematical theory of solid mechanics has traditionally focused on the models of continuum mechanics, which is in stark contrast to the vast scientific literature employing atomistic models, particularly in the physics and materials science communities, to study material behavior. Only the past few years have seen the beginning of an effort to establish the mathematical foundations of atomistic models of solids, including the foundations of numerical algorithms and the connections to coarse-grained descriptions (e.g., continuum models).

Crystal defects play an important role in determining material parameters. For example, dislocations are the origin of plasticity; inclusions and other types of defects can "pin" dislocations, and cause hardening. The modeling of crystal defects is a broad scientific field that spans many spatial and temporal scales, from quantum mechanical models of nuclei to effective continuum theories of plasticity; and many disciplines, including mathematical modeling, mechanics, and scientific computation. For this workshop we focused on the interplay between the discrete structure of defect cores and the elastic fields through which they interact with their environment, and the roles of mathematical analysis and numerical computations.

Over the past decade there has been increasing interest in the mathematical analysis community on atomistic multi-scale methods, starting from atomistic descriptions of materials. The focus of this research effort has been the rigorous derivation of effective continuum models from atomistic models. Some of the main achievements in this area include proofs of crystallization, rigorous understanding of the Cauchy–Born approximation, and rigorous asymptotic results on effective dislocation models.

In the numerical analysis community there has recently been much interest in the development and analysis of atomistic-to-continuum coupling methods. These are a class of numerical coarse-graining techniques used for the efficient atomistic simulation of material defects in large computational cells. There exists a wide range of techniques in this class, and the effort of numerical analysts has led to a clear picture of the key approximations made, the reliability of the various approaches, and the challenges that remain to be overcome.

Much of the rigorous analytical work has focused on the derivation of continuum elasticity from atomistic models. Even when defects are considered, the need for a detailed understanding of the discrete core structure is usually circumvented by making simplifying assumptions on the models. The stated aim of this workshop was to fill this gap and to begin a systematic study of the atomistic structure of crystal defects, by providing a platform for close interaction between engineering and materials science, numerical simulation, and mathematical analysis.

28.2 Recent Developments and Open Problems

The modelling and simulation of crystalline defects is a broad field. Here, we focus on some concrete areas of current activity in the mathematics community as well as scientific numerical methodologies. Yet, the techniques of numerical analysis are ideally suited to identifying the main sources of errors in such numerical simulations, thus identifying bottlenecks on where to focus new developments.

28.2.1 Numerical analysis of multi-scale methods

Atomistic and multi-scale simulation are indispensable components of modern materials science research, as is evidenced by the award of the 2013 Nobel Prize in Chemistry for the development of such simulation techniques. Until very recently there has been next to no mathematical foundation underpinning these techniques.

While there were a few earlier contributions, the numerical analysis theory of multi-scale methods began in earnest around 2008 with a number of papers appearing at the same time, from different groups. The focus has been on developing a rigorous theory of atomistic-to-continuum coupling methods, a paradigm case of a multi-scale scheme. Briefly, the idea is that a crystalline region containing a defects (or multiple defects) is modelled atomistically, while the surrounding crystalline bulk is treated by a continuum model. The key component in such a simulation is the "handshake" mechanism, the biggest difficulty being the transition from a non-local (atomistic) to a local (continuum) model. Such methods have been under development in the computational science community since the early 80's.

The numerical analysis theory has made some remarkable achievements: separation of the different sources of error (far-field boundary condition, continuum model, coarse-graining, and coupling) and characterisation and benchmarking of the different coupling mechanisms, identification of "universally stable" coupling mechanisms. All this has been achieved within a rigorous mathematical context. Further, the theoretical results have led to highly optimised formulations and prototype implementations with quasi-optimal convergence rates. See [1, 2] and references therein.

While challenging open problems remain in the field of zero-temperature atomistic/continuum coupling, much of the attention has recently turned towards two new frontiers: coarse-graining at finite temperature (see § 28.2.2) and coupling between quantum mechanics and molecular mechanics. The significant difficulty in the latter is that quantum mechanics is an inherently long-ranged theory which makes the non-local to local transition particularly challenging.

28.2.2 Coarse-graining of materials at finite temperature

While the extraction of continuum theories from deterministic discrete models is conceptually clear thanks to tools such as the Cauchy-Born rule the connection between the corresponding finite temperature systems and the continuum limits is less obvious. Finite temperature versions of standard tools such as the Cauchy-Born rule or stability are still in the process of development. As a result, many fundamental question are still awaiting mathematical treatment. Examples include the existence for solid phases at finite temperature, theoretical prediction of aging rates, and characterisation of thermodynamic parameters such as heat conductivity in terms of atomistic properties.

Current efforts concentrate mainly on static problems, key challenges are the characterization of nucleation energies and properties of the solid phases. Recent progress has been the result of the introduction of multiscale methods such as renormalisation groups, finite-range decompositions. Most results are of perturbative nature, e.g. the characterisation of elastic moduli.

The theoretical research efforts are complemented by the challenge to design efficient simulation strategies for materials at finite temperature. Key ideas in this direction are the quasi-continuum method which has been originally designed in the context of minimum energy problems. Recent ideas by Tadmor, Luskin, Perez,and Voter lead to generalisations of the methods so that finite-temperature cases can be simulated as well. This progress is the result of a careful localisation of the partition function. See, e.g., [6, 7] for early references in this field.

A relatively recent development is the idea to supplement the standard approach of deriving effective equations of motion based on theoretical analysis with methods from Machine Learning. Here the complex model responses are treated probabilistically in the sense that one tries to automatise the construction of statistical models which predict the model responses.

28.2.3 Rigorous mathematical theory of dislocations

The characterisation of plastic material flow in terms of the microscopic material models is one of the holy grails in Material Science. The key step is the characterisation of the density and mobility of dislocations. Macroscopic laws like plastic harding are closely linked to dislocation mobility, which depends heavily on entanglement of the dislocation. Even a phenomenological statistical description is not available.

It is noteworthy that any discussion of dislocation structures is hampered by the presence of many length-scales. The first scale is given by the atomic structure of the core, and the energy contributions resulting from geometric properties such as curvature and climb. The second scale emerges from the spatial distribution of the dislocations, e.g. in the form of walls or networks. A third scale is introduced by the fact that plastic deformation itself will introduce internal structure. Well-known examples of this effect are elasto-plastic microstructures and strain-gradient plasticity.

The application of variational methods has recently lead to significant progress for static problems. It has been shown that (simple) dislocations can be interpreted as critical points in atomistic models for crystals [3]. This opens the possibility to characterize the strength of the pinning forces in terms of the depth and the geometry of the local energy well.

A related problem is the structure of dislocation walls (pile-ups) near grain boundaries, which is strongly influenced by the properties of the boundary, the interaction strength between the dislocations and the temperature. Progress has been achieved by several independent groups who managed to characterise the main patterns which are experimentally observed in terms of the scaling properties of the ground state energies.

Recently, much attention has been focussed on the study the microscopic evolution of dislocations. It would be highly desirable to derive standard macroscopic (rate-independent) evolution equation from discrete dislocation dynamics.

28.2.4 Simulation and Sampling with Molecular Dynamics

Molecular dynamics (MD) offers a robust and clear methodology for exploring a variety of physical systems at, for example, constant energy or temperature. MD models can retain full atomistic detail or be coarse grained. Up to the choice of physical approximations, their simulation output can be interpreted as, next to a laboratory experiment, the gold standard against which other methods should be compared. MD simulations allow practitioners to see how individual realizations of the system evolve and respond to thermal fluctuations and external forcing, and to sample equilibrium distributions, allowing for the computation of thermodynamic quantities. Important thermodynamic quantities include reaction rates for both defect migration in crystalline structures and changes of conformations in molecules.

Though simple to implement, the computational cost of MD often renders it impractical for either exploring the evolution of the system or computing thermodynamic quantities. Physical systems are often ripe with metastable regions in configuration space. When the system enters such a region, it may take a relatively long time to exit it, only to enter some other metastable region. For comparison, the typical time step in an MD simulation is that of a femtosecond, but the escape from a metastable region could be as much as a nanosecond. At the same time, interesting physical changes in the system might require transitions through many such metastable states, with time scales of microseconds or longer. For computing thermodynamic quantities, many such metastable regions must be visited to accurately sample the equilibrium distribution.

Over the years, there has been significant effort to develop approximations and algorithms that overcome metastability. One of the most celebrated such approximations is Transition State Theory (TST), which is robust in the case that the temperature of the system is sufficiently low and/or the energy barriers between states is sufficiently high. Using harmonic approximations, TST allows for the estimation of reaction rates amongst metastable regions which can form the basis of a kinetic Monte Carlo (KMC) model. However, not all systems have adequate scale separation for the harmonic approximation to hold, putting limitations on its applicability. Additionally, KMC models, based on TST, cannot capture correlated events in an atomistic system, such as the rapid transition over multiple energy barriers due to inertia.

A variety of other algorithms have appeared in the last two decades, including accelerated molecular dynamics, Wang-Landau sampling, nested sampling, adaptive KMC, Markov state models, and milestoning, which aim to improve upon TST. These methods are the result of decades of experience by MD practitioners and their physical intuition, along with some of the ideas that originate in TST. While these have allowed users to explorer larger systems, on longer time scales, the grand challenge remains simulating high dimensional systems over extended (laboratory) time scales.

Recently, an effort emerged on the part of mathematicians, particularly numerical analysts, applied probabalists, and scientific computing specialists, to build a rigorous, mathematical, foundation for coarse-grained dynamics and sampling schemes; see e.g. [4, 5].

28.3 Presentation Summaries

We had presentations on a wide range of topics related to the modelling, simulation and analysis of crystalline defects, with considerable overlap between speakers and topics:

- Numerical analysis of multiscale schemes: B. Vankoten, A. Shapeev, A. Binder, D. Trinkle, F. Legoll
- Models: G. Csanyi, P. Vorhees
- Temperature, free energy, Hot-QC:: A. Shapeev, D. Perez, P. Vorhees, C. Reina, F. Legoll
- Electronic structure aspects: E. Cances, F. Nazar, D. Trinkle, G. Csanyi
- Sampling, Stochastic homogenisation, variance reduction: G. Simpson, V. Ehrlacher, W. Minvielle, X. Blanc
- Analytical structure of defects: A. Garroni, F. Nazar, B. Vankoten, B. Schmidt, A. Binder
- Dislocation modelling: A. Garroni, C. Hall, D. Trinkle, P. Vorhees

We summarize all talks in alphabetical order:

Andrew Binder spoke about the Surface Cauchy-Born Method, an inexpensive multiscale technique for modelling surface effects. Surface effects can play a significant role in the determination of material properties on smaller scales. Despite the fact that surface effects are most influential in smaller systems, the systems may still be large enough that simulating the system atomistically will be computationally infeasible. The surface Cauchy-Born method was designed to efficiently model such systems and improve upon the regular Cauchy-Born method by better capturing surface effects. Binder showed the striking result that, while from a numerical analysis perspective, there is no reason to suspect improved accuracy of the SCB model, however, that there is a small physical parameter with respect to which the method does improve over classical Cauchy–Born.

Xavier Blanc spoke about elliptic problems in homogenization of periodic structure with defects. He presented an approach to approximate both at the coarse and fine scale the solution to an elliptic equation with oscillatory coefficients when this coefficient consists of a ”nice”, say periodic (the crystalline environment), function that is locally perturbed (the defect). The approach is based on computing a local defect profile given as the solution to an equation similar to the corrector equation in classical homogenization, but it is now posed in an infinite domain. The well-posedness of that equation were explored in various functional settings depending upon the locality of the perturbation, and decay estimates on the corrector were shown.

Eric Cances gave an introductory talk on electronic structure density functional theory for crystals with local defects. He started by presenting some simplified electronic structure models, Thomas-Fermi-Weizsäcker and reduced Hartree-Fock, as stepping stones towards the commonly employed Kohn-Sham density functional theory and the Hartree-Fock model, and surveyed the state of the art in their mathematical theory. He then presented analyses of situations with defects, both the case of a single defect and of a random distribution of local defects. For example a striking result is that the TFW model cannot model charged defects. Cances concluded by mentioning open problems in this field including, e.g., the treatement of dislocations, or random defects with Coulomb interaction.

Gabor Csanyi presented the construction of highly accurate interatomic potentials using machine learning techniques. The most significant difficulty in extending quantum mechanical simulation techniques to larger length and time scales is that all exact formulations of quantum mechanics are non-local. Indeed it seems that the fundamental difference between the simplest semi-empirical quantum mechanical model (e.g. Tight Binding) and the most complicated classical model (at least for insulators) is that the quantum model involves some global operation over the entire system, like diagonalizing the whole Hamiltonian. Great strides have been made in making this less and less painful, principally by taking advantage of the sparse nature of the Hamiltonian and the density matrix, which can be considered to be a form of weak locality of the quantum model. However, it has long been known (indeed universally assumed and implicitly taken advantage of), that in most systems, there is a much stronger locality, namely that the forces, trajectories and general properties of an atom are not very dependent on the configuration of atoms far away. This motivates the construction of “interatomic potentials”. These are mostly made by trial, error and guesswork. The GAP technique, which Csanyi presented, created interatomic potential automatically and rigourously using only the quantum mechanical data itself as input together with reasonable and universal assumptions about the smoothness and locality of the potential energy surface.

Virginie Ehrlacher discussed the approximation of effective coefficients in stochastic homogenization using a boundary integral approach. A very efficient algorithm has recently been introduced by Cances, et al. to approximate the solution of implicit solvation models for molecules. The main ingredient of this algorithm relies on the clever use of a boundary integral formulation of the problem to solve. In her talk, Ehrlacher presented how such an algorithm can be adapted in order to compute efficiently effective coefficients in stochastic homogenization for random media with spherical inclusions. To this end, she defined new approximate corrector problems and approximate effective coefficients and derived convergence results for this new formulation. Some numerical test cases illustrated the behaviour of this method.

Adriana Garroni gave an introduction to the mathematical analysis of dislocation models beginning from an atomistic description. She described an atomistic model for straight screw dislocations in different types of crystalline structure, for simplicity only treating anti-plane deformation. In this case the problem reduces to a two dimensional discrete model governed by a periodic potential. Garroni then study the asymptotic expansion of the energy of the system in the context of Γ-convergence as the lattice spacing tends to zero, where she identified the classical continuum elasticity model. Further, she then introduced a notion of effective gradient flow for the defects that account for the glide directions of the crystal.

Cameron Hall discussed formal asymptotic methods for connecting discrete models of dislocations with a continuum dislocation density model, focusing on the problem of dislocation pileup. A major challenge in multiscale modelling is to find the appropriate connections between the models that are relevant at different scales. This is especially difficult when trying to connect discrete models that track individual particles (whether they be atoms, discrete dislocations, or some other particle) with continuum models that deal with properties on a larger scale, such as deformation gradients and dislocation densities. Hall showed that a very effective way of approaching the problem of connecting these two scales is to use methods from classical asymptotics, such as the asymptotic approximation of sums using the Euler-Maclaurin summation formula, the method of multiple scales, and the method of matched asymptotics. In particular, he demonstrated how Euler-Maclaurin summation can be used to exploit regularity in the arrangement of particles to obtain the continuum model that is associated with a given discrete model. Then, he discussed how matched asymptotics can be used to analyse some cases where the assumptions required for Euler-Maclaurin summation break down, leading to discrete-scale boundary layer regions. From an applied perspective, these methods are useful because they demonstrate which physical interactions are important on which material scales, as well as giving a systematic framework for developing continuum models and canonical discrete models from a fundamentally discrete problem. From the perspective of mathematical analysis, these methods are also valuable because they give a way of finding ansatzes that can form the basis for establishing the convergence of energies via more rigorous methods.

Legoll, Frederic spoke about the calculation of defect formation (free) energy by a QCM-type approach. The formation free energy of defects is the difference between the free energy of an atomistic system with defects (computed in the canonical ensemble) and the free energy of the same system without any defects. This free energy difference, in the limit of asymptotically large systems, is a quantity of important practical interest, e.g., it determines the density of defects in the crystal. In practice, these quantities are difficult to compute as they require sampling extremely high-dimensional energy landscapes, and approximate models are normally employed. In this talk Legoll discuss the accuracy of a quasicontinuum type approach when computing these quantities.

William Minvielle spoke about variance reduction, via a control variate approach, for the homogenization of a random, linear elliptic second order partial differential equation set on a bounded domain in $\mathbb{R}^d$. The random diffusion coefficient matrix field $A(\frac{x}{\varepsilon}, \omega)$ is assumed to be uniformly elliptic, bounded and stationary ("periodic in law"). In the limit when $\varepsilon \to 0$, the solution of the equation converges to that of a homogenized problem of the same form, the coefficient field of which is a deterministic and constant matrix $A^\star$ given by an average involving the so-called corrector function that solves a random auxilliary problem set on the entire space. In practice, the corrector problem is approximated on a bounded domain Q_N as large as possible. A by-product of this truncation procedure is that the deterministic matrix $A^\star$ is approximated by a random, apparent homogenized matrix $A^\star_N(\omega)$. Minvielle therefore introduced a variance reduction approach to obtain practical approximations of $A^\star$ with a smaller variance in order to reduce the statistical error.

Faizan Nazar presented new results on locality of interaction in the Thomas-Fermi-von Weizsäcker electronic structure model. The TFW model is the paradigm example of an orbital-free density functional theory. The interaction between nuclei is obtained by solving a nonlinear PDE (eigenvalue problem) incorporating kinetic energy of the electron density and Coulomb interactions between electrons-electrons and electrons-nuclei. The model is inherently non-local; however, Nazar showed that the interaction between nuclei is always effectively local, i.e., it decays exponentially with distance between particles. He then applied this result to an analysis of crystalline defects in the TFW model.

Perez, Danny talked about the accuracy of kinetics in Coarse-Grained Molecular Dynamics. Multiscale methods that allow for a significant reduction of the number of dynamical degrees of freedom compared to conventional molecular dynamics are in principle ideally suited to simulate the long time dynamics of large systems. Indeed, the reduced computational cost associated with the integration of the equations of motion should enable the extension of the timescale horizon amenable to direct simulation. It is therefore important to assess the accuracy with which the long-time evolution is preserved upon coarse-graining. However, kinetics has of yet received much less attention than dynamics (e.g., wave reflection coefficients) or thermodynamics. In this talk, Perez showed how to quantify the error induced in Harmonic Transition State Theory (HTST) rates by the coarse-graining process. He then applied these results to the Coarse-Grained Molecular Dynamics (CGMD) formalism of Rudd and Broughton, providing both lower and upper bounds on the error on the HTST rates in terms of spectral characteristics of the atomistic and coarse-grained Hamiltonians and of the elastic response of the system. Within this framework he was able to identify and physically interpret the sources of error and present guidelines to determine the appropriate level of coarse-graining.

Celia Reina spoke about a self-consistent atomistic-phase field model for the study of Ge nanocrystallization. In her talk, Reine developed a new multiscale model for phase transformation in a heat bath at constant temperature. The model consists of a thermodynamically consistent phase field model that reproduces exactly the interface energetics and kinetics of atomistically computed crystallization fronts. As an additional feature, the interface thickness may be chosen arbitrarily large while preserving this exact atomistic-to-continuum coupling, in the case of flat interfaces. By extension this leads to controllable model errors in terms of interface curvature. This approach delivers a highly efficient multiscale computational model. As an application of this multiscale approach, Reina studied the interplay between nucleation and growth in the nano-crystallization of amorphous Ge. She demonstrated simple scaling laws between the mean radius of crystallized Ge grains, the nucleation rate and the time of crystallization.

Bernd Schmidt spoke about the passage from atomistic models to continuum theory in a crystal cleavage context. In his talk, Schmidt discussed the behavior of atomistic models in general dimensions under uniaxial tension and investigated the system for critical fracture loads. He demonstrated a rigorous proof that in the discrete-to-continuum limit the minimal energy satisfies a particular cleavage law with quadratic response to small boundary displacements followed by a sharp constant cut-off beyond some critical value, a behaviour that had been conjectured (with some controversy), but only now rigorously proven. Moreover, Schmidt showed that the minimal energy is attained by homogeneous elastic configurations in the subcritical case and that beyond critical loading cleavage along specific crystallographic hyperplanes is energetically favorable. For some simplified situations he was also able to provide a complete characterization of the energy minimizing configurations

Simpson, Gideon described a relative entropy preconditioner for Markov chain Monte Carlo simulations. One of the challenges in using Markov Chain Monte Carlo methods to sample from a target distribution, such as the distribution of trajectories in a molecular dynamics problem, is finding a good proposal distribution. An ideal prior distribution would both be easy to sample from and have a high acceptance rate in the Metropolis step of the algorithm. This latter property ensures that the Markov chain will rapidly explore the configuration space under the target distribution. In this talk, Simpson presented work on functionalized Gaussian priors which are preconditioned to minimize the distance, with respect to relative entropy, to the target measure and showed exciting applications to path sampling.

Alexander Shapeev presented his recent ideas on evaluating the accuracy of (coarse-grained) defect calculations at finite temperature. While the analysis of accuracy for the calculation of crystalline defects at zero temperature has recently seen rapid development and major milestones, the corresponding finite temperature theory is wide open. In this talk, Shapeev presented a new and potentially fruitful approach to this issue. In order to continue to employ largely analytical (as opposed to probabilistic) methods he proposed to estimate the error of a coarse-grained calculation relative to an exact calculation by expanding both in termperature to arbitrary order. The errors in the expansion coefficents would then yield information on the coarse-graining error. He demostrated this principle on a non-trivial 1D example.

Dallas Trinkle discussed lattice Green function methods for electronic structure calculations in the presence of a dislocation. Flexible boundary condition for dislocations in bulk and in boundaries rely on accurate computation of the lattice Green function (LGF) from first-principles data. Previously, the lattice Green function for a perfect crystal was calculated directly from the bulk force constants, and applied to the relaxation of dislocations. However, that relies on the perfect LGF as an approximation to the LGF for the dislocation; even absent changes in the local force constants between atoms, a dislocation introduces a topological change in the connectivity of atoms (corresponding to a Burgers circuit). Trinkle showed a new numerical approach that accounts for the topology change of a dislocation, and estimated the error in previous calculations from the perfect LGF. He also discussed open or ill-understood issues connected to Green's functions for edge dislocations and challenges in obtaining optimal rates of convergence.

Brian Van Koten presented an error analysis of blended quasicontinuum methods for the simulation of defects at zero temperature. The BQC method is an atomistic/continuum coupling designed to simulate crystallographic defects. Van Koten presented an error analysis of the method valid for point defects in 2D or 3D crystals and also for straight screw dislocations. He showed a unique (in this field) "universal stability" result, that as long as the defect is stable in the atomistic model, BQC can simulate the defect accurately.

Peter Vorhees (Northwestern) spoke about the phase field crystal model, with particular applications to low-angle grain boundaries. Phase field crystal (PFC) models have been used to describe a wide range of phenomena from grain growth to solidification and dislocation motion in crystals. The strength of the method lies in its ability to follow the atomic scale motion over diffusive timescales. Peter Vorhees examined the evolution of the dislocation structure of a grain boundary and the local atomic displacements of atoms near the boundary during grain growth. He showed that the atomic scale structure of the boundary gives rise to qualitatively new grain growth kinetics as well as both grain rotation and translation. The grain translation is a result of the climb, glide, and interactions of the dislocations that comprise the grain boundary.

28.4 Scientific Progress and Outcome of the Meeting

The purpose of the meeting was not to solve major open problems, but to grow a new community and find common ground for collaboration, in particular across disciplines and subdisciplines, as well as targets to meet over the coming years. In this respect it was felt to be a resounding success by all participants.

Below are a representative (strict) subset of new ideas and collaborations that arose during this workshop:

- The talk of Vorhees served to show-case the potential of phase-field models for crystals. Here the objective is to derive approximations of single-particle marginal distributions related to the random process of the atomic positions at finite temperature. Phase field crystals are obtained by approximating of those marginal distributions by semi-linear elliptic equations. Thanks to an extensive mathematical theory of semi-linear equations it is possible to simulate the phase-field equations efficiently and thereby study the emerging properties of the underlying materials. A proper mathematical understanding of the derivation, simplification and simulation of phase field equations is still in its infancy. It is certain that the study of those questions will influence future developments in applied analysis.

- Dallas Trinkle's talk inspired a discussion to generalise the numerical analysis of atomistic/continuum coupling to QM/MM coupling schemes. He showed how even for relatively simple static problems (computing the equilibrium state of a dislocation) constructing a highly accurate QM/MM scheme is non-trivial. A further question that arose is how to optimally distribute computational resources. Further discussion between Trinkle and other participants have led to new research projects, and potential for future collaboration.

- Gideon Simpson's talk demonstrated how, in the case of path sampling, some of the challenges of sampling high-dimensional configurations can be overcome. This led to a discussion with Gabor Csanyi and others, on how to incorporate these techniques into sampling configurations (rather than paths). The conclusion of this discussion is that the seemingly canonical approach will not achieve this, but that some interesting technical questions must first be answered. There are plans for further collaboration.

- Gabor Csanyi's talk on the construction of highly accurate interatomic site energies raised the open problem of how to treat long-range forces (Coulomb and related) in this context. A concrete suggestion of Shapeev has led to a collaboration with plans for future implementation.
- Eric Cances presented the state of the art in the mathematical analysis of electronic structure of defects. Among the open problems he mentioned in his talk is the treatement of dislocations. Faizan Nazar's talk show-cased an improvement of a technique that will likely lead to tackling this in the near future.
- Shapeev's talk on defects in 1D chains at finite temperature triggered a half-day discussion between Shapeev, Theil and Schmidt. The result of the discussion was the insight that transfer-operator methods are equivalent to harmonic approximations provided the relevant profiles are known in advance.
- A particular highlight of the workshop was the chance encounter between Theil and Arnold Neumaier who participated in the parallel meeting on rigorous verification. Thanks to the discussion it became clear that computer aided constraint satisfaction methods can play an important role to determine the structure of atomistic defects. It was agreed to study the double kissing problem (Maximal number of neighbors of two touching spheres) in order to establish the feasibility of the concept.
- Comments from three attendant PhD students:

  "As a result of my participation in the BIRS workshop, I have gained a greater understanding of the physical models used in electronic structure theory. In particular, I have learned how they may be used in the context of analyzing defects such as for determining the decay rate of the change in the electronic density functions due to the defect. Finally, I have gained a greater understanding of other defects that are examined in this research field and their interest to material scientists."

  "At BIRS, I learnt about current work on treating defects, including approaches using homogenisation theory, work on understanding surface effects and the current state of considering defects in crystals using Density Functional Theory, which is directly relevant to my area of research. I also had the opportunity to discuss my work and other related problems with the participants, which was very beneficial for me."

  "The Banff workshop was a great place for me to learn about recent advances in material science; I specifically enjoyed contributions from the atomistic perspective. I am also very grateful to the organizers to give me the opportunity to present my work. I was delighted to meet with the leading scientists in the field. As a young researcher this is a great occasion to build new collaborations."

Participants

Binder, Andrew (University of Minnesota)
Blanc, Xavier (Universit Paris Diderot)
Cances, Eric (Ecole des Ponts and INRIA)
Csanyi, Gabor (Cambridge)
Ehrlacher, Virginie (Ecole des Ponts - ParisTech and INRIA)
Garroni, Adriana (Universita‘ di Roma Sapienza)
Hall, Cameron (Oxford University)
Legoll, Frdric (Ecole Nationale des Ponts et Chaussees)
Luskin, Mitchell (University of Minnesota)
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Nazar, Faizan (University of Warwick)
Ortner, Christoph (University of Warwick)

Perez, Danny (Los Alamos National Laboratory)
Reina, Celia (University of Pennsylvania)
Schmidt, Bernd (Augsburg University)
Shapeev, Alexander (University of Minnesota)
Simpson, Gideon (Drexel University)
Theil, Florian (University of Warwick)
Trinkle, Dallas (University of Illinois)
Van Koten, Brian (University of Chicago)
Voorhees, Peter (Northwestern University)

Bibliography

[1] X. H. Li, C. Ortner, A. Shapeev and B. Van Koten. Analysis of blended atomistic/continuum hybrid methods. arXiv:1404.4878.

[2] M. Luskin and C. Ortner. Atomistic-to-continuum-coupling. Acta Numerica, 2013

[3] Roberto Alicandro, Lucia De Luca, Adriana Garroni, Marcello Ponsiglione. Metastability and Dynamics of Discrete Topological Singularities in Two Dimensions: A Γ-Convergence Approach. Arch. Ration. Mech. Anal. **214**, 2014.

[4] Tony Lelievre, Mathias Rousset, Gabriel Stoltz. Free Energy Computations — A Mathematical Perspective. Imperial College Press 2010.

[5] G. Simpson and M. Luskin. Numerical analysis of parallel replica dynamics. ESAIM: Math. Model. Numer. Anal. **47**, 2013.

[6] L. M. Dupuy, E. B. Tadmor, R. E. Miller, R. Phillips. Physical Review Letters, 2005.

[7] Woo Kyun Kim, Ellad Tadmor, Mitchell Luskin, Danny Perez, and Art Voter. Hyper-QC: An accelerated finite-temperature quasicontinuum method using hyperdynamics. Journal of the Mechanics and Physics of Solids **63**:94112, 2014.

Chapter 29

Rigorously Verified Computing for Infinite Dimensional Nonlinear Dynamics (14w5098)

September 21 - 26, 2014

Organizer(s): Jean-Philippe Lessard (Université Laval), Konstantin Mischaikow (Rutgers University), Siegfried Rump (Hamburg University of Technology), Jan Bouwe van den Berg (VU University Amsterdam), JF Williams (Simon Fraser University)

All participants contributed to this report:

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- Marcio Gameiro, University of São Paulo at São Carlos
- Chris Groothedde, VU University Amsterdam
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- Maxime Murray, Université Laval
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- Michael Plum, Karlsruhe Institute of Technology
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- Ray Sheombarsing, VU University Amsterdam
- Jan Bouwe van den Berg, VU University Amsterdam
- Thomas Wanner, George Mason University

- JF Williams, Simon Fraser University
- Piotr Zgliczynski, Jagiellonian University

29.1 Overview of the Field

Partial differential equations are at the core of the mathematical description of the world around us: from Schrödinger's equation in quantum mechanics to the Navier-Stokes equations in fluid dynamics, from the reaction-diffusion equations governing biochemistry to the Black-Scholes equation in mathematical finance.

The nonlinear nature of many of these equations makes their analysis challenging. Two complementary approaches are used to investigate such problems. On the one hand, one can exploit geometric and topological ideas to perform a global analysis. This provides robust qualitative information. Ideally this is coupled with numerical calculations, which offer detailed quantitative information and clear pictures of the solutions, but the information from the numerics is local (in parameter space) and non-rigorous.

Dramatic advances in algorithms, analysis, code, and computer speed and memory have opened the possibility of utilizing the power and robustness of topological and analytic methods to rigorously verify computational results. For questions related to nonlinear dynamics the most significant results, e.g. [1, 2], are associated with finite dimensional systems. Computer assisted proofs of the existence of low dimensional dynamical structures, e.g. fixed points, periodic orbits, heteroclinic and homoclinic orbits, can be used as building blocks in global analysis, either using gluing methods from dynamical systems theory or via Morse-Conley-Floer theory. In this way local, rigorously verified, numerical solutions form the seeds of information from which additional global understanding can be gained.

Moreover, encouraging first steps for infinite dimensional systems are starting to appear. In this workshop we explored the challenges that lie ahead in applying these techniques to fully fledged problems in the theory of infinite dimensional nonlinear dynamical systems, with a particular emphasis on nonlinear partial differential equations.

Rigorous verification goes far beyond an a posteriori analysis of numerical computations. In a nutshell, verification methods are mathematical theorems formulated in such a way that the assumptions can be rigorously verified on a computer. Indeed, it requires an a priori setup that allows analysis and numerics to go hand in hand: the choice of function spaces, the choice of the basis functions/elements and Galerkin projections, the analytic estimates, and the computational parameters must all work together to bound the errors due to approximation, rounding and truncation sufficiently tightly for the verification proof to go through. On top of that, for high and infinite dimensional problems additional aspects arise. On the analysis side, we need to deal with much subtler and more involved truncation estimates and, for connecting orbits, with high or infinite dimensional invariant manifolds. On the algorithm side, we must find suitable pre-conditioners and develop efficient interval-arithmetic based algorithms. Finally we need to understand how to tie these computational results to the geometric and topological ideas of global nonlinear analysis that form the framework for our understanding of nonlinear dynamics.

29.2 Presentations

We had presentations at the start of each morning and afternoon session (except for Wednesday afternoon, when we hiked up Sulphur Mountain).

1. Jean-Philippe Lessard, Rigorously verified computing for infinite dimensional nonlinear dynamics: a functional analytic approach
2. Siegfried Rump, Computer-assisted proofs using floating point arithmetic using the new INTLAB
3. Jay Mireles-James, Fixed point approach to rigorous validated computation of connecting orbits in infinite dimensions
4. Piotr Zgliczynski, Geometric methods in the integration of evolutionary problems in infinite dimension
5. Michael Plum, Computer-assisted existence and multiplicity proofs for semilinear elliptic boundary value problems

6. Christian Reinhardt, Rigorous numerics using Chebyshev series
   and
   Jacek Cyranka, Some results on global attractors of certain parabolic PDEs and a 2D convection-diffusion PDE

7. Arnold Neumaier, Rigorously covering all solutions of infinite-dimensional equations

Additionally, on Monday the PhD students introduced themselves in a sequence of short talks:

1. Ray Sheombarsing, Rigorous numerical methods for dynamical systems

2. Andréa Deschênes, Coexistence of hexagons and rolls

3. Jonathan Jaquette, Parametrizing Invariant Manifolds for Flows in Banach Spaces

4. Chris Groothedde, Rigorous numerics

5. Maxime Murray, The suspension bridge equation

6. Aleksander Czechowski, Periodic orbits of the FitzHugh-Nagumo equations — a computer assisted proof

7. Maxime Breden, Rigorous numerics for a tridiagonal dominant operator

29.3 Outcome of the Meeting

The main goal when structuring this workshop was to create plenty of opportunities for interaction and collaboration. After each lecture we had a central meeting to make a list of possible subjects to work on, such as an open problem or a particular technique (adding and removing subjects to/from the list as the week went on). We then democratically selected three topics for discussion. The remainder of the morning or afternoon was spent in breakout sessions: smaller subgroups came together to exchange ideas. Some topics were discussed just once, others multiple times. The results of the nine selected topics are summarized below.

29.3.1 Software for rigorous verification of PDEs

The functional analytic approach to rigorous verification of PDEs is still a new field but has progressed theoretically, and gained sufficient researchers. While scientific software is a necessary product of research in rigorously verified computing, a conscious effort is needed to collect and share the disparately developed software. By having a community curated collection of code, we hope to encourage researchers to improve their coding practices and allow for a greater degree of software-reusability.

We have some preliminary ideas for good practice for computer assisted proofs in this area such as:

- Readable, commented code
- Documentation to accompany publicly available code
- Variable names and algorithmic implementations in the code should match those the accompanying paper
- Scripts reproducing any and all figures in the accompanying paper should also be publicly available.

All aspects of a proof must be clear to a reader of both the paper and public code. All results should be completely reproducible!

There is no reason to try and enforce a standard language or coding style on the community. Instead we intend to create a wiki to share work in a common place that is open to all and editable by all. By developing a wiki-based repository maintained by the community, its continued existence will not be dependent on any one person or group. We hope that good practice will develop from researchers have good examples to follow and start from.

Initially the wiki will primarily be a repository for papers, codes and links. We hope that over time we can include an index of methods, subroutines, problems, etc., so that people can quickly find what they are looking for.

It is also important to start looking at the functional analytic approaches in comparison to the more geometric approach. We need to compare problems with those that can be done with CAPD to find where which approach is better and where the two methods are complimentary. Additionally we plan to collect test examples such as descriptions and implementations of simple rigorous ODE integrators, examples of continuation proofs and other standard infinite-dimensional problems. These examples can then be used by newcomers, allowing for a more open and inviting introduction to the field of rigorously verified computations than previously possible.

Finally, we identified several directions for common software needs, such as a rigorous FFT algorithm and rigorous continuation wrappers.

29.3.2 Fast Fourier Transform

For a number of the problems discussed in our workshop the practical computation of rigorous error bounds uses the Fast Fourier Transform (FFT). As the name suggests it is a fast version of the Discrete Fourier Transform (DFT) for converting time (or space) data into a frequency domain and vice versa. There are a number of algorithms for converting an n-vector by FFT, and those algorithms are especially efficient if n is a power of 2.

On a broader scale the computation of rigorous error bounds requires, in particular, the estimation of rounding errors. Rather than doing that for each operation individually it is very useful not to use plain floating-point arithmetic but to handle the estimates by special data types, for example, interval arithmetic.

To address operations on such new data types using traditional programming language C or Fortran and corresponding software is quite cumbersome. This can be solved by using Matlab. This very widely used programming environment offers an operator concept. That in turn allows to write operations including rigorous error estimates at a level close to mathematical notation. This is true for scalars, vectors, matrices and other spaces.

A convenient Matlab toolbox to address required operations with rigorous error bounds is INTLAB, the Matlab toolbox for reliable computing. A number of participants in the workshop use INTLAB. For some reason the Fast Fourier Transform is not (yet) included in INTLAB. It turned out during the workshop that first, FFT with rigorous error bounds is very important and second, there is an existing routine which works correctly but, however, is rather slow.

One main reason for weak performance is the fact that Matlab interprets the code. On the one hand this allows to write a code close to the mathematical specification. However, on the other hand, interpretation may slow down computations significantly. This can be avoided by vectorizing Matlab code. In that case the computing time of a single operation can be much larger than the interpretation time of that single operation, thus diminishing the interpretation overhead.

The existing routine for the FFT was vectorized to a certain degree, but more could be done. As a result of the workshop a new routine verifyfft for the forward and inverse FFT with rigorous error bounds was developed and distributed among the participants. For small vector lengths the computing was reduced by a factor of more than 100, for larger vector lengths even by a factor 1000 and more.

Moreover, often many vectors have to be transformed at a time. In that case it is superior to put the vectors into a matrix and to transform all columns of the matrix at once. This kind of vectorization improves the performance again by an order of magnitude for moderate vector lengths.

Both the existing and the new routine compute verified inclusions of the true result. The results of the existing routine are pretty accurate, i.e. the bounds are narrow. An additional effort was spend to improve the width of the bounds. For moderate vector lengths the improvement is about two orders of magnitude.

The workshop helped to identify the FFT with verified error bounds as a crucial operation in many of the algorithms for computing rigorous error bounds for continuous problems. The new routine will be included in INTLAB.

29.3.3 Nonexistence Proofs for Dynamical Systems

This discussion focused on the question of whether one can compute the entire solution set for problems of the type $F(x) = 0$, $x \in X$ where X is a Banach space. This involves not only locating and verifying solutions, but also ruling out solutions in the remainder of X. Ruling out additional solutions, or showing the nonexistence of solutions, requires a number of reductions for infinite-dimensional problems. This may include using analytical methods to determine feasible bounds of the solution set in X and using computational methods to refine this set by locating regions on which one can prove that no solution exists.

We discussed two prior results to motivate our more general discussion. Day and Kalies (2013) used two sets of bounds (labeled *global* and *point-wise*) together with computational outer approximation techniques to bound and refine a covering of the maximal invariant set for a class of integrodifference equations with smooth nonlinearities. Cyranka and Zgliczyński (arXiv:1403.7170, 2014) used analytical bounds and computations of absorbing sets to prove that a unique equilibrium solution is globally asymptotically stable (hence, ruling out additional solutions) for the viscous Burgers equation.

One of the outcomes of the further discussions was the recognition that it is possible to reduce (under favorable conditions) the problem of a rigorous enclosure of all solutions of equations in a Banach space with reasonable tolerances to a finite-dimensional constraint satisfaction problem (CSP) whose solution gives the desired information about the original problem. If a low number of degrees of freedom suffice to give a reasonable approximate description of the problem, if the number of solutions is not too large, and if these solutions are not overly sensitive to perturbations of the problem then the CSP is expected to be solvable in a reasonable amount of time by off-the-shelf rigorous branch-and-bound methods for constraint satisfaction problems. The resulting rigorous error bounds for the solutions of the infinite-dimensional problem are then expected to be reasonable. This resulted in a lecture by Arnold Neumaier on Thursday afternoon, and a manuscript written during the meeting.

Several software packages exist for solving factorable CSPs with complete rigor: COCONUT, GloptLab, ANTIGONE, Couenne, ICOS, and GlobSol. In each case, the user only needs to provide an appropriate text file describing the constraints and to select appropriate options for steering and stopping the solver. The prize-winning solver BARON also solves constraint satisfaction problems, but relies on unverified techniques that may lead to inaccurate coverings and even to the loss of solutions.

As one possible test case the group briefly discussed the diblock copolymer model, which is one of the standard equations describing micro-phase separation in materials. It is a fourth-order parabolic partial differential equation, which arises as a regular perturbation of the well-studied Cahn-Hilliard model. The model is a gradient system, so the study of its global dynamics reduces to understanding its global attractor. It was shown in Johnson, Sander, and Wanner (2013) that the diblock copolymer bifurcation diagram is considerably more complicated than that of the Cahn-Hilliard model. At the same time, low-dimensional projections of the flow seem to provide reasonable approximations of the dynamics in interesting parameter regimes. As a test case, the group created GAMS input files for a three-dimensional projection of the model, and used BARON through the NEOS server to perform a comprehensive sweep of the equilibrium structure at a particular parameter value. BARON resolved all fifteen equilibrium solutions of the model in a few minutes, in accordance with the results of Johnson, Sander, and Wanner (2013).

29.3.4 Approximate inverse of infinite dimensional tridiagonal operators

Consider a tridiagonal linear operator of the form

$$J = \begin{pmatrix} D & & & 0 & & \\ & & \lambda & & & \\ & \lambda & \mu_m & \lambda & & \\ 0 & & \lambda & \mu_{m+1} & \lambda & \\ & & & \ddots & \ddots & \ddots \end{pmatrix}, \tag{29.3.1}$$

where D is a finite dimensional $m \times m$ matrix, λ is a large constant and $|\mu_k| \to \infty$ as $k \to \infty$. An operator of the form (29.3.1) occurs in several contexts, and obtaining explicit bounds on its inverse, or constructing a good approximate inverse is a key step in many rigorous computational methods aimed at studying infinite dimensional nonlinear problems. We considered two separate situations.

Non uniqueness phenomena in a convection-diffusion 2D PDE model

Consider the following convection-diffusion 2D PDE model

$$P\boldsymbol{u} \cdot \nabla \boldsymbol{u} - \Delta \boldsymbol{u} = \lambda \boldsymbol{F}(x), \qquad \boldsymbol{u}\colon \mathbb{T}^2 \to \mathbb{R}^2,\ \boldsymbol{F}\colon \mathbb{T}^2 \to \mathbb{R}^2, \tag{29.3.2a}$$

where $P\boldsymbol{u}$ is the Helmholtz projector onto the zero divergence subspace, i.e. $P\boldsymbol{u} = \boldsymbol{u} - \nabla \text{div}\left(\Delta^{-1}\boldsymbol{u}\right)$, and $\mathbb{T}^2$ is the two dimensional torus. This is a toy model related with 2D incompressible Navier-Stokes equations. Our goal in studying this problem is to explore the non uniqueness phenomena – generically embedded in fluid dynamics models. In particular, we aim at answering the question of multiplicity of solutions with respect to the parameter λ. For the particular choice of forcing

$$F(x) = (2\sin x_2, 2\sin x_1),$$

when $\lambda \gg 1$, the stable solution can be decomposed into the dominant part $(2\lambda \sin x_2, 0)$, and the remainder $\widetilde{u}_\lambda$, i.e.

$$u_\lambda = (2\lambda \sin x_2, 0) + \widetilde{u}_\lambda. \tag{29.3.3}$$

After this formula is plugged into (29.3.2), the linear part takes the form of the operator

$$L(\widetilde{u}) = 2\lambda \sin x \widetilde{u}^2 + \Delta \widetilde{u}^2,$$

which is of tridiagonal form as in (29.3.1) with $\mu_k = -1 - (k-1)^2$ in Fourier's basis.

Results and conjectures

The problem of bounding $\|L_\lambda^{-1}\|$ (in an operator norm) is crucial for establishing the existence of u_λ – solution of (29.3.2) asymptotically for large λ values, which we conjecture is true. Our current research in progress revealed that if we consider a finite k-dim truncation of the operator L_λ ($P_k L_\lambda$) its norm can be bounded

$$\|(P_k L_\lambda)^{-1}\|_\infty < C/\sqrt{\lambda},$$

where the constant C does not depend on both of the truncation dim. k and the parameter λ. On the workshop we realized that this bound probably holds even for the inverse of the infinite dim operator L_λ, and this could help us progress with our conjecture.

Chebyshev series for the study of BVP

When using Chebyshev series to compute solutions to boundary value problems (BVP), we derive an infinite dimensional nonlinear operator whose derivative is of the form (29.3.1), where the off diagonal term λ consists essentially of a time rescaling constant multiplied by the first Chebyshev coefficients of the numerical approximation.

Hence, for BVP arising in fast-slow systems or posed on long time domains, the off diagonal term will be large and hence should not be ignored when constructing an approximate inverse. During the week, we discussed about possibilities to adapt the work of [Breden, Desvillettes and Lessard, Rigorous numerics for nonlinear operators with tridiagonal dominant linear parts, preprint, 2014] to this context. Since there, the operators considered have unbounded off diagonal terms, we believe that the method should in principle be adapted.

29.3.5 Bifurcations

We discussed the problem of finding bifurcation points in infinite-dimensional parameter-dependent zero-finding problems

$$F(b,\lambda)=0,$$

for $F : B \times \Lambda \to B$.

Among other things, we designed a general setup in the spirit Lyapunov-Schmidt reduction and considered variations thereon. Furthermore, we discussed the inherent problems surrounding of finding bifurcation-points in an asymmetrical setting using validated numerical techniques, i.e. singularities of the derivative, pitchfork, period-doubling etc. Finally, we considered several examples, such as the pitchfork's normal form, the Swift-Hohenberg equation and a system of reaction-diffusion equations considered by J.-P. Lessard, and M. Breden.

Lyapunov-Schmidt-type method

More precisely, we considered a singular zero-finding problem $F(b_0,\lambda_0)=0$ with a one-dimensional kernel

$$N=\ker(D_bF(b_0,\lambda_0)),$$

and one-dimensional co-range Y, whose complement is given by

$$R=\operatorname{ran}(D_bF(b_0,\lambda_0)).$$

Using the splittings $B=N\oplus X$ and $B=R\oplus Y$ one defines the one-dimensional projections $P : B \to N$ and $Q : B \to Y$. Consequently, the system $F(b,\lambda)=0$ can be written equivalently as

$$\begin{aligned} QF(P(b)+(I-P)(b),\lambda)&=0\\ (I-Q)F(P(b)+(I-P)(b),\lambda)&=0. \end{aligned}$$

The benefit of this construction is that the function $\Phi : N \times X \times \Lambda$, given by

$$\Phi(n,x,\lambda)=(I-Q)F(n+x,\lambda)$$

has a non-singular derivative (with respect to x) at n_0, x_0, λ_0 given by

$$D_x\Phi(n_0,x_0,\lambda_0)=(I-Q)D_xF(n_0+x_0,\lambda_0).$$

By the implicit function theorem, this implies that there exists a function ϕ defined on a neighbourhood of $(n_0,\lambda_0)\in N\times\Lambda$, such that

$$\Phi(n,\phi(n,x),\lambda)=0,$$

for all (n,λ) in this neighbourhood.

Using this, we can define the bifurcation function

$$g(n,\lambda)=QF(n+\phi(n,\lambda),\lambda),$$

whose derivatives can be used to determine the characteristic behaviour of the bifurcation. Crucial in this discussion is the verified computation of the function ϕ, which can be done for instance in the setting of radii-polynomials.

An alternative approach was considered based on regularizing the problem in the following way. Instead of splitting the space, one can augment the system by considering the problem given by

$$\begin{aligned} F(b,\lambda) - \kappa y &= 0 \\ \psi(b) - \mu &= 0. \end{aligned}$$

In this system y must be taken from the co-range of $DF(b_0, \lambda_0)$ and ψ is a suitably chosen monitor function, typically the function used to plot the bifurcation diagram.

This new system is non-singular and by solving it we can rigorously compute expressions for

$$\begin{aligned} b &= b(\kappa, y) \\ \kappa &= \kappa(\lambda, \mu). \end{aligned}$$

By studying the null set of κ, one can identify a neighbourhood of the bifurcation diagram and by subsequently considering the sign changes of κ one can verify the existence of a bifurcation branch contained in this neighbourhood. It should be noted that this technique usually is unable to rigorously verify the existence of a bifurcation point in cases where an inherent symmetry of the system cannot be exploited.

Asymmetrical systems

In addition, we also discussed the identification of bifurcations in settings where symmetry is either absent or not immediately obvious. Primarily, we considered this problem in the context of the pitchfork bifurcation. When such a bifurcation occurs, a symmetry in the system (usually given by the fact that F is an odd function) can be exploited in order to rigorously construct the bifurcation branch by dividing out the singularity of the system. This can then be used to prove the existence of a bifurcation point on this branch.

In cases where symmetry is not present, this cannot be done. In generic bifurcations, it is usually impossible to distinguish between two non-intersecting bifurcation branches and an actual pitchfork. We briefly discussed a method of finding bifurcation points by considering small perturbations of the original system, by adding a parameter to the system.

Examples

In conclusion, we considered several examples of systems in which bifurcations play a role. In particular, we briefly considered the pitchfork bifurcation's normal form while studying the problem of asymmetrical system.

In addition we also considered how our Lyapunov-Schmidt type method could be applied to the Swift-Hohenberg equation as well as a system of reaction-diffusion equations previously considered by J.-P. Lessard, and M. Breden.

29.3.6 Exploiting smoothing property of parabolic PDEs in rigorous numerics

Consider the problem

$$u_t(t,x) = Lu + N(u, Du, \dots, D^r u), \tag{29.3.4}$$

on some compact domain $\Omega \subset \mathbb{R}^n$ with some boundary conditions, where L - smoothing operator, Laplacian or its power with a correct sign and $r < s$, where s the order of L.

The smoothing properties of the time evolution of (29.3.4) are well known. When the periodic boundary conditions for (29.3.4) are considered, then in the Fourier basis $\{\exp(ikx)\}_{k\in\mathbb{Z}^n}$ the effect of smoothing gives rise for tail isolation for the sets of the form $W \oplus \Pi_{|k|>M} B(0, \frac{C}{|k|^s})$. This makes it possible to design a rigorous integrator for such system.

Two crucial facts in the construction of the integrator are

- L is diagonal in the Fourier basis, hence $\exp^{Lt}$ is known explicitly;
- the following lemma holds:

  Lemma 29.3.1 *Let $s > s_0$. If $|a_k| \leq C/|k|^s$, $|a_0| \leq C$, then there exists $D = D(C, s)$*

  $$|N_k| \leq \frac{D}{|k|^{s-r}}, \qquad |N_0| \leq D.$$

  This is in fact a statement about regularity, namely if a is of "class C^s" (plus bounds) then $N(a)$ is of "class C^{s-r}" (plus bounds).

For other boundary conditions and domains usually we do not have the eigenfunctions basis and Lemma 29.3.1 appears not to be true. This probably excludes the possibility of the component-wise isolation with arbitrary decay power s. However it is quite possible that we will have an isolation, if in the tail we consider balls in some norms. Instead of (29.3.4) we think it is worth trying to analyze its integral form

$$u(t) = \exp(Lt)u(0) + \int_0^t \exp(L(t-t'))N(u(t'), Du(t'), \dots)dt' \tag{29.3.5}$$

Observe that $\exp(Lt)$ is the Green function for the problem (29.3.4) with $N \equiv 0$.

We can rewrite (29.3.5) as follows

$$u(t,x) = \int_\Omega G(t,x')u_0(x')dx' + \int_0^t dt' \int_\Omega dx' G(t-t', x-x')N(u(t',x')) \tag{29.3.6}$$

We see two possibilities of splitting of our phasespace, $X \oplus Y$, into 'main modes' X and the tail Y

- using approximate leading eigenfunctions for L generating X and estimating action of L on $Y = X^\perp$. The techniques used by Plum and his coworkers can be helpful in obtaining this goal. On the other side it not obvious how to exploit the smoothing property.
- assuming some knowledge of G (some bounds which allow to derive the smoothing property) following the approach developed by Nakao we set $X = S_h$ and $Y = S_h^\perp$ where S_h is obtained as the projection trough some interpolation. Hopefully in this setting the isolation property can be analytically established. This requires study of two topic: developing bounds for the projection error in various norms and function spaces and the Green function for the linear problem.

We think that it will be worth to look at a problem on the disk, where the eigenfunctions are known (Bessel functions) but apparently Lemma 29.3.1 is not true. There we should learn how to achieve an isolation and this new insight will likely allow us to attack other problems.

29.3.7 Eigenvalue enclosures and exclosures

In various contexts of rigorous computations, but also of more general analytical problems, information about the spectrum of given selfadjoint or non-selfadjoint eigenvalue problems is of crucial importance. For example, when the stable and the unstable manifold of a dynamical system shall be suitably controlled by rigorous computations, information about the location of eigenvalues in certain parts of the complex plane is required. Also in norm computations for linear operators eigenvalue bounds play an important role.

For selfadjoint eigenvalue problems, eigenvalues below the essential spectrum can be characterized variationally e.g. by Poincare's min-max-principle. Based on such characterizations, finite dimensional matrix eigenvalue problems can be put up, the eigenvalues of which are upper or lower bounds for the eigenvalues of the given (usually infinite dimensional) eigenvalue problem. These matrix eigenvalue problems can be solved rigorously by means of well-established linear algebra software, as e.g. INTLAB. The eigenvalue bounds obtained in this way are index-wise, and thus in particular also guarantee that the regions (on the real line) between the enclosing intervals are free of eigenvalues, i.e. they also give eigenvalue exclosures.

For non-selfadjoint eigenvalue problems, the situation is more complicated since no useful variational eigenvalue characterizations are available. Here, after a suitable reformulation of the problem, fixed-point arguments can be used to rigorously enclose single eigenvalues in the complex plane, and also for computing compact complex regions which are free of eigenvalues, i.e. eigenvalue exclosures.

For the more special case of linear operators acting in spaces of (real or complex) sequences, which therefore are directly representable as infinite dimensional matrices, also Gerschgorin-type eigenvalue enclosures can be considered. In particular when the off-diagonal entries are "small" (measured in the corresponding sequence-space norm), such bounds are often quite satisfactory. For example, in case of the Kot-Schafer model such Gerschgorin-type bounds are sufficient to obtain the desired information about the number of eigenvalues located inside or outside the complex unit disk, as needed for controlling the stable and the unstable manifold.

It will be of major interest for future investigations to identify larger classes of operators, also out side the class of operators in sequence spaces, for which Gerschgorin-type eigenvalue bounds give appropriate information.

29.3.8 Perturbation Arguments in the Method of Radii Polynomials

Many problems in analysis are solved by formulating a zero finding problem for a function between appropriate Banach spaces. Indeed this was a recurring theme in a number of the sessions and many of the lectures at this workshop. A number of researchers at the workshop have used the method of radii-polynomials in order to organize computer assisted zero finding arguments. This method begins with a particular numerical approximate solution, a particular choice of approximate inverse for the problem, and a choice of the Banach space on which the solution is desired. One constructs a "Newton-like" operator and aims to shows that the operator is a contraction in some neighborhood of the approximate solution.

Based on these choices the method of radii polynomials is a strategy for obtaining bounds on the smallest and largest neighborhoods about the approximate solution on which the Newton-like operator is a contraction mapping. The radii of these balls appear as the roots of some polynomial equations with coefficients determined by the data of the problem. The size of the smallest of the neighborhoods gives a rigorous bound on the truncation error. The size of the largest neighborhood gives isolation bounds for the solution. Continuity of the radii polynomials aids in the smooth connection one computer assisted proof to another. In addition, information about the isolation of the solution is sometimes exploited to aid in mathematically rigorous continuation arguments.

This session considered the possibility of applying the radii-polynomial argument directly to the projected finite dimensional problem and then using some weaker perturbative argument to obtain a (possibly non-unique) solution of the infinite dimensional problem. We discussed the possibility of using the isolation information from the finite dimensional radii polynomial argument in order to facilitate the perturbative step. The participants observed that when the Newton like operator has certain smoothing properties then the perturbative argument seems to goes through. The argument is based on the Schauder theorem and requires some bounds on the difference between the projected and infinite dimensional map. The advantage of this approach is that projection errors for the derivative of the infinite dimensional map are not needed. The disadvantage is of course the loss of uniqueness.

Many problems considered in applied mathematics have the smoothing properties required for this argument. The participants also discussed the possibility that in some problems it may be possible to recover the uniqueness by some regularity/bootstrap arguments. Further consideration is required in order to determine if the proposed approach will lead to solution of problems not solvable by current methods. It does seem clear that the argument could be used in some cases to simplify some computer assisted proofs.

29.3.9 Fast-Slow systems

Fast-slow systems are difficult to analyse using rigorous numerics due to the presence of different time scales. In the singular limit, complementary topological-based techniques can be used to describe the dynamics for all $\varepsilon \in (0, \varepsilon_0]$, for some (very) small explicit ε_0. The problem to be solved is then to develop a rigorous numerical procedure for continuing the solution starting at $\varepsilon = \varepsilon_0$. In this regime the topological technique no longer works. Moreover, since ε_0 is (very) small, the time scale separation still hampers general continuation techniques. Hence, an approach adapted to fast-slow systems is needed.

We identified a hierarchy of problems:

1. <u>0th order</u>: the limit where a periodic orbit tends to a homoclinic one, so that part of the trajectory is close to an equilibrium (a 0-dimensional slow manifold).

2. <u>1st order</u>: trajectories that alternately follow one-dimensional slow manifolds and fast transitions between these.

3. <u>2nd order</u>: the case in which the slow manifold is of dimension two or higher, so that part of the problem is to determine <u>which</u> orbit on the slow manifold is being shadowed.

Concerning the 0th order problem, we focused on the functional analytic approach (in particular, using domain decomposition and Chebyshev series) for the Lorenz system. Several ideas were mentioned.

- Reparameterize time for the part of the trajectory that is close to the equilibrium and find a way to do this automatically (to be able to do continuation).
- Use splines near the equilibrium, as different bases functions can be used on each domain.
- Use normal forms (a la Tucker) to give a phase-space description near the equilibrium and combine that with a boundary value problem, which in turn can be solved by using the Chebyshev series.
- Combine the idea of normal forms with the choice of appropriate basis functions for the part of the trajectory near the equilibrium, i.e., try to lift the normal approach to function space.

Naturally, the 0th order problem has been solved before, using several methods (including CAPD). The goal of looking for new approaches is to use these as stepping stones for the 1st (and later 2nd) order problem. Concerning the latter, the ideas were obviously less concrete:

- Explicitly split the problem into several boundary values problems, each dealing with either a fast part or a slow part, so that time can be appropriately rescaled on each piece.
- Construct a parameterized normal form near the slow manifold. Here one could either use the slow manifold of the singular limit or a persisting slow manifold for small $\varepsilon > 0$.

Bibliography

[1] Oscar E. Lanford, III, A computer-assisted proof of the Feigenbaum conjectures, Bull. Amer. Math. Soc. (N.S.) **6** (1982), 427–434.

[2] Warwick Tucker, A rigorous ODE solver and Smale's 14th problem, Found. Comput. Math. **2** (2002), 53–117.

Chapter 30

Vojta's Conjectures (14w5129)

September 28 - October 3, 2014

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This report was prepared by David McKinnon, who takes sole responsibility for the contents.

30.1 Overview of the Field

In his seminal work [16], Paul Vojta opened the door to a vast network of correspondences between Nevanlinna Theory and Diophantine geometry, culminating in a set of sweeping conjectures that aimed at unifying a huge swath of number theory and arithmetic geometry. Vojta's work provided a framework and context for a variety of powerful results in number theory, a new proof of an old conjecture, and illuminated the path forward to new results in virtually every area of arithmetic geometry.

The two fields united by Vojta's conjectures have a long history, although Diophantine geometry, by its nature, is much older, dating back – in a sense at least – to ancient Greece. The modern part of the story therefore cannot have a clear beginning, but a convenient starting point is the chain of results begun by Liouville in his 1844 paper ([7]).

Theorem 30.1.1 (Liouville 1844) *Let α be a real algebraic number, and let $d = [\mathbb{Q}(\alpha) : \mathbb{Q}]$. There are only finitely many rational numbers p/q such that:*

$$\left|\alpha - \frac{p}{q}\right| \leq \frac{1}{q^d}$$

Liouville's central observation was that a rational number cannot get too close to an algebraic one. Liouville applied his theorem to construct the first concrete example of a transcendental number, by finding a real number that, for any d, could be approximated better than his theorem prescribes for an algebraic number. This kind of clever application of Diophantine geometry to transcendence theory continues to this day – in work of Adamczewski and Bugeaud (see [1]), for example.

Liouville's result, revolutionary though it was, was not best possible for $d \geq 3$. (It is sharp for $d = 1$ and $d = 2$.) In particular, the exponent d on the right hand side is much larger than necessary for large d. A famous chain of results followed to improve this, starting with Axel Thue in 1909 ([15]). He reduced the exponent from d to $d/2+1+\varepsilon$. Carl Siegel reduced the exponent further to $2\sqrt{d}$, in 1921 ([14]), and in 1947 Freeman Dyson reduced it still further to approximately $\sqrt{2d}$ ([5]).

However, none of these results were optimal, even though they all had profound applications to arithmetic geometry. The capstone theorem of this line of research was the 1955 masterwork of Klaus Roth ([11]).

Theorem 30.1.2 (Roth 1955) *Let α be a real algebraic number. There are only finitely many rational numbers p/q such that:*

$$\left|\alpha - \frac{p}{q}\right| \leq \frac{1}{q^{2+\varepsilon}}$$

The value of $2+\varepsilon$ for the exponent is known to be the best possible because of the continued fraction expansion of α, which gives an infinite number of rational approximations of α with exponent 2. So Roth's Theorem, it would seem, is the end of the story.

Except, of course, that whenever a mathematical problem is solved, several more problems arise. For example, the left side of the inequality in Roth's Theorem is phrased in terms of the usual archimedean distance. What happens if one uses a p-adic distance instead? (The exponent of $2+\varepsilon$ is unchanged – see [10].) Or a finite product of distances instead of just one? (Same exponent again, essentially – see [10] again.)

A much deeper generalization of Roth's Theorem was found in 1970 by Wolfgang Schmidt (see [12]). Roth's Theorem is essentially a one-dimensional statement, about approximations on the line. Schmidt's theorem vastly extended the scope, to approximations in arbitrary finite dimensions. It was generalized in [13] to the following.

Theorem 30.1.3 (Subspace Theorem) *Let k be a number field with ring of integers $\mathcal{O}_k$, and let $n \geq 1$ be a positive integer. Let S be a finite set of places of k. For each $v \in S$ and each $i \in \{0,\ldots,n\}$, let $L_{v,i}$ be a linear form in $n+1$ variables with algebraic coefficients, and assume that for each v, the forms $L_{v,0},\ldots,L_{v,n}$ are linearly independent.*

Choose $\varepsilon > 0$, and let Q be the set of all $s \in \mathcal{O}_k^{n+1}$ satisfying

$$\prod_{v\in S}\prod_{i=0}^{n}|L_{v,i}(s)|_v < \left(\max_{v|\infty,\, i}|s_i|_v\right)^{-\varepsilon}$$

where $|\cdot|_v$ denotes the absolute value associated to v and s_i denotes the ith coordinate of s.

Then Q is contained in a finite union of hyperplanes of k^{n+1}.

This was the state of the art in Diophantine geometry when Paul Vojta formulated his conjectures. The other half of the story is in Nevanlinna theory, which was the source of the key inspiration.

Nevanlinna theory was inspired by a result of Hadamard in 1896, probably, although he did not publish a proof of it. Hadamard noted that the logarithm of the maximum modulus of an entire function inside the circle $|z| = r$ grows at least as fast as the number of zeroes of f inside the circle, as a function of r. The key breakthrough was made by Nevanlinna, however, when he replaced the notion of maximum modulus with a counting function, enabling him to deal with general meromorphic functions instead of entire functions. (See [9] for details.) To state Nevanlinna's results, we need some additional terminology and notation.

- For any real valued function A, define $A^+(x) = \max\{A(x), 0\}$.
- Let : $\mathbb{C} \to \mathbb{C}$ be a meromorphic function.
- For any $a \in \mathbb{C}$, define the proximity function of f at a to be $m(a,r) = \int_0^{2\pi} \log^+ \left|\frac{1}{f(re^{i\theta})-a}\right| \frac{d\theta}{2\pi}$.

- Define the proximity function of f at infinity to be $m(\infty, r) = \int_0^{2\pi} \log^+ \left| f(re^{i\theta}) \right| \frac{d\theta}{2\pi}$.
- For any complex number a and positive real number r, define $n(a, r)$ to be the number of zeroes of $f - a$ inside the circle $|z| = r$.
- Define $n(\infty, r)$ to be the number of poles of f inside $|z| = r$.
- For any complex number a, define the counting function of f at a to be the integral $N(a, r) = \int_0^r n(a, s) \frac{ds}{s}$.
- Similarly, define the counting function at infinity to be $N(\infty, r) = \int_0^r n(\infty, s) \frac{ds}{s}$.
- Define the characteristic function of f to be $T(r) = \int_0^{2\pi} \log^+ \left| f(re^{i\theta}) \right| \frac{d\theta}{2\pi} + N(\infty, r)$.
- Define $n_1(r)$ to be the number of ramification points of f in the disk $|z| < r$.
- If 0 is not a ramification points of f, define $N_1(r) = \int_0^r n_1(r) \frac{dr}{r}$.

Nevanlinna's First Main Theorem states:

Theorem 30.1.4 (First Main Theorem) *For any meromorphic function $f \colon \mathbb{C} \to \mathbb{C}$, and any complex number a, $N(a, r) + m(a, r) = T(r) + O(1)$.*

Nevanlinna's much deeper Second Main Theorem is as follows.

Theorem 30.1.5 (Second Main Theorem) *For any distinct complex numbers $a_1, \ldots, a_n$, the following inequality holds outside a set of bounded measure:*

$$\sum_{i=1}^{n} m(a_i, r) \leq 2T(r) - N_1(r) + O(\log rT(r))$$

The Second Main Theorem deals with an arbitrary finite set of complex numbers rather than just one, and involves the derivative of f in a highly nontrivial way through the term $N_1(r)$. The third member of Nevanlinna's trio of foundational theorems is the defect relation.

Theorem 30.1.6 (Defect relation) *For any non-constant meromorphic function $f \colon \mathbb{C} \to \mathbb{C}$, we have the following inequality:*

$$\sum_{a \in \mathbb{C}} \mathit{liminf}_{r \to \infty} \frac{m(a, r)}{T(r)} \leq 2$$

These notions have been generalised to higher dimensions – and arbitrary smooth varieties – by various authors. The higher dimensions have appeared in both the domain and the codomain of the meromorphic maps, but we will concentrate on the codomain in this report. In order to do this, we must define the basic objects in higher dimensions.

- Let V be a smooth projective variety defined over $\mathbb{C}$.
- Let $f \colon \mathbb{C} \to V$ be a non-constant meromorphic function.
- Let D be a normal crossings divisor on V.
- A Weil function for D is a function $\lambda_D \colon (V - \text{Supp}(D))(\mathbb{C}) \to \mathbb{R}$ such that if f is a local defining function for D, then $\lambda_D + \log |f|$ is continuous.
- The proximity function for D is $m_f(D, r) = \int_0^{2\pi} \lambda(f(re^{i\theta})) \frac{d\theta}{2\pi}$

- The counting function for D is $N_f(D,r) = \sum_{0<|z|<r} \mathrm{ord}_z f^*D \cdot \log \frac{r}{|z|} + \mathrm{ord}_0 f^*D \cdot \log r$
- The characteristic function (or height function) for D is $T_{D,f}(r) = m_f(D,r) + N_f(D,r)$.

With these definitions, the First Main Theorem becomes a tautology, although the fact that T depends only on the linear equivalence class of D rather than the particular divisor is also well known (and not immediate) – see Proposition 11.6 of [17] for a proof.

The generalised Second Main Theorem, however, is still unknown. It is apparently originally due to Griffiths, but [17] contains a thorough discussion. For the statement used below (taken from [17]), we assume that K is the canonical line bundle on V, and A is an ample line bundle on V.

Conjecture 30.1.7 *(a) The inequality*

$$m_f(D,r) + T_{K,f}(r) \le O(\log^+ T_{A,f}(r)) + o(\log r)$$

holds for all holomorphic curves $f\colon \mathbb{C} \to V$ with Zariski dense image, except for r lying in a set of finite Lebesgue measure. (b) For any $\varepsilon > 0$, there is a proper Zariski closed subset Z of X (depending only on X, D, A, and ε) such that the inequality

$$m_f(D,r) + T_{K,f}(r) \le \varepsilon T_{A,f}(r) + C$$

holds (except for r lying in a set of finite Lebesgue measure) for all nonconstant holomorphic curves $f\colon \mathbb{C} \to V$ whose image is not contained in Z, and for all $C \in \mathbb{R}$.

Vojta's critical insight was to realise that there were deep connections to be made between these various theorems and the objects they describe. Vojta's dictionary between the two fields contains the following correspondences:

- A meromorphic function $f\colon \mathbb{C} \to \mathbb{C}$ corresponds to an infinite set of elements of a number field k.
- The characteristic function $T(r)$ corresponds to the height function $h(b) = \frac{1}{[k:\mathbb{Q}]} \sum_v \log^+ \|b\|$.
- Let S be a finite set of places of k. Then there are analogues of m and N for the Diophantine case:
  $m(a,b) = \frac{1}{[k:\mathbb{Q}]} \sum_{v \in S} \log^+ \|b\|$
  $N(a,b) = \frac{1}{[k:\mathbb{Q}]} \sum_{v \notin S} \log^+ \|b\|$

The correspondence extends to theorems as well. Roth's Theorem corresponds to the Defect Relation in Nevanlinna theory, using the correspondences described above. The First Main Theorem in Nevanlinna theory becomes a simple statement about the height of an algebraic number, following immediately from the definition. The Second Main Theorem in Nevanlinna theory, however, becomes something much, much deeper, which Vojta called his Main Conjecture.

To state the Main Conjecture, we need to define some notation.

- Let V be a smooth projective variety defined over k.
- Let D be a normal crossings divisor on V, also defined over k.
- Let K be the canonical divisor class on V.
- Let A be a big divisor class on V.
- Let ε be any positive real number.
- Let S be a finite set of places of k.

Conjecture 30.1.8 (Vojta's Main Conjecture) *There is a proper Zariski closed subset Z of V, depending on V, D, k, A, ε, and S, such that for all $P \in V(k)$ with $P \notin Z$, we have*

$$m(D,P) + h_K(P) \leq \varepsilon h_A(P) + O(1)$$

where the implied constant in the $O(1)$ does not depend on P.

This conjecture is a generalization of the Subspace Theorem, and therefore of all the other theorems in Diophantine geometry described so far. It also generalises Siegel's Theorem for curves, Faltings' Theorem (originally the Mordell Conjecture), and the Bombieri-Lang conjecture for varieties of general type. Vojta's Main Conjecture is known to imply many of the major conjectures in modern Diophantine geometry, including the abc Conjecture, Hall's Conjecture (see [16] for details on these two), and the Batyrev-Manin Conjecture for varieties of non-negative Kodaira dimension (see [8]). It also has deep consequences in transcendence theory and on the distribution of integral and rational points on algebraic varieties.

30.2 Recent Developments and Open Problems

Boris Adamczewski and Yann Bugeaud reignited interest in applying Vojta-like ideas to transcendence theory with their paper [1], which uses the Subspace Theorem to the complexity of the b-ary expansions of irrational numbers, and in particular proving the transcendence of irrational automatic numbers. To explain their results more fully, we need some definitions.

Let $b \geq 2$ be an integer, and let $x = 0.a_1a_2a_3\ldots$ be a real number, expressed in base b. That is, we have $x = \sum_i a_i b^{-i}$, with $a_i \in \{0,\ldots,b-1\}$. The complexity function of x in base b is a function $\rho_x \colon \mathbb{Z}_{\geq 1} \to \mathbb{Z}$, where $\rho_x(n)$ is the number of distinct strings of digits $d_1 \ldots d_n$ of length n that appear somewhere in the b-ary expansion of x. That is, a string $d_1 \ldots d_n$ contributes to $\rho_x(n)$ if and only if there is some integer j such that $d_i = a_{i+j}$ for all $i \in \{1,\ldots,n\}$. To convert this measure of complexity into a number, one can estimate the growth of $\rho_x(n)$ as a function of n. Rational numbers will have $\rho_x(n) = O(1)$, because their b-ary expansions are periodic. Adamczewski and Bugeaud, by contrast, showed that irrational algebraic numbers have complexity functions that grow faster than any linear functions: (see [1])

Theorem 30.2.1 *Let $\alpha \in (0,1)$ be an irrational algebraic number, and let $b \geq 2$ be an integer. The b-ary complexity function $\rho_\alpha(n)$ of α satisfies*

$$\lim_{n\to\infty} \frac{\rho_\alpha(n)}{n} = \infty$$

This means that any real number whose complexity function grows linearly (or more slowly) must either be rational or transcendental. In particular, automatic numbers are well known to have complexity functions that are $O(n)$, and are therefore either rational or transcendental. In particular, the irrational automatic numbers are all transcendental.

This theorem was derived from an earlier result of Adamczewski, Bugeaud, and Luca ([2]).

Theorem 30.2.2 *Let $\alpha \in (0,1)$ be a real number, and let $b \geq 2$ be a positive integer. Assume that for every positive integer N and every $\varepsilon > 0$ there are two identical disjoint sequences of digits of length at least εN in the first N digits of the b-ary expansion of α. Then $alpha$ is either rational or transcendental.*

Pietro Corvaja and Umberto Zannier, together with a variety of other authors, discovered an ingenious new method of applying the Subspace Theorem to the question of determining the distribution of integral points on algebraic varieties. The following theorem appears in [4].

Theorem 30.2.3 *Let V be a smooth projective surface defined over a number field k, and let $U \subset \mathbb{A}^n$ be a nonempty affine subset of V. Let $D_1,\ldots,D_r$ be effective (but not necessarily irreducible) divisors on V supported* *on $V - U$. Assume that no two of the D_i have a common component, and that no three of the D_i have a common point. Assume that for some integers $a_1, \ldots, a_r, n$, $D = a_1 D_1 + \ldots + a_r D_r$, we have*

$$\frac{\sum_{k=0}^{\infty} h^0(nD - kD_i)}{nh^0(nD)} > a_i$$

for all i. Then for any finite set of places S of k, the set of S-integral points on U is not Zariski dense.

Many authors have followed up on these ideas, and have improved the results. A particularly impressive example was obtained independently by Autissier ([3]) and Levin ([6]).

Theorem 30.2.4 *Let V be a smooth projective surface defined over a number field k, and let $U \subset \mathbb{A}^n$ be a nonempty affine subset of V. Let $D_1, \ldots, D_r$ be effective (but not necessarily irreducible) divisors on V supported on $V - U$. Assume that no two of the D_i have a common component, and that no three of the D_i have a common point. If $r \geq 4$, then for any finite set S of places of k, the S-integral points of U are not Zariski dense.*

In a still different direction, David McKinnon ([8]) proved that Vojta's conjectures imply the Batyrev-Manin conjectures for an arbitrary smooth projective variety of non-negative Kodaira dimension. In particular, he proves this implication for a $K3$ surface, which has a particularly interesting role in the conjectures.

To state the main theorem, we must first describe the Batyrev-Manin conjecture for a $K3$ surface. It gives a conjectural description of the distribution of rational points on the surface, in terms of the height density. In particular, let X be a $K3$ surface defined over a number field k. For any real number B, and for any subset U of X, let $N_U(B)$ be the number of k-rational points of U of height at most B. The Batyrev-Manin Conjecture states that

Conjecture 30.2.5 *Let $\varepsilon > 0$ be any positive real number. Then there is a nonempty Zariski open subset $U(\varepsilon) \subset X$ such that*

$$N_{U(\varepsilon)}(B) = O(B^{\varepsilon})$$

In this conjecture, we are using the multiplicative height rather than the logarithmic one used earlier. Note also that the conjecture implies that the surface X is presented as a subvariety of projective space, in order to define the height functions. This corresponds to a choice of (very) ample divisor on X, and this dependence is often made explicit.

It is known that $K3$ surfaces contain rational curves, and it is widely believed that the number of such curves is always infinite. Certainly there are examples of $K3$ surfaces that contain an infinite number of rational curves, and in many of these there are infinitely many such curves defined over k. In these cases, the surface X will contain curves which violate the Batyrev-Manin inequality, and so these curves must be in the complement of the set $U(\varepsilon)$ for small enough ε. These curves will turn out to be related to the exceptional sets Z that appear in Vojta's Conjecture.

In [8], McKinnon proves the following theorem.

Theorem 30.2.6 *Let X be a smooth, projective surface of nonnegative Kodaira dimension, defined over a number field k. Assume that Vojta's Main Conjecture for general cycles is true for any variety birational to a subvariety of $X \times X$. Then for every $\varepsilon > 0$ and ample divisor L on X, there is a nonempty Zariski open subset $U(\varepsilon) \subset X$ such that*

$$N_{U(\varepsilon),L}(B) = O(B^{\varepsilon}).$$

In particular, Vojta's Main Conjecture implies the Batyrev-Manin Conjecture for $K3$ surfaces.

Vojta's Main Conjecture for general cycles is a natural generalization of Vojta's Main Conjecture, with the slightly relaxed hypothesis that the divisor D might have codimension larger than one. The normal crossings condition is generalised to demanding that the cycle D be contained in a divisor with normal crossings. This generalization of Vojta's Main Conjecture is an immediate consequence of the original. See [8] for details.

30.3 Presentation Highlights

The workshop was filled with interesting presentations. The workshop was inaugurated by three introductory talks by Paul Vojta, Frédéric Campana, and Aaron Levin, who set the stage for the week to come. Vojta's talk laid out the conceptual framework for his conjectures, and outlined recent developments in broad terms. Campana reported on the progress of research in Vojta's conjectures as they apply to certain kinds of fibrations, and in particular on the effect of non-reduced components of singular fibres on the distribution of rational points. After lunch, Levin gave an excellent overview of the recent impressive results on integral points deriving from clever applications of the Subspace Theorem by Corvaja, Levin, and Zannier.

Ekaterina Amerik described joint work with Frédéric Campana on the characteristic foliation on smooth divisors in holomorphically symplectic manifolds. Let D be a smooth divisor in a holomorphically symplectic manifold X. Then D carries a rank-one foliation obtained as a kernel of the restriction of the symplectic form to D. It is called the characteristic foliation. Hwang and Viehweg have proved that when D is of general type, the foliation cannot be algebraic (unless in the trivial case when X is a surface). On the other hand, it is easy to see that the foliation is algebraic when D is uniruled. She explained what happens in the case when D is not uniruled. In particular, if X is an irreducible holomorphic symplectic manifold (that is, simply connected and such that the holomorphic symplectic form is unique up to a constant), she and Campana proved that the characteristic foliation is never algebraic in this case. The main new ingredient for their results is the observation that the canonical bundle of the orbifold base of the family of leaves must be torsion. This implies, in particular, the isotriviality of the family of leaves.

Yann Bugeaud spoke about connections of Vojta's conjectures to transcendence theory. A few years after Roth's fundamental breakthrough, Cugiani proved a theorem with the same conclusion, except with the ε replaced by a function $q \mapsto \varepsilon(q)$ that decreases very slowly to zero, provided that the sequence of rational solutions to $|\xi - p/q| < q^{-2-\varepsilon(q)}$ is sufficiently dense, in a suitable sense. He described an alternative, and much simpler, proof of Cugiani's Theorem and extended it to simultaneous approximation.

William Cherry gave an excellent survey of the non-Archimedean analog of Nevanlinna's theory of value distribution initiated by Ha Huy Khoai, focussing on similarities to and differences from the complex case. He also discussed the work of An, Levin, and Wang which introduces a Vojta like analogy between non-Archimedean analytic curves and integral points over the rationals and imaginary quadratic number fields. Finally, he also surveyed criteria for degeneracy of non-Archimedean analytic maps from the affine line into algebraic varieties and highlight an open problem whose solution might shed some light on the Green-Griffiths conjecture in complex geometry.

Pietro Corvaja, one of the major contributors to the recent impressive theorems on integral points, gave a presentation about joint work with Thomas Tucker, Vijay Sookdeo, and Umberto Zannier on integral points in orbits for a two-dimensional dynamical system. Let K be a number field, let $f : \mathbb{P}_1 \dashrightarrow \mathbb{P}_1$ be a nonconstant rational map of degree greater than 1, let S be a finite set of places of K, and suppose that $u, w \in \mathbb{P}_1(K)$ are not preperiodic under f. We prove that the set of $(m, n) \in \mathbb{N}^2$ such that $f^{\circ m}(u)$ is S-integral relative to $f^{\circ n}(w)$ is finite and effectively computable. This may be thought of as a two-parameter analog of a result of Silverman on integral points in orbits of rational maps. This issue can be translated in terms of integral points on an open subset of $\mathbb{P}_1^2$; then one can apply a modern version of the method of Runge, after increasing the number of components at infinity by iterating the rational map. Alternatively, an ineffective result comes from a well-known theorem of Vojta.

A very deep and comprehensive presentation came from Jan-Hendrik Evertse, surveying recent results and open problems relating to the Subspace Theorem. Let $L_i = \sum_{i=1}^{n} \alpha_{ij} X_j \ (i = 1 \ldots n)$ be n linearly independent linear forms with algebraic coefficients (from $\mathbb{C}$), and let $c_1 \ldots c_n$ be reals. Denote by $\|\mathbf{x}\|$ the maximum norm of $\mathbf{x} \in \mathbb{Z}^n$. Consider the system of inequalities

$$|L_i(\mathbf{x})| \leq \|\mathbf{x}\|^{c_i} \ (i = 1 \ldots n) \quad \text{in } \mathbf{x} \in \mathbb{Z}^n. \tag{30.3.1}$$

The following result is equivalent to Schmidt's Subspace Theorem from 1972:

Assume that $c_1 + \cdots + c_n < 0$. Then the set of solutions of (30.3.1) is contained in finitely many proper linear subspaces of $\mathbb{Q}^n$.

The proofs of the Subspace Theorem given so far are ineffective, in that they do not allow to compute the subspaces containing the solutions. But work of Vojta (1989), Schmidt (1993) and Faltings and Wüstholz (1994) implies that Schmidt's Subspace Theorem can be refined as follows:

Assumptions being as above, there is an effectively computable, proper linear subspace T^{exc} of $\mathbb{Q}^n$ such that (30.3.1) has only finitely many solutions outside T^{exc}. Moreover, T^{exc} can be chosen from a finite collection independent of $c_1 \dots c_n$.

Here, the method of proof does not allow to compute the solutions outside T^{exc}. But one can prove the following 'semi-effective' result. Assume that the coefficients of $L_1 \dots L_n$ have heights at most H, and that they generate a number field K of degree D. Further, let $c_1 + \cdots + c_n \leq -\delta$ with $0 < \delta < 1$, and $\max(c_1 \dots c_n) = 1$. Then one can show that for the solutions $\mathbf{x} \in \mathbb{Z}^n$ of (30.3.1) outside T^{exc} one has

$$\|\mathbf{x}\| \leq \max\left(B^{\text{ineff}}(n, K, \delta),\ H^{c^{\text{eff}}(n,D,\delta)}\right),$$

where c^{eff} is effectively computable, B^{ineff} not effectively computable from the method of proof, and both constants depend only on the parameters between the parentheses.

Evertse posed as an open problem to replace the above bound by one in which B^{ineff} depends on D instead of K. This would have various interesting consequences, of which he mentioned a few during the talk.

Kálmán Győry gave a survey of some recent results, partly obtained jointly with A. Berczes and J.-H. Evertse on various classes of Diophantine equations, including unit equations and some of their generalizations, Thue equations, superelliptic equations with unknown exponents, discriminant equations and their applications. Their results make effective several ineffective results of Lang and others, and generalize many earlier results established over number fields.

Gordon Heier discussed joint work with Aaron Levin regarding a generalization of the Schmidt subspace theorem (and Cartan's Second Main Theorem) in the setting of not numerically equivalent divisors. His presentation fit beautifully into the framework of the workshop, reinforcing the link between Nevanlinna theory (or, more generally, value distribution theory) and Diophantine geometry.

Khoa Nguyen presented joint research with Thomas Tucker, Dragos Ghioca, and Chad Gratton about primitive and doubly primitive divisors in dynamical sequences. Let K be a number field or a function field of characteristic 0, let $\varphi(z) \in K(z)$ having degree at least 2 and let $\alpha \in K$ such that the orbit $\{\varphi^n(\alpha)\}_{n\geq 0}$ is infinite. Consider the question: (A) except trivial counter-examples, is it true that for all sufficiently large n, the element $\varphi^n(\alpha)$ has a prime divisor $\mathfrak{p}$ that is not a divisor of $\varphi^k(\alpha)$ for every $k < n$. Ingram and Silverman are the first to consider this question in such generality. They even go further and ask: (B) except trivial counter-examples, is it true that for all $m \geq 0$ and $n > 0$ such that $m + n$ is sufficiently large, the element $\varphi^{m+n}(\alpha) - \varphi^m(\alpha)$ has a prime divisor $\mathfrak{p}$ that is not a divisor of any $\varphi^{M+N}(\alpha) - \varphi^M(\alpha)$ for $M < n$ or $N < n$. Later on, Faber and Granville modify question (B) somewhat and provide certain evidence towards it.

Nguyen explained how the abc Conjecture (well known to be a consequence of Vojta's conjectures) implies that both questions have an affirmative answer. In the function field case their result is unconditional; when using a deep result of Yamanoi (previously conjectured by Vojta), he showed that $\mathfrak{p}$ appears with multiplicity 1.

In his presentation on the radical of polynomial values, Hector Pasten pointed out that it is known that the abc conjecture gives a good lower bound for the radical of $F(n)$ in terms of n, for any fixed polynomial F without repeated factors. He further explained related results where one is interested in lower bounds in terms of F rather than n. This leads to new applications of the abc conjecture, such as counting square free values of polynomials at prime arguments (which also uses results of Green, Tao and Ziegler about arithmetic progressions of primes), and some consequences in undecidability questions (related to Hilbert's tenth problem).

Min Ru's presentation was about quantitative geometric and arithmetic results for complements of divisors. He introduced, for an effective divisor D on a smooth projective variety X, the notion of Nevanlinna constant. He then explained his proof of a quantitative result, in terms of the Nevanlinna constant of D, which extends the Subspace Theorem to D in X. He also derived the counterpart in Nevanlinna theory. The result recovers the recent important results in this direction, including the results of Corvaja-Zannier, Evertse-Ferretti, Levin, Ru etc., as well as deriving new results. The notion of "Nevanlinna constant of D" gives a unified description of the quantitative geometric and arithmetic properties of (X, D).

Amos Turchet presented a proof of the function field version of Lang-Vojta Conjecture on algebraic hyperbolicity for complements of very generic quartics in the projective plane with at most normal crossing singularities. The proof relies on a deformation argument applied to the known case for three components divisors (proved by Corvaja and Zannier) and uses a reformulation of the problem via moduli spaces of logarithmic stable maps as introduced by Q. Chen and Abramovich.

Paul Vojta himself gave a second talk, more focussed on a specific area of research, namely toric geometry and Dyson's lemma. In 1989, he proved a Dyson lemma for products of two smooth projective curves of arbitrary genus. In 1995, M. Nakamaye extended this to a result for a product of an arbitrary number of smooth projective curves of arbitrary genus, in a formulation involving an additional "perturbation divisor." In 1998, he also found an example in which a hoped-for Dyson lemma is false without such a perturbation divisor. This talk will present work in progress on eliminating the perturbation divisor by using a different definition of "volume" at the points under consideration. The proof involves toric and toroidal geometry, and this is reflected in the statement as well.

Felipe Voloch followed up his lively and heavily-debated contribution to the open problem session (described in the next section) by discussing some results and speculations about the number of rational points on curves of genus bigger than one over global fields. In particular, he described the result obtained jointly with R. Concei and D. Ulmer, where he showed that the number of rational points on (non-isotrivial) curves of fixed genus over a fixed function field can be arbitrarily large.

As grand finale to the workshop, Julie Tzu-Yueh Wang proved the rank one case of Skolems Conjecture on the exponential local-global principle for algebraic functions, and discussed its analog for meromorphic functions.

30.4 Scientific Progress Made

In addition to the various presentations, there were a great number of research collaborations that were initiated or continued at the workshop. Ekaterina Amerik and Frédéric Campana, for example, were working tirelessly on their joint project described by Amerik in her talk. McKinnon and Yongqiang Zhao also made substantial progress in their research collaboration, and in general the BIRS lounge and reading room were seldom empty during the evening, filled with workshop participants.

The most palpable evidence of scientific progress at the meeting, however, was made at the open problem session on Monday afternoon. Participants spent roughly an hour proposing interesting open questions to attack, and suggested ways of approaching their colleagues open problems (and sometimes their own!) The problems proposed, together with some of the discussion about them, were recorded and distributed to all participants of the workshop, including the two who were, at the last minute, prevented from attending by circumstances beyond their control.

Felipe Voloch opened the session by asking if most curves are hyperelliptic.

There are several senses in which this question might be interpreted.

Consider the moduli space M_g of genus g curves over $\mathbb{Q}$, and let h be a height function on M_g. Is

$$\lim_{H\to\infty} \frac{\#\{x \in M_g(\mathbb{Q}) : h(x) \leq H \text{ and } x \text{ is hyperelliptic}\}}{\#\{x \in M_g(\mathbb{Q}) : h(x) \leq H\}} = 1?$$

If so, is there a special locus on M_g whose rational points dominate this count by height? For example, the locus of points corresponding to hyperelliptic curves is of dimension $2g-1$, and the trigonal locus (curves admitting a 3 to 1 morphism to the projective line) is of dimension $2g+1$.

However, this interpretation considers two curves to be isomorphic if they are isomorphic over $\overline{\mathbb{Q}}$. What about $\mathbb{Q}$-isomorphism classes, in which curves are equivalent only if they are isomorphic over $\mathbb{Q}$? There are several ways in which one might count such classes.

First, one might count with respect to naive height in some pre-specified embedding such as a fixed pluricanonical embedding. One might also count by the conductor, or by the Faltings height.

Junjiro Noguchi's question was more technical and specific. Lang's conjecture over number fields states: If X is a projective algebraic variety defined over a number field k and $X_{\mathbf{C}}$ is Kobayashi hyperbolic, then $X(k)$ is finite. An analogue of this over function fields is as follows: Let $f : X \to C$ with a finite subset $S \subset C$ be a morphism of compact varieties with $\dim C = 1$ such that fibers $X_t = f^{-1}t$ are Kobayashi hyperbolic for $t \in C \setminus S$. Moreover, assume a boundary condition (BC) that $X|_{C \setminus S}$ is hyperbolically embedded into X along the boundary fibers $X_t, t \in S$, then the analogue of Lang's conjecture holds (Noguchi, 1985, 1992); i.e., if the set of sections of $f : X \to C$ is Zariski dense, then it is flat, $X \cong C \times X_0$, and there are only finitely many dominant maps from a fixed variety Y onto X_0.

Is it really necessary to assume (BC) or can this hypothesis be omitted? If $\dim X/C = 1$, then (BC) is not necessary.

A second question is the following. Let Y be a fixed compact complex space. Consider $(f; X)$, where X is a compact Kobayashi hyperbolic complex space and $f : Y \to X$ is a surjective holomorphic map. Is the set of such $(f; X)$ finite?

Noam Elkies asked a question more firmly rooted in Diophantine geometry. For which n are there nontrivial maps from $\mathbb{C}$ to the Fermat surface $F_n : w^n + x^n + y^n + z^n = 0$? For $n > 4$ for which the answer is "yes", what are the maps?

For all n, there are trivial maps from $\mathbb{C}$ to F_n, corresponding to lines on the surface. For $n < 4$ or $n = 4$ the surface is rational or K3, and the images of rational maps from $\mathbb{C}$ are dense. For $n > 8$ there are no nontrivial maps, by an argument involving the Wronskian; the same argument excludes nontrivial rational maps for $n = 8$.

For $n = 5$, such maps do exist. Intersect F_5 with the plane $w + x + y + z = 0$, and remove the three lines such as $w + x = y + z = 0$ to get a residual conic. Alas this conic is isomorphic with $\alpha^2 + \beta^2 + \gamma^2 = \mathbb{C}$, and hence has no rational points; still, it is a rational curve, and thus the image of a rational map from $\mathbb{C}$.

For $n = 6$, there are elliptic curves, and thus holomorphic maps, because $(x^2+x-1)^3+(x^2-x-1)^3 = 2(x^6-1)$ and $\mathbb{C}(x, \sqrt{x^2 + x - 1}, \sqrt{x^2 - x - 1})$ is a genus-1 function field. For example, there are infinitely many primitive integer solutions of $w^6 + 2x^6 + 125y^6 = 2z^6$, parametrized by an elliptic curve over $\mathbb{Q}$.

Are these maps, and their images under $\mathrm{Aut}(F_n)$, all of the nontrivial maps from $\mathbb{C}$ to F_n for $n = 5, 6$? And what is the answer for $n = 7$ and $n = 8$?

Bjorn Poonen's contribution was the following. Let X be a general genus 2 curve (say, over $\mathbb{C}$). Let $P \in X$ be a general point. Is there an unramified cover $f\colon Y \to X$ such that there is a nonconstant rational function on Y with divisor supported on $f^{-1}P$?

William Cherry returned the session more firmly to the realm of Nevanlinna theory. Let $X \to B$ be a morphism of smooth varieties such that the generic fiber is a smooth curve of genus $g \geq 2$, and let X_B^n be the n^{th} fiber power of X over B.

A theorem of Caporaso, Harris, and Mazur states that for n large enough, X_B^n dominates a variety of general type. Thus Lang's conjecture implies uniform boundedness of rational points on X: there exists $B(\mathbb{Q}, g)$ such that $\#C(\mathbb{Q}) \leq B(\mathbb{Q}, g)$ for all smooth curves of genus g defined over $\mathbb{Q}$.

Does the Caporaso, Harris, and Mazur correlation theorem have any function theoretic consequences? For example, if X is equipped with a Hermitian metric, does CHM imply some kind of uniform bound on $|f'(0)|_h$ for holomorphic maps f from the unit disc into the fibers X_b of X?

Furthermore, there are theorems in arithmetic geometry that bound the number of solutions to a Diophantine equation without also bounding the height of those solutions. Are there any function-theoretic analogues of any such theorems?

There was much discussion of these questions through the week, and definite progress has been made. In particular, one of the problems was completely solved – by Bjorn Poonen – and we are hopeful that this list of problems will inspire more work in the future.

30.5 Outcome of the Meeting

The Banff International Research Station is a terrific place to do mathematics. The location is peaceful and inspiring, the staff are efficient, friendly, and helpful, and the facilities are first class. This workshop was one of the first to be organised explicitly around Vojta's conjectures, and was a total success, including the planning of a meeting in 2017 on the same theme by Aaron Levin, David McKinnon, and Thomas Tucker. There has already been success in attacking the problems from the open problem session, and several research collaborations were started or significantly continued during the week. A complete success.

Participants

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Bibliography

[1] Adamczewski, B. and Bugeaud, Y.,On the complexity of algebraic numbers I, Ann. of Math. (2), to appear.

[2] Adamczewski, B., Bugeaud, Y., and Luca, F., Sur la complexité des nombres algébriques, C. R. Math. Acad. Sci. Paris **339** (2004), 11-14.

[3] Autissier, P., Sur la non-densité des points entiers, Duke Math. J. **158** (2011), no. 1, 13-27.

[4] Corvaja, P., Zannier, U., On integral points on surfaces, Ann. of Math. (2) **160** (2004), 705-726.

[5] Dyson, F., The approximation to algebraic numbers by rationals, Acta Mathematica **79** (1947), 225-240. doi:10.1007/BF02404697

[6] Levin, A., Generalizations of Siegel's and Picard's theorems, Ann. of Math. (2) **170** (2009), no. 2, 609-655.

[7] Liouville, Nouvelle démonstration d'un théorème sur les irrationnelles algébriques, Comptes rendus hebdomadaires des séances de l'Académie des sciences, Tome XVIII, séance de 20 mai 1844, 910–911.

[8] McKinnon, D., Vojta's Conjecture implies the Batyrev-Manin Conjecture for K3 surfaces, Bull. Lond. Math. Soc. **43** (2011), no. 6, 1111–1118.

[9] Nevanlinna, R., Le Théorème de Picard-Borel et la théorie des fonctions méromorphes, Chelsea, 1929.

[10] Ridout, D., The p-adic generalization of the Thue-Siegel-Roth theorem, Mathematika **5** (1958), 40-48. doi:10.1112/s0025579300001339

[11] Roth, K. Rational approximations to algebraic numbers, Mathematika **2** (1955), 1-20, 168. doi:10.1112/S0025579300000644

[12] Schmidt, W., Diophantine Approximation, Lecture Notes in Mathematics **785**, Springer-Verlag, Berlin, 1980.

[13] Schlickewei, H. P., The p-adic Thue-Siegel-Roth-Schmidt theorem, Archiv der Math. **29** (1977), 267–270.

[14] Siegel, C., Approximation algebraischer Zahlen, Mathematische Zeitschrift **10** (3) (1921), 173-213. doi:10.1007/BF01211608

[15] Thue, A., Über Annäherungswerte algebraischer Zahlen, Journal für die reine und angewandte Mathematik **135** (1909), 284-305. doi:10.1515/crll.1909.135.284

[16] Vojta, P., Diophantine Approximations and Value Distribution Theory, Lecture Notes in Mathematics **1239**, Springer-Verlag, New York, 1987.

[17] Vojta, P., Part III of Arithmetic geometry, Lectures from the C.I.M.E. Summer School held in Cetraro, September 1015, 2007. Edited by Pietro Corvaja and Carlo Gasbarri. Lecture Notes in Mathematics **2009**, Springer-Verlag, Berlin; Fondazione C.I.M.E., Florence, 2011.

Chapter 31

Sparse Representations, Numerical Linear Algebra, and Optimization (14w5003)

October 5 - 10, 2014

Organizer(s): Gitta Kutyniok (Technische Universität Berlin), Michael Saunders (Stanford University), Stephen Wright (University of Madison-Wisconsin), Özgur Yilmaz (University of British Columbia)

31.1 Overview of the Field

Sparse representations of functions and data have become crucial for a wide range of applications in technology and science, such as data analysis, imaging, and the construction of efficient solvers for ODEs and PDEs. With many important recent developments in frame theory and compressed sensing, the understanding of the underlying mathematics has grown substantially, and connections to other mathematical fields have started to evolve. Examples include the use of compressed sensing techniques for model reduction in numerical linear algebra, novel optimization algorithms for compressed sensing and image processing problems, and the design of regularization functions that yield the desired type of sparsity in the solutions of reconstruction problems.

The key idea of sparsity is that functions and signals arising naturally in many contexts can be described using only a small number of significant terms in a suitable basis or frame. This observation lies at the heart of many lossy compression techniques such as JPEG or MP3. Interestingly, sparsity is useful not only for compression purposes, but also in the design of sensing and sampling techniques for capturing signals. Under suitable conditions, sparse high-dimensional signals can be recovered efficiently from what would previously have been considered a highly incomplete set of measurements. This discovery is the basis of the field of compressed sensing. It has led to a paradigm change in information theory and has caused great excitement across many areas of science and engineering.

One key to the success of compressed sensing in many application areas is the generation of data-dependent sparsifying systems, customarily termed "dictionary learning." Because of the highly complex nature of this problem, the mathematical theory is in the early stages of development, and fundamental new ideas are still needed. A key property that ensures the occurrence of sparse expansions is the redundancy of these systems—i.e., these are complete systems that are linearly dependent. This is the focus of study in frame theory, which examines various aspects of redundancy as a mathematical concept. Frame theory has already impacted the area of applied harmonic analysis and sparse approximation; yet we are only beginning to grasp a fundamental understanding of redundancy measures.

Numerical linear algebra provides the mathematical foundation for stable computational algorithms based on matrix operations, with a myriad of applications ranging from signal and image processing, optimization, through data mining and model reduction, to ODE and PDE solvers. Indeed, it can be said that numerical linear algebra is at the foundation of computational science. Not only is efficient linear algebra important in algorithms for solving compressed sensing and frame analysis problems, but the fields interact in another way: Compressed sensing principles can be used to reduce extreme size linear systems that result from real-world applications, to the point where they become tractable for classical linear algebra algorithms. The first studies in linear algebra model-reduction using compressed sensing have just appeared. There is a world of new possibilities to be explored in this area.

Efficient algorithms for solving the optimization formulations of sparse approximation problems have been an area of intense research during the past five years. Indeed, Candés and Tao's foundational discovery in compressed sensing was that a seemingly intractable formulation of the sparse reconstruction problem could under certain assumptions be replaced by an equivalent convex (and highly structured) optimization formulation. This observation, which lent theoretical support to the use of ℓ_1 and total-variation functions as devices for inducing desired structure in the solutions of optimization problems, opened the door to a burst of work on optimization algorithms that exploit the specific structure of the sparse reconstruction problems. Cross-fertilization with other areas, particularly computational statistics and machine learning, has led to an exciting body of interdisciplinary work that has great potential for continued growth and development.

31.2 Recent Developments and Open Problems

The subject of the workshop is rife with interesting open problems, the scope of which only seems to grow as the area is developed. We mention several themes along these lines that were addressed in the workshop.

- As the size and complexity of data sets increases, the demands on algorithms continue to grow. There is a continuing need for algorithmic innovations to tackle enormous problems efficiently; we cannot rely solely in improvements in computational hardware. This issue arose in many guises during the meeting: Herrmann's massive geophysical data sets; Balzano's real-time processing of structure-from-motion data; Willett's use of online learning techniques; and the use of randomized algorithms, hierarchical matrix representations, and new perspectives on preconditioning in linear algebra problems of extreme scale.

- The theoretical and algorithmic breakthroughs in sparse recovery problems during the past decade have been astonishing, and several important practical applications have been identified. But much remains to be done in making sparse recovery truly practical across the full range of potential applications. Issues that need to be addressed include weakening of the too-strong assumptions on incoherence and restricted isometry that underlie the effectiveness of convex relaxations, the fact that observations are quantized, the need to calibrate uncertain sensing matrices as part of the recovery process, the rapid degradation of recovery algorithms as noise levels and observational coherence increase, and the extremely large size and incompleteness of some data sets. Algorithms and formulations need to be made more robust and self-calibrating while maintaining their efficiency across broader regimes. Devices such as dimension reduction and nonconvex formulations must be employed where relevant.

- Phase retrieval—the recovery of phase information about a complex signal from measurements of its magnitude—was proposed 25 years ago as one of the original grand challenge problems in computational science. It is a central problem in crystallography, and thus in structural biology. The obvious optimization formulations of the problem are notoriously nonconvex. But we have seen this before: sparse recovery problems are intractable in their obvious formulations, but yield to powerful convex relaxations in certain regimes. Recent works have explored connections between sparse reconstruction techniques and phase retrieval, and have shown that it is possible to find global minima of nonconvex formulations of the latter problem in some circumstances. It is likely that much more can be said by bringing the full range of experience over the past decade with sparse reconstruction to bear on phase retrieval. Further successes along these lines may have an enormous impact.

- A great deal has been accomplished with convex formulations, which can be solved efficiently with optimization algorithms. But we may be reaching the limits of this methodology: It is increasingly apparent that nonconvex formulations are more powerful in many settings, and more broadly applicable. (Even in the most elementary formulations of variables selection in statisical regression, nonconvex penalties give better results that the popular ℓ_1 penalty over a wide range of problems.) It has been noted, however, that nonconvexity does not necessarily connote intractability. Some nonconvex optimization formulations have global minimizers that are easily found by standard algorithms. In others, clever presolving techniques or algorithmic innovations yield either the global minimizer or provably accurate approximations to it. We lack a great deal of understanding about this phenomenon of seemingly "tractable" nonconvex formulations. Is there some underlying convex structure, perhaps in a higher-dimensional embedding? If so, how can we recognize this structure, characterize the problems that have this structure, and exploit it in algorithms? Several talks at the meeting touched on this theme, including Strohmer's keynote, and Chandrasekaran's relaxation hierarchy for signomial polynomials.
- An enduring mystery in the current burst of activity in "big data" is the unreasonable effectiveness of deep learning (multilayer neural networks) in speech, vision, and many other applications of machine learning. At least one speaker at the meeting (Mixon) discussed an interpretation of deep learning in terms of scattering transforms. It is quite possible that frame theory can provide valuable insight into this topic, which is one of the hottest topics in data science today.

31.3 Presentation Highlights

The talks consisted of four longer keynote talks, with each presenting an introduction to one of four research areas: compressed sensing, frame theory, numerical linear algebra, and optimization. Twenty shorter talks presented a bouquet of topics, most of which were related to employing sparsity as prior information.

Below, we discuss the presentations according to their specific focus, each time starting with the keynote talk. Most presentations covered at least two of our four targeted areas.

31.3.1 Compressed Sensing

Thomas Strohmer (**Keynote Talk**) presented an introduction to compressed sensing and pointed out probable future directions for this research area. In the first part, he discussed how compressed sensing provides a methodology to solve the problem of reconstructing a sparse signal exactly from an underdetermined system of linear equations in a computationally efficient manner via convex optimization. He presented the key ingredients of compressed sensing and extensions such as matrix completion, incoherence, and various notions of sparsity. In the second part, which focussed on current challenges and possible opportunities, he discussed the chasm between discrete and continuous models; self-calibrating compressed sensing and uncertainty mitigation; and fast and provable nonconvex algorithms related to sparsity.

Laura Balzano considered low-dimensional linear subspace approximations to high-dimensional data, which have applications when missing data is inevitable because of difficulties in collecting it. She described recent results on estimating subspace projections from incomplete data, including convergence guarantees and performance of the GROUSE algorithm (Grassmannian Rank-One Update Subspace Estimation) [1]. She explained the relationship between GROUSE and an incremental SVD algorithm, and presented results for GROUSE on problems in computer vision.

Felix Herrmann focussed on the area of exploration seismology and its formulation as a PDE-constrained inverse problem. The main challenges are extremely large data sets ($\approx 10^{15}$ measurements), large sets of unknowns ($\approx 10^9$ variables), and the hyperbolic PDEs themselves. He presented two competing approaches developed by his group, respectively based on optimization and compressed sensing [18, 13]. Both approaches utilize randomized dimension-reduction techniques to reduce the number of PDE solves, but they differ in how they control the errors.

Rayan Saab focussed on compressed sensing and frame theory. He considered the question of reconstruction from quantized compressed sensing measurements—a natural question because in the digital era, an acquisition process is typically followed by quantization. He first discussed a novel approach to handle quantization of frame coefficients by a post-processing step consisting of a discrete random Johnson-Lindenstrauss embedding of the integrated bit-stream. Near-optimal approximation accuracy as a function of the number of bits used can be shown for this method, and it holds for a large class of frames including smooth frames and random frames [11]. He then showed that the same encoding scheme applied to quantized compressed sensing measurements yields near-optimal approximation accuracy as a function of the bit-rate. A different reconstruction scheme is needed but it still uses convex optimization.

Jared Tanner focussed on algorithmic aspects of compressed sensing and matrix completion. He presented a novel algorithm that balances low per iteration complexity with fast asymptotic convergence. He proved numerically that this approach has faster recovery time than any other known algorithm, both for small-scale problems and for massively parallel GPU implementations. His method, named conjugate gradient iterative hard thresholding [2], is based on the classical nonlinear conjugate gradient algorithm.

Vladimir Temlyakov discussed greedy sparse approximation in Banach spaces with respect to redundant dictionaries [9]. He considered the design and analysis of such greedy methods, including Lebesgue-type inequalities to measure efficiency. He introduced a generalization of the RIP concept in a Hilbert space to dictionaries in a Banach space, and analyzed the Weak Chebyshev Greedy Algorithm—a generalization of the Orthogonal Greedy Algorithm (Orthogonal Matching Pursuit).

Rachel Ward focussed on matrix completion. Former results in this area typically required that the underlying matrix satisfy a restrictive structural constraint on its row and column spaces, and the subset of elements is then sampled uniformly at random. She showed that any $n \times n$ matrix of rank r can be exactly recovered from as few as $O(nr \log^2 n)$ randomly chosen elements, provided the random choice follows a specific biased distribution based on leverage scores of the underlying matrix. She proved that this specific form of sampling is in a certain sense nearly necessary, and presented three ways the results can be used when the leverage scores are not known in advance [8].

Rebecca Willett studied the problem of tracking dynamic point processes on networks, which is not a classical compressed sensing problem but bears some resemblance. Cascading chains of interactions are a salient feature of many real-world social, biological, and financial networks. Typically, only individual events associated with network nodes can be observed, usually without knowledge of the underlying dynamic network structure. Rebecca asked the question of tracking how such events within networks influence future events. She uses techniques from online learning frameworks and a multivariate Hawkes model to encapsulate autoregressive features of observed events within a network. With no prior knowledge of the network, her method performs almost as well as would be possible with complete knowledge [10].

31.3.2 Frame Theory

Dustin Mixon (**Keynote Talk**) presented an introduction to frame theory— the study of overcomplete yet stable expansions. One focus is to design frames for diverse applications, each with its own evaluation criteria (tightness, symmetry, incoherence, fast transforms, or signal model representation). Applications include time-frequency analysis, compression, and machine learning.

Pete Casazza discussed his work on the problem of phase retrieval: recovery of a vector from the absolute values of its inner products against a family of measurement vectors. The problem has been well studied in mathematics and engineering. A generalization exists in engineering: recovery of a vector from measurements consisting of norms of its orthogonal projections onto a family of subspaces. Pete provided several characterizations of subspaces that yield injective measurements—hence phase retrieval is potentially possible—and through a concrete construction proved that phase retrieval in this general case can be achieved with $2M-1$ projections of arbitrary rank [3]. He also raised and provided (partial) answers to questions on the minimal number of subspaces to have injectivity and how closely this problem compares to the usual phase retrieval problem with families of measurement vectors.

31.3.3 Numerical Linear Algebra

Daniel Kressner (**Keynote Talk**) presented a survey about the role of sparsity and low rank in numerical linear algebra. He pointed out that one of the key drivers of developments in numerical linear algebra has traditionally been the need for solving large-scale linear systems and eigenvalue problems. These arise naturally from finite difference or finite element discretizations of partial difference equations. The matrices involved are typically sparse, suggesting Krylov subspace methods and sparse direct solvers. Other types of data-sparsity have also gained importance, such as the low-rank structure of hierarchical matrices and hierarchically semi-separable matrices. Exploiting approximate sparsity in the desired solution is another direction of research that links numerical linear algebra with other disciplines, especially optimization.

Felix Krahmer presented a randomized algorithm for approximating matrix-vector multiplication, with the goal of computing dictionary representations. The algorithm makes heavy use of approximate spherical designs, and its proof of performance is based on Johnson–Lindenstrauss projections.

Dominique Orban spoke on linear algebra for matrix-free optimization. Sequential quadratic programming, augmented Lagrangian, and interior-point methods all need to solve symmetric saddle-point linear systems, which become symmetric quasi-definite with the help of regularizaiton. He discussed different forms of the equations for computing search directions in optimization, and iterative methods that exploit their structure.

Fred Roosta-Khorasani focussed on Monte-Carlo methods for the estimation of the trace of an implicit matrix A (one that is known only via matrix-vector products). In many applications, A is symmetric positive semi-definite, and the trace is estimated by averaging quadratic forms of A with random vector realizations from a suitable probability distribution. He focussed on the Gaussian distribution and derived bounds on the number of matrix-vector products required to guarantee a probabilistic bound on the relative error, revealing direct connections between the performance of the Gaussian estimator, the rank of the matrix, and its stable-rank [16].

Martin Stoll studies problems from PDE-constrained optimization in which controls with a certain sparsity are preferred. In his approach, in addition to the classical sparsity term a directional sparsity term is added. His talk focussed on the development of preconditioners for saddle-point systems and their use within Krylov subspace solvers. Typically this requires robust approximations to the relevant Schur complement.

Zdeněk Strakoš and Jörg Liesen gave a sequence of two talks on the general topic of sparsity, local and global information in numerical solution of PDEs. They first noted that in the finite element method (FEM) for discretizing partial differential equations (PDEs), the finite-dimensional piecewise polynomial approximation subspaces are generated using locally supported basis functions that typically vanish on all but a small number of elements determining the decomposition of the domain. This leads to sparsity in the matrix representation of the discretized operator. When iterative methods (such as Krylov subspace methods) are applied to solve the resulting algebraic problem, sparsity of the discretized matrix does not automatically mean an advantage, and the matter should be considered within the context of the original infinite-dimensional mathematical model. Normally, a transformation (preconditioning) of the discretized problem is needed to assure fast convergence. Preconditioners incorporating coarse space information (such as multilevel preconditioners or domain decomposition techniques) are often efficient because they handle naturally the global exchange of information between various parts of the domain. The key point of this talk was the interplay between the local discretization and global algebraic computation. The speakers interpret algebraic preconditioning as transformation of the discretization basis and simultaneous change of the inner product in the associated function space. Moreover, they compare the distribution of the algebraic and discretization errors over the domain, and interpret the algebraic error as a possible change of the discretization basis [12, 14].

Jean-Philippe Vert spoke on the introduction of new matrix norms for structured matrix estimation. Non-smooth convex penalties are currently state-of-the-art for estimating sparse models through convex optimization procedures such as the lasso. He showed that a norm introduced by Xiao, Zhou, and Wu (2010) is an atomic norm that is optimal in a certain sense for estimating matrices with orthogonal columns. He then showed that the (k, q)-trace norm, a new convex penalty for estimating low-rank matrices with sparse factors, outperforms the L_1 norm and other norms, especially for sparse principal component analysis [15].

31.3.4 Optimization

Michael Friedlander (**Keynote Talk**) spoke about algorithms for sparse optimization. He described the fundamental building blocks and surveyed some of the main research directions in this area, noting that convex optimization plays a key role.

Sasha Aravkin presented a general variational framework that allows efficient algorithms for denoising problems, where a functional is minimized subject to a constraint on fitting the observed data. The framework applies to vector recovery (sparse optimization) and matrix recovery (matrix completion and robust PCA). He discussed performance aspects and noted that the efficiency of his approach relies on efficient first-order solvers. For matrix recovery, novel ideas in factorized and accelerated first-order methods were incorporated into the variational framework.

Coralia Cartis was concerned with line-search methods—an important class of algorithms for unconstrained non-convex optimisation that rely on approximately computing a local descent direction and a step along this direction in such a way that sufficient decrease is achieved. To ensure that sufficient decrease is possible, the direction must satisfy certain requirements. In large-scale applications, meeting the requirements may be prohibitively expensive. Coralia presented global convergence rates for a line-search method based on random models and directions whose quality is ensured only with certain probability. In the convex and strongly convex case, she could improve those results. She finished by presenting a probabilistic cubic regularisation variant that allows approximate probabilistic second-order models and showed improved complexity bounds compared to probabilistic first-order methods.

Venkat Chandrasekaran focussed on signomial programs (SPs): optimization problems consisting of an objective and constraints specified by signomials (sums of exponentials of linear functionals of a decision variable). Such programs are non-convex optimization problems in general, but some instances of NP-hard problems can be reduced to SPs. He described a hierarchy of convex relaxations that provide successively tighter lower bounds on the optimal value in SPs. The approach relies on the observation that the relative entropy function provides a convex parametrization of certain sets of globally nonnegative signomials with efficiently computable nonnegativity certificates. The sequence of lower bounds converges to the global optimum for broad classes of SPs [6].

Mark Schmidt proposed the stochastic average gradient (SAG) method for optimizing the sum of a finite number of smooth convex functions. As for stochastic gradient methods, the iteration cost is independent of the number of terms in the sum. By incorporating a memory of previous gradient values, he improves the convergence rate of SAG from $O(1/k)$ to a linear convergence rate of the form $O(p^k)$ for some $p < 1$. Some good practical properties are achieved. The method supports regularization and sparse datasets, it allows an adaptive step-size and has a termination criterion, it allows mini-batches, and its performance can be improved by non-uniform sampling [17].

Ewout van den Berg presented a hybrid quasi-Newton projected-gradient method for the optimization of convex functions over a polyhedral set. He described applications such as the lasso, bound-constrained optimization, and optimization over the simplex.

31.4 Scientific Progress Made and Outcome of the Meeting

The meeting proved very successful. Participants from the four different communities interacted closely as planned. Many participants mentioned to us that they greatly enjoyed the excellent talks, the fruitful discussions, the inspiring atmosphere at BIRS, and the tireless support of the BIRS staff. Several asked us if another meeting of this type could be held, with invited representatives from the same four research areas.

Let us summarize the impact of our meeting.

- Initiation of communication between the four research areas

  A main goal of our workshop was to invite people from the four research areas of compressed sensing, frame theory, numerical linear algebra, and optimization, with sparse representations being the common factor. This BIRS workshop was a unique opportunity to initiate a fertile discussion among those representatives. The four keynote talks indeed provided excellent introductions to the respective research areas. These and the shorter talks led to many vivid debates, showing that all groups highly benefitted from being exposed to different methodologies and ideas. We can report that these discussions led to several new collaborations within the four groups.

- Intensification of new directions in the field

  Various new directions both theoretical and applied were presented during talks and vividly discussed afterwards. One main new direction is the utilization of randomized algorithms for numerical linear algebra problems such as matrix-vector multiplication, but related to sparsity. This direction requires a close interaction among essentially all four research areas. It is currently in its beginning stage, and far more developments can be expected in the near future. As further directions, also at the beginning stage, we especially mention a general framework for PDE solvers that balances discretization aspects and numerical linear algebra considerations such as preconditioning (Zdeněk Strakoš and Jörg Liesen). The workshop was a unique opportunity to discuss the most recent results and stimulate these directions.

- Discussion of interactions across research areas

  Since a main goal of the workshop was to bring together the aforementioned key areas required for sparsity methodologies in data sciences, we put a particular focus on interactions across research areas. The four keynote talks were one main approach to implement improved each participant's understanding of the other three areas. Another approach was two discussion sessions, one of which was about notational issues. It turned out that it is indeed a major obstacle for many researchers to read publications from other areas. We then assembled a collection of notational problems in the sense of notations used in the other areas with a very different meaning. This made everybody aware of the fact that notation has to be carefully thought through, especially when aiming to have a readership in a different research area.

- Discussion of methodologies

  Several talks made the audience aware of methods being present in other areas that might be useful in their own work as well. One example was the range of optimization approaches for sparse recovery presented by members of the optimization community such as Michael Friedlander and Ewout von den Berg, which will be highly beneficial for participants working in compressed sensing. The talk by Thomas Strohmer discussed various obstacles that are still present in compressed sensing, such as self-calibrating compressed sensing, which, as he pointed out, can only be overcome by methodologies from other areas. Also, many problems in frame theory can be regarded as problems in numerical linear algebra, yet those two communities almost never interact. The workshop permitted open discussion of methods that could assist other communities, such as the diverse preconditioners described by Daniel Kressner.

- Introduction of young scientists

  Several of our participants were young and very promising scientists, such as Ewout von den Berg, Martin Stoll, and even Dustin Mixon. The workshop gave them an exceptional chance to present themselves and get in contact with the leading researchers not only in their own field but also in the three other research areas, and also to broaden their horizon. After the workshop, we received excited feedbacks from this group, voicing the general opinion that this was a unique opportunity.

- Manifestation of the future direction of the field

  Since this workshop brought together the main leaders in the four research areas of compressed sensing, frame theory, numerical linear algebra, and optimization with sparse representations, with particular focus on the common element of sparse representations, it presented the chance to debate and perceive the future directions of this field. Intense discussions took place right after most talks, as well as during the two scheduled general discussion sessions. Interesting open problems and possible future research directions came up. We therefore expect this workshop to have a signal effect that will significantly influence the future research in this field, in particular by bringing the four research areas more closely together.

As particular topics that came up in the discussion session we mention the following. Large-scale computations are still a major topic, as indicated in Felix Herrmann's talk. This led to a vibrant discussion of how methods can be developed to solve such problems in an efficient and robust (to noise) way. In particular, Felix met with several linear algebra people to derive an approach that will be greatly beneficial for his truly huge problems. On the theoretical side, the question arose of to what extent Hilbert space methods should be extended to the Banach space setting, to allow a more general viewpoint and to include L^p spaces in a natural way.

Participants

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Bibliography

[1] L. Balzano, B. Recht, and R. Nowak, High-dimensional matched subspace detection when data are missing, Proceedings of IEEE International Symposium on Information Theory (ISIT) (2010), 1638–1642.

[2] J. Blanchard, J. Tanner, and K. Wei, Conjugate Gradient Iterative Hard Thresholding: observed noise stability for compressed sensing, IEEE Transactions on Signal Processing. Accepted (2014).

[3] J. Cahill, P.G. Casazza, J. Peterson, and L. Woodland, Phase retrieval by projections, arXiv preprint, arXiv:1305.6226 [math.FA]

[4] E. Candès and B. Recht, Exact matrix completion via convex optimization, Foundations of Computational Mathematics **9** (2009), 717–772.

[5] E. Candès, J. Romberg, and T. Tao, Robust uncertainty principles: Exact signal reconstruction from highly incomplete frequency information, IEEE Transactions on Information Theory **52** (2006), 489–509.

[6] V. Chandrasekaran and P. Shah, Relative entropy relaxations for signomial optimization, arXiv preprint, arXiv:1409.7640 [math.OC]

[7] S. S. Chen, D. L. Donoho, and M. A. Saunders, Atomic decomposition by basis pursuit, SIAM Journal on Scientific Computing **20** (1998), 33–61.

[8] Y. Chen, S. Bhojanapalli, S. Sanghavi, and R. Ward, Completing any low-rank matrix, provably, arXiv preprint, arXiv:1306.2979 [stat.ML]

[9] V. N. Temlyakov, Sparse approximation and recovery algorithms in Banach spaces, Forum of Mathematics, Sigma, **2** (2014), e12 doi:10.1017/fms.2014.7

[10] E.C. Hall and R. M. Willet, Tracking dynamic point processes on networks, arXiv preprint arXiv:1409.0031 [stat.ML]

[11] M. Iwen and R. Saab, Near-optimal encoding of finite frame expansions, Journal of Fourier Analysis and Applications **19** (2013), 1255–1273.

[12] J. Màlek and Z. Strakoš, Preconditioning and the Conjugate Gradient Method in the Context of Solving PDEs. SIAM Spotlights Series, SIAM, Philadelphia, 2014.

[13] H. Mansour, F. J. Herrmann, and Ö. Yılmaz, Improved wavefield reconstruction from randomized sampling via weighted one-norm minimization, Geophysics **78** (2013), V193–V206.

[14] J. Papež, J. Liesen, and Z. Strakoš, Distribution of the discretization and algebraic error in numerical solution of partial differential equations, Linear Algebra and Its Applications **449** (2014), 89–114.

[15] E. Richard, G. Obozinski, and Jean-Philippe Vert, Tight convex relaxations for sparse matrix factorization, arXiv preprint, arXiv:1407.5158 [stat.ML]

[16] F. Roosta-Khorasani and U. Ascher, Improved bounds on sample size for implicit matrix trace estimators, arXiv preprint, arXiv:1308.2475 [cs.NA]

[17] M. Schmidt, N. Le Roux, and F. Bach, Minimizing finite sums with the stochastic average gradient, arXiv preprint, arXiv:1309.2388 [math.OC]

[18] T. van Leeuwen and F. J. Herrmann, 3D frequency-domain seismic inversion with controlled sloppiness , SIAM Journal on Scientific Computing **36** (2014), S192–S217.

[19] S. J. Wright, R. D. Nowak, and M. A. T. Figueiredo, Sparse reconstruction by separable approximation, IEEE Transactions on Signal Processing **57** (2009), 2479–2493.

Chapter 32

Optimal Cooperation, Communication, and Learning in Decentralized Systems (14w5077)

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The problem of optimal decision-making in decentralized systems arises in different application domains, including smart grids, cyber-physical systems, communication networks, machine learning, and information processing in organizations. Traditionally, these application domains have been investigated by different research communities, and each community has developed its own set of mathematical tools and theories to address optimal decentralized decision making. This workshop was the first of its kind, where researchers from these different communities were given an opportunity to be exposed to new ideas, angles, and perspectives on decentralized decision-making.

32.1 Overview of the Field, Recent Developments and Open Problems

Cooperation and coordination in decentralized systems. In decentralized systems, no decision maker (DM) knows the information known to all other DMs, yet all DMs must cooperate to achieve a common, system-wide objective. Multiple approaches have been used in the literature to achieve cooperation and coordination; they include: (a) Identifying optimality conditions so that a solution can be obtained by all DMs based on their local information (either using mathematical programming or dynamic programming); (b) Identifying projected sub-problems that are solved at each DM and iterating after exchanging information (either through a pricing mechanism or through explicit data communication subject to constraints) to reconcile the results.

Role of communication in decentralized systems. Communication or information-exchange is an important aspect of decentralized decision making because of the following: (a) Communication generates common knowledge among DMs. Such a common knowledge is useful for dynamic programming (see the previous bullet) and learning (see the next bullet). (b) When the DMs have an incentive to communicate, the global optimization problem is usually non-convex; while if such an incentive is absent, e.g., in static and partially nested teams, the global optimization problem may be convex. Thus, on one hand, the incentive to communicate makes the decentralized optimization problem harder. On the other hand, the presence of communication sometimes facilitates a dynamic programming decomposition, e.g., in partial history sharing. (c) Economic and technological constraints often impose a restriction on information exchange, which in turn imposes restrictions on the solution approaches.

Learning in decentralized systems. When the DMs communicate, they exchange information in order to reduce their uncertainty. This process of uncertainty reduction is generically referred to as learning. Existing research on learning in decentralized systems is along two complementary directions: (a) Bayesian learning (and its variants), which models the process by which the DMs form and refine their probabilistic beliefs about other DMs (including their knowledge, their strategies, etc.) and about the overall state of nature relevant to the problem at hand, assuming that all DMs conform to certain axioms of rational behavior; and (b) Non-Bayesian learning or learning by boundedly rational agents, which model the process of learning in repeated or sequential situations in the presence of various resource and complexity constraints. Bayesian learning describes the situation in which the DMs know the system model, so all the uncertainty arises due to the presence of other DMs, as well as due to local nature of communication; by contrast, bounded rationality deals with situations in which the system model is not completely known, so the DMs need to learn the model based on their local observations.

32.2 Presentation Highlights

Each day of the workshop featured several 40-minute technical talks, as well as several 50-minute overview talks. Most talks on each day were centered around one broad theme.

32.2.1 Day 1: Learning, stability, and games in multiagent Markovian environments

Overview talk – VIKRAM KRISHNAMURTY: *Social learning and active sensing.* Vikram opened up the workshop with an overview talk about structural results for partially observed Markov decision processes in multi-agent systems when individual agents perform *social learning*, i.e., they aggregate their private noisy signals about the global system state with the signals they receive from their neighbors in the network. He illustrated the key ideas using three specific examples: (1) constrained optimal social learning problem, where the onset of herding (i.e., agents exhibiting preference for nearly the same action) is delayed by agents sharing full information; (2) change detection when individual agents perform social learning; and (3) some recent (but incomplete) work by Vikram and collaborators on social networks where diffusion approximations are made resulting in a controlled Markovian system.

TARA JAVIDI: *Noisy Bayesian active learning.* Following the theme of learning in a Markovian environment, Tara discussed the problem of noisy Bayesian active learning, where we are given a class of functions and a sample space. An unknown function in this class assigns a label to any sample in the sample space, and the result of a label query on any sample is corrupted by independent stochastic noise. The goal is to identify the function that generates the labels with high reliability using as few label queries as possible, by selecting the queries adaptively in a strategic manner. Previous work on Bayesian active learning has revolved around a specific algorithm, the so-called Generalized Binary Search (and its variants for the noisy case), and provided upper bounds on the number of queries required by these sampling strategies. Tara first presented a converse result, characterizing the smallest number of queries that must be made by *any* adaptive algorithm as a function of the structure of the function class, the noise model, and the required reliability. The proof of this result relied on a blend of techniques from statistics, stochastic control theory, and information theory. She then revisited Generalized Binary Search and similar schemes in light of the converse result and showed that, in general, these schemes are suboptimal. She presented and analyzed an alternative strategy for sample collection based on DeGroot's notion of information utility: at each time step, this strategy queries the label of a sample which maximizes the so-called Extrinsic Jensen–Shannon divergence, which was recently introduced by Tara and her collaborators.

Overview talk – TAMER BAŞAR: *Stochastic dynamic games and intricacy of information structures.* In spite of decades-long past research activity on stochastic dynamic/differential games, there still remain some outstanding fundamental questions on the existence, uniqueness, and characterization of non-cooperative equilibria when players have access to noisy state information. Tamer's overview talk identified these questions, along with the underlying challenges, and addressed a number of them within specific contexts. One of the questions is related to the notion of certainty equivalence (CE), which is well-understood in single-player games (that is, stochastic control problems) but not in stochastic dynamic games, even if all players receive state information through a common (noisy) channel. Following a general overview of CE in stochastic control, Tamer discussed it in the context of two-player zero-sum stochastic differential/dynamic games (ZSSDGs) when the players have access to state information through a common noisy measurement channel — in both continuous time and discrete time. For the discrete-time case, the channel is also allowed to fail sporadically according to an independent Bernoulli process, leading to intermittent loss of measurements, and the players are allowed to observe past realizations of this process. Within this framework, Tamer presented a complete analysis of a parametrized two-stage stochastic dynamic game in terms of existence, uniqueness and characterization of saddle-point equilibria (SPE). Tamer then used the insight provided by the analysis of this game to obtain SPEs for three classes of differential/dynamic games: (i) linear-quadratic-Gaussian (LQG) zero-sum differential games with common noisy measurements, (ii) discrete-time LQG zero-sum dynamic games with common noisy measurements, and (iii) discrete-time LQG zero-sum dynamic games with intermittently missing perfect state measurements. In all of these cases, CE is a generalized notion, requiring two separate filters for the players, even though they have a common communication channel. There was a brief discussion of some extensions, such as (i) multi-player ZSSDGs, with teams playing against teams, where agents in each team do not have identical information, and (ii) nonzero-sum stochastic differential games, with asymmetric information among the players. The overview talk was concluded with a discussion of the mean-field approximation and the simplifications it brings at both the conceptual and analytical levels.

ALI BELABBAS: *Hurwitz graphs: algorithmic and probabilistic aspects.* Design of distributed control systems involves careful balancing of the complexity of the information structure against such desirable properties as stability, controllability, etc. Ali presented a mathematical formalization of this trade-off in the context of continuous-time distributed linear systems. The information structure (communication pattern between agents) in such a system is described by the locations of the nonzero entries in the system matrix. The question is: given the desired locations of the nonzero entries, does there exist at least one matrix that conforms to a desired information structure and is also *Hurwitz stable* (all of its eigenvalues have strictly negative real parts). This motivates the definition of a *Hurwitz space* as a vector space of square matrices that contains Hurwitz matrices. The talk focused on the design of Hurwitz vector spaces. After a brief overview of the main known results in the area, Ali presented new sufficient conditions guaranteeing that a vector space containing a Hurwitz subspace is itself Hurwitz. In the second part, he provided polynomial-time algorithms based on these sufficient conditions. He concluded the talk by discussing probabilistic aspects of Hurwitz spaces, where the locations of nonzero entries are chosen at random, and connected the emergence of Hurwitz property to monotone threshold phenomena in random graphs.

MICHEL DE LARA: *Smart power systems, renewable energies and markets: the optimization challenge.* Michel's talk was focused on concepts, models, and mathematical and numerical methods allowing to formalize and to treat issues concerning sustainability and precaution in the management of natural resources and of the environment. Specifically, he discussed mathematical concepts, such as controlled dynamical systems in discrete time, equilibrium and stability, viability and invariance, intertemporal optimality, stochastic and robust control; specific analysis and design methods, such as linearization, maximum principle, and dynamic programming; and simulation tools and algorithms. Throughout the talk, he focused on examples related to the exploitation of renewable or exhaustible resources and to greenhouse gases mitigation and proposed a common framework of sequential decision-making in this context.

SEAN MEYN: *Randomized policies for mean field control with application to automated demand response.* Sean's talk continued with the same theme as Michel de Lara's talk. Renewable energy sources such as wind and solar power have a high degree of unpredictability and time-variation, which makes balancing demand and supply challenging. One possible way to address this challenge is to harness the inherent flexibility in demand of many types of loads. At the grid-level, ancillary services may be seen as actuators in a large disturbance rejection problem. Sean argued that a randomized control architecture for an individual load can be designed to meet a number of objectives: The need to protect consumer privacy, the value of simple control of the aggregate at the grid level, and the need to avoid synchronization of loads that can lead to detrimental spikes in demand. He described new design techniques for randomized control of such systems, following a three-step program:

1. A parameterized family of average-reward MDP models is introduced whose solution defines the local randomized policy. The balancing authority broadcasts a common real-time control signal to the loads; at each time, each load changes state based on its own current state and the value of the common control signal.
2. The mean field limit defines an aggregate model for grid-level control. Special structure of the Markov model leads to a simple linear time-invariant (LTI) approximation. The LTI model is passive when the nominal Markov model is reversible.
3. Additional local control is used to put strict bounds on individual quality of service of each load, without impacting the quality of grid-level ancillary service.

Examples of application include chillers, flexible manufacturing, and even residential pool pumps. Sean demonstrated, through simulation, how pool pumps in Florida can supply a substantial amount of the ancillary service needs of the Eastern U.S.

Overview talk – VENKAT ANANTHARAM: *The objective method as a tool in large systems.* The objective method, also called the method of local weak convergence, is a technique to describe the local experience of a typical agent in a large interacting system through the solution of a recursive equation. Unlike the popular mean field limit method, it allows one to retain the essence of the locality of the interaction instead of modeling it away. This tool has so far been largely developed by probabilists and mathematicians in their quest to understand long range interactions in models motivated by physics and computer science. This tool appears to be potentially also of great value for understanding the role of interactions in control,communications, and other system-theoretic applications. Venkat provided an introduction to this technique, with illustrative examples revolving around distributed resource allocation.

ROLAND MALHAME: *A class of interference induced games: Asymptotic Nash equilibria and parameterized cooperative solutions.* Roland's talk focused on a multi-agent systems with linear stochastic individual dynamics and individual linear quadratic ergodic cost functions. The individuals partially observe their own states. Their cost functions and initial statistics are a priori independent, but they are coupled through an interference term (the mean of all agents' states), entering each of their individual measurement equations. While in general for a finite number of agents, the resulting optimal control law may be a non-linear function of the available observations, Roland showed that, for certain classes of costs and dynamic parameters, optimal separated control laws obtained by ignoring the interference coupling are asymptotically optimal when the number of agents goes to infinity, More generally though, optimal separated control laws may not be asymptotically optimal, and can in fact result in unstable overall behavior. Roland described a way of mitigating this via a class of parameterized decentralized control laws whereby the separated Kalman gain is treated as the arbitrary gain of a Luenberger-like observer. He characterized system stability regions and the nature of optimal cooperative control policies within the considered class, and presented some results of numerical simulations.

BILL SANDHOLM: *Large deviations and stochastic stability in the small noise double limit.* Bill Sandholm's talk was also on the subject of multi-agent games, but from the viewpoint of evolutionary dynamics. He described a model of stochastic evolution under general noisy best-response protocols, allowing the probabilities of suboptimal choices to depend on their payoff consequences. The focus of his talk was on behavior in the small-noise double limit: we first take the noise level in agents' decisions to zero, and then take the population size to infinity. He showed that, in this double limit, escape from (and transitions between) equilibria can be described in terms of solutions to certain continuous optimal control problems. These were used in turn to characterize the asymptotics of the stationary distribution, and thus to determine the stochastically stable states. He then presented a class of examples, where the control problems can be solved explicitly – three-strategy coordination games that satisfy the marginal bandwagon property and that have an interior equilibrium, and choices governed by the logit rule. He gave evidence for the conjecture that this should remain true for other classes of games and other choice rules.

PRAKASH NARAYAN: *Interactive multiterminal communication.* Shifting gears a bit, Prakash presented an information-theoretic perspective on communication in multi-agent systems. Information-theoretic models for multiuser source and channel coding usually take the communication between multiple terminals to be "simple," i.e., noninteractive. On the other hand, studies of multiparty function computation, especially in computer science, emphasize the useful role of interactive communication. Prakash described basic structural properties of interactive communication and presented "Single-shot" bounds for the amount of common randomness, i.e., shared information, that can be generated among the terminals using such communication.

32.2.2 Day 2: Decentralized systems with partial observations, sequential decompositions, and sufficient statistics.

The first three talks, starting with an overview talk by Shlomo Zilberstein and followed by Matthijs Spaan and Frans Oliehoek, focused on decentralized partially observable Markov decision processes (DEC-POMDPs) from a computer science and artificial intelligence (AI) perspective.

Overview talk – SHLOMO ZILBERSTEIN: *Cooperative multi-agent planning in partially observable uncertain worlds.* Coordinating the operation of a group of decision makers or agents in stochastic environments is a long-standing challenge in AI. Decision theory offers a normative framework for optimizing decisions under uncertainty, but due to computational complexity barriers, developing decision-theoretic planning algorithms for multiagent systems has been a serious challenge. Shlomo described a range of recently developed formal models and algorithms to tackle this problem, largely based on extensions of MDPs and POMDPs. Exact algorithms shed light on the structure and complexity of the problem and offer valuable building blocks for approximation methods. He described a number of effective approximation techniques that use bounded memory, sampling, and randomization. These methods can produce high-quality results in a variety of application domains such as mobile robot coordination and sensor network management. He also examined the performance of these algorithms and describe current research efforts to further improve their applicability and scalability.

MATTHIJS SPAAN: *Multi-agent planning under uncertainty with communication.* Next, Matthijs presented decision-theoretic approaches to multiagent planning under uncertainty, formalized as extensions of the POMDP model. In cooperative settings, communication between agents has the potential to significantly improve team performance. For instance, a higher degree of coordination can often be obtained by sharing local information. A common objective, however, is to minimize the level of communication required for satisfying performance. Matthijs discussed different models of communication that have been explored and paired them with appropriate solution techniques. A particular focus was on multi-robot planning problems, in which quality restrictions on the communication network need to be taken into account.

FRANS OLIEHOEK: *Exploiting structured representation in multi-agent sequential decision making.* While the framework of DEC-POMDPs gives a principled formalization of multi-agent decision-making problems, computing optimal plans for them is computationally intractable (NEXP-complete). In order to try and scale-decision making to larger problems involving more agents, researchers have tried to exploit different forms of structure which may be present across many mult-iagent applications. Frans surveyed two types of approaches to exploiting structure in mult-iagent decision problems. The first type was based on methods from (distributed) constraint optimization. Essentially, these methods try to exploit conditional independence between agents. The second type was based on the insight that, even in the case of two agents that directly influence each other, not all details of the policies may be relevant for the coordination process. That is, rather than coordinating at the level of (joint) policies, it may be possible to coordinate at the more abstract level of (joint) influences of such policies.

Overview talk – MIHAILO JOVANOVIC: *Sparsity-promoting optimal control of distributed systems.* Mihailo's talk, delivered from the perspective of a control theorist, was about the design of feedback gains that achieve a desirable tradeoff between quadratic performance of distributed systems and controller sparsity. (Similar ideas were explored by Ali Belabbas during Day 1.) He first identified sparsity patterns of the feedback gains by incorporating sparsity-promoting penalty functions into the optimal control problem, where the added terms penalize the number of communication links in the distributed controller. He then showed how to optimize feedback gains subject to structural constraints determined by the identified sparsity patterns. In the first step, the sparsity structure of feedback gains is identified using the alternating direction method of multipliers, an algorithm well-suited to large optimization problems. This method alternates between promoting the sparsity of the controller and optimizing the closed-loop performance, which allows us to exploit the structure of the corresponding objective functions. Even though the standard quadratic performance index is in general a nonconvex function of the feedback gain, we identify several classes of convex problems. In this case, the corresponding synthesis problem can be formulated as a semidefinite program for which we develop efficient customized solvers. Several examples were provided to demonstrate the effectiveness of the developed approach.

WING S. WONG: *Systems for open interaction.* For the majority of distributed multi-agent systems reported in the literature the system objective is uniquely defined. However, there are many real-life examples in which the system objective could depend on the choices selected by the agents that are unknown to each other. Wing's talk designated these as systems for open interaction. Control design of such systems does not follow the classic paradigm, and is intimately tied with communication issues. Wing reported results on optimal control design for some concrete systems and used them to illustrate a number of fundamental issues of interest for cooperative decentralized systems.

RAHUL JAIN: *The art of sequential optimization via simulations.* Sequential optimization is a common thread that emerges in the context of decentralized decision-making. Rahul presented a natural framework for simulation-based optimization and control of MDPs. The idea is very simple: Replace the Bellman operator that appears in the dynamic programming recursion by its 'empirical' variant wherein the expectation is replaced by a sample average approximation. This leads to a *random* Bellman operator. Rahul introduced several notions of probabilistic fixed points of such random operators, and showed their asymptotic equivalence. He then established convergence of empirical Value and Policy Iteration algorithms by a stochastic dominance argument. The mathematical technique introduced by Rahul is useful for analyzing other iterated random operators (and not just the empirical Bellman operator), and may also be useful in random matrix theory. The idea can be generalized to asynchronous dynamic programming, and is also useful for computing equilibria of zero-sum stochastic games. Preliminary numerical results showed better convergence rate and runtime performance than stochastic approximation/reinforcement learning, or any other commonly used schemes.

ADITYA MAHAJAN: *The common information approach to decentralized stochastic control.* Many modern technological systems, such as cyber-physical systems, communication, transportation and social networks, smart grids, sensing and surveillance systems are informationally decentralized. A key feature of informationally decentralized systems is that decisions are made by multiple decision makers that have access to different information. This feature violates the fundamental assumption upon which centralized stochastic control theory is based, namely, that all decisions are made by a centralized decision maker who has access to all the information and perfectly recalls all past observations and decisions/actions. Consequently, techniques from centralized stochastic control cannot be directly applied to decentralized stochastic control problem primarily for the following reason. In centralized stochastic control, the controllers belief on the current state of the system is a *sufficient statistic* for decision making. A similar sufficient statistic does not work for decentralized stochastic control because controllers have different information and hence their beliefs on the state of the system are not consistent. Nevertheless, two general approaches that use ideas from centralized stochastic control theory have been used for the solution of decentralized control problems: (i) the person-by-person approach; and (ii) the designers approach. Aditya gave a detailed discussion of the features and merits of these approaches, as well as some illustrative examples, such as control problems with delay-sharing, control-sharing, and mean-field information sharing.

SANJAY LALL: *Sufficient statistics for multi-agent decisions.* Continuing in the same vein, Sanjay described a notion of sufficient statistics for decision, estimation or control problems involving multiple players. As in the classical single-player setting, sufficient statistics contain all of the information necessary for the players to make optimal decisions. In the multi-agent setting, he showed how to construct such sufficient statistics via a convex relaxation of the feasible set of the corresponding decision problem. He proved that that these statistics may be updated recursively, and may be constructed by appropriately composing the corresponding single-player statistics. He also presented algorithms for this construction when the information pattern is defined by an appropriate graph.

NUNO MARTINS: *Distributed estimation over shared networks: optimal event-based policies.* Nuno focused on the design of distributed estimation systems that are composed of multiple non-collocated components. A shared network is used to disseminate information among the components. He discussed recent results that characterize the structure of certain optimal policies for the case in which the number of components exceeds the maximal number of simultaneous transmissions that the network can accept. In order to obtain a tractable framework for which design principles can be characterized analytically, he consider at most two estimators that rely on information sent to them by two sensors that access dissimilar measurements. He showed the optimality of certain threshold-based policies, established a connection with a problem of optimal quantization for which the distortion is non-uniform across representation symbols, presented numerical approaches, discussed interpretations of the results, and listed related open issues.

BAHMAN GHARESIFARD: *On the convergence of strategic interaction dynamics on networks.* Bahman presented a proof of the following result: piecewise-linear best-response dynamical systems with strategic interactions are asymptotically convergent to their set of equilibria on any weighted undirected graph. He discussed various features of these dynamical systems, including the uniqueness and abundance properties of the set of equilibria and the emergence of unstable equilibria. He also introduced the novel notions of *social equivalence* and *social dominance* for such dynamics on directed graphs, and demonstrated some of their interesting implications, including their correspondence to consensus and chromatic number of partite graphs.

32.2.3 Day 3: Information and learning in multi-agent cooperation and competition.

Overview talk – JASON MARDEN: *The role of information in multi-agent coordination.* The goal in networked control of multi-agent systems is to induce desirable collective behavior through the design of local control algorithms. The information available to the individual agents, either attained through communication or sensing, invariably defines the space of admissible control laws. Hence, informational restrictions impose constraints on achievable performance guarantees. Jason talked about one such constraint with regards to the efficiency of the resulting stable solutions for a class of networked resource allocation problems with submodular objective functions. When the agents have full information regarding the mission space, the efficiency of the resulting stable solutions is guaranteed to be within 50% of optimal. However, when the agents have only localized information about the mission space, which is a common feature of many well-studied control designs, the efficiency of the resulting stable solutions can be $1/n$ of optimal, where n is the number of agents. Consequently, in general such schemes cannot guarantee that systems consisting of n agents can perform any better than a system consisting of a single agent for identical environmental conditions. Jason presented an algorithm that overcomes this limitation by allowing the agents to communicate minimally with neighboring agents.

GÜRDAL ARSLAN: *Learning algorithms for stochastic dynamic games.* Gürdal first provided an overview of the literature on learning in static and dynamic games and made the point that there do not exist decentralized learning algorithms for dynamic games which are uncoupled (that is, which do not require the decision maker's to share any information) which converge to equilibria. Generalizing the notion of *weakly acyclic games* for static games to dynamic games, he introduced a decentralized Q-learning algorithm which is guaranteed, first probabilistically and then (through annealing) almost surely, to equilibria. Such games include dynamic team problems and potential games.

DAVID LESLIE: *Two-timescales game-theoretical learning with continuous action spaces.* Much work on learning in games has focused on the discrete-action case. However, in the contexts of both economics and control applications, the action set is frequently continuous (such as the price of a good, the position, or power level of a component of the system). David talked about a framework for learning in games with continuous actions sets, and introduced the necessary stochastic approximation theory with which such processes can be analyzed. He then demonstrated how this theory can be extended to a two-timescales system, in which the values of actions can be estimated, and strategies adapted, without any player actually observing the actions or rewards of any other. This results in a system where 'individual action learners' can converge successfully to approximate Nash equilibria, in zero-sum games and potential games.

JOHANNES HÖRNER: *Dynamic Bayesian games.* Johannes focused on characterizing an equilibrium payoff subset for Markovian games with private information as in the limit of vanishing discount factor. Monitoring is imperfect, transitions may depend on actions, types may be correlated and values may be interdependent. The focus was on equilibria in which players report truthfully. This characterization generalizes that for repeated games, reducing the analysis to static Bayesian games with transfers. With correlated types, results from mechanism design apply, yielding a folk theorem (or general feasibility theorem). With independent private values, the restriction to truthful equilibria is without loss, except for the punishment level; if players withhold their information during punishment-like phases, a "folk theorem" obtains also.)

BEHROUZ TOURI: *TS graph approach to evolutionary stability.* Behrouz revisited the theory of evolutionary stability for population games in finite populations. He provided two illustrative examples showing that (i) games with no evolutionarily stable strategy can admit a cloud of dominating set of strategies emerging from the selection-mutation process, and (ii) there are games with a unique evolutionarily stable strategy which, interestingly, becomes extinct in the selection-mutation dynamics. He generalized the conventional theory of evolutionary stability and showed how a cloud of strategies can emerge in the selection-mutation dynamics. The key object in our development is the Transitive Stability (TS) graph of the population dynamics. Behrouz demonstrated that all the strategies, except those of the extreme vertices of the associated TS-graph, become extinct in the mutation-selection process.

ALEX OLSHEVSKY: *Linear-time consensus.* Alex described a protocol for the average consensus problem on any fixed undirected graph whose convergence time scales linearly in the total number nodes n. The protocol is completely distributed, with the exception of requiring each node to know an upper bound on the total number of nodes which is correct within a constant multiplicative factor. He discussed applications of this protocol to questions in decentralized optimization and multi-agent control connected to the consensus problem. In particular, we develop a distributed protocol for minimizing an average of (possibly nondifferentiable) convex functions. Under the same assumption as above, and additionally assuming that the subgradients of each term in the average have norms upper-bounded by some constant L known to the nodes, after T iterations our protocol has error which is $O(L\sqrt{n/T})$.

SHREYAS SUNDARAM: *Spectral and structural properties of random graphs with applications to consensus dynamics on networks.* Shreyas' talk focused on some recent results on spectral and structural properties of large-scale random graphs that play a role in certain classes of coordination and consensus dynamics on networks. He started with a commonly studied class of Laplacian dynamics where the asymptotic rate of convergence is given by the second smallest eigenvalue (also known as the algebraic connectivity) of the graph Laplacian matrix. We provide a characterization of the algebraic connectivity of certain random graphs,including some results pertaining to interdependent networks that highlight the relative importance of edges between and within communities in the network. We then consider a variant of Laplacian dynamics where one or more nodes in the network keep their state fixed at certain values – such scenarios occur in the case of diffusion dynamics with stubborn agents.The rate of convergence in such settings is given by the smallest eigenvalue of the grounded Laplacian matrix of the network; we give explicit characterizations of this eigenvalue for various random graphs. Finally, we study a class of dynamics where each node in the network ignores the most extreme values in its neighborhood before averaging the rest, and propose a topological property known as "robustness" to characterize networks where such dynamics will lead to consensus. We show that this notion of robustness is much stronger than classical metrics such as connectivity, but that these properties coincide in certain random graph models (Erdős-Renyi, 1-D geometric, and preferential attachment graphs).

MAXIM RAGINSKY: *Online discrete optimization in social networks with inertia.* Recently, there has been a great deal of interest in modeling and analysis of collective information processing by networks of locally interacting entities with limited information. On the theoretical front, this circle of problems has deep connections to ideas from game theory, statistical physics, and discrete probability. Maxim described a model of online (i.e., real-time) discrete optimization by a social network consisting of agents that must choose actions to balance immediate time-varying costs against a desire to act according to some default myopic strategy. The costs are generated by a dynamic environment, and the agents lack ability or incentive to construct an a priori model of the environment's evolution. The global cost of the network decomposes into a sum of individual and pairwise interaction terms, and at each time step each agent is informed only about its own cost and the pairwise costs in its immediate neighborhood. The overall objective is to minimize the worst-case regret, i.e., the difference between the cumulative real-time performance of the network and the best performance that could have been achieved in hindsight with full centralized knowledge. Maxim presented an explicit strategy for the network based on the Glauber dynamics and showed that it achieves favorable scaling of the regret in terms of problem parameters under a Dobrushin-type mixing condition. The proof relied on ideas from statistical physics, as well as on recent developments in the theory of Markov chains in metric spaces, specifically Yann Ollivier's notion of positive Ricci curvature of a Markov operator.

ANDRAS GYÖRGY: *Online learning in Markov Decision Processes with changing reward sequences.* Andras talked about consider online learning in finite stochastic Markovian environments, where at each time step a new reward function is chosen by an oblivious adversary. The goal of the learning agent is to compete with the best stationary policy in hindsight in terms of the total reward received. Two variants of the problem were considered: the online stochastic shortest path problem and learning in unichain Markov decision processes. Several low-complexity algorithms were proposed, for both the full-information and the bandit-feedback settings, which achieve almost optimal performance under different assumptions on the Markov transition kernel. In the case of full-information feedback, the results presented by Andras complement existing results, while in the bandit feedback he gave the first low-complexity algorithms achieving optimal performance. Some of the algorithms were based on distributed learning, where separate learning agents were used for each state of the MDP, while others were completely centralized. Andras compared these approaches and discussed how different levels of synchronization and information sharing affects performance.

CSABA SZEPESVARI: *Online learning under delayed feedback.* In distributed, networked systems, feedback arrives in a delayed fashion. The question then arises how this will affect the learning speed of various algorithms. Csaba talked about some recent results concerning this effect in the framework of online learning with partial monitoring, which includes both full-information feedback, as well as bandit information feedback, as special cases. He then described novel results concerning the impact of delay on the regret, both for adversarial and stochastic settings. These results showed that, while for the adversarial setting the cost of the delay increases the regret in a multiplicative way, in the stochastic setting the increase is only additive. He described meta-algorithms that transform, in a black-box fashion, algorithms developed for the non-delayed case into ones that can handle the presence of delays in the feedback loop. Modifications of the well-known UCB algorithm were also developed for the stochastic multi-armed bandit problem with delayed feedback, with the advantage over the meta-algorithms that they can be implemented with lower complexity. Remaining open problems are discussed at the end.

VIANNEY PERCHET: *Blackwell approachability in (stochastic) games.* Vianney gave a unified presentation of standard frameworks for Blackwell approachability, both in full and partial monitoring, by defining a new abstract game, called the purely informative game, where the outcome at each stage is the maximal information players can obtain, represented as some probability measure. Objectives of players can be rewritten as the convergence (to some given set) of sequences of averages of these probability measures. He presented new results extending the approachability theory developed by Blackwell. This new abstract framework enables us to characterize approachable sets with a remarkably simple and clear reformulation for convex sets. Translated into the original games, those results become the first necessary and sufficient condition under which an arbitrary set is approachable and they cover and extend previous known results for convex sets. He also described a specific class of games where, thanks to some unusual definition of averages and convexity, one can obtain a complete characterization of approachable sets along with rates of convergence.

32.2.4 Day 4. Information and communication constraints in decentralized systems.

Overview talk – SERDAR YÜKSEL: *Quantization for stabilization, optimization and approximation in networked control.* In this three-part talk, Serdar discussed three ways in which quantization appears in stochastic control and networked control. The first area is on stabilization under information constraints, for which quantization is essential. For non-linear stochastic systems, he presented lower and upper bounds on information transmission rates required for stabilization in the sense of asymptotic stationarity, which in the case of linear systems turn out to be equal, and established the connection with a well-known limitation theorem due to Bode interpreted for non-linear systems. The second area is on optimization under quantization constraints, where he presented structural and existence results for optimal quantization policies. Explicit solutions were obtained for the application of these results to Linear Quadratic Gaussian systems. Finally, in the third part, he presented the problem of approximation in stochastic and networked control, where the action sets available to a controller are restricted to be finite. Asymptotic optimality of controllers which only can select from finitely many actions, as the size of the sets increase to infinity, was established, and under further conditions on the controlled Markov chains, explicit rates of convergence bounds were established. These bounds are tight in the sense of *order-optimality* for a class of systems and cost functions.

ANANT SAHAI: *Information theory and decentralized control.* Networked control systems require an interdisciplinary study of information, control and probability. In his talk, Anant discussed the interaction of information and control theories for networked control systems. Viewing the control plant as the source to a noisy channel, he presented a novel look at arriving at the requirements on channel reliabilities for stochastic stabilization. He then studied erasure channels extensively and discussed the limitations in imperfections in the sensor-controller channel and the controller-plant channel, and showed that the optimal networked control problems are not robust to uncertainties in the information channel.

CÉDRIC LANGBORT: *On myopic strategies in dynamic adversarial team decision problems.* Cedric discussed game theoretic aspects in networked control and dynamic team problems, where there are decision makers with mis-aligned objective functions. In the context of a large class of cost functions, including the celebrated Witsenhausen's counterexample problem, the quadratic source-channel coding problem as well as variations of such quadratic cost functions, he discussed the optimality and sub-optimality of linear policies, and quantization based strategies for such problems. When uncertainty in the system model is included, he made the point that for a class of team/game problems, when the uncertainty as seen by a decision maker is quantitatively large, myopic strategies (non-strategic policies which are oblivious to other decision makers) may perform very well and be indeed optimal for a class of quadratic problems.

OHAD SHAMIR: *Information constraints in distributed and online learning.* Many machine learning approaches are characterized by information constraints on how they interact with training data. One prominent example is communication constraints in distributed learning, while other examples include memory and sequential access constraints in stochastic optimization and online learning, and partial access to the underlying data (such as in multi-armed bandits). However, in a statistical learning setting, we have little understanding how these information constraints fundamentally affect the learning performance, without making assumptions on their semantics. Ohad discussed these issues, and described how a single set of results sheds some light on them, simultaneously for different types of information constraints and for different learning settings.

VIVEK BORKAR: *Gossip and related algorithms.* Vivek concluded the workshop by describing some of his recent work on gossip and related distributed algorithms, highlighting some possible future directions.

32.3 Scientific Progress Made and Outcome of the Meeting

The main outcome of the workshop workshop was to provide an opportunity for researchers from different communities (stochastic control, economics, information theory, and machine learning) working on optimal decentralized decision-making to exchange ideas and learn new mathematical tools and techniques (used by other communities). This was an intense week, and each day was packed with many talks looking at a wide variety of decentralized decision-making problems using a broad array of tools from probability theory, information theory, systems and control, game theory, optimization, and artificial intelligence. Nevertheless, there were plenty of discussions among the participants during the coffee breaks and after dinner, and through many email communications after the workshop, and we believe that ultimately the workshop succeeded in bringing to the fore various connections between the solution approaches of the different communities, fostering future collaborations, and providing an improved understanding of optimal decentralized decision-making. Since this was the first workshop of this kind on the topic of decentralized decision-making, we expect to see the fruits of collaboration between the participants in the near future; in the meantime, here are some impressions of the workshop from several participants:

Excellent workshop, idyllic surroundings. Feel recharged.

Vivek Borkar
Electrical Engineering, Indian Institute of Technology Bombay

Thanks a lot for the invitation to Banff. I learnt a great deal, thanks to you. Hopefully we will get more chances to interact, stay in touch.

Johannes Hörner
Economics, Yale University

The workshop was well organized, gathering scholars from different disciplines, which opened new angles for me.

Michel De Lara
CERMICS, Ecole des Ponts ParisTech

The BIRS workshop was an outstanding experience. The opportunity to interact with and learn from the top researchers in the field, against the idyllic backdrop of the Canadian Rockies, was very memorable. I am very glad that places such as BIRS and the Banff Centre exist to facilitate the exchange and pursuit of knowledge.

Shreyas Sundaram
Electrical and Computer Engineering, University of Waterloo

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Arslan, Grdal (University of Hawaii)
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Chapter 33

Particle-Based Stochastic Reaction-Diffusion Models in Biology (14w5103)

November 9 - 14, 2014

Organizer(s): Daniel Coombs (University of British Columbia), Mark Flegg (Monash University), Samuel Isaacson (Boston University), Per Lötstedt (Uppsala University), Linda Petzold (University of California Santa Barbara)

33.1 Overview of the Field

Throughout the twentieth century, biological and medical research was centered within the laboratory. The development of detailed mathematical models of cellular systems was hindered by a need for quantitative measurements of cellular processes and insufficient computer resources. In recent years, the combination of new experimental techniques and exponential improvements in computer technology has made the construction and study of such models possible. These mathematical models have the potential to provide biological and medical research with predictive power. A quantitative scientific paradigm is developing in which the theoretical predictions of mathematical models provide complementary tools that can help guide laboratory experiments. Such is the importance of simulation techniques to the future of fields including molecular biology, cellular biology and systems biology that a full quantitative numerical model of a cell has been labeled as one of the "grand challenges of the 21st century"[24].

Mathematical models have been used during the last decade to model a number of biological processes, including gene regulation, molecular signaling, cell division and molecular transport. The development of these models has been motivated by the aforementioned advances in experimental techniques, which have revealed that many processes in cell and molecular biology are inherently stochastic [6]. This stochasticity can provide a challenge that must be compensated for to allow proper function, such as the inherent noisiness of gene expression [19]. Stochasticity can also drive biological function, facilitating phenotypic diversity of cellular populations and driving evolution.

At the scale of a single cell, stochasticity becomes important due to low copy numbers of biological molecules, such as mRNA and proteins, that take part in bio-chemical reactions driving cellular processes [19]. When trying to describe such biological processes traditional (mean-field, coarse-grained) deterministic models for the concentration of chemical species, given by systems of ordinary differential equations (ODEs) or partial differential equations (PDEs), are often inadequate, exactly because of these low copy numbers. Stochastic models are necessary to account for small particle numbers (intrinsic noise) and extrinsic noise sources. Often the complexity of these models depends crucially on several key bio-chemical reactions, and whether they are diffusion-limited or reaction-limited. In the latter case, one can describe the processes by adopting the framework of Markov jump processes [10] and stochastic differential equations (SDEs) [1] (chemical master and Fokker Planck equations), while in the former one needs to adopt the framework of stochastic reaction-diffusion models, including the lattice reaction-diffusion master equation (RDME) [14], stochastic partial differential equations (SPDEs) and particle-based Brownian dynamics models [7].

Many fundamental biological processes involve spatially distributed components in which diffusion–limited reactions play a key role. Examples include the diffusion of proteins within microdomains and lipid bilayers; the propagation of trans-membrane potentials across cellular membranes; the movement of cells within tumors; and the transmission of chemical signals from the cell surface to regulatory sites in the nucleus. As such, models that explicitly resolve the spatial transport of molecules within cells can help to understand the influence of subcellular structure, spatially distributed signaling compartments, and cell shape on such processes [13, 16, 17]. In recent years, particle-based stochastic reaction-diffusion models have been used to develop mathematical models which both account for noise in the chemical reaction process, and incorporate the explicit diffusion and reaction of proteins and mRNAs within cells. There are two primary particle-based models that have been used: variants of the diffusion limited reaction model due to Smoluchowski [21, 15], and the reaction-diffusion master equation (RDME) [9].

In the former molecules are modeled as points or spheres undergoing Brownian motion. First order reactions of the form $\mathrm{A} \to \mathrm{B}$, are modeled as basic Poisson processes, with each molecule of type A having a probability per time to convert into a molecule of species B. When considering second order reactions of the form $\mathrm{A} + \mathrm{B} \to \mathrm{C}$ several variants of the Smoluchowski model have been proposed. In the original, pure–adsorption model [21] two molecules react instantly upon reaching a fixed separation, a model parameter called the reaction-radius. Depending on the underlying biological system being studied, this parameter will be the sum of the physical "radii" of the two molecules, or can be an empirical parameter chosen to fit certain experimentally determined statistics of the reaction process [2]. A more general partial–adsorption model then allows for the possibility of non-reactive encounters, where two reactants may sometimes reflect off each other when their separation equals the reaction radius. Finally, a third variant popularized by Doi posits that the two reactants may react with a specified probability per unit time when their separation is less then a reaction radius. Mathematically, the two Smoluchowski reaction models lead to Dirichlet and Robin boundary conditions in the associated Forward Kolomogorov equations describing the evolution of the probability density for a chemical system to be in a specified state. In contrast, the Doi model leads to interaction functions within the associated Forward Kolmogorov equation.

In contrast to the Smoluchowski type models, in the RDME space is discretized into a lattice, with molecular diffusion approximated by continuous-time random walks on the lattice. First order reactions are modeled identically to the Smoluchowski models, while bimolecular reactions occur with fixed probabilities per unit time for two reactants located at the same lattice site. The Smoluchowski model is often considered a more microscopic model, with the RDME interpreted as a mesoscopic scale coarse graining of Smoluchowski type models.

There has been a large body of work in the last decade to develop numerical methods capable of accurately and efficiently simulating the stochastic processes described by these models. The development of these numerical methods has been motivated largely by specific biological systems studied within individual research groups. As a result, a wide variety of numerical methods have been developed to simulate specific biological systems, with a wide variety of extensions of the base models. These extensions allow for more realistic biological features, including complex domain geometries; spatial transport by advection–diffusion or drift–diffusion; non-elementary chemical reaction mechanisms; and molecular crowding.

Broadly speaking, there are three general classes of numerical methods that have been widely studied. The First Passage Kinetic Monte Carlo (FPKMC) [18, 4] and Green's Function Reaction Dynamics (GFRD) [25, 23] methods can generate exact realizations of the stochastic process described by the Smoluchowski model, while time-step based Brownian Dynamics (BD) methods approximate this process [2, 8]. The Gillespie method [10] can be used to generate exact realizations of the stochastic process described by the RDME. Whilst a great deal of literature exists on the analysis of these methods, there are few detailed comparisons of their relative merits, and no 'gold standard' has been established. Part of the reason why no gold standard approach has been identified in the literature is the disjointed, interdisciplinary nature of the research. Understanding the usefulness, efficiency and accuracy of the various algorithms requires careful studies by computer scientists, mathematicians, physicists, chemists and biologists, who have had limited opportunities for collaboration in this space. Another reason why no gold standard has been established is because the various approaches are dichotomous and difficult to compare objectively.

Typically, numerical methods based on the Smoluchowski model allow for high precision since each molecule/particle is represented separately and traced exactly in space. The cost of such high precision is the requirement that each reaction/interaction must be simulated separately. Thus, the computational cost of these methods grow rapidly as the number of molecules/particles (and individual trajectories) increase, and also as the number of possible reactant combinations increase. Once the number of molecules within a domain become sufficiently large (or concentrated), the computational cost of Smoluchowski-based numerical methods can be prohibitively high. RDME-based Gillespie methods, on the other hand, are generally more computationally efficient at high particle counts as only the copy number of molecules within each compartment is tracked; the position of individual molecules within each compartment are not distinguished. Despite their computational efficiency, Gillespie methods may introduce unphysical computational artifacts. This is due to the discretization of the domain into a lattice, random walk approximations of the underlying diffusion processes, and choice of mechanism for modeling bimolecular reactions. It is difficult to objectively value accuracy over efficiency or vice versa to model problems as diverse as those in biology. Some biological systems may fluctuate between low concentrations and high concentrations in both space and time and to achieve acceptable levels of accuracy using current technology and computational resources it is important to improve our understanding of how these approaches may be hybridized, taking the best of both approach.

True to the rather fractured/diverse nature of the community, a wide variety of publicly available simulation packages have been developed to facilitate the study of cellular processes, each based on a different variant of the aforementioned methods. Some of the more popular programs include Smoldyn [2], SpatioCyte [3], URDME [5], MesoRD [11], STEPS [12], Lattice Microbes [20], MCell [22] and GFRD [25]. At the BIRS workshop, each of these simulation methodologies were represented and open problems were discussed.

33.2 Recent Developments and Open Problems

We highlight four broad areas, corresponding to the four main session topics of the workshop:

1. **Biological Models and Analytical Approximations:** In the last 10-20 years, a broad body of work has been developed to understand the dynamics of non-spatial models for biological systems. Here the underlying mathematical models are typically given by ODEs, SDEs, or integer-valued jump processes. For such systems we have gained a deep understanding of the types of dynamical behavior that can occur and how these dynamics depend on critical system parameters and network topology. For example, the possibility of multi-stability in deterministic ODE models for cellular processes can now be predicted in many cases from network topology. More recently such results have begun to be adapted to the stochastic regime, where deterministic chemical concentrations are replaced by jump processes for the number of molecules of each chemical species.

   In contrast to these well-mixed models, in spatially extended models the types of dynamical behaviors that can arise, and methods for predicting them are much less developed. Moreover, there are few general results on how explicitly accounting for spatial transport in biochemical systems might influence the predicted behavior of previously non-spatial models. One reason such questions are less well-developed in the context of spatial models is due to a much reduced set of well-developed tools for the general analysis of these systems. For stochastic jump-process models of chemical systems we have a large collection of exact and approximate techniques for analytically investigating system behavior. These include exact transform and solution methods for simple systems, network-theory based approaches, and asymptotic methods based on separation of timescales. In particular, a rigorous hierarchy of mathematical models have been established to show how "large volume" expansions can lead from stochastic jump process models, to SDE models, and ultimately to deterministic ODE models. In contrast, no similar complete and rigorous theory has been developed for spatially extended particle-based reaction-diffusion models.

One area where analysis of particle-based reaction-diffusion models has made substantial progress in recent years is in estimating timescales for various reaction processes. A large body of asymptotic methods have been developed to estimate mean first passage times across a variety of particle-based reaction-diffusion models. One general theme in the development of these methods is that the "reaction-radius" at which two proteins may interact is generally a very small parameter relative to the typical size of cellular domains, and the typical distance between reactive molecules. These methods have provided insight into a variety of biological problems, from how proteins search for DNA bindings sites through to how molecules are trafficked to receptors in synaptic spines.

2. **Mesoscopic Methods and Modeling:** While quite popular for modeling biological systems, there are several practical challenges in using lattice reaction-diffusion master equation (RDME) models. One difficultly arises from the underlying discretization of space, which introduces a purely numerical parameter, the lattice spacing, into RDME-based models. While the RDME can be shown to converge back to the Smoluchowski continuous-space particle model for systems with only linear reactions, bimolecular reactions are lost in the RDME as the lattice spacing is taken to zero. This difficultly arises as molecules are treated as point particles, that may only react when located at the same lattice site within the RDME. As the lattice spacing is taken to zero one obtains point particles moving by Brownian motion, which can only react when located at the same point. Since the probability for two diffusing molecules to ever have the same position is zero, bimolecular reactions are lost. To overcome this challenge the RDME is usually postulated to only be an appropriate model for lattice spacings that are sufficiently large that bimolecular reactions can be adequately resolved, while also sufficiently small that the approximation of Brownian as a continuous–time random walk on the lattice is accurate. As discussed in the workshop, a number of groups have recently investigated over what range of lattice spacings this approximation is robust, how to broaden the range of lattice spacings over which the RDME provides an accurate approximation to continuous–space particle models, and how to modify the RDME model to provide a similar lattice-based stochastic reaction-diffusion model that actually converges back to continuous-space models as the lattice spacing is taken to zero.

   A second major challenge in the use of RDME–based models is in how to efficiently generate realizations of the associated stochastic process. The well-known Gillespie method (i.e. stochastic simulation algorithm or kinetic Monte Karlo method) can generate exact realizations of the stochastic process associated with the RDME [14]. While there is an enormous body of work developing optimized versions of the Gillespie method for well-mixed chemical systems, there are only a few methods that have been optimized for the RDME. Here the simulation of spatial movement of molecules as continuous-time random walks is usually the dominant computational cost, often requiring more then 90% of simulation time. In recent years several methods have been proposed to help optimize this component of RDME simulations, including methods that approximate the random walks of individual molecules by only resolving the net motion of molecules between two lattice sites, by replacing the random walks with various continuous diffusion methods, by grouping together many diffusive hops into one event, and by optimized data structures to efficiently sample and update the location and time of the next diffusive hopping event.

3. **Particle-Based Methods and Modeling:** Timestep based Brownian Dynamics (BD) methods are one of the most popular stochastic reaction-diffusion methods for studying biological systems. In their most basic formulations these methods provide first-order (in the timestep) approximations to the underlying particle dynamics that are relatively easy to implement, but can be computationally demanding when taking small timesteps to adequately resolve the dynamics of cellular processes. To overcome this challenge a number of improved BD methods have been proposed in recent years to facilitate the use of large timesteps, while still accurately resolving important statistics of the underlying stochastic reaction-diffusion processes [8].

   In sufficiently dilute systems the First Passage Kinetic Monte Carlo Method was recently developed to provide exact realizations of the stochastic process associated with the Smoluchowski model [4]. While this method provides substantial computational savings for dilute systems in simplified geometries, it is not competitive with BD methods for more dense systems in which molecules are tightly packed, or when the domain geometry is tortuous. As presented at the workshop, a number of groups have recently developed variants of the method that allow for more general methods of spatial transport then diffusion, while sacrificing the exactness of the underlying simulation algorithm.

4. **Multiscale Methods and Modeling:** Current particle-based stochastic reaction-diffusion methods can accurately simulate hundreds of thousands to perhaps millions of reacting and diffusing molecules over timescales of several hours. To achieve the simulation of cellular processes that occur over longer timescales, such as the cell cycle, and over length scales of mammalian cells, multiscale methods are needed to automatically resolve model components at the coarsest acceptable level of physical resolution. In recent years researchers have begun to investigate how to achieve such couplings, proposing a number of methods to allow for multiscale couplings across interfaces separating different regions of space, or allow for resolving different reactions or chemical species at different physical scales. Examples of the former include coupling across an interface a particle model in one region of a domain to deterministic reaction-diffusion PDE models in a second region, or similar couplings between microscopic Smoluchowski models and mesoscopic RDME models. For the latter, several groups have investigated how to accurately resolve different components of a given physical system at different scales in a manner that is consistent with a fully particle-based model.

33.3 Presentation Highlights

The workshop brought together theorists and experimentalists investigating spatially distributed stochastic processes in cell and molecular biology, with researchers developing techniques for the analysis of mathematical models and related numerical methods. One particular emphasis was models involving spatial transport and chemical reactions, which often span multiple time and length scales. Applications to biological processes such as gene expression, immunological receptor signaling, and signal transduction were discussed to illustrate the types of biological problems for which accurate and efficient stochastic spatio-temporal methods are needed.

Below we highlight, in the presenter's own words, several talks from each of the workshop's four sessions:

Session on Biological Models and Analytical Approximations:

Speaker: **Jun Allard** (University of California Irvine)
Title: *Mechanics of diffusing surface molecules modulates T cell receptor sensitivity*
Abstract: Receptors on the surface of cells control many cellular processes. An important class of receptors, e.g., T-cell receptors, attach to molecules that are anchored to other cells or surfaces, and remain poorly understood. The T-cell receptor complex spans 15 nanometers, while other nearby molecules spans ~ 40 nanometers. Since all these molecules are mobile on the two-dimensional cell surface, the size differential has been proposed to lead to spatial segregation (mediated by the mechanical properties of the cell membranes) that triggers immune signaling. I will present a nanometer-scale mathematical model that couples membrane elasticity with compressional resistance and lateral mobility of molecules. We find robust supradiffusive segregation. The model predicts a time-dependent tension on the receptor leading to a nonlinearity which could enhance the receptors ability to make precise immune decisions. Understanding the full life-cycle of receptor dynamics raises questions involving surface diffusion of a population of molecules, and I will present open problems along with computational estimates and their biological importance.

Speaker: **Daniel Coombs** (University of British Columbia)
Title: *Random violence: A stochastic approach to cell cytotoxicity*
Abstract: This talk is about our recent work on the delivery of effector molecules from immune cells such as T and Natural Killer cells. These cells release fairly small numbers of molecules that induce cell death, into the tightly

defined region of contact with a target cell (the ”immunological synapse”). I will explain the background biology and the leading hypothesis of how this process works. I will then show how we used a spatial stochastic algorithm to analyze whether the hypothesis is correct and outline future experimental work. This research was done jointly with Daniel Woodsworth (BC Cancer Research Centre).

Speaker: **Andreas Hellander** (Department of Information Technology, Uppsala University)
Title: *Accuracy of the Michaelis-Menten approximation when analyzing effects of molecular noise*
Quantitative biology relies on the construction of accurate mathematical models, yet the effectiveness of these models is often predicated on making simplifying approximations that allow for direct comparisons with available experimental data. The Michaelis-Menten approximation is widely used in both deterministic and discrete stochastic models of intracellular reaction networks, due to the ubiquity of enzymatic activity in cellular processes and the clear biochemical interpretation of its parameters. However, it is not well understood how the approximation applies to the discrete stochastic case or how it extends to spatially inhomogeneous systems. We study the behavior of the discrete stochastic Michaelis-Menten approximation as a function of system size and show that significant errors can occur for small volumes, in comparison with a corresponding mass action system. We then explore some consequences of these results for quantitative modeling. One consequence is that fluctuation-induced sensitivity, or stochastic focusing, can become highly exaggerated in models that make use of Michaelis-Menten kinetics even if the approximations are excellent in a deterministic model.Another consequence is that spatial stochastic simulations based on the reaction-diffusion master equation can become highly inaccurate if the model contains Michaelis-Menten terms.

Session on Mesoscopic Methods and Modeling:

Speaker: **Stefan Engblom** (Uppsala university)
Title: *Mesoscopic Stochastic Modeling: Diffusion Operators, Multiphysics Couplings, and Convergence*
Abstract: In this talk I will discuss stochastic modeling in the reaction-transport framework from various viewpoints. I shall initially be concerned with diffusion-controlled reactions targeting applications mainly in molecular cell biology. I will briefly review the basic setup and conditions for the validity of this type of modeling. In particular I will discuss the properties of the diffusion transport operator.

I will next discuss an application example from outside the diffusion-controlled domain, namely an approach towards multiphysics modeling of neuronal spiking activity affected by stochastic channel fluctuations. This example serves as a reminding illustration that questions of convergence are not that straightforward to answer.

Speaker: **Anastasios Matzavinos** (Brown University)
Title: *Dissipative particle dynamics simulations of polymer networks*
Abstract: Networks of entangled or cross-linked polymers, such as the actin cytoskeleton, are ubiquitous in phenomena pertaining to cellular and molecular biology. In many cases, the structure of these networks is dynamically altered by the mechanical feedback of biological lipid membranes and cytoplasmic flows. However, current modeling and computational approaches neglect such mechanical feedbacks for the sake of computational tractability.

In this talk, we present a *dissipative particle dynamics* approach to simulating the meso-scale dynamics of polymer networks. Our simulations explicitly include mechanical interactions with other meso-scale structures (e.g., lipid membranes) and cytoplasmic flows. We compare the results of our approach to those of Brownian dynamics simulations. We also discuss ongoing work on stochastic homogenization, bridging the gap between the meso-scale description and macroscopic models of bulk mechanical properties.

Speaker: **Kevin Sanft** (University of Minnesota)
Title: *Scaling properties of exact simulation algorithms for spatially discretized stochastic reaction-diffusion processes*
Abstract: Stochastic reaction-diffusion processes are widely used to model biochemical systems. Discretizing the spatial domain leads to a discrete state, continuous time Markov jump process that can be described by the reaction-diffusion master equation. Solutions to the master equation are approximated by generating exact trajectories using

variants of the Gillespie algorithm. The choice of simulation formulation and underlying data structures has a dramatic effect on computational efficiency. In this talk, I will show how the optimal algorithm choice depends on the number and relative timescales of the transition channels. For very large problems, memory hierarchy effects lead to scaling properties that differ from the asymptotic analysis, which influences the optimal simulation algorithm parameters.

Session on Particle-Based Methods and Modeling:

Speaker: **Steven Andrews** (Fred Hutchinson Cancer Research Center)
Title: *The Smoldyn simulator: overview, applications, and hybrid simulation*
Abstract: Smoldyn is a particle-based cell biology simulator which represents proteins or other molecules of interest as individual spheres. These particles diffuse, undergo chemical reactions with each other, and interact with membranes and other surfaces in ways that closely mimic reality. In particular, all interaction rates are quite accurate. Smoldyn is easy to use and supports a wide variety of features. Several colleagues and I recently used Smoldyn to investigate transcription factor dynamics in cell nuclei to determine what processes enable transcription factors to locate their target genes quickly. In agreement with prior results, we found that non-specific binding and then diffusion along DNA accelerates target gene finding through a process called the antenna effect. Additionally, we found that intersegmental transfer also accelerates target gene finding; here, a transcription factor transfers directly from being non-specifically bound on one DNA segment to being non-specifically bound on an adjacent DNA segment. In separate work, Martin Robinson and I recently added adjacent-volume hybrid simulation capability to Smoldyn. Here, space is partitioned into adjacent continuum and lattice regions, which are simulated with particle-based and spatial Gillespie type methods, respectively. These enable simulations to represent high levels of detail where required but lower detail (and faster computation) elsewhere.

Speaker: **Samuel Isaacson** (Boston University)
Title: *Lattice Approximation of Spatially-Continuous Particle-Based Stochastic Reaction-Diffusion Models*
Abstract: We derive a lattice, continuous-time jump process approximation of a spatially-continuous, interaction-function based stochastic reaction-diffusion model. The new model has the benefit of treating diffusion and linear reactions in exactly the same manner as the reaction-diffusion master equation (RDME). Moreover, in the limit of coarse meshes it can be shown that the RDME approximates this model. Unlike the RDME, this new, convergent reaction-diffusion master equation model (CRDME) retains bimolecular reactions in the limit that the mesh spacing approaches zero, converging to the underlying interaction-function model. The CRDME therefore offers alternatives to both Brownian Dynamics (BD) methods for solving the interaction-function model, and coupled RDME-BD methods that attempt to overcome the loss of bimolecular reactions in the RDME for small mesh sizes.

Speaker: **Frank Noe** (Free University of Berlin)
Title: *interacting-Particle Reaction-Diffusion (iPRD) dynamics*
Abstract: In cellular signal transduction, what happens where and when? Addressing this question requires to deal with protein interactions that involve low copy numbers, precise stoichiometry, the spatiotemporal arrangement within molecular machines. While modern experimental techniques such as super-resolution microscopy are taking giant leaps towards watching cells in action with molecular resolution, computer simulation is still facing the challenge of combining physical detail with computational efficiency. Here we propose the interacting-Particle Reaction-Diffusion (iPRD) approach. iPRD is a fusion of particle-based reaction-kinetics and molecular dynamics including particle-interactions aiming at simulating cellular signal transduction with rigorous physical approach. I will present the theory and methodology, briefly sketch our ReaDDy implementation of iPRD and hint to some biological applications.

Session on Multiscale Methods and Modeling:

Speaker: **Ruth Baker** (Oxford University)
Title: *Adaptive multi-level Monte Carlo methods*
Abstract: Discrete-state, continuous-time Markov models are widely used in the modelling of biochemical reaction

networks. Their complexity generally precludes analytic solution, and so we rely on Monte Carlo simulation to estimate system statistics of interest. Perhaps the most widely used method is the Gillespie algorithm. This algorithm is exact but computationally complex. As such, approximate stochastic simulation algorithms such as the tau-leap algorithm are often used. Sample paths are generated by taking leaps of length tau through time and using an approximate method to generate reactions within leaps. However, tau must be held relatively small to avoid significant estimator bias and this significantly impacts on potential computational advantages of the method.

The multi-level method of Anderson and Higham tackles this problem by cleverly generating a suite of sample paths with different accuracy in order to estimate statistics. A base estimator is computed using many (cheap) paths at low accuracy. The bias inherent in this estimator is then reduced using a number of correction estimators. Each correction term is estimated using a collection of (increasingly expensive) paired sample paths where one path of each pair is generated at a higher accuracy compared to the other. By sharing randomness between these paired sample paths only a relatively small number of pairs are required to calculate each correction term.

In the original multi-level method, paths are simulated using the tau-leap technique with a fixed value of tau. This approach can result in poor performance where the reaction activity of a system changes substantially over the timescale of interest. By introducing a novel, adaptive time-stepping approach we extend the applicability of the multi-level method to such cases. In our algorithm, tau is chosen according to the stochastic behaviour of each sample path. We present an implementation of our adaptive time-stepping multi-level method that, despite its simplicity, performs well across a wide range of sample problems.

Speaker: **Radek Erban** (University of Oxford)
Title: *From Molecular Dynamics to Particle-based Stochastic Reaction-Diffusion Models*
Abstract: I will discuss all-atom and coarse-grained molecular dynamics (MD) models with the aim of developing and analysing multiscale methods which use MD simulations in parts of the computational domain and (less detailed) particle-based stochastic reaction-diffusion models in the remainder of the domain. Applications using all-atom MD include intracellular dynamics of ions and ion channels. Applications using coarse-grained MD include protein binding to receptors on the cellular membrane, where modern stochastic reaction-diffusion simulators of intracellular processes can be used in the bulk and accurately coupled with a (more detailed) MD model of protein binding which is used close to the membrane.

Speaker: **Christian Yates** (University of Bath)
Title: *A PDE/compartment-based hybrid method for simulating stochastic reaction-diffusion systems*
Abstract: Spatial reaction-diffusion models have been employed to describe many emergent phenomena in biological systems. The modelling technique for reaction-diffusion systems that has predominated due to its analytical tractability and ease of simulation has been the use of partial differential equations (PDEs). However, due to recent advances in computational power, the simulation, and therefore postulation, of computationally intensive individual-based models has become a popular way to investigate the effects of noise in reaction-diffusion systems.

The specific stochastic model with which we shall concern ourselves are known as ‘compartment-based’. These models are characterised by a discretisation of the computational domain into a grid/lattice of discrete voxels between which molecules can jump. Molecules are considered to be well-mixed in each one of these voxels and can react stochastically with other molecules in their voxel with prescribed rates.

In a wide variety of biological situations, stochasticity due to low copy numbers is relevant only in particular regions of the domain. In other regions, copy numbers are sufficiently high that mean field models suffice to capture the important dynamics. Such conditions necessitate the development of hybrid models in which some areas of the domain are modeled using a continuum representation and others using an individual-based representation.

In this talk we develop hybrid algorithms which couple a PDE in one region of the domain to a compartment-based model in the other. Rather than balancing flux at the interface, we use a method which is similar to the ghost-cell method. Characteristic of this method is the individual treatment of particles as they cross the interface. A small region of the PDE domain adjacent to the compartment-based region is allowed to contribute particles to the compartment-based regime. When particles cross over the interface into this pseudo-compartment from the

compartment-based regime a step-function with the mass of a single particle is added. We test our hybrid method in a variety of different scenarios and analyse the error introduced in each case.

33.4 Scientific Progress Made

Discussions at the workshop identified a number of future research directions and important problems to be investigated.

After the speaker presentations outlined in Section 3, there was a panel discussion where a number of important issues were discussed specific to the research and software development community present. The panel discussions were lead by leaders from the major simulation software groups. Simulation approaches to modelling stochastic reaction-diffusion processes are quite varied and each approach has advantages and disadvantages from a numerical standpoint. Some issues that need to be taken into account by modellers when using these numerical approaches are accuracy, computational complexity and data management, and the ease with which the approach may be implemented in parallel. There are currently no standard test problems for assessing these qualities, which is just part of the reason it is very difficult to compare different approaches and choose the most appropriate one for a given model system. In a discussion lead by E. de Schutter a number of important problems were identified which prohibit the establishment of a community standard against which algorithms may be compared and tested. Whilst some of these problems had simple solutions others remain as open problems. One of the problems that was identified was the need for the standards to be valued by the community. This discussion was the first organised discussion of this problem by the community and an important step to establishing a common scientific language to report findings. An online forum was set up to encourage future communication within the community on important issues such as this.

The structure and order of the workshop speakers played an important role in stimulating critical discussion and identifying important problems for future work. Open problems were easily identifiable by focusing on specific topics such as biological models and open problems in the feasibility of the methods to simulating real biological systems, and then specifically focusing on modelling techniques. The limitations of both particle-based methods and mesoscopic methods were summarised well in the final section which focused on hybrid modelling approaches. These limitations need to be addressed by the community before the modelling techniques available to researchers are capable of simulating very complex biological systems such as a human cell. Segmenting the workshop subject content in this way lead to critical discussions and the development of new collaborations. For example, organizer S. Isaacson has two projects that were stimulated by discussions at the workshop: 1. Determining how reversible reactions should be modeled in general particle-based models to preserve key physical properties such as detailed balance, and 2. Developing asymptotic methods to provide analytic approximations to the solutions of particle-based stochastic reaction-diffusion models (in collaboration with conference participant Jay Newby). For both these projects manuscripts are now in preparation for submission.

33.5 Outcome of the Meeting

The workshop offered a unique opportunity for the wider scientific community working on mathematical biology, systems biology, numerical analysis, computational methods, and stochastic analysis to exchange ideas and work collaboratively in order to tackle the many challenging open problems of this field. These include researchers from mathematics (probabilists, numerical analysts, and applied mathematicians), statistics, computational science, physics, biology, engineering, and systems biology. The interactions between these researchers are expected to lead to the development of better mathematical and computational methods with which to study biological processes, and new insights into specific systems arising in cell and population biology. The workshop also introduced a number of more junior researchers to the broader international community of scientists interested in particle-based stochastic reaction-diffusion models.

The meeting also identified the growing importance for the community to congregate and discuss future directions on a more regular basis. A workshop was organised for the community in Cambridge in 2016 and discussions have already started for holding another meeting in Australia in 2018. Prior to the Particle-Based Stochastic Reaction-Diffusion Models in Biology workshop at BIRS, research in this area was fragmented and progress was reported in small groups separately by mathematicians, computer scientists, computational biologists etc. The importance of meeting as an interdisciplinary community to establish shared research goals was widely recognized as a key outcome from the workshop. This in turn stimulated ongoing efforts to continue holding bi-annual meetings on Particle-Based Stochastic Reaction Diffusion models.

Participants

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Bibliography

[1] D. Anderson and J. Mattingly, A weak trapezoidal method for a class of stochastic differential equations, *Communications in Mathematical Sciences* **9** (2011), no. 1, 301–318.

[2] S. Andrews and D. Bray, Stochastic simulation of chemical reactions with spatial resolution and single molecule detail. *Phys Biol* **1** (2004),137–151.

[3] S. Arjunan and M. Tomita, A new multicompartmental reaction-diffusion modeling method links transient membrane attachment of E. coli MinE to E-ring formation. *Systems and Synthetic Biol* **4** (2010), 35–53.

[4] A. Donev, V. Bulatov, T. Oppelstrup, G. Gilmer, B. Sadigh, and M. Kalos, A first-passage kinetic Monte Carlo algorithm for complex diffusion–reaction systems, J. Comp. Phys. **229** (2010),3214–3236.

[5] S. Engblom, L. Ferm, A. Hellander and P. Lötstedt, Simulation of stochastic reaction-diffusion processes on unstructured meshes. *SIAM J Sci Comput* **31** (2009), 1774–1797.

[6] M. Elowitz, A. Levine, E. Siggia, and P. Swain, Stochastic gene expression in a single cell, *Science* **297** (2002), 1183–1186.

[7] R. Erban and S. J. Chapman, Stochastic modelling of reaction-diffusion processes: algorithms for bimolecular reactions, Physical Biology **6** (2009), no. 4, 046001.

[8] J. Lipkova , K. Zygalakis, S. J. Chapman, and R. Erban,Analysis of Brownian Dynamics simulations of reversible bimolecular reactions, SIAM J. Appl. Math. **71** (2011), 714.

[9] C. W. Gardiner, K. J. McNeil, D. F. Walls, and I. S. Matheson, Correlations in stochastic models of chemical reactions, J. Stat. Phys. **14** (1976), 307.

[10] D. T. Gillespie, Exact stochastic simulation of coupled chemical-reactions, J. Phys. Chem. **81** (1977), 2340–2361.

[11] J. Hattne, D. Fange and J. Elf, Stochastic reaction-diffusion simulation with MesoRD, *Bioinformatics* **21** (2005), 2923–2924.

[12] I. Hepburn, W. Chen, S. Wils and E. De Schutter, STEPS: efficient simulation of stochastic reaction-diffusion models in realistic morphologies. *BMC Syst Biol* **6** (2012), 36.

[13] S. A. Isaacson, D. M. McQueen and C. S. Peskin, The influence of volume exclusion by chromatin on the time required to find specific DNA binding sites by diffusion, PNAS **108** (2011), 3815–3820.

[14] S. Isaacson and C. Peskin, Incorporating diffusion in complex geometries into stochastic chemical kinetics simulations, SIAM Journal on Scientific Computing **28** (2006), no. 1, 47–74.

[15] J Keizer, Nonequilibrium statistical thermodynamics and the effect of diffusion on chemical reaction rates, J. Phys. Chem. **86** (1982),5052–5067.

[16] Muñoz-García J., Neufeld Z., Kholodenko B. N., and Sauro H. M. (2009), Positional information generated by spatially distributed signaling cascades, PLoS Comp. Biol. **5**, no. 3:e1000330.

[17] S. Neves, P. Tsokas, A. Sarkar, E. Grace, P. Rangamani, S. Taubenfeld, C. Alberini, J. Schaff, R. Blitzer, I. Moraru, R. and Iyengar, Cell shape and negative links in regulatory motifs together control spatial information flow in signaling networks, Cell **133** (2008), 666–680.

[18] T. Opplestrup, V. Bulatov, A. Donev, M. Kalos, G. Gilmer and B. Sadigh, First-passage kinetic Monte Carlo method. *Phys Rev E* **80** (2009),066701.

[19] J. Paulsson, Summing up the noise in gene networks, *Nature* **427** (2004), 415–418.

[20] E. Roberts, J. E. Stone, and Z. Luthey-Schulten, Lattice Microbes: high-performance stochastic simulation method for the reaction-diffusion master equation, J. Comput. Chem. **34** (2013).

[21] M. V. Smoluchowski, Mathematical theory of the kinetics of the coagulation of colloidal solutions, Z. Phys. Chem. **92** (1917), 129–168.

[22] J. Stiles and T. Bartol, Monte Carlo methods for simulating realistic synaptic microphysiology using MCell. *Computational Neuroscience: Realistic Modeling for Experimentalists* (E. Schutter, ed.), CRC Press, (2001) pp: 87–127.

[23] K. Takahashi and S. Tănase-Nicola and P. R. ten Wolde, Spatio-temporal correlations can drastically change the response of a MAPK pathway, PNAS **107** (2010), 2473–2478,

[24] M. Tomita, Whole-cell simulation: a grand challenge of the 21st century. *Trends Biotechnology* **19** (2001), 205–210.

[25] J. van Zon and P. R. ten Wolde, Green's-function reaction dynamics: a particle-based approach for simulating biochemical networks in time and space. *J Chem Phys* **123** (2005), 234910.

Chapter 34

Algorithms for Linear Groups (14w5031)

November 16 - 21, 2014

Organizer(s): Jon F. Carlson (University of Georgia), Bettina Eick (University of Braunschweig), Alexander Hulpke (Colorado State University), Eamonn O'Brien (University of Auckland)

34.1 Overview of the Field

The development of algorithms for the study of matrix groups is a very active area of computational group theory. It is a rapidly growing research topic with many highly interesting recent results and challenging open problems. Its overall goal is to develop effective algorithms to investigate and classify matrix groups of various types. The research in this area has interesting links to abstract group theory, representation theory, the theory of matrix algebras as well as to computer science and the general theory of efficient algorithms. Further, it has applications in areas such as crystallography, coding theory, number theory, topology, and cryptography.

Matrix groups are subgroups of a general linear group over a field. The design of algorithms for matrix groups depends heavily on the underlying field. In the case of finite fields, the "matrix group recognition project" has made significant progress in the development of algorithms to investigate the structure of a matrix group given by generators. This meeting considered the status of this major international research project and surveyed the open problems that still need to be resolved. In the case of infinite fields, the situation is much more difficult and less well understood at the current time. This meeting had a number of talks on recent advances in different aspects on this still wide open research topic. This may be considered as an important initial step forward.

We include a brief overview on the research topic of algorithms for matrix groups below. For details on the various aspects of this research topic we refer to the surveys by O'Brien [21]; Kantor & Seress [15]; Leedham-Green [16]; Babai, Beals & Seress [4]; Neunhöffer & Seress [19]; and Detinko, Eick & Flannery [9]. We also note that the Handbook of Computational Group Theory [14] contains an introduction to the topic.

34.2 Developments and Open Problems

The meeting witnessed the confluence of different strands of mathematics that in the past interacted on an ad-hoc basis, but rarely, if ever, came together in a broader context.

34.2.1 Matrix Group Recognition

The catalyst for enabling this broad interaction has been the ”matrix group recognition project”, which for the last two decades has been one of the major of areas of study in computational group theory. This research project is now reaching fruition, moving from a self-motivated project towards becoming a crucial tool for the computation with groups.

It has benefited from contributions by many researchers from various different areas of mathematics. Put succinctly, the problem is this: Given a small collection of invertible $n \times n$ matrices, for some $n > 0$, defined over a finite field K, provide effective algorithms to describe the structure of the group that they generate. In other words, one wants to identify the group from the representation that is provided by the action of the matrices on the vector space of row vectors.

Aschbacher [1] described the maximal subgroups of the general linear groups and other finite classical groups. This classification of maximal subgroups underpins the matrix group recognition project: the first step of this recognition is to determine a maximal subgroup in which the considered group is contained. For example, it is easily determined if the representation fixes some proper non-trivial subspace and thus is reducible. In this case, a maximal subgroup containing the given group is determined. At the same time, this type of recognition of the matrix group gives rise to a decomposition of the group into smaller matrix groups and thus allows for a recursive application of the method.

Aschbacher's classification of maximal subgroups shows that every subgroup of $\mathrm{GL}(n, K)$ lies in a subgroup that is in at least one of nine classes. The first seven classes are characterized by geometric conditions such as being reducible, being definable over a smaller field or having the representation imprimitive or tensor induced. The starting point of the the project was the development of algorithms that run in polynomial time to recognise membership in a specific class and exploit the natural linear action of the group on the underlying vector space. The remaining two classes are classical groups in their natural representation and other absolutely irreducible tensor-indecomposable representation of simple groups.

Here the aim is to ”constructively recognise” the group: obtain an effective isomorphism between the given copy of the group and a “standard” copy of the associated simple group. If such an isomorphism is available, then it allows us to translate known data (for example, its conjugacy class representatives) from the standard copy to the input copy.

At the meeting the lecture by Charles Leedham-Green

summarized

the progress on the project. The goal of constructing a chief series of the linear group is essentially now realised. At the present time, there is a nearly complete implementation of the resulting algorithms available in the computer algebra system MAGMA. Leedham-Green suggested in his lecture that it is now appropriate for a unified push to create an alternative implementation in the system GAP. The advantages of having a second implementation are significant, both from the standpoint of correctness by providing the ability to check results, and the development of new ideas and refinements. It also would provide general access to what is increasingly viewed as a central piece of infrastructure for computational group theory. A meeting of some of the participants was held one evening at the workshop for the purpose of planning this second implementation.

34.2.2 Maximal subgroups of Classical Groups

To utilize the reduction process of matrix group recognition to simple composition factors, one needs to understand the ninth class in Aschbacher's classification, consisting of maximal subgroups of classical groups that are not identifiable by some geometric property.

Understanding this class would have widespread applications, for example to matrix group recognition and, more generally, broadening the range of applicability of many algorithms for the structural investigations of matrix groups. It would also allow an explicit determination of maximal subgroups of the classical groups, which has been a long-standing problem of intense interest in finite group theory.

The recent monograph by Bray, Holt and Roney-Dougal [7] is a first step in this direction by offering a complete classification of the maximal subgroups of classical groups of degree at most 12; the results of this are already being exploited in many algorithms.

A non-geometric maximal subgroup of a classical group must satisfy certain conditions on its generalized Fitting subgroup and the action of that Fitting subgroup on the natural module of the classical group. The generalized Fitting subgroup is generated by the largest nilpotent subgroup and the maximal normal semisimple subgroup. Recent developments in the field have put a premium on finding the maximal subgroups in this class. Kay Magaard reported on progress in this direction. His latest work has taken the form of looking for obstructions to maximality, that is, subgroups lying between a given subgroup and a classical group. The focus of his work has been on obstructions that are sporadic simple groups.

The pervasive presence of classical groups, and matrix representations of simple groups, was seen in the work of several other participants.

34.2.3 Isomorphism testing

The constructive isomorphism test required for simple composition factors is a special case of the more general problem of algorithmic determination of an isomorphism between two finite groups. Efficient algorithms to test if two groups are isomorphic or to reduce a collection of groups to isomorphism type representatives have a wide range of applications in group theory. For example, such methods provide a basis for the classification of groups of small order, see [6]. The currently available algorithms to test isomorphism for finite p-groups [13] and finite groups in general [8] make significant use of algorithms for matrix groups over finite fields and hence are an important application of such algorithms.

At the workshop two talks addressed aspects of the isomorphism problem directly. Peter Brooksbank spoke on a new algorithm for testing isomorphism of p-groups of genus 2. These are groups of small nilpotency class. Any effort at a solution immediately encounters difficult problems in the area of algorithms for matrix groups.

Alice Niemeyer spoke on a closely related problem. She considered the question of how to construct finite p-groups whose automorphism groups map onto prescribed matrix groups and presented an interesting solution to this problem.

The problem of solving the isomorphism problem for matrix groups is still wide open even for finite matrix groups; this can be considered as a major challenge in this area.

34.2.4 Infinite Fields

Over infinite fields the analysis of matrix groups by computational methods is far more difficult than it is over finite fields. Generically, such a task may be intractable and it is know that some fundamental problems, such as the membership problem, may be undecidable in general for arbitrary infinite matrix groups. On the other hand such groups play an important role in many applications, and even solutions for particular classes of groups are therefore highly welcome. Several participants reported on progress for particular classes.

The Tits alternative and applications. A dividing line between the possible and impossible here appears to be given by the Tits Alternative [22], a theorem which asserts that a finitely generated matrix group is either has a solvable normal subgroup of finite index or has a non-abelian free subgroup. The Tits Alternative has been shown to be algorithmically verifiable; see [10, 5]. Its solution relies on the outcome of the "matrix group recognition project" to study finite images. The class of solvable-by-finite matrix groups seems to be accessible for algorithmic methods. For example, an algorithm of Assmann & Eick [2] decides if a rational virtually solvable group is also virtually polycyclic.

The class of matrix groups that contain a non-abelian free subgroup is significantly harder to investigate. Even deciding if a matrix group with two generators is free on these two generators is an open problem. In the meeting a first step towards computations with free matrix groups was reported by Markus Kirschmer, see [12].

Arithmetic groups. Arithmetic groups are matrix groups which are defined as a variety of a polynomial ideal. It is known that each integral arithmetic group is finitely generated.

A first main goal in the algorithmic investigation of such groups is to find generators of such a group. Willem de Graff discussed how to solve this problem if the considered group is unipotent or abelian.

Dane Flannery extended these solutions to consider solvable matrix groups.

Alla Detinko presented a survey on recent advances on arithmetic subgroups that have the congruence subgroup property. Here again finite images, treated by matrix group recognition, are a crucial component.

Lattices and unit groups. Crystallographic groups are rational matrix groups that preserve a lattice. Karel Dekimpe reported on the problem of determining a small, or even a minimal, generating set for a crystallographic group, utilizing methods from computational group theory. This intriguing problem still has no general algorithmic solution.

Gabriele Nebe showed how the classical algorithm of Voronoi can be used in a new application to determine normalizers of finite matrix groups and unit groups of orders. The structure of unit groups of integral group rings was discussed by Eric Jespers.

34.2.5 Open problems.

John Dixon (Ottawa, Canada) presented a very interesting lecture on "Some open problems in linear groups". We list some of his suggested problems in the following.

(1) Given elements x, y of prime order p in the general linear group $\mathrm{GL}(n, \mathbb{C})$, what can be said about the subgroup $\langle x, y\rangle$ which they generate. It is known that if $\langle x, y\rangle$ is finite then it is abelian.

Does this gives any information about the infinite case?

(2)

A matrix $x \in \mathrm{GL}(n, F)$ is cyclic if its minimal polynomial has degree n. Cyclic matrices play a role in computational questions in linear groups. An open problem due to Thompson asks whether there is always a permutation matrix u such that ux is cyclic.

(3)

Determining whether a linear group is free is an important problem in computational study of infinite linear groups. Is there some sense in which almost all pairs of elements of $\mathrm{GL}(n, \mathbb{Q})$ generate a free group? Is the set of such pairs Zariski-dense in $\mathrm{GL}(n, \mathbb{Q}) \times \mathrm{GL}(n, \mathbb{Q})$?

(4)

Is it possible to generate (approximately) uniformly random conjugacy classes in a finite group without generating random elements? In other words is the former problem easier that the latter?

(5)

Let $s\colon G \to \mathrm{GL}(n, \mathbb{C})$ be a representation of a finite group. There are cases when it would be useful to find c in the group ring $\mathbb{C}G$ such that c is easily computed from a given set of generators of G and $s(c)$ has rank 1 (or nullity 1). How can we do this?

34.3 A summary of presentations

The following is a summary of the broad themes covered by the individual lectures at the meeting.

Matrix Group Recognition. Charles Leedham-Green (London, UK) presented a major lecture on ”The matrix group recognition project; where do we go from here?” This was the first lecture of the Ákos Seress day. The speaker noted that the matrix group recognition is (with small gaps that are being filled) fully functional and available in MAGMA, see [3]. Some theoretical problems, such as reliance on integer factorisation and discrete logarithms, remain but only cause problems in extreme cases. He presented five directions for future work:

improve performance; increase functionality; incorporate modular representation theory; use the software; produce a version in GAP.

The talk, as well as an evening discussion, focused on the last of these objectives.

Alex Ryba (New York, US) presented a lecture on ”Tensor Decompositions”. It is related to one of the more difficult issues of the matrix group recognition project. He introduced an algorithm to determine all decompositions of a matrix as a tensor product of smaller representations. The method involves a polynomial reduction to the Pure Tensor Problem:

Given a subspace of a tensor product determine all pure tensors in the subspace. He discussed some issues with the running time of the algorithm; it currently relies on use of Gröbner basis techniques and so does not run in polynomial time. He concluded by raising the following intriguing questions:

Is “matrix recognition” in the NP complexity class?

An answer to this latter question seems tantalizingly close.

If so, is “matrix recognition” NP complete? This is not implausible, given some of the characteristics it shares with known NP complete problems, and would make it an interesting problem from a computer science point of view.

Bill Kantor (Eugene, US) introduced new results obtained with another participant, Martin Kassabov (Cornell, US) which allow for efficient constructive recognition of a black box group isomorphic to $\mathrm{PSL}(2, q)$where q is even. There is related work by Borovik and Yalçınkaya for q odd. This is a critically important base case for many algorithms.

Arithmetic Groups. Willem de Graaf (Trento, Italy) lectured on “Generators of arithmetic groups”.

Let G be an algebraic matrix group defined over $\mathbb{Q}$ and let $G(\mathbb{Z})$ denote the subgroup consisting of the elements with coefficients in $\mathbb{Z}$. This group, and subgroups of $G(\mathbb{Q})$ commensurable with it, are arithmetic subgroups of G. A major problem in algorithmic matrix group theory is to determine a finite set of generators for $G(\mathbb{Z})$. While a finite generating set exists, it remains a difficult problem to construct one. The speaker discussed some examples where such is known: unit groups of number fields (an algorithm of Buchmann (1990) solves the problem); unit groups of quaternion algebras (algorithms go back to Ford (1925)); the unit groups of group rings (there are several constructions of subgroups of finite index of the unit group, starting with work of Bass (1966)). He presented a solution to the problem where G is unipotent or diagonalizable. The first part is joint work with Pavan, and the second with Faccin and Plesken. The algorithm for the problem in the diagonalizable case can be used to find generators of units groups of integral abelian group rings.

Alla Detinko (Galway, Ireland) lectured on ”Algorithms for arithmetic groups: a practical approach”. She presented a survey of recent results in joint work with Flannery and Hulpke on computing with arithmetic subgroups which have the congruence subgroup property, giving most consideration to arithmetic subgroups of the special linear group. She discussed decidability of fundamental algorithmic problems, and presented a general technique to handle algorithmically this class of groups. Applying that technique, it is possible to solve a number of computational problems such as membership testing, the orbit-stabilizer problem, and finding algorithms to investigate subnormal structure of arithmetic subgroups.

Dane Flannery (Galway, Ireland) lectured on “Integrality and arithmeticity of solvable linear groups”.

He described an algorithm to decide whether a finitely generated subgroup H of a solvable algebraic group G is arithmetic. The algorithm incorporates procedures by de Graaf *et al.* to compute a generating set of an arithmetic subgroup of G. He introduced a simple new algorithm for integrality testing of finitely generated solvable-by-finite linear groups over $\mathbb{Q}$. This enables one to decide whether the index $|H : H_{\mathbb{Z}}|$ is finite. Another component of the main algorithm requires the determination of torsion-free ranks of solvable finitely generated subgroups of $\mathrm{GL}(n, \mathbb{Q})$, which uses an algorithm developed by Detinko, Flannery, and O’Brien.

Structure and characters for finite groups. A number of lectures were given on various aspects of finite group theory and group representation theory that use computational methods. The work on these problems has contributed significantly to other areas of computational group theory.

Robert Wilson’s (London, UK) lecture, entitled “Black box groups and the Monster”, considered how methods developed initially for solving hard problems for sporadic groups have migrated into general-purpose software. Examples are Sims’ machinery of base and strong generating set for permutation groups (applied by Sims to groups such as the Baby Monster, in which one cannot even write down permutations), or the Meataxe, originally designed by Parker and Thackeray for constructing the sporadic group J_4.

The speaker discussed how methods developed by him and several collaborators for computing in the Monster, of order approximately 10^{53} and probably the single most interesting matrix group, but whose matrices were too big to write down, are now used in other situations. One example is the use of involution centralizer methods in the matrix group recognition project.

Kay Magaard (Birmingham, UK) lectured on ”Quasisimple overgroups of quasisimple irreducible subgroups of classical groups”. He discussed finding maximal subgroup of finite classical groups. This is a problem that has implications for many areas of computational group theory. Suppose that X is a finite classical group with natural module $V = k^m$. In 1984 Aschbacher defines eight families of “geometric” subgroups of X. The maximal subgroups of X that are not in a geometric family are distinguished by the structure and action on V of their generalized Fitting subgroups. Building on the earlier work of Kleidman and Liebeck and the 2012 work of Bray, Holt and Roney-Dougal, a full classification of the maximal subgroups of the finite classical groups can be achieved by answering the very challenging question: When is a non-geometric subgroup H maximal in X?

The possible obstructions to the maximality of non-geometric H in X, that is subgroups G where $H < G < X$, must lie in one of the geometric classes and the group H must be sporadic, alternating, or of Lie type.

Magaard surveyed research on obstructions to maximality as well as introducing some new results, mainly concerning cases where $H = J_1$ or where H is of Lie type.

Rebecca Waldecker (Halle, Germany) reported on joint work with Magaard on “Permutation groups where nontrivial elements have few fixed points”. The motivation for the work is a better understanding of the automorphism groups of Riemann surfaces. It is known that the automorphism group of a compact Riemann surface X of genus at least 2 is finite, and one way to prove this uses the so-called Weierstrass points, a finite set of geometrically significant points on X on which the automorphism group acts. To identify nontrivial automorphisms fixing at least 5 such points they investigate permutation groups where all non-trivial elements have at least two, three, or four fixed points, aiming to describe precisely those finite simple groups which occur in these cases. Waldecker sketched some typical arguments, and discussed other related questions needing resolution.

A lecture by Klaus Lux (Tucson, US) discussed ”Character tables of trivial source modules”. Trivial source modules are direct summands of permutation modules and play a central role in several conjectures in representation theory, for example the celebrated Alperin weight conjecture. Conveniently, there are only finitely many indecomposable trivial source modules.

The speaker discussed methods to determine a trivial source character table (as introduced by Benson and Parker) computationally and demonstrated these for the Mathieu groups and the Higman-Sims group. The computational techniques use a variety of GAP packages, for example the basic package for basic algebras.

Groups of Lie Type. Several lectures at the workshop concentrated on structure and representations of these finite simple groups.

Arjeh Cohen (Eindhoven, Netherlands) reported on joint work with Don Taylor (Sydney, Australia) on ”Row Reduction for Twisted Groups of Lie type”. This represented an extension of earlier work (also with Murray) on an algorithm for a finite group G of untwisted Lie type and an irreducible G-module M over a field of the same characteristic as G.

Given a linear transformation A on M, and the coefficients of the highest weight λ of the representation, it decides whether A is in the image of G; if so, it finds a preimage of A in polynomial time in $\log q$, subject to the existence of a discrete log oracle for $GF(q)$.

Gerhard Hiss (Aachen, Germany) lectured on “Imprimitive representations for quasisimple classical groups”. He reported on a joint project with Magaard. In previous work with Husen, they classified the imprimitive (not induced from smaller subgroups) ordinary irreducible representations of finite groups of Lie type arising from algebraic groups with connected centers. This excludes some quasisimple classical groups such as the special linear groups or the spin groups. The new project applies results of the former, Clifford theory and Lusztig’s generalized Jordan decomposition of characters to the classification of the imprimitive representations for quasisimple classical groups.

Free Groups as Matrix Groups. Markus Kirschmer (Aachen, Germany) lectured on “The explicit membership problem for discrete free subgroups of $\mathrm{PSL}(2, \mathbb{R})$”, joint work with Eick and Leedham-Green. Computing with matrix groups over infinite rings is much more complicated than working with matrix groups over finite fields. For example, the membership problem is undecidable in general. However, for subgroups of $\mathrm{PSL}(2, \mathbb{R})$ the situation is much better since there are powerful geometric methods available.

Kirschmer presented a practical method which uses the Ping-Pong Lemma to solve the membership problem in this case.

Classical Groups. Cheryl Praeger (Perth, Australia) lectured on “Generating finite classical groups by elements with large fixed point spaces”. She discussed a body of work, comprising her collaboration with Seress and others over the past decade. It relates to work of many other researchers in the discipline. She discussed problems arising in the analysis of the constructive recognition algorithm of Leedham-Green and O’Brien [17] for classical groups in odd characteristic and natural representation, specifically in finding balanced involutions and constructing their centralizers.

This work was followed by several papers on generation of such classical groups by a sequence of balanced involutions.

Constructive recognition for finite classical groups in even characteristic is more difficult.

Innovative new procedures developed by Neunhöffer and Seress, and by Dietrich, Leedham-Green, Lübeck & O’Brien [11] have solved the problem with two rather different approaches. Justifying either of these new methods requires proof that the groups can be generated efficiently by elements with large fixed point spaces. A fundamental problem involved the generation of a classical group in dimension $2n$ over a field of order q by so-called ’good elements', namely elements with an n-dimensional fixed point space, and with order divisible by a primitive prime divisor of $q^n - 1$. The lecture described estimates, obtained in her work with Seress and Yalçınkaya, for the probability that two random conjugates of a good element generate the classical group, and how this result is employed in the design of the algorithms.

Discrete groups and unit groups. Several lectures presented advances in techniques for studying discrete groups and unit groups of algebras.

Gabriele Nebe (Aachen, Germany) lectured on "Computing unit groups of orders".

Let Λ be an order in some semisimple rational algebra A. Its unit group $\Lambda^\times$ is a finitely presented group. In joint work with Braun, Coulangeon, and Schönnenbeck, she applied an algorithm first developed by Voronoi in 1900 in the context of reduction theory of integral lattices to compute generators and relations of $\Lambda^\times$. Additional data obtained from Voronoi's algorithm can be used to solve the word problem in these generators.

The algorithm has applications in many contexts. For example, it can be used to determine generators for the normalizer of a finite integral matrix group as shown by Opgenorth (2001); it also can be employed to calculate the automorphism group of a lattice of signature $n, 1$ as described by Mertens (2009).

Nebe reported on a recent implementation to handle certain unit groups of orders including all orders in rational division algebras. For quaternion algebras it improves substantially the existing implementation in MAGMA.

A lecture by Eric Jespers (Brussels, Belgium)

surveyed methods to determine the unit group of an integral group ring of a finite group. In many circumstances, it is possible to determine a subgroup of finite index in such a unit group, but the full group of units is known in comparatively few cases only. He also discussed a structure theorem for the unit group for some classes of finite groups.

Crystallographic Groups. Karel Dekimpe (Leuven, Belgium) lectured "On the number of generators of a crystallographic group". A Bieberbach group is a torsion-free crystallographic group and these groups are the fundamental groups of the compact flat Riemannian manifolds.

Each such group has a natural matrix representation and this is usually used to compute with such a group. There exist upper bounds on the rank of an n-dimensional crystallographic group Γ in case the holonomy group is a p-group.

In a joint paper with Penninckx (2009), the speaker proved that if the holonomy of Γ is elementary abelian, then Γ can be generated by n elements

The result raises the question whether every n-dimensional Bieberbach group (or even every torsion-free polycyclic-by-finite group of Hirsch length n) can be generated by n elements. In this direction, the speaker together with Adem, Petrosyan and Putrycz proved (2012) that such a group

Γ can be generated by $a(n-\beta_1)/(p-1)+\beta_1$ elements, where $a = 2$ if $p \leq 19$ otherwise $a = 3$, and β_1 is the rank of $Z(\Gamma)$, which equals the torsion-free rank of $\Gamma/[\Gamma, \Gamma]$.

Abstract Groups and Algebras. Gretchen Ostheimer (New York, US) lectured on "Recognizing torsion-free nilpotent groups as direct products", joint work with Baumslag and Miller.

She described an algorithm to decide if a given finitely generated torsion-free nilpotent group is decomposable as the direct product of two non-trivial subgroups, and, if so, to compute such a decomposition.

Alice Niemeyer (Perth, Australia) lectured on "Symmetric p-groups".

In 1978, Bryant and Kovács showed that for every subgroup H of $\mathrm{GL}(d, p)$ for a prime p there is a finite p-group P such that the automorphism group of P induces a subgroup on the Frattini quotient $P/\Phi(P)$ which is isomorphic to H. Their proof demonstrates the existence of such a p-group by considering sufficiently large quotients to terms of the exponent-p lower central series of the free group F on d generators. In joint work with Bamberg, Glasby and Morgan, the speaker has considered maximal subgroups of GL(d, p) for odd primes p and $d \geq 4$ and they show that in many cases it is only necessary to consider exponent-p class 3 quotients of F to find such a p-group.

Alastair Litterick (Auckland, New Zealand) lectured on ”Non-Completely Reducible Subgroups of Exceptional Algebraic Groups”.

The subgroup structure of algebraic groups has been heavily studied recently, with applications to finite groups of Lie type and elsewhere. An approach due to Serre generalizes concepts from representation theory by replacing GL(V) by another reductive algebraic group G. This leads naturally to the concept of a subgroup being 'G-completely reducible'.

Litterick presented recent joint work with Thomas, which classifies connected, reductive, non-G-completely reducible subgroups when G is of exceptional type and the ambient characteristic is good for G. Techniques employed vary from standard Lie theory and representation theory of reductive groups to non-abelian cohomology and computational methods.

Tobias Moede (Braunschweig, Germany) lectured on ”Coclass theory for nilpotent associative algebras”.

The talk concerned joint work with Eick.

Coclass theory is a highly successful tool in the classification of finite p-groups. For a finite-dimensional nilpotent associative algebra A of class c, its coclass is defined as $\dim(A) - c$.

One can visualize the algebras of a given coclass r by a coclass graph $\mathcal{G}_{\mathbb{F}}(r)$. The vertices in this graph correspond one-to-one to isomorphism types of finite-dimensional nilpotent associative $\mathbb{F}$-algebras of coclass r and there is a directed edge $A \to B$ if $A \cong B/B^{cl(B)}$. Moede presented an algorithm to determine finite parts of the associated coclass graphs and exhibited some examples.

He gave a structural description for the infinite paths in these graphs and used this to determine which coclass graphs have finitely many maximal infinite paths.

Automorphisms and isomorphisms of finite groups. The problems of constructing the automorphism group of a finite group and of testing for isomorphism between two finite groups are both important and difficult. Indeed, the problems seem most difficult for very restricted classes of groups.

Three lectures at the workshop introduced new methods for dealing with these and related problems.

Peter Brooksbank (Lewisburg, US) lectured on “Testing isomorphism of p-groups of genus 2”.

He began by noting that testing isomorphism of p-groups of class 2 and exponent p is widely believed to be no less difficult than the general problem.

Such a group has genus 1 if its center has order p; these are the extraspecial groups and it is elementary to decide isomorphism for this class. The speaker and collaborators considered the genus 2 case, where centers have order p^2. While only a modest step away from extraspecial groups, testing isomorphism for this class requires dramatically different ideas.

Brooksbank presented two approaches towards computing the automorphism groups of such groups, the critical step toward solving the isomorphism problem. The first is based on methods of Vishnevetskii and is particular to genus 2 groups. The second uses the more general adjoint-tensor method. Using a combination of the two algorithms, they test isomorphism of genus 2 groups of order N in time (almost) polynomial in $\log(N)$.

A lecture on “A new isomorphism test for groups” was presented by James Wilson (Fort Collins, US).

He introduced new structures that highlight properties of automorphism groups of finite groups. A subset of the techniques already reveals new characteristic subgroups in about 80% of the groups order at most 2000 in the Small Groups Library of Besche-Eick-O'Brien.

The first idea is to introduce a more relaxed notion of a filter for groups, one that can be updated when new characteristic subgroups are found. The speaker defined a filter over an arbitrary pre-ordered commutative monoid. Each filter determines an associated graded Lie algebra. Furthermore every characteristic filter induces a filter on the automorphism group. Finally, the Lie algebra of the filter on the automorphism group maps canonically to the derivations of the associated graded algebra of the original group. At this point the problem of group automorphisms is reduced to understanding the autotopisms between the homogeneous components of a graded algebra. Exact sequences are determined that explain the structure of the autotopism group in relation to class groups.

On a related subject, Josh Maglione (Fort Collins, US) lectured on "Finding chief series in large unipotent groups of Lie type". The nilpotent groups, $T(r,q)$ of Lie type T and rank r, have a canonical characteristic series of length $O(r^2)$ with q-bounded factors, and this applies also to almost all quotients. Compared to the standard lower central series of length $O(r)$, these new series give strong computational speedups on problems such as constructive recognition and isomorphism testing, and answer a long-standing demand for practical improvements for calculating automorphism groups. An implementation of these ideas using machinery from from the "matrix group recognition project" computes this structure in one minute of CPU time for groups of order about 2^{80}.

34.4 Some notes about the meeting

The workshop had forty-one participants. There were twenty-five lectures. Many of the lectures were short, each approximately 15 minutes. The lecture schedule was kept purposefully light in order to allow for discussions among the participants which were lively and fruitful.

The meeting was diverse geographically:

eleven participants from North America;

two from South America;

twenty-three from Europe;

and five from Australia and New Zealand.

There were eight women among the participants, six of whom were speakers. Four participants were graduate students or had received their degree within the last year, three of these spoke. The weather was wonderful and the scenery in Banff was spectacular.

The workshop featured a special day in memory of Ákos Seress who was one of the original applicants to organize the meeting.

Unfortunately, Ákos passed away a year before the meeting. There were four lectures on the special day given by Peter Brooksbank, Bill Kantor, Charles Leedham-Green, and Cheryl Praeger. All four distinguished speakers had close associations with Ákos. At the meeting, a volume of the *Journal of Algebra*, edited by Bill Kantor and Charles Leedham-Green, dedicated to the memory of Ákos and published just in time for the meeting was displayed.

34.5 Discussions and future directions

In addition to the lectures, there were a variety of discussions held at the meeting. A major working session was devoted to the organization of a GAP implementation of the matrix group recognition algorithms. A problem session was held at the meeting in which additional interesting open problems were discussed.

Moreover, there were many discussions and meetings of small groups held at the meeting. In these, many interesting new research avenues were discussed and new collaborations on joint research interests were created. These will, without doubt, lead to many new and interesting research projects and new publications, thus enhancing the research in computations with matrix groups significantly.

We gratefully acknowledge the wonderful facilities offered by the Banff Center to host meetings of this kind. It is the mixture of highly stimulating lectures and many associated informal discussions that take place in such an environment that makes a meeting of this kind such a success and a memorable experience.

Participants

Brooksbank, Peter (Bucknell University)
Carlson, Jon (University of Georgia)
Cohen, Arjeh (Eindhoven)
Corr, Brian (University of Western Australia)
de Graaf, Willem (University of Trento)
Dekimpe, Karel (KU Leuven Kulak)
Detinko, Alla (National Univeristy of Ireland Galway)
Dietrich, Heiko (Monash University)
Dixon, John D. (Carleton University)
Eick, Bettina (Technische UniversitŁt Braunschweig)
Flannery, Dane (National University of Ireland, Galway (Ireland))
Hiss, Gerhard (RWTH Aachen University)
Horn, Max (Justus-Liebig-UniversitŁt Gieen)
Hulpke, Alexander (Colorado State University)
Jespers, Eric (Vrije Universiteit Brussel)
Kantor, William (Brookline, MA)
Kassabov, Martin (Cornell University)
Kirschmer, Markus (RWTH Aachen University)
Leedham-Green, Charles (Queen Mary College London)
Litterick, Alastair (University of Auckland)
Lbeck, Frank (RWTH Aachen)
Lux, Klaus (University of Arizona)
Magaard, Kay (University Birmingham)
Maglione, Josh (Colorado State University)
Malle, Gunter (Technische UniversitŁt Kaiserslautern)
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Pfeiffer, Markus (University of ST. Andrews)
Praeger, Cheryl (The University of Western Australia)
Roney-Dougal, Colva (University of St Andrews)
Rossmann, Tobias (UniversitŁt Bielefeld)
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Schillewaert, Jeroen (Imperial College London)
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Taylor, Don (University of Sydney)
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Wilson, James (Colorado State University)
Wilson, Robert (Queen Mary London)

Bibliography

[1] M. Aschbacher, On the maximal subgroups of the finite classical groups, Invent. Math. **76** (1984), 469–514.

[2] B. Assmann and B. Eick, Testing polycyclicity of finitely generated rational matrix groups, Math. Comp.**76** (2007), 1169–1682.

[3] H. Bäärnhielm, D. Holt, C.R. Leedham-Green, E. A. O'Brien, A practical model for computation with matrix groups, J. Symb. Comp., **68** (2015), 27–60.

[4] L. Babai, R. Beals, Á. Seress, Polynomial-time theory of matrix groups, STOC'09 – Proceedings of the 2009 ACM International Symposium on Theory of Computing, 55–64, ACM, New York, 2009.

[5] R. Beals, Improved algorithms for the Tits alternative, In Groups and Computation III (Columbus OH, 1999), (A. Seress and W. M. Kantor, eds.), Ohio State Univ. Math. Res. Inst. Publ. **8**, 63–67, de Gruyter, Berlin, 2001.

[6] H. U. Besche, B. Eick and E. A. O'Brien, A millenium project: constructing small groups, Internat. J. Algebra Comput., **12** (2002), 623–644.

[7] J. N. Bray, D. F. Holt, C. M. Roney-Dougal. The maximal subgroups of the low-dimensional finite classical groups. London Mathematical Society Lecture Note Series, 407. Cambridge University Press, Cambridge, 2013.

[8] J. J. Cannon and D. F. Holt, Automorphism group computation and isomorphism testing in finite groups, J. Symb. Comput., **35** (2003), 241–267.

[9] A. S. Detinko, B. Eick and D. L. Flannery, Computing with matrix groups over infinite fields, In Groups St. Andrews 2009 in Bath. Volume 1, London Math. Soc. Lecture Note Ser., **387**, 256–270, Cambridge Univ. Press, Cambridge, 2011.

[10] A. Detinko, D. F. Flannery and E. A. O'Brien, Algorithms for the Tits alternative and related problems, J. Algebra, **344** (2011), 397–406.

[11] H. Dietrich, C, R, Leedham-Green, F. Lübeck and E. A. O'Brien, Constructive recognition of classical groups in even characteristic, J. Algebra **391** (2013), 227–255.

[12] B. Eick, M. Kirschmer and C. R. Leedham-Green, The constructive membership problem for discrete free subgroups of rank 2 of $SL_2(\mathbb{R})$, London Math. Soc. J. Comput. Math., **17** (2014), 345–359.

[13] B. Eick, C. R. Leedham-Green and E. A. O'Brien, Constructing automorphism groups of p-groups, Comm. Alg., **30** (2002), 2271–1195.

[14] D. F. Holt, B. Eick and E. A. O'Brien, Handbook of computational group theory, Discrete Mathematics and its Applications (Boca Raton), Chapman & Hall/CRC, Boca Raton, FL, 2005.

[15] W. M. Kantor and A. Seress, Black box classical groups Memoirs of the Amer. Math. Soc., **708**, American Mathematical Society, 2001.

[16] C. R. Leedham-Green, The computational matrix group project, In Groups and Computation III (Columbus OH, 1999), (A. Seress and W. M. Kantor, eds.), Ohio State Univ. Math. Res. Inst. Publ. **8**, 229–247, de Gruyter, Berlin, 2001.

[17] C. R. Leedham-Green and E. A. O'Brien, Constructive recognition of classical groups in odd characteristic, J. Algebra, **322** (2009), 833–881.

[18] G. Nebe and W. Plesken, Finite rational matrix groups, Memoirs of the Amer. Math. Soc., **116**, American Mathematical Society, 1995.

[19] M. Neunhöffer and Á. Seress, A data structure for a uniform approach to computations with finite groups. ISSAC 2006, 254261, ACM, New York, 2006.

[20] E. A. O'Brien, Isomorphism testing for p-groups, J. Symb. Comput., **17** (1994), 133–147,

[21] E. A. O'Brien, Algorithms for matrix groups, Groups St Andrews 2009 in Bath, Volume 2, 297323, London Math. Soc. Lecture Note Ser., **388**, Cambridge Univ. Press, Cambridge, 2011.

[22] J. Tits, Free subgroups in linear groups, J. Algebra **20** (1972), 250-270.

Chapter 35

14w5136 Algebraic and Model Theoretical Methods in Constraint Satisfaction (14w5136)

November 23 - 28, 2014

Organizer(s): Manuel Bodirsky (Dresden Technical University), Andrei Bulatov (Simon Fraser University), Dugald MacPherson (University of Leeds), Jaroslav Nešetřil (Charles University)

35.1 Overview of the field and the structure of the workshop

The aim in a constraint satisfaction problem (CSP) is to find an assignment of values to a given set of variables, subject to constraints on the values which can be assigned simultaneously to certain specified subsets of variables. CSPs are used to model a wide variety of computational problems in computer science, discrete mathematics, artificial intelligence, and elsewhere, and they have found numerous applications in those areas. Several very successful approaches to study the complexity and algorithms for constraint satisfaction problems have been developed over the last decade. One of the most fruitful uses universal algebra. So far the bulk of research on the CSP has been done assuming the variables can take only a finite number of values. The infinite CSP, in which this restriction is removed, has much stronger expressive power, but is also much harder to study. Two recent discoveries made it possible to transfer some techniques, in particular the algebraic approach, from the finite to some classes of the infinite CSP. The first one is the expansion of the algebraic approach onto infinite domain CSPs by Bodirsky and Nešetřil. The universal algebraic approach rests on the observation that primitive positive definability in finite structures can be characterized by polymorphisms. The second one is a surprising connection between topological dynamics and Ramsey theory discovered by Kechris, Pestov, and Todorcevic [14]. This is highly relevant in the context of constraint satisfaction, since the universal-algebraic approach is particularly powerful for omega-categorical structures that are definable in ordered Ramsey structures.

In contrast to finite domain CSPs the study of infinite domain CSPs through algebra and model theory is still in its infancy, and many directions, problems, and hypotheses are yet to be identified. The workshop therefore focuses on the interaction of three areas of mathematics and computer science:

- Universal Algebra and its applications in the finite CSP,

- Infinite CSP and its algebraic theory,
- Model Theory and Topological Dynamics.

This workshop brought together for the first time researchers from these three areas to explore the implications of this new connection between them.

Along with 19 contributing 1- and 0.5-hour talks highlighted in subsequent sections, the workshop featured three tutorials corresponding to the three main areas, aiming to bring up the participants' background to the level necessary to understand the contributing talks. The tutorials were given by M.Pinsker on "Constraint satisfaction problems on infinite domains", by P.Cameron on "Synchronization, graph endomorphisms, and some remarkable graphs", and by R.Willard on "Universal algebra and CSP".

35.2 Universal algebra and finite CSP

In the theoretical study of CSPs that has witnessed a rapid growth over the last decade, the principal research problems are: to determine the computational and descriptive complexity of constraint problems and to develop efficient algorithms for solving CSPs whenever such algorithms exist. The main focus of research has been the computational and descriptive complexity of finite domain CSPs, in which the set of possible values of variables is finite. The quest for a classification of CSPs restricted by a constraint language has been guided by the dichotomy conjecture posed in 1993 by Feder and Vardi [2]. This conjecture claims that any CSP of this type is either polynomial time solvable, or NP-complete; despite significant progress this conjecture remains unresolved. The bulk of research done towards resolving the dichotomy conjecture uses connections between the complexity of CSPs with restrictions on the allowed constraints, and concepts from universal algebra. More specifically, the complexity of CSPs is determined by the properties of polymorphisms, multi-ary operations that can be viewed as generalized symmetries of constraints. This universal-algebraic approach to CSPs has not only greatly assisted in the study of CSP complexity, but vitalizes the field of universal algebra since it raises questions that are of central importance in the study of finite algebras.

35.2.1 Presentation Highlights

Linear Datalog and k-permutability = symmetric Datalog

Alexandr Kazda reported on recent progress on characterizing low complexity CSPs. Datalog is a Prolog-like language that allows one to talk about relational structures. Given a relational structure $\mathbf{A}$, there is a Datalog program that decides CSP($\mathbf{A}$) if and only if CSP($\mathbf{A}$) can be solved by local consistency methods. Such structures are well understood. By restricting the kinds of rules a Datalog program can use, one obtains first linear and then symmetric Datalog languages. Characterizing the CSPs solvable by these fragments of Datalog is an open problem.

Kazda showed that if $\mathbf{A}$ is a finite relational structure whose algebra of polymorphisms is k-permutable for some k and CSP($\mathbf{A}$) can be solved using linear Datalog, then CSP($\mathbf{A}$) can be solved by symmetric Datalog (which is weaker). This supports the conjecture that CSP($\mathbf{A}$) is solvable by symmetric Datalog iff the algebra of polymorphisms of $\mathbf{A}$ is semidistributive and k-permutable for some k.

The basic CSP reductions revisited

Libor Barto revisited the classic reductions between fixed template CSPs over a finite domain. These reductions are based on three constructions on relational structures: forming images under unary endomorphisms, adding singletons to cores, and pp-interpretation. On the algebraic side, these reductions are usually interpreted in the following (or some equivalent) way: the complexity (computational or descriptive) of CSP($\mathbf{A}$) depends only on the idempotent Maltsev conditions satisfied by the core of $\mathbf{A}$. Barto offers a sharper interpretation: the complexity of CSP$(\mathbf{A})$ depends only on the linear Maltsev conditions satisfied by $\mathbf{A}$.

Absorption and directed Jonsson terms

Ralph McKenzie improved the known characterizations of conditions on the congruence lattice through specific term operations. He proved that every congruence distributive variety has directed Jónsson terms, and every congruence modular variety has directed Gumm terms. These directed terms have the property that they respect every absorption witnessed by the original Jónsson or Gumm terms. This result is directly equivalent to a strong absorption theorem (formulated differently for CD and CM varieties.) These results were already known for locally finite varieties, but it is a surprise that they hold for unrestricted varieties as well. The absorption theorems have interesting applications in a broader domain.

The absorption theorem in question was proved by Libor Barto for finite algebras with Jonsson terms, as a main step toward his proof that a finitely related finite algebra with Jonsson terms has a near unanimity term operation. Marcin Kozik used this to prove that a finite algebra has Jonsson terms iff it has directed Jonsson terms: that is, $J_1(x, y, z), \ldots, J_n(x, y, z)$ satisfying equations $J_i(x, y, x) = x, J_1(x, x, y) = x, \ldots, J_n(x, y, y) = y$, and $J_i(x, x, y) = J_{i+1}(x, y, y)$ for $1 \le i < n$. Both results are now extended to arbitrary (not locally finite) algebras, and shown that they are fundamentally the same result.

Optimal strong Maltcev conditions for congruence meet-semidistributivity

Matthew Moore provided new characterizations of locally finite, congruence meet-semidistributive varieties. These varieties have been characterized by numerous Maltcev conditions and, recently, by two strong Maltcev conditions. The new work provides three new strong Maltcev characterizations and a new Maltcev characterization each of which improves the known ones in some way.

Counting Matrix Partitions

Martin Dyer discussed recent work on the counting version of the Matrix Partition problem. Matrix partitions are a generalisation of graph homomorphisms. They were introduced into the context of structural graph theory, and are equivalent to homomorphisms of trigraphs, as introduced by Chudnovsky. The decision version of this problem was investigated in [3].

Descriptive Complexity of approximate counting CSPs

Victor Dalmau reported on several results related to the descriptive complexity of counting CSPs. Motivated by Fagin's characterization of NP, Saluja et al. [4] have introduced a logic based framework for expressing counting problems. In this setting, a counting problem (seen as a mapping C from structures to non-negative integers) is 'defined' by a first-order sentence ϕ if for every instance A of the problem, the number of possible satisfying assignments of the variables of ϕ in A is equal to $C(A)$. The logic $RH\Pi_1$ has been introduced by Dyer et al. [5] in their study of the counting complexity class #BIS. The interest in the class #BIS stems from the fact that, it is quite plausible that the problems in #BIS are not #P-hard, nor they admit a fully polynomial randomized approximation scheme. In this talk we shall present some results concerning the definability of counting constraint satisfaction problems #CSP(H) in the monotone fragment of $RH\Pi_1$.

The other side of the CSP

Hubie Chen studied the CSPs restricted by the left-hand side, formulated as the relational homomorphism problem over a set of structures $\mathbf{A}$, wherein each instance must be a pair of structures such that the first structure is an element of $\mathbf{A}$. He presented a comprehensive complexity classification of these problems, which strongly links graph-theoretic properties of $\mathbf{A}$ to the complexity of the corresponding homomorphism problem. In particular, he defined a binary relation on graph classes and completely describe the resulting hierarchy given by this relation. This binary relation is defined in terms of a notion which is called graph deconstruction and which is a variant of the well-known notion of tree decomposition. Then he used this graph hierarchy to infer a complexity hierarchy of homomorphism problems which is comprehensive up to a computationally very weak notion of reduction, namely, a parameterized form of quantifier-free reductions. He obtained a significantly refined complexity classification of left-hand side restricted homomorphism problems, as well as a unifying, modular, and conceptually clean treatment of existing complexity classifications, such as the celebrated classifications by Grohe et al. [6, 7, 8].

Constant-factor approximable finite-valued CSPs

Andrei Krokhin presented new results on the approximability of minimization problems related to CSP, namely the (finite-)valued constraint satisfaction problems (VCSPs) and their special case, the minimum constraint satisfaction problems (Min CSPs), all with a fixed finite constraint language Γ. The main focus is on characterising such problems that admit a constant-factor approximation algorithm.

A recent result of Ene et al. says that, under a mild technical condition, the basic LP relaxation is optimal for constant-factor approximation for VCSPs unless the Unique Games Conjecture fails. Krokhin showed that the characterisation problem for VCSPs reduces to the one for Min CSPs, and then used the algebraic approach to the CSP to characterise constraint languages such that the basic LP has a finite integrality gap for the corresponding Min CSP. We also show how this result can in principle be used to round solutions of the basic LP relaxation, and how, for several examples that cover all previously known cases, this leads to efficient constant-factor approximation algorithms. Finally, we improve the above mentioned UG-hardness of constant-factor approximation to NP-hardness for a class of Min CSPs.

Necessary Conditions for Tractability of Valued CSPs

Stanislav Zivny gave a talk on a Galois connection for weighted clones. The connection between constraint languages and clone theory has been a fruitful line of research on the complexity of constraint satisfaction problems. In a recent result, Cohen et al. [12] have characterised a Galois connection between valued constraint languages and so-called weighted clones. In his talk Zivny studied the structure of weighted clones. We extend the results of Creed and Zivny from [13, 12] and provide necessary conditions for tractability of weighted clones and thus valued constraint languages. We demonstrate that some of the necessary conditions are also sufficient for tractability, while others are provably not.

35.2.2 Open Problems

- Are the following problems decidable?

  Given operations $f_1, \ldots, f_k$ and a relation R on a finite set A:

  1. Is the clone generated by $f_1, \ldots, f_k$ equal to the clone of functions preserving R, i.e., is $\mathrm{Clo}(f_1, \ldots, f_k) = \mathrm{Pol}(R)$?
  2. Is the clone generated by $f_1, \ldots, f_k$ finitely related, i.e., is $\mathrm{Clo}(f_1, \ldots, f_k) = \mathrm{Pol}(S)$ for some relation S on A?
  3. Is the clone of R-preserving operations finitely generated, i.e., is $\mathrm{Pol}(R) = \mathrm{Clo}(g_1, \ldots, g_l)$ for some $l \in \mathbb{N}$ and operations $g_1, \ldots, g_l$ on A?
  4. Is there a finite bound on the essential arities of operations in $\mathrm{Pol}(R)$?

- Let A be an (infinite) algebra that has a n-ary WNU, does A have to have a Taylor operation of low arity? Ie. does there exist a sequence of algebras $A_1, A_2, \ldots$ such that i has an i-ary WNU, but the minimum arity of a Taylor term in A_i tends to infinity as i increases?
- Characterise the class of relational structures A such that $CSP(A)$ can be solved by linear Datalog.
- Given a finite idempotent algebra (by tables of its operations), is it possible to decide in polynomial time whether the algebra admits a minority operation?
- One very interesting open problem is surjective CSP on the template with universe $\{1, 2, 3\}$ and relation $\{(a, b, c) \mid |\{a, b, c| \leq 2\}$.

  It appears in the survey on surjective homomorphism problems by Bodirsky, Kara, and Martin [1].

35.3 Ramsey Theory and Model Theory

The increasing emphasis on CSPs with infinite domains (see the next section), and in particular on CSPs whose domain is an ω-categorical first order structure, has led to close interactions with parts of model theory, Ramsey theory, permutation group theory (and extensions to transformation monoids), and topological dynamics. One goal, for infinite structures which give natural CSPs, is to classify the CSPs for templates which are interpretable in them. This takes various forms. A first goal might be to classify the reducts of a given template M up to first-order interdefinability, or equivalently to classify the closed supergroups of the automorphism group. A classification of reducts of M up to positive-primitive interdefinability corresponds to classifying the clones (closed topologically in the clone of all polymorphisms of the set M) which contain the clone of polymorphisms of M.

Approaches to these problems, in recent papers of Bodirsky, Pinsker, and co-authors, mostly use structural Ramsey theory for classes of finite relational structures, as developed by Nešetřil, Rödl and others since the 1970s. A class $\mathcal{C}$ of finite structures is a Ramsey class if for an $A \leq B$ in $\mathcal{C}$ and positive integer k, there is $D \in \mathcal{C}$ such that for any function f from the collection of copies of A in D to $\{1, \ldots, k\}$, there is a copy B' of B in D such that f is constant on the copies of A in B'. Under reasonable conditions, if $\mathcal{C}$ is a Ramsey class then there is a homogeneous structure (a countably infinite structure such that any isomorphism between finite substructures extends to an automorphism) whose age (the collection of finite structures which embed in it) equals $\mathcal{C}$. This subject has major connections to a further current topic, topological dynamics (the study of continuous actions of topological groups on compact spaces). In particular, if G is a closed permutation group on a countable set M, then G is extremely amenable (i.e. every continuous action on a compact space has a fixed point) if and only if G is the automorphism group of a homogeneous totally ordered structures on M whose age is a Ramsey class. This equivalence (in both directions) has been used in results classifying reducts.

The meeting included a 3-lecture tutorial by Pinsker describing the connections of this field to CSPs (see Section 4), a somewhat related 3-lecture tutorial by Cameron on synchronisation and transformation monoids, and several other talks.

35.3.1 Presentation Highlights

Synchronization, graph endomorphisms, and some remarkable graphs (tutorial)

A transformation monoid on a set (here assumed finite) is synchronizing if it contains an element of rank 1, that is, an element whose image has cardinality 1. This tutorial by Cameron on synchronizing monoids and permutation groups described recent work, motivated ultimately by a conjecture of Cerny on reset words in finite state automata, on a topic with some connection to robot design. A permutation group G on a finite set Ω synchronizes the map $f : \Omega \to \Omega$ if the transformation monoid $\langle G, f \rangle$ is synchronizing. A key goal is to characterize synchronizing permutation groups.

Given a transformation monoid M on set X, the graph of M, denoted $\mathrm{Gr}(M)$, has vertex set X, with vertices v, w adjacent if and only if there is no $f \in M$ with $f(u) = v$. Then $M \leq \mathrm{End}(\mathrm{Gr}(M))$, and furthermore $\mathrm{Gr}(\mathrm{End}(\mathrm{Gr}(M))) = \mathrm{Gr}(M)$. Useful information is encoded by $\mathrm{Gr}(M)$ – for example, the minimal rank of an element of M equals the clique number and chromatic number of $\mathrm{Gr}(M)$. Cameron used $\mathrm{Gr}(M)$ to give a characterization of synchronizing transformation monoids. He noted a result of Rystsov that a permutation group G on a set of size n is primitive (that is, preserves no proper non-trivial equivalence relation on X) if and only if it synchronizes every map of rank $n - 1$. Thus, every synchronizing permutation group on a set of size at least 3 is primitive (and every 2-transitive permutation group is synchronizing). The converse is false, but Araújo has conjectured that every primitive permutation group is almost synchronizing, i.e. synchronizes every non-uniform map (map with fibres not all of the same size).

Cameron described very recent work with Araújo and Betz around this conjecture, showing for example that every primitive group of rank at least n synchronizes every map of rank at least $n - 4$, and every non-uniform map of rank at most 4. He described some remarkable recent counterexamples to Araújo's conjecture, and gave modified conjectures and related results.

Simple homogeneous structures

Koponen described recent work on homogeneous structures over a finite relational language which have the model-theoretic property of simplicity, a combinatorial condition defined by Shelah which guarantees that there is a notion of independence with strong properties. A strengthening of simplicity is supersimplicity, and there are open questions whether every ω-categorical supersimple structure has finite rank (SU-rank, akin to a dimension), and whether every simple structure homogeneous over a finite relational language is supersimple. Koponen sketched recent proofs of these conjectures for structures which are homogeneous over a finite binary language. He described several further results (some joint with Ahlman) on binary homogeneous structures under strong extra assumptions on the behaviour of independence, and posed several problems.

Classifying homogeneous structures

Cherlin described a range of classification results and conjectures, from the last 40 years, on homogeneous structures. He gave an overview of the deep structural results of Lachlan on finite homogeneous structures over a finite relational language, and of the classifications of homogeneous graphs (Lachlan-Woodrow) and digraphs (Cherlin), homogeneous ordered graphs (Cherlin), and a recent conjecture on finite homogeneous binary structures. He also described a conjectured classification of metrically homogeneous graphs (graphs which become homogeneous when binary predicates are added to express distance) and gave evidence for this conjecture.

Ramsey classes with algebraic closure and forbidden homomorphisms

Hubicka gave an overview of Ramsey classes, and focussed his talk on the question: does every structure homogeneous over a finite relational language have a Ramsey lift (an expansion to a structure whose age is a Ramsey class), and more generally whether certain classes of finite structures have a 'Ramsey lift'. For example, by 2014 work this is known for each of the $2^{\aleph_0}$ homogeneous digraphs. He described several recent results, some joint with Nešetřil, showing that certain structures have Ramsey lifts. Part of the talk was motivated by certain ω-categorical structures identified by Cherlin, Shelah, and Shi (1998), with an associated locally finite notion of algebraic closure.

Continuity of homomorphisms to the clone of projections

Pongracz gave an introduction to (topological) clones of polymorphisms of ω-categorical structures. A key result of Bodirsky and Pinsker says that if Γ is an ω-categorical structure, then a structure Π is primitive positive interpretable in Γ if and only if there is a continuous clone homomorphism from the polymorphism clone $\mathrm{Pol}(\Gamma)$ to **1**, the trivial clone consisting only of projections. Pongracz described several recent results in this area, for example joint work with Bodirsky and Pinsker showing that if Γ is homogeneous over a finite relational language, then if there is a homomorphism from a closed 'canonical' clone of polymorphisms of Γ (containing Aut(Γ)) to **1** then there is a continuous one. This gives a dichotomy result for closed canonical clones.

35.3.2 Open Problems

- Find new interesting permutation groups G on an infinite set X which, for some $k \geq 4$, are k-transitive but not $(k+1)$-transitive. It is easy to give Fraïssé constructions with such automorphism groups, but there are open test questions. Is there a homogeneous relational structure with 4-transitive not 5-transitive automorphism group such that the age of M has no infinite antichains? Or such that $f(n)$, the number of isomorphism types of n-element substructures, grows no faster than exponentially? Or such that the first order theory of M does not have the 'independence property'? There are Fraïssé constructions of 3-transitive not 4-transitive permutation groups with all these properties (though the known examples are all somehow linked).

  There is evidence that the 3-4 boundary is significant. For example there are sharply 3-transitive infinite permutation groups, but, by a theorem of M. Hall, no sharply 4-transitive ones. These questions are linked to that of Pongracz below.

- For $n = 4$, is there an ω-categorical structure Δ_n with n-transitive automorphism group, such that Aut(Δ_n) has a proper subflow in its action on the space LO of all total orderings of Δ_n – i.e. can there be a closed Aut(Δ_n)-invariant proper non-empty subset of LO? If yes, can this be done for all n? Can it be done so that Δ_n is Ramsey?

- Given finite tournaments $T_1, \ldots, T_k$, is there a decision procedure to tell whether there is an infinite antichain (under embeddability) in the collection of all finite tournaments which do not embed any of $T_1, \ldots, T_k$? The corresponding problem for permutation patterns has also been investigated.

- Suppose that M is a homogeneous but not binary relational structure. Which if any of the following implications are true?

$$M \text{ is simple} \Rightarrow M \text{ is supersimple} \Rightarrow M \text{ has finite SU-rank.}$$

- Suppose that M is a (binary) homogeneous (super)simple relational structure (with finite SU rank) (extra assumptions in parentheses optional). Can such a structure M interpret a non-trivial pregeometry?

- Suppose M is binary, homogeneous, primitive, simple, and 1-based. Must M be a binary random structure? What if we remove '1-based'?

- It appears that in the known examples of a set K of finite relational structures with a 0–1 law and ω-categorical almost sure theory T_K, T_K is homogenizable and simple. Are there reasonable conditions on K which guarantee this?

- Which homogeneous/homogenizable (simple) structures M can be 'constructed' as probabilistic limits of finite structures?

35.4 Infinite-Domain CSPs

In infinite domain constraint satisfaction, there are two major directions: the first is the generalisation of the universal-algebraic approach to finite domain CSPs to large classes of CSPs with infinite domains. The natural context here is the class of ω-categorical structures, since for those structures the complexity of the CSP is captured by the polymorphisms of the template.

The second major direction is the study of CSPs for templates that are of general interest in computer science and mathematics, which might not be ω-categorical. A typical example is the feasibility problem for linear programs over $\mathbb{R}$ or the max-atoms problem (which is polynomial-time equivalent to mean payoff games, a notorious problem of open computational complexity).

Michael Pinsker's tutorial addressed the first of those two directions, providing a detailed introduction to the universal-algebraic approach to CSPs for ω-categorical templates. Of direct relevance for this approach are the results that have been presented by Barto, and by Pongracz, reported above. But also the Ramsey lift questions treated in the talk of Hubicka are important in this context. The second direction was also well represented by talks of Barnaby Martin and Johan Thapper.

35.4.1 Presentation Highlights

Pinsker

The introduction of Michael Pinsker to the universal-algebraic approach to infinite-domain CSPs had three parts:

- In the first part he first described why the complexity of the CSP for ω-categorical templates only depends on the polymorphism clone of the template, introducing the necessary model theoretic background. He illustrated the class of problems that can be modelled in this way by graph satisfiability problems.
- In the second part Michael took a further abstraction step, considering the clone of polymorphisms only as a topological clone, and finally as an abstract clone. For ω-categorical structures, the topological polymorphism clone is closely related to the pseudovariety generated by the polymorphism algebra, and he explained how this link becomes important for proving NP-hardness of CSPs. In fact, the complexity of an ω-categorical CSP only depends on the topological polymorphism clone. In this part, Pinsker also covered an important tool for studying automorphism groups and endomorphism monoids, namely Ramsey theory.
- In the third and final part, Pinsker treated model-complete cores, which are the ω-categorical pendants to cores of finite structures. Having all these concepts available, he could present a precise formulation of a dichotomy conjecture that holds for a very broad class of ω-categorical structures. He closed with other open problems that could be relevant to solve this dichotomy conjecture.

Martin

Barnaby Martin presented a classification of the computational complexity of CSPs where the template has domain $\mathbb{Z}$, and where all relations are first-order definable over $(\mathbb{Z}; \mathrm{succ})$, that is, the integers with the successor function. The complexity classification is complete under the assumption that the Feder-Vardi conjecture is true. The motivation to study reducts of $(\mathbb{Z}; \mathrm{succ})$ is that this structure is probably the most fundamental structure with a finite relational signature that is not ω-categorical.

The surprising message of Martin's talk is that the universal-algebraic approach can be adapted even to this setting. Even though that we do not have an a priori argument that polymorphisms capture the computational complexity of the CSP in this setting, it turns out that, a posteriori, having obtained the classification, we see that this is the case. Indeed, the tractable cases are described by polymorphisms of the template, or a saturated extension of the template, that satisfy certain equations, as in the case of finite domain CSPs.

Thapper

Johan Thapper reported on joint work with Peter Jonsson which investigates polynomial-time tractable variants of the linear program feasibility problem. More specically, they looked at CSPs whose template contains the relation defined by $x + y = z$, and an arbitrary finite set of semilinear relations. For a large subclass of these templates, Thapper and Jonsson identified the boundary between tractable and hard CSPs. To handle the new tractable problems, they introduced a notion of affine consistency and an accompanying algorithm that can be used to decide satisfiability.

35.4.2 Open Problems

- Is every homomorphism from a polymorphism clone to the clone of projections **1** continuous with respect to the topology of pointwise convergence?
- Can every homogeneous structure be expanded by finitely many relations such that the resulting structure is still homogeneous and additionally Ramsey?
- Classify $\mathrm{CSP}(\Gamma)$ for all reducts Γ of the universal homogeneous permutation.
- Classify the complexity of all problems in MMSNP_2. The logic MMSNP is monotone monadic SNP, a fragment of existential second-order logic closely related to finite domain CSP. MMSNP_2 is the generalisation of this logic by restricted existential quantification (à la Courcelle) over higher-ary relations. All the problems in this class correspond to CSPs with ω-categorical templates.
- Does every semi-algebraic extension of linear program feasibility which is not semilinear simulate a sums-of-roots problem?
- Do CSPs for reducts of $(\mathbb{Z}; \mathrm{succ}, y = 2x)$ have a non-dichotomy?
- Do CSPs for reducts of $(\mathbb{Z}; 0, \mathrm{succ})$ have a non-dichotomy?

35.5 CSP Related Areas

The methods from the Constraint Satisfaction problem, universal algebra and model theory have also been used in numerous applications some of which have also been presented at the workshop.

35.5.1 Further Presentation Highlights

Dvorak

Zdenek Dvorak studied the restriction of Boolean CSPs where the incidence graph of the constraints is planar. This restriction on the input instances can make some NP-hard Boolean CSPs easy, for instance the problem Not-all-equal 3-SAT. When the template is not preserved by the map $x \mapsto -x$, hard CSPs remain hard. Otherwise, some additional CSPs become feasible via algorithms for finding maximal matchings. Dvorak presented a precise conjecture about the border between NP-hardness and tractability in this setting: if the CSP is 'matching-realizable', it is in P, otherwise NP-complete. The conjecture has been verified for all templates with relations of arity at most five.

Osssona de Mendez

Patrice Osssona de Mendez presented joint results with Jarik Nešetřil on restricted dualities: a class $\mathcal{C}$ has all restricted dualities if every connected structure F has a dual D for $\mathcal{C}$, that is, F does no homomorphically map to D, and every $G \in \mathcal{C}$ maps to D if and only if F does not map to G. De Mendez and Nešetřil showed that every graph class with bounded expansion has all restricted dualities. For the case when $\mathcal{C}$ is the class of positive instances of a CSP, they found a necessary and sufficient condition for having all restricted dualities.

Algebraic Algorithms for the Inference Problem in Propositional Circumscription

Michal Wrona reported on new algorithms for the Inference problem. Circumscription, introduced by McCarthy [9], is perhaps the most important formalism in nonmonotonic reasoning. The inference problem for propositional circumscription in multi-valued logics may be defined in constraint-based way as follows. Let $(D; \leq)$ be a partial order on domain D and Γ a constraint language over D. An instance of the general minimal constraint inference problem $(\mathrm{GMININF}(\Gamma, (D; \leq)))$ is a set of constraints C over variables V and relations in Γ, a partition of V into three sets of variables: P that are subject to minimizing, Q that must maintain the fixed value and Z that can vary, and a constraint ψ over domain D. The question is whether every minimal solution to C is a solution to ψ.

The classification of the complexity of four variants of this problem where $D = \{0, 1\}$ and $0 < 1$ (propositional circumscription in Boolean logic) has been completed in [10]. Each version of GMININF exhibit a trichotomy among Π_2^P -complete, coNP-complete and problems solvable in polynomial time. In two versions: the most general one $(\mathrm{GMININF}(\Gamma, (D; \leq)))$ and $\mathrm{VMININF}(\Gamma, (D; \leq))$, where Q is always $\emptyset$, the complexity is fully captured by the clone of polymorphisms of Γ. To the best of our knowledge, in the full generality, GMININF has been studied so far only in [11] which focuses on the complexity dichotomy between Π_2^P-complete problems and those contained in coNP for the three element domain. The question of whether there are any interesting polynomial classes of languages is left open. We answer this question affirmatively by providing three such classes of languages for GMININF and three for VMININF for arbitrarily large finite domains. These classes fully generalize two-element tractable classes from [DHN12] and are defined by closures under certain polymorphisms. Therefore the algorithms we provide for them are fully algebraic. We believe that it is the first but serious step towards obtaining trichotomies for GMININF and VMININF for restricted cases such as the three element domain or conservative languages.

35.6 Comments of participants, and further research

Comments on the meeting were received afterwards from the participants, all positive about the stimulation of the meeting, the scientific organisation, and the hosting by BIRS and the Banff Centre. Several mentioned further projects initiated at the workshop. For example, Cameron and Hartman began a project on homogenizability of line graphs. Through suggestions of Dalmau, Dvorak made progress on the classification problem for planar Boolean CSPs. Pinsker made progress on a project with Barto, and with Goldstern solved a problem which will enable them to finish a paper with Shelah. Others mentioned new interactions, new problems which caught their attention for future work, and the general value of the workshop in breaking down barriers between fields (universal algebra, CSPs, combinatorics, model theory).

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Bibliography

[1] Manuel Bodirsky, Jan Kára, Barnaby Martin. The complexity of surjective homomorphism problems - a survey. Discrete Applied Mathematics, 160(12): 1680-1690 (2012)

[2] T.Feder, M.Vardi. Monotone monadic SNP and constraint satisfaction. In STOC, pages 612-622, 1993.

[3] T.Feder, P.Hell, S.Klein, R.Motwani. List Partitions. SIAM J. Discrete Math, 16(3): 449-478 (2003)

[4] S.Saluja, K.Subrahmanyam, M.Thakur. Descriptive Complexity of #P Functions. J. Comput. Syst. Sci., 50(3): 493-505 (1995)

[5] M.E.Dyer, L.A.Goldberg, C.S.Greenhill, M.Jerrum. The Relative Complexity of Approximate Counting Problems. Algorithmica, 38(3): 471-500 (2003)

[6] M.Grohe. Computing crossing numbers in quadratic time. In STOC pages 231-236, 2001

[7] M.Grohe. The Complexity of Homomorphism and Constraint Satisfaction Problems Seen from the Other Side. In FOCS pages 552-561, 2003

[8] M.Grohe. The complexity of homomorphism and constraint satisfaction problems seen from the other side. J. ACM, 54(1) (2007)

[9] J.McCarthy. Circumscription — A form of non-monotonic reasoning. Artificial Intelligence, 13: 27–39 (1980).

[10] A.Durand, M.Hermann, and G.Nordh. Trichotomies in the complexity of minimal inference. Theory Comput. Syst., 50(3):446–491, 2012

[11] G.Nordh, P.Jonsson. An algebraic approach to the complexity of propositional circumscription. In LICS, pages 367–376, 2004

[12] D.A.Cohen, M.C.Cooper, P.Creed, P.G.Jeavons, S.Zivny. An Algebraic Theory of Complexity for Discrete Optimization. SIAM J. Comput., 42(5): 1915-1939 (2013)

[13] P.Creed, S.Zivny. On Minimal Weighted Clones. In CP pages 210-224, 2011

[14] A.S.Kechris, V.G.Pestov, and S.Todorcevic. Fraïssé limits, Ramsey theory, and topological dynamics of automorphism groups. Geom. Funct. Anal., 15(1), 106–189 (2005)

Chapter 36

Cohomological Realizations of Motives (14w5074)

December 7 - 12, 2014

Organizer(s): James D. Lewis, University of Alberta (Contact Organizer), Rob de Jeu, (VU University Amsterdam), E. Javier Elizondo, (Universidad Nacional Autonoma de Mexico, Ciudad Universitaria), Paulo Lima-Filho, (Texas A&M), Deepam Patel, (IHES/Purdue University), Pedro Luis del Angel, (Center of Investigations in Mathematics, MX)

36.1 Overview of the Field

The subject of motives is arguably the most fascinating and far reaching goals of Grothendieck's legacy. Grothendieck's unifying vision had to do with what all cohomology theories have in common. Perhaps contrary to popular misconception, Grothendieck did propose an explicit candidate construction of a category of motives, as documented by Manin. The problem is that to move forward with his construction, one needed the full strength of number of conjectures (Grothendiek's standard conjectures (see [Kl])). The standard conjectures, as well as the related celebrated Hodge ([Lew1]) and Tate conjectures are still unresolved. But this has not stopped the progress towards constructing suitable candidate motivic cohomology theories meeting the original goal of Grothendieck's vision. Indeed the input of D. Quillen's higher K-theory K_m in algebraic geometry (generalizing Grothendieck's K_0) led to a natural candidate for motivic cohomology (absolute motivic cohomology). Although K_0 has a cycle theoretic description in terms of a cycle group (classical Chow groups), it was through the work of S. Bloch [Blo] that a cycle theoretic description of K_m in terms of higher Chow groups led to an explosion of activity on the subject. A key milestone in the development of motivic cohomology is Voevodsky's revolutionary construction of motivic cohomology, which incorporates the powerful homological machinery necessary to meet the original goal of Grothendieck. The most spectacular recent success of the idea of motives was Voevodsky's proof of the Milnor conjecture for which he received the Fields medal in 2002. More generally, Rost-Voevodsky have announced a proof of the Bloch-Kato conjecture, which was later written up by C. Weibel [We]. In both proofs, Voevodsky's triangulated category of "mixed" motives is an essential tool.

It seems that the (once almost completely conjectural) picture of motives is becoming more tangible. Until recently, even the existence of a good category of mixed motives was conjectural whereas now we have various constructions of such a category due to Voevodsky, Nori (unpublished), Levine, Hanamura, and others. That is, we are beginning a phase where things are concrete enough that motives can be used as a tool for answering questions rather than simply forming a language in which to express some of the most difficult unsolved conjectures in algebraic geometry and related areas.

As with many other great mathematical ideas, the reasons for studying motives morphed over time. Our best attempts to "calculate" motivic cohomology into something more earthly, viz., via cohomological realizations, is the subject of this workshop. Historically, the subject of regulators (a regulator being a "realization" of motivic cohomology), which encompasses cohomological realizations, and from the number theoretic side, began with the works of Dirichlet, Dedekind, and on the geometric side with the works of Abel and Jacobi. The geometric aspects would be later fortified by the monumental works of Weil and Griffiths. At a later stage, it was the more recent works of S. Bloch and A. Beilinson that elevated the subject of regulators to a whole new level. These other important applications of motives to problems in algebraic geometry have had a much broader impact reaching into algebraic number theory and representation theory via the Langlands' program. Furthermore, recent results exhibit a connection between motives, periods and physics, as for example seen from the collaborative works of S. Bloch and D. Kreimer.

The timeliness of this workshop fits in beautifully with a number of recent developments particularly on the subject of regulators. The Beilinson Hodge theoretic realizations of motivic cohomology, have been explicitly worked out in detail by M. Kerr, J. D. Lewis, S. Mueller-Stach [KLM], and together with recent developments by K. Kato and S. Usui on logarithmic Hodge structures, the techniques are in place for degeneration arguments as well. R. de Jeu and J. D. Lewis have found an interpretation of the recent Bloch-Kato theorem to a version of the Hodge conjecture for Milnor K-theory [dJ-L]. More recent works on Hodge realizations of Voevodsky's motivic cohomology (as well as real variants) are due to P. L. Filho and P. des Santos, and J. D. Lewis. Then there is the recent work by M. Walker, et al, on morphic cohomological realizations. One also has the p-adic syntomic regulator realizations, with some recent progress by A. Besser and M. Asakura. While it would be unrealistic to include the works of all the major contributors in the subject, no less significant are the recent works due to C. Deninger, W. Raskind, R. Sreekantan, C. Schoen, J.-L. Colliot-Thélène, P. Griffiths and M. Green, G. Pearlstein and P. Brosnan, et al, that are having a major impact on this subject.

36.2 Logistics, and the Overall Program

The choice of title of this workshop served as a broad enough umbrella to include a number of areas that interact with the subject of motives, such as regulators, Hodge theory [De] or number theory, some aspects of Physics connect to Calabi-Yau varieties, or that connected to Feynman integrals, motivic cohomology, as so forth. And yet we limited our scope so as to involve meaningful exchange amount the various groups involved here, given the limitation in time.

A number of guiding principles ensured the successfulness of this workshop, namely:

• We limited the number of talks per day (four), except for the half day (two). This allowed for adequate time for those to meet in break-a-way rooms for collaborations. Indeed, some of those collaborations were newly established, being a result of the talks (more on this later). Ironically, this did not result in denying anyone the opportunity to give a talk. For the most part, the senior people were more than happy to let our mid-career colleagues (some of whom are at the top of their fields!) present their results.

• Although there is a dearth of females working in this subject (or for that matter mathematics!), three of the female participants did indeed plan and give very interesting talks; one of which may further solidify some collaboration between J. Lewis and B. Kahn (see $\bullet_e$ below).

• By the nature of the organizing committee, this conference engaged a number of top rate colleagues of different nationalities (outside of N. America, those include hispanic (Spain/Mexico), Japan, China, India, Russia, Europe, and so forth). There was also a significant component from Alberta, due to some prejudices in hiring at the UofA. Another important point is that BIRS is within rather easy reach of UofA, making it very easy for candidates there to accept invitations.

• Every attempt was made to ensure that the participation at this conference would be maximal. Indeed, the organizers aggressively sought promising researchers to fill the vacant slots on our participant list.

• We generally like to open and close the conference with very good speakers. Bruno Kahn was the opening speaker, and we ended with Stefan Gille. Stefan Gille, being local (Alberta) turned out to be a natural choice, as many others had to leave earlier on Friday to catch a plane. Still, those many others wanted to attend his talk, albeit resulting in a reduced audience. Apart from all of this, attendance at each talk was excellent, which indicated a desire from various research groups of colleagues to learn what each other was doing. We also avoided concentrations of particular topics on any one day, allowing people to fully focus on a particular topic if they so desired, but also ensuring good cross-fertilization between topics.

36.3 Recent Developments and Open Problems

36.3.1 Recent developments.

To the layperson, a regulator can be thought of as a generalization of the logarithm. In its current incarnation, the precise definition is that it is a map from the K-theory of an algebraic variety to a cohomology theory. There are for example Betti realizations (related to the Hodge conjecture), l-adic, Hodge (such as in Beilinson-Deligne absolute Hodge cohomology), and so forth. This is well documented in [Ja2]. All such realizations can equivalently called regulators but with a caveat: our current understanding of motivic cohomology, as well as a correct definition of the category of mixed motives, is still lacking, and is included in our workshop. Indeed, besides Voevodsky, Nori has also presented a version of motivic cohomology. In both instances, how does one compute extension classes? As abstract as this sounds, the repercussions would be revolutionary (e.g., related to the kernel and image of the classical Abel-Jacobi map, and so forth...).

$\bullet_0$ (Number theory) The naive concept of a regulator being a generalization of the logarithm, is in fact typical of new developments in recent years. For example, Deninger's interpretation of Mahler measures in terms of real regulators involving mixed motives and expressed in terms of special values of polylogarithms, is a decisive development in number theory.

$\bullet_1$ (Physics) The interpretation of Feynman integrals in terms in regulators of cycles (periods) leading to multiple zeta values and polylogarithms, along the lines of Bloch, Kreimer, and more recently using the regulator formulas of Kerr-Lewis-Mueller-Stach [KLM], and Kerr-Lewis [K-L] and Kerr-Doran [D-K], has significantly had an impact in this area of Mathematical Physics. There is also the works by Griffiths-Green-Kerr [GGK], Doran, Pearlstein-Brosnan, Robbles, Usui-Kato on period domains in Hodge theory, and their impact on Calabi-Yau Geometry and Mirror symmetry (these domains serve as spaces capturing the images of variational regulators (normal functions) at the boundary.

$\bullet_1'$ (Period domains) Although mentioned in $\bullet_1$, it is a separate subject by itself, and has connections to $\bullet_2$ below.

$\bullet_2$ (Classical Hodge conjecture) Further to the previous paragraph is the work of Griffiths-Green on singularities of normal functions (variational regulators), based on a key observation of Richard Thomas, has led to a new and interesting re-interpretation of the classical Hodge conjecture[1]. Much of this has also been raised at a new level by the works of Pearlstein-Brosnan-Schnell [BPS].

$\bullet_3$ (Beilinson-Hodge conjecture) The formulation of the amended Beilinson Hodge conjecture has evolved significantly over the years by S. Saito-Asakura [A-K], Lewis-de Jeu [dJ-L], Lewis-de Jeu-Patel (to appear, revisiting [SJK-L]), Arapura [A-K] and can be viewed as a top down approach to the classical Hodge conjecture, as it involves all the higher K-groups of complex varieties. It not only can connections to the Bloch-Kato theorem, but these generalized Hodge conjectures play a deep role in the conjectures about the zero loci of cycle induced normal functions, particularly being invariant under an absolute Galois action.

$\bullet_4$ (Revisting the classical Hodge conjecture - arithmetic considerations) The works of Voisin over the past 10 years have made it abundantly clear that any conceivable generalization of the Hodge conjecture beyond the category of complex algebraic varieties, is false. If one were dealing with the category of compact complex manifolds, then the key ingredient of being projective algebraic is the notion of polarization (Kodaira). Having said this, something more elementary (viz., on an earthly level) is at work here, and was observed and exploited independently by

[1]If X is a projective algebraic manifold, then there is a decomposition of singular cohomology $H^\bullet(X,\mathbb{Q})\otimes\mathbb{C}=\oplus_{p+q=\bullet}H^{p,q}(X)$ into pieces depending only on the the complex structure of X. For an integer $r\geq 0$, the Hodge conjecture states that $H^{2r}(X,\mathbb{Q})\cap H^{r,r}(X)$ is generated by the fundamental classes of algebraic cycles of codimemention r in X. An arithmetic variant of this is the celebrated Tate conjecture.

many, including Nori, Bloch, Beilinson, Deligne, Esnault, Griffiths, Green, Lewis [Lew2], M. Saito, S. Saito, M. Asakura [A], Schoen, Kerr [K-L], Raskind, Voisin, et al.; that being the notion of spreads. Consider any complex scheme X (of finite type, etc.). Working with the coefficients of the polynomials defining X, one can spread X to a smooth family $\rho : \mathcal{X} \to S$ over a number field k for which $\mathcal{X} \times_{k(S)} \mathbb{C} = X$. If X is complete, then one can work with a (conjectural) regular model of $\mathcal{X}$ over the ring of integers in k, which would involve the world of Arakelov geometry. This obviously leads one in the world of arithmetic geometry. Griffiths-Green, Lewis, Asakura-M. Saito, Lewis-Kerr, independently exploited this idea in terms of developing a candidate "Bloch-Beilinson filtration" on the K-groups of a complex projective variety X, which measures the "complexity" of these groups. This spread idea already served a precursor to the notion of arithmetic variations of Hodge structures, which was independently studied by Griffiths-Green, and the Japanese school, including M. Saito, S. Saito and M. Asakura. The meeting of these two schools occurred at the 1998 NATO conference in Banff; a pivotal point in the creation of BIRS.

In the late 1970's Deligne introduced the notion of absolute Hodge classes on Betti cohomology (as well as l-adic). With regard to projective algebraic manifolds $X = X/\mathbb{C}$, any element $\sigma \in \mathrm{Gal}(\mathbb{C}/\mathbb{Q})$ acts on the arithmetic de Rham cohomology of X in a functorial way (hence by the work of Serre, on classical de Rham cohomology), but $\sigma : X \to X^\sigma$ is not continuous, unless σ is either the identity or complex conjugation. Thus σ does not define a map on the level of $\mathbb{Q}$-Betti cohomology, albeit it does preserve algebraic cycles. The subspace of Hodge classes $= H^{2r}(X, \mathbb{Q}) \cap H^{r,r}(X)$ preserved under $\mathrm{Gal}(\mathbb{C}/\mathbb{Q})$ is called the space of absolute Hodge class. Deligne proved that X is an Abelian variety, then $H^{2r}(X, \mathbb{Q}) \cap H^{r,r}(X)$ is absolute Hodge. One conjectures that for any projective algebraic manifold X, all Hodge classess are absolute Hodge, that being implied by the classical Hodge conjecture. Using the idea of $\mathbb{Q}$-spreads of a proiective algebraic manifold X, together with an interpretation of Deligne's ideas in this context (involving a Noether-Lefschetz locus), and Deligne's global invariant cycle theorem, Voisin showed that if every Hodge class on a projective algebraic manifold is absolute Hodge, then the classical Hodge conjecture can be reduced to those X of the form $X = X_0 \times \mathbb{C}$, where X_0 is defined over a number field.

$\bullet_5$ (Beilinson/Bloch regulator to Deligne cohomology) In 1995 [Go], Goncharov provided an explicit description of the regulator of a projective algebraic manifold X to real Deligne cohomology, and more generally to integral Deligne cohomology as well. That there are often mistakes in Goncharov's work is no surprise to anyone in this field. For instance, as first observed by Lewis, his regulator to integral Deligne cohomology is clearly flawed. An amended version appeared in [KLM] involving polylogarithmic currents, where we tacitly acknowledged that his real regulator is correct. Indeed in Matt's thesis [K], it is proven that it would be correct if one adopted a cubical representation of the higher K theory of X. But the Goncharov regulator is defined simplicially, and as first discovered by Matt, there are serious issues about his formula , with consequences involving a number of works. A paper soon to be submitted by Matt, Lewis and Patrick (Matt's student) [BKLP] provides the definitive formula, and truly qualifies as a new development. (See the present highlights below.)

$\bullet_6$ (Zero locus of admissible normal functions associated to variations of mixed Hodge structures) The work of Cattani-Deligne-Kaplan [CDK] on the algebraicity of the Noether-Lefschetz locus of Hodge classes on a family of projective algebraic manifolds (associated to a variation of Hodge structure) represented a significant milestone towards evidence in favour of the Hodge conjecture. The extension of these results to variations of mixed Hodge structures, is both a significant and highly non-trivial result, due to Pearstein-Brosnan-Schnell [BPS]. This plays a role in the open problem $\bullet_b$ below.

$\bullet_7$ (Essential dimension and related topics) The work of Nikita Karpenko, et al., on incompressibility, and its application to essential dimension, which also interacts with the theory of motives, has significantly evolved over the last few years.

36.3.2 Open problems

$\bullet_a$ The original Griffiths program on using normal functions as a line of attack on the classical Hodge conjecture, has been generalized to the higher K-groups, vis-á-vis the Beilinson-Hodge conjecture, and beyond that, using a concept of arithmetic normal functions (See [K-L], [L]). Is there an analog of the Griffith-Green program in $\bullet_2$ involving singularities of normal functions to this generalized situation? (The extension of Voisin's program in $\bullet_5$ is already done [L].)

$\bullet_b$ Take a cycle-induced arithmetic normal function, where the cycle arises from the K theory of a smooth projective X/k, $k \subseteq \mathbb{C}$. Is the zero-locus of that normal function defined over $\overline{k}$? This involves ongoing work of Lewis-Pearlstein. Some evidence in support of this appears in [L].

$\bullet_c$ Given a choice of universal family of polarized K3 surfaces, it is shown in [CDKL], based on Kodaira-Spencer deformation theory, that the "imaginary" of the K_1 regulator (also called transcendental regulator) for a general K3 surface of Picard rank ≤ 19, is non-zero. The holy grail is the situation where a given algebraic K3 surface has maximal Picard rank 20, and hence where deformation theory cannot be applied. We suspect it is non-zero. The problem then is to prove or disprove this.

$\bullet_d$ The classical Hodge conjecture is known to be false if one replaces $\mathbb{Q}$-coefficients by $\mathbb{Z}$-coefficients. The first counter-example was due to Atiyah-Hirzebruch [A-H], involving the existence of torsion non-algebraic integral classes. This was fascinating result at that time, given the fact that in codimension one, the classical Hodge conjecture holds with $\mathbb{Z}$-coefficients (Lefschetz (1,1) theorem). Turning the clock ahead 60 years, we now have a better understanding of this situation. Indeed the Bloch-Kato theorem implies that all torsion is supported in codimension one. Thus in higher codimension, it is conceptually easier to understand the phenomena of torsion non-algebraic integral classes. Later, it was discovered by Kollar that non-torsion, non-algebraic integral classes also exist. In recent years Voisin, J.-L. Colliot-Thélène, et al, have studied this phenomena in more detail, as to when to anticipate an integral version holding. The problem then is to consider an analogue of this for the Beilinson-Hodge conjecture. Some work in this direction appears in [dJ-L], as well as the appendix provided by Asakura.

$\bullet_e$ The Griffiths group is a very important invariant associated to K_0 of projective algebraic manifolds. It was a landmark result appearing in [Gr], using his program on normal functions. Indeed it may still be the most important accomplishment using normal functions. Philosophically speaking, a similar object is the notion of K_1 indecomposable classes, which can also be derived from a generalized program in $\bullet_a$. One fantasy of Lewis-Kahn is that there should be a direct connection between these two groups. One possible route goes back to Bloch, and A. Collino [Co], involving the degeneration of a K_0 class in a family of varieties to a K_1 class (and one can go even further to degenerating to a K_2 class). We were reminded of this idea in Jaya Iyer's talk, and Bruno Kahn quickly jumped on this idea as well. The central problem then is to connect a series of invariants, beginning with the Griffiths group at the K_0 level, to higher K theory.

36.4 Presentation Highlights

Our first speaker, Bruno Kahn, discussed the generalized Hodge and Tate conjectures for products of elliptic curves. It should be pointed out that a Grothendieck amended version of a generalized Hodge conjecture (and subsequent Tate analog) has been known for a long time. These new results were well presented and were certainly appealing to those in Hodge theory, as well as those experts on the Tate side (Rob de Jeu, W. Raskind, Mao Sheng, M. Asakura,,...). Susama Agarwala's talk on graphical motives, is very much connected to the mixed Tate motive regulator calculations appearing in $\bullet_1$. Ravindra's talk is very much connected to Nori connectivity (see [P]), the import of which is a step in the direction of a weak Lefschetz theorem for Chow groups (K_0 case). Such a theorem would be a consequence of the famous Bloch-Beilinson conjecture on the injectivity of the rational regulator on K_0 of smooth varieties defined over number fields. At the present time, this conjecture remains elusive. Matilde Lalin gave a very appealing lecture on recent developments on Mahler measures, and implicitly indicated the role of Deninger's observation that the Mahler measures are explained in terms of regulators of periods. Matt Kerr presented joint work with Lewis on the simplicial regulator to $\mathbb{Q}$-Deligne cohomology, and pointed out the errors by Goncharov indicated in $\bullet_5$. Jaya Iyer's interesting talk on the degeneration of the Gross-Schoen algebraic cycle, is what led Kahn and Lewis to revisit the ideas in $\bullet_e$. Chuck Doran's talk, which is in the realm of $\bullet_1$, also has some underpinnings with $\bullet_c$. M. Asakura's talk also has similar connections to $\bullet_c$. Pearlstein's talk, which was very well received, pertains directly to the subject in $\bullet_1'$. Roy Joshua's talk dealt with t-structures, which goes back to Verdier's introduction of triangulated categories, and the problem of placing derived categories in a category-theoretic context. A partial solution to this problem, due to Beilinson, Bernstein and Deligne in the 1980's, was to impose a t-structure on the triangulated category D. Mao Sheng is an expert in both Hodge theory in characteristic zero, and its analogues in positive characteristic. This was clearly reflected in his talk. The contact organizer (Lewis) has spent time with Mao in China, discussing the wide range potential of arithmetic techniques in Lewis's recent works on regulators. Pablo Pelaez's work deals with filtrations on Chow groups, for which there are many such possibilities. The basic problem is to measure the "complexity" of Chow groups, and this can only be achieved via filtrations, as reflected by the title of his talk. Goncalo Tabuada's talk was an interesting albeit highly technical invitation to non-commutative motives of separable algebras over a field k.

Phillipe Gille's talk, which is somewhat in the spirit of the research areas of Nikita and Stefan (below), dealt with certain homogeneous spaces X vover a field k for which $X(k) \neq \emptyset$.

The last two talks on Friday (given by our local colleagues in Edmonton), by Stefan Gille by Nikita Karpenko, attracted the interests of most participants, albeit a reduced audience due to travel itinerary issues. For this reason alone, we feel a need to mention their works in greater detail.

Nikita Karpenko's research deals with difficult and significant problems about algebraic cycles and motives of projective homogeneous varieties, their decompositions into simple pieces and their applications in the theory of algebraic groups. This was clearly evident in his well received talk on incompressibility of products of projective homogeneous varieties. A smooth projective variety X is called incompressible if every rational map from X into itself is dominant. The canonical dimension cdim X is a measure for the incompressibility of X. This positive integer is always smaller or equal than the dimension of X, and equal dim X if and only if X is incompressible. It is in general quite a task to show that a given variety is incompressible, or to compute the canonical dimension of it. However there exists a slightly weaker and more accessible notion, the so called p-incompressiblity, where p is a prime number, of a smooth and projective variety. This property is measured by the canonical p-dimension, which has been computed for many projective homogeneous varieties (for semisimple algebraic groups). All these results have strong implications on the cycles over such varieties, and applications to algebraic problems as for instance isotropy questions about algebras with involutions.

The last talk, by Stefan Gille, attracted the interests of K-theorists, on the Milnor-Witt groups of local rings. Milnor-Witt groups $K_n^{MW}(F)$, n an integer, of a field F show up as certain homotopy groups in Morel and Voevodsky's A^1-homotopy theory. Hopkins and Morel have found a nice presentation of these groups by generators and relations. This definition can be naively extended to local rings similar as the definition of Milnor K-Theory of fields extends to local rings. Morel has shown that for a field F of characteristic not 2 the n-th Milnor-Witt group of F is the pull-back of the nth Milnor K-group of F and the nth power of the fundamental ideal of the Witt ring of F over the nth Milnor K-group of F modulo 2. We have proven that the same holds for a regular local ring R which contains an infinite field of characteristic not 2. The proof uses a recent result of one of us which describes the nth fundamental power of the fundamental ideal in the Witt ring of such a ring. The proof of this presentation uses in turn a recent theorem of Panin and Pimenov on the existence of strictly isotropic vectors over such regular local rings. A corollary of our theorem is that the nth unramified Milnor-Witt group of such a regular local ring is equal the nth Milnor-Witt group of the ring for all integers n. This implies in particular that the unramified Milnor-Witt groups of smooth and proper schemes over an infinite field of characteristic not 2 are a birational invariant.

36.5 Scientific Progress Made

The contact organizer has initiated three projects, and invitations abroad (India, Japan, Mexico, N. America) as a direct result of this meeting. Judging by the interactions among other participants, one can well imagine a lot of new lines of research as a direct result of communication, and the interesting lectures that were presented. In particular several others initiated new connections/topics/invitations and discussions (there certainly was a lot of interaction between some of those seen more often at meetings in this field, and some that were perhaps more from other fields (Agarwala, Tabuada, for example). This is a great formula to produce good mathematics, and much of which can be expected to lead to fruition.

36.6 Outcome of the Meeting

The high intensity of this workshop, the broad range of participants approaching motives from various angles, and the good quality of the lectures, made this workshop a great experience, and a testament to the value of the BIRS facility; particularly with the backdrop of a bustling town and stunning scenery! Having said this, the real outcome of the meeting really lies in the future.

36.7 A Recommendation

The desire for mostly all participants to attend all talks was very apparent, and should be accommodated if feasible. Our main concern was the final day of the conference, where attendance was skewed due to travel itineraries. Perhaps an option is to stay overnight on the final day (viz., at a reduced cost, with or without meals) which could make a big difference.

36.8 Final Comment

The staff at BIRS were very professional, and certainly made our life agreeable at BIRS!

Participants

Agarwala, Susama (Oxford University)
Asakura, Masanori (Hokkaido University)
Brosnan, Patrick (University of Maryland)
Burgos Gil, Jose Ignacio (ICMAT)
Chen, Xi (University of Alberta)
Chernousov, Vladimir (University of Alberta)
de Jeu, Rob (VU University Amsterdam)
Dos Santos, Pedro (Instituto Superior Tcnico Lisbon)
Elizondo, E. Javier (Universidad Nacional Autonoma de Mexico, Ciudad Universitaria)
Gangl, Herbert (Durham University)
Gille, Stefan (University of Alberta)
Gille, Philippe (Universit Claude Bernard Lyon 1)
Girivaru, Ravindra (University of Missouri St. Louis)
Goswami, Souvik (University of Alberta)
Iyer, Jaya (Institute of Mathematical Sciences,India)
Joshua, Roy (Ohio State University)

Kahn, Bruno (Centre national de la recherche scientifique)
Karpenko, Nikita (University of Alberta)
Kerr, Matt (Washington University in St. Louis)
Kimura, Shun-ichi (Hiroshima University)
Lalin, Matilde (Universit de Montral)
Lewis, James (University of Alberta)
Lima-Filho, Paulo (Texas A&M University)
Mendez, Hector (University of Alberta)
Nagel, Jan (Universite de Bourgogne)
Pal, Suchandan (Univ. of Michigan)
Patel, Deepam (IHES)
Pearlstein, Gregory (Texas A&M)
Pelaez, Pablo (UNAM)
Raskind, Wayne (Wayne State Univ.)
Rivera Arredondo, Carolina (Universit degli Studi di Milano)
Sheng, Mao (University of Science and Technology of China)
Tabuada, Gonalo (MIT)
Tong, Zhang (University of Alberta)
Weibel, Chuck (Rutgers University)
Wilson, Glen (Rutgers, The State University of New Jersey)
Zhong, Changlong (University of Alberta)

Bibliography

[A-K] Arapura, D., Kumar, M. Beilinson-Hodge cycles on semiabelian varieties. Math. Res. Lett. **16**, (2009), no. 4, 557–562.

[A] Asakura, M. Motives and algebraic de Rham cohomology, in: The Arithmetic and Geometry of Algebraic Cycles, Proceedings of the CRM Summer School, June 7-19, 1998, Banff, Alberta, Canada (Editors: B. Gordon, J. Lewis, S. Müller-Stach, S. Saito and N. Yui), NATO Science Series **548** (2000), Kluwer Academic Publishers.

[A-H] Atiyah, M., Hirzebruch, F. Analytic cycles on complex manifolds, Topology **1** (1962), 25-45.

[A-S] Asakura, M., Saito, S. Beilinson's Hodge conjecture with coefficients, in Algebraic Cycles and Motives, Vol. 2, Edited by J. Nagel and C. Peters, LNS **344**, London Math. Soc., (2007), 3-37.

[Be1] Beilinson, A. *Notes on absolute Hodge cohomology*, in Applications of Algebraic K-Theory to Algebraic Geometry and Number Theory, Contemporary Mathematics **55**, part 1, AMS, Providence 1986, 35-68.

[Be2] Beilinson, Higher regulators and values of L-functions, J. Sov. Math. **30** (1985), 2036-2070.

[Blo] Bloch, S. *Algebraic cycles and higher K-theory*, Adv. Math. **61** (1986), 267–304.

[BKLP] Burgos, Kerr, Lewis, Patrick. In progress.

[Co] A. Collino, Griffiths' infinitesimal invariant and higher K-theory on hyperelliptic Jacobians, J. Algebraic Geom. **6** (1997), 393 -415.

[dJ-L] de Jeu, R., Lewis, J. D. (with an appendix by M. Asakura), Beilinson's Hodge conjecture for smooth varieties. J. K-Theory **11** (2013), no. 2, 243-282.

[De] Deligne, P. *Théorie de Hodge, II, III,* Inst. Hautes Études Sci. Publ. Math. No. **40** (1971), 5-57; No. **44** (1974), 5-77.

[Gr] Griffiths, P. *On the periods of certain rational integrals, I&II*, Annals of Math. **90** (1969), pp. 460-541.

[GGK] M. Green, P. Griffiths, M. Kerr, Matt, Néron models and limits of Abel-Jacobi mappings, Compos. Math. **146** (2010), no. 2, 288 - 366.

[Ja2] Jannsen, U., Mixed Motives and Algebraic K-Theory, Lecture Notes in Math. **1000** (1990), Springer-Verlag, Berlin.

[CDK] Cattani, E., Deligne P., and Kaplan, A. *On the locus of Hodge classes,* J. Amer.Math. Soc. **8** (1995), 483-506.

[Kl] Kleiman, S. *Algebraic cycles and the Weil conjecture,* Dix Exposes sur la cohomologie es schemes, North-Holland (1968), pp. 359 - 386.

[KLM] Kerr, M., Lewis, J. D., Müller-Stach, S. *The Abel-Jacobi map for higher Chow groups,* Compos. Math. **142** (2006), no. 2, 374-396.

[K-L] Kerr, M., Lewis, J. D. *The Abel-Jacobi map for higher Chow groups, II,* Invent. Math. **170** (2007), no. 2, 355-420.

[Lew1] Lewis, J. D., A Survey of the Hodge Conjecture. Second edition. Appendix B by B. Brent Gordon. CRM Monograph Series, **10**. American Mathematical Society, Providence, RI, 1999. xvi+368 pp.

[Lew2] Lewis, J. D., A filtration on the Chow groups of a complex projective variety, Compositio Math. **128** (2001), no. 3, 299-322.

[Lew3] Lewis, J. D., Abel-Jacobi equivalence and a variant of the Beilinson-Hodge conjecture, J. Math. Sci. Univ. Tokyo **17** (2010), 179-199.

[Lew4] Lewis, J. D., Arithmetic normal functions and filtrations on Chow groups, Proc. Amer. Math. Soc. **140** (2012), no. 8, 2663-2670.

[K] M. Kerr, His outstanding thesis. Princeton, 2003. 350 pages.

[P] Paranjape, K. Cohomological and cycle-theoretic connectivity, Ann. of Math. (2) **139** (1994), no. 3, 641-660.

[Sa] Saito, S. Beilinson's Hodge and Tate conjectures, in Transcendental Aspects of Algebraic Cycles, Edited by S. Müller-Stach and C. Peters, LNS **313**, London Math. Soc., (2004), 276–290.

[SJK-L] Kang, S-J., Lewis, J. D. Beilinson's Hodge conjecture for K_1 revisited, Cycles, motives and Shimura varieties, 197-215, Tata Inst. Fund. Res. Stud. Math., Tata Inst. Fund. Res., Mumbai, 2010.

[We] Weibel, C. The norm residue isomorphism theorem, Topology **2**, (2009), 346-372.

Two-day Workshop Reports

Chapter 37

Alberta Number Theory Days VI (14w2192)

April 18 - 20, 2014

Organizer(s): Clifton Cunningham (University of Calgary), Habiba Kadiri (University of Lethbridge), Soroosh Yazdani (University of Lethbridge)

Objectives achieved:

This was the sixth edition of Alberta Number Theory Days. Previous conferences took place in Lethbridge (2008), Calgary (2009), and BIRS (2010, 2011, 2013). This friendly meeting gathers the number theorists of the Alberta Universities to interact and exchange ideas once a year.

This year, we wanted to have more invited speakers so that our community (and in particular our students) would be exposed to some new research themes. At the same time we wanted to showcase the research done in Alberta. We had a total of fifteen talks: four external speakers, six from Calgary, four from Lethbridge, and one from Alberta. We scheduled our conference just before the Women In Numbers Conference at BIRS and invited three of their participants to join us: Jennifer Balakrishnan (Oxford), Kate Stange (Colorado), and Ila Varma (Princeton). We also invited Nils Bruin (SFU) to give a presentation.

We have an increasing number of young female researchers and it was important to reflect this in both the schedule and the list of participants. This year, one third of the speakers and participants were female. Moreover of the fifteen talks presented, six were by female speakers, and among those three by students.

Another goal of the conference was to give the opportunity to young researchers to present their research. For many of them it was their first presentation outside their university and a first introduction to a wider research community. It was stimulating for them to gain feedback from senior researchers and broaden their connections to new colleagues as well. Of the fifteen talks presented, four were by faculty, six were by postdoctoral fellows, and five were by students.

Scientific highlights:

This year there were many interesting talks. Highlights included the talks by Jennifer Balakrishnan (Oxford), Kate Stange (Colorado), and Ila Varma (Princeton).

Jennifer Balakrishnan presented research with Amnon Besser and Steffen Müller on integral points of hyperelliptic curves. She discussed their work on a non-abelian Chabauty method. Chabauty's method provides a tool for bounding the number of rational points on a curve X and for finding p-adic approximations of the points. Chabauty's original method applies to the case when the genus of X is greater than the Mordell-Weil rank of the Jacobian of X. Recent deep work of Minhyong Kim gave a generalization which allows the removal of the restriction on the genus in certain cases. Building on Kim's work, Balakrishan and her coauthors have proven a formula for the component at p of the p-adic height pairing to a sum of iterated Coleman integrals. She discussed this formula and also presented several numerical examples.

Ila Varma spoke about her exciting joint work with recent Fields medalist Manjul Bhargava on the mean number of 3-torsion elements in the class groups of quadratic orders. This is a generalization of a classic theorem of Davenport and Heilbronn. Many of the conference participants were excited to hear about this impressive work which is related to Bhargava's groundbreaking work in the geometry of numbers.

Another highlight was Kate Stange's very interesting work on the Bianchi groups of $\mathrm{PSL}_2(\mathcal{O}_K)$ where $\mathcal{O}_K$ is the ring of integers of a number field K. The images of $\mathbb{R}$ under $\mathrm{PSL}_2(\mathcal{O}_K)$ are circles. Stange shows that there is a natural bijection between these circles and certain ideal classes of the orders of K. Furthermore, she relates the curvature of 'tangent' circles by the norm form.

Speakers:

Jennifer Balakrishnan (Mathematics, University of Oxford)
Title: *Integral points on hyperelliptic curves via quadratic Chabauty*.
Abstract: We discuss explicit computations of p-adic line integrals (Coleman integrals) on hyperelliptic curves and some applications. In particular, we relate a formula for the component at p of the p-adic height pairing to a sum of iterated Coleman integrals. We use this to give a Chabauty-like method for computing p-adic approximations to integral points on such curves when the Mordell-Weil rank of the Jacobian equals the genus. This is joint work with Amnon Besser and Steffen Müller.

Jean-Francois Biasse (Mathematics and Statistics, University of Calgary)
Title: *Subexponential class group and unit group computation for large degree number fields*
Abstract: Class group and unit group computation are two of the four major tasks postulated by Zassenhaus. This occurs in particular in the resolution of some Diophantine equations and the numerical study of some unproven conjectures. Computing class group and unit group was known to be feasible in subexponential time for classes of number fields of fixed degree since the work of Buchmann. In this talk, we will see how to extend this result to classes of number fields of arbitrary degree.

Jeff Bleaney (Mathematics and Computer Science, University of Lethbridge)
Title: *Valuations of net polynomials*
Abstract: Let K be a number field with ring of integers $\mathcal{O}_K$, and Let E/K. For $\mathbf{v} = (v_1, v_2, \ldots, v_r) \in \mathbb{Z}^r$, and $\mathbf{P} = (P_1, P_2, \ldots, P_r) \in E(K)^r$, we have $\mathbf{v} \cdot \mathbf{P} := v_1 P_1 + v_2 P_2 + \cdots + v_r P_r = \left(\frac{A_{\mathbf{v}\cdot\mathbf{P}}}{D^2_{\mathbf{v}\cdot\mathbf{P}}}, \frac{B_{\mathbf{v}\cdot\mathbf{P}}}{D^3_{\mathbf{v}\cdot\mathbf{P}}} \right)$.
On the other hand, there exist polynomials $\Psi_{\mathbf{v}}(\mathbf{P}), \Phi_{\mathbf{v}}(\mathbf{P})$, and $\Omega_{\mathbf{v}}(\mathbf{P})$ such that $\mathbf{v} \cdot \mathbf{P} = \left(\frac{\Phi_{\mathbf{v}}(\mathbf{P})}{\Psi^2_{\mathbf{v}}(\mathbf{P})}, \frac{\Omega_{\mathbf{v}}(\mathbf{P})}{\Psi^3_{\mathbf{v}}(\mathbf{P})} \right)$. By generalizing a theorem of Ayad, we show that for all but finitely many primes $\mathfrak{p} \subset \mathcal{O}_K$, the $\mathfrak{p}$-adic valuation $\nu_{\mathfrak{p}}(\Psi_{\mathbf{v}}(\mathbf{P})) = \nu_{\mathfrak{p}}(D_{\mathbf{v}\cdot\mathbf{P}})$.

Nils Bruin (Mathematics, Simon Fraser University)
Title: *Genus 2 curves with* $(3,3)$*-isogenies and 3-torsion in Sha*
Abstract: We parametrize genus 2 curves with a maximal isotropic $(\mathbb{Z}/3)^2$ in their Jacobian, together with an explicit description of the associated isogeny. This allows us to perform $(3,3)$-isogeny descent on various simple principally polarized abelian surfaces and exhibit non-trivial 3-part in their Tate-Shafarevich groups. This is joint work with Victor Flynn and Damiano Testa.

Diane Fenton (Mathematics and Statistics, University of Calgary)
Title: *A generalization of Artin's conjecture*
Abstract: Artin's primitive root conjecture is an old and well-studied problem in number theory. It conjectures that, for a constant a not a perfect square and not -1, a is a primitive root mod p for infinitely many primes p and, furthermore, gives a conjectural density for these primes. Artin's conjecture has been proved subject to the generalized Riemann hypothesis, but remains unresolved for any single value of a. We will explain why algebraic number theory expects Artin's conjecture to be true and discuss a generalization of Artin's conjecture that has interesting applications to ranks of apparition in divisibility sequences.

Hugo Labrande (Mathematics and Statistics, University of Calgary)
Title: *Isogeny computation using a complex analytic method*
Abstract: Isogenies are maps between two abelian varieties that have a finite kernel and preserve the group law. Those maps have been studied for various purposes, from point counting to order computation, as well as faster resolution of the discrete logarithm problem. Algorithms to compute explicitly those maps exist for genus 1 elliptic curves (e.g. Vélu's formulae), and recent work (Cosset-Robert) allowed computations of isogenies between genus 2 hyperelliptic curves. We outline here a method to compute isogenies between elliptic curves over finite fields, using computation of isogenies between elliptic curves defined over the complex field. This method brings together a few well-known mathematical results, as well as some recent advanced algorithms; it is expected to generalize gracefully to hyperelliptic curves of genus 2.

Sebastian Lindner (Mathematics and Statistics, University of Calgary)
Title: *Fast Divisor Tripling*
Abstract: Our main objective is to improve efficiency of low-genus hyperelliptic curve cryptosystems via alternative scalar multiplication algorithms and new explicit formulas. The basic operations in the divisor class group over a hyperelliptic curve are scalar multiplications, in other words adding a divisor to itself a fixed number of times. Divisor arithmetic on low-genus hyperelliptic curves is done by using explicit formulas described in terms of finite field operations. One way to increase efficiency is to use a double base algorithm for scalar multiplication where you represent the scalar as a sum of powers of two and three. The efficiency of using this algorithm over a single base algorithm becomes advantageous if you have fast explicit tripling formulas. We have produced explicit tripling formulas that are computationally faster than any other combination of doubling and adding, giving an increase in efficiency over all when using double base representation algorithms for scalar multiplication in the divisor class group.

Allysa Lumley (Mathematics and Computer Science, University of Lethbridge)
Title: *New bounds for* $\psi(x;q,a)$
Abstract: Let a, q be relatively prime integers. Then consider

$$\psi(x;q,a) = \sum_{\substack{n\le x \\ n\equiv a(\bmod q)}} \Lambda(n).$$

We discuss new explicit bounds for $\psi(x;q,a)$, which provide an extension and improvement over the bounds given in the previous work of Ramaré and Rumely. This article introduces two new ideas. We smooth the prime counting function and use the partial verification of GRH by Platt along with an explicit zero-free region given by Kadiri. This is joint work with Habiba Kadiri.

Nathan Ng (Mathematics and Computer Science, University of Lethbridge)
Title: *Large deviations of sums of independent random variables and prime number error terms*
Abstract: Aurel Wintner initiated the study of limiting distributions of error terms in prime number theory. These error terms may be modelled by certain infinite sums of independent random variables. In the 1980's Montgomery and then Montgomery-Odlzyko proved upper and lower bounds for the probability that sums of independent random variables are large. In this talk I will present some theorems which provide more precise upper and lower

bounds for these large deviations. Our results can be used to make a conjecture on the sizes of certain prime number error terms. This is joint work with Amir Akbary and Majid Shahabi.

James Parks (Mathematics and Computer Science, University of Lethbridge)
Title: *One-level density of families of elliptic curves and the Ratio Conjectures*
Abstract: In this talk we use the Ratios Conjecture to obtain closed formulas for the one-level density for two families of L-functions attached to elliptic curves. We find that the one-level scaling density for the second family is the sum of the Dirac distribution and the even orthogonal distribution. This seems to be a new phenomenon, caused by the fact that the curves we consider in the second families have odd rank.

Manish Patnaik (Mathematics and Statistics, University of Alberta)
Title: *Automorphic Forms on Loop Groups*
Abstract: The Langlands-Shahidi method is used to study L-functions of cusp forms on a group G_o by analyzing the Fourier coefficients of certain Eisenstein series on a larger group G. We shall explain some elements of this construction in the case when G_o is a finite-dimensional Lie group and G is an infinite-dimensional loop group. Joint work in parts with A. Braverman, H. Garland, D. Kazhdan, and S.D. Miller.

Renate Scheidler (Mathematics and Statistics, University of Calgary)
Title: *Explicit One-Dimensional Infrastructure in Function Fields of Arbitrary Degree*
Abstract: Infrastructure arithmetic is a useful tool for computing invariants of global fields. To apply this tool effectively, a framework of explicit and efficient ideal arithmetic is essential. To date, such arithmetic is only available in certain extensions of small degree, where the infrastructure machinery has been used extensively and successfully for computing class numbers and regulators, and even for cryptographic applications. In this talk, we describe fast infrastructure arithmetic for global function fields of arbitrary degree that support one-dimensional infrastructures, i.e. have two in finite places. This scenario has no analogue in number fields, where one-dimensional infrastructures occur only in real quadratic, complex cubic and totally complex quartic extensions. Our description includes connections with Riemann-Roch spaces and Mahler's geometry of Puiseux series, explicit baby step and giant step arithmetic, and run time results of these algorithms. This is joint work with my former doctoral student Adrian Tang (Google Inc.).

Kate Stange (Mathematics, University of Colorado)
Title: *Here a circle, there a circle, everywhere a circle circle.*
Abstract: Motivated by questions about Apollonian circle packings, I'll present a simple way to add geometry to a collection of ideal classes of orders in an imaginary quadratic field K. The images of $\mathbb{R}$ under $\mathrm{PGL}_2(\mathcal{O}_K)$ are circles shown to be naturally in bijection with certain ideal classes of the orders of $\mathcal{O}_K$. The relevant conductor can be read off from the curvature of the circle. For most K, any two circles are either pairwise disjoint or tangent. The conductors of 'tangent' ideal classes relate to the values of the norm form. This leads to a 'lattice Descartes rule' for Apollonian circle packings and a simple description of the curvature quadratic forms associated to such packings.

Ander Steele (Mathematics and Statistics, University of Calgary)
Title: *Shintani cocycles and p-adic measures*
Abstract: The Shintani cocycle on $\mathrm{GL}_n(\mathbb{Q})$, as constructed by R. Hill, gives a cohomological interpretation of special values of zeta functions for totally real fields of degree n. In this talk, we specialize Hill's cocycle to a cocycle valued in a space p-adic pseudo-measures and determine which specializations yield actual measures. As an application, we will give a new construction of p-adic L-functions of totally real fields in the spirit of Cassou Noguès and Barsky.

Ila Varma (Mathematics, University of Princeton)

Title: *The mean number of 3-torsion elements in the class groups of quadratic orders*
Abstract: In joint work with Manjul Bhargava, we determine the mean number of 3-torsion elements in the class groups of quadratic orders, when quadratic orders are ordered by their absolute discriminants. In 1971, Davenport-Heilbronn determined the mean number of 3-torsion elements in the class groups of *maximal* quadratic orders. I will describe Davenport-Heilbronn's original proof and the alterations (including inputs from ring class field theory) we make to extend their theorem to all orders.

Participants

Akbary, Amir (University of Lethbridge)
Aryan, Farzad (University of Lethbridge)
Balakrishnan, Jennifer (University of Oxford)
Bauer, Mark (University of Calgary)
Bedard, Robert (University of Lethbridge)
Biasse, Jean-Francois (University of Calgary)
Bleaney, Jeff (University of Lethbridge)
Bruin, Nils (Simon Fraser University)
Cunningham, Clifton (University of Calgary)
DeQuehen, Victoria (McGill University)
Felix, Adam (University of Lethbridge)
Fenton, Diane (University of Calgary)
Gherga, Adela (University of Lethbridge)
Guy, Richard (The University of Calgary)
Kadiri, Habiba (University of Lethbridge)
Kumar, Manoj (University of Lethbridge)
Labrande, Hugo (University of Calgary/ISPIA, INRIA Nancy)
Langlois, Marie-Andree (University of Calgary)
Lindner, Sebastian (University of Calgary)
Lumley, Allysa (University of Lethbridge)
Ng, Nathan (University of Lethbridge)
Parks, James (University of Lethbridge)
Patnaik, Manish (University of Alberta)
Roe, David (University of British Columbia)
Scheidler, Renate (University of Calgary)
Stange, Katherine (University of Colorado, Boulder)
Steele, Ander (University of Calgary)
Varma, Ila (Princeton University)
Yazdani, Soroosh (University of Lethbridge)

Chapter 38

Ted Lewis SNAP Math Fair Workshop (14w2197)

April 25 - 27, 2014

Organizer(s): Sean Graves, (University of Alberta), Tiina Hohn (Grant MacEwan University), Ted Lewis (SNAP Foundation)

The SNAP Foundation is a non-profit organization whose mandate is to encourage the development of mathematics learning resources at the classroom level with very little retraining of the teaching staff, with very flexible budgets, and by utilizing the energy and natural curiosity of the students themselves. The main theme of the BIRS workshop was, What is a SNAP math fair and how to organize a math fair in your classroom. The speakers mostly consisted of teachers/educators who shared their math fair experiences and success stories.

The first SNAP type math fair was designed in Edmonton by Mike Dumanski and Andy Liu in 1997-1998. Since then, a large number of schools in Alberta and beyond have adapted the SNAP math fair to their needs. The SNAP program has been spread through similar workshops and conferences, and mainly by teachers themselves.

SNAP received its initial funding from the Canadian Mathematical Society and from private donations. PIMS, the Pacific Institute for the Mathematical Sciences, has been a long time financial supporter of our math fairs. BIRS, the Banff International Research Station, has provided funding for the BIRS math fair workshops that have been held in Banff on a regular basis. Currently, our major supporter is Thinkfun - a company that develops a variety of excellent puzzles.

This year marked the eleventh annual Ted Lewis SNAP Math Fair Workshop at BIRS. Some of the feedback from elementary teachers is given below:

I had a terrific time with the group! Thanks for sharing all of the ideas and puzzles!

Thank you so much for the invitation to the SNAP Math Fair Conference! I am absolutely thrilled with the possibilities I have to bring math alive in my classroom and school. I am so excited to spread the information, websites and puzzles that I was able to gather at the conference. I greatly enjoyed hearing the various perspectives on math fairs and can't wait to plan one of my own. Please keep me on your mailing list and inform me of other SNAP activities that I could participate in.

Thank you for organizing this event. I know that my kids love playing games, so any new ones are always welcomed in my room. It was fun as always and it hurt my brain just a bit.

Participants

Akinwumi, Michael (University of Alberta)
Alcock, Jazz (St. Gerard Elementary)
Alfano, Dan (Telus World of Science Edmonton)
Brogly, Katherine (St. Gerard Elementary)
Campbell, Cathy (Bessie Nichols School, Edmonton Public Schools)
Froese, Heidi (Allendale School)
Gagnon, Lynn (St. Martha School)
Graves, Sean (University of Alberta)
Hoffman, Janice (Edmonton Public Schools)
Hohn, Tiina (MacEwan University)
Ikari, Cindy (Rutland Middle School)
Isaac, Vince (St. Teresa)
Jones, Carolyn (Centre for Education)
Korah, Lyn (Edmonton Public Schools)
Kotyk, Nicole (Evergreen Elementary School)
Kristiansen, Joel (St Gerard school)
Lewis, Ted (SNAP Mathematics Foundation)
Marion, Sam (TELUS World of Science - Edmonton)
Mclellan, Brandy (Calgary Catholic School District)
Morin, Matthew (Keyano College)
Morrill, Ryan (University of Alberta)
Myers, Lisa (Calgary Catholic School Board)
Nastos, James (University of British Columbia Okanagan)
Naturkach, Christine (St. Gerard Elementary)
Pasanen, Trevor (University of Alberta)
Sartorelli, Toni (Johnny Bright School)
Truong, Richard (Edmonton Public Schools)

Chapter 39

Algebraic design theory with Hadamard matrices: applications, current trends and future directions (14w2199)

July 11 - 13, 2014

Organizer(s): Robert Craigen (University of Manitoba), Dane Flannery (National University of Ireland, Galway), Hadi Kharaghani (University of Lethbridge)

The meeting began 8.30am on 12 July 2014 and concluded at noon on 13 July. Invited and contributed lectures (of 50 and 20 minutes respectively) were delivered by leading experts, and a lengthy problem session ran on the second day. There were 32 participants from more than 25 institutions in Australia, Canada, Croatia, Hungary, Iran, Ireland, Japan, Poland, Singapore, Spain, Turkey, and the USA. Early stage researchers, especially graduate students, were well represented.

39.1 Overview of the Field

As formulated in [3, 4], algebraic design theory emphasizes the use of algebraic techniques and viewpoints to solve problems in combinatorial design theory. The focus is on 'pairwise combinatorial designs', such as Hadamard matrices and their generalizations; these are rich in applications to areas such as coding and communications theory, quantum physics and computing, to name just a few.

Several long-standing problems concern the existence question: whether for every allowable order there are any designs of the specified type. Perhaps the most famous of these is the existence conjecture for Hadamard matrices; and a special case for Hadamard matrices that are circulant type. B.Schmidt, a participant at the meeting, has made remarkable progress towards resolution of the circulant conjecture, and it seems likely that he will eventually settle it (in the negative) [5, 6].

Another important kind of problem is enumeration or classification. Typically these are most prominent in cases when existence is trivial or easily proved. Even here, however, sophisticated algebraic tools are required to produce manageable classifications. The use of modern computer algebra systems such as MAGMA [1] is vital in generating lists.

39.2 Recent Developments and Open Problems

Two of the foremost researchers on existence problems for Hadamard matrices, W. Orrick and B. Schmidt, delivered presentations and shared their expertise in numerous conversations with other participants. Classification problems for complex Hadamard matrices and generalized Hadamard matrices over groups are powered by applications in quantum physics and computing; this area was represented by K. Życzkowski. Other very recent applications featured prominently: to coding theory (V. Tonchev) and compressed sensing (P. O Catháin).

39.3 Presentation Highlights

C. Colbourn outlined a general framework for permutation covering problems, and an algorithm for constructing them.

R. Craigen talked about constructions for circulant and group-developed generalized weighing matrices. This is work with Warwick de Launey, who is a founder of algebraic design theory and a continuing major influence on the subject.

W. Orrick spoke on Hadamard's maximal determinant problem—another major unsolved problem in the field. The question is: what is the largest determinant of a $\{\pm 1\}$-matrix of (arbitrary) order n? Much progress towards its solution has been made by Orrick and his co-authors. He surveyed various constructions and proofs of maximality.

Lander's conjecture states that if G is an abelian group of order v containing a difference set of order n, and p is a prime dividing v and n, then the Sylow p-subgroup of G must be non-cyclic. B. Schmidt discussed attempts to construct counterexamples to Lander's conjecture.

V. Tonchev spoke on special classes of Hadamard matrices, such as Bush-type matrices, and generalized Hadamard matrices over groups. He also described results on related combinatorial designs and codes.

Talks by early stage researchers included those by Darcy Best on parity of transversals in Latin squares, and by Ferenc Szöllősi, on the recent closure of the final existence questions for weighing matrices of weight 9.

39.4 Scientific Progress Made

The meeting culminated in a lively and highly productive problem session. Single-page writeups of new interesting problems arising out of the work presented at both this meeting and the preceding one in Lethbridge (ADTHM 2014) were compiled and discussed during this session. In no particular order, the following problems were raised.

- R. Craigen proposed a problem of studying $\bmod m$ Hadamard matrices of order 256 for $m \leq 256$ to produce helpful new insights about modular questions and potential progress toward the current smallest outstanding case of existence of Hadamard matrices. Known special cases and general approaches were discussed.
- P. Leopardi asked about graphs whose edge-sets can be partitioned into two or three strongly regular subgraphs, isomorphic via an isomorphism of the underlying graph. These correspond to an important class of combinatorial designs related to Hadamard matrices.
- D. Goyeneche and K. Życzkowski suggested that an Orthogonal Array OA(r, N, d, k) be called irredundant if, when any k columns are removed, all remaining r rows are distinct. They ask for a list and characterization of irredundant OAs at low orders, and for a characterization of "local equivalence" of orthogonal arrays corresponding to local equivalence of orthogonal states (a deep question arising from quantum information theory).
- M. Matolcsi and K. Życkowski define "Almost Hadamard matrices" (AHM), slightly perturbed from $\{\pm 1\}$-matrices (distance defined using matrix norms) and exhibiting orthogonality, i.e., $AA^\top = nI$. They pose four problems (much discussion ensued).

- Find an infinite family of these in which the distance goes to 0 as $n \to \infty$.
- Improve known numerical algorithms for AHM, particularly for large values of n.
- Experiment with known and new techniques in order $n = 667$ and other small, likely difficult, orders.
- When such a matrix can be 2-valued, explore replacement by 1 and -1 (heuristics suggest that previously unknown Hadamard matrices may arise in this way).

* A. Rao spoke on "Alltop functions", which provide powerful ways to construct difference sets, Hadamard matrices, and mutually unbiased bases (MUBs). She posed four problems: find new families (these are currently rare); identify whether certain classical families are equivalent; determine whether inequivalent Alltop functions generate inequivalent MUBs; and analyse the new Alltop functions discussed in her talk, relative to correlation measure.

* P. Ó Catháin gave a surprising lemma about the number of nonzero entries in linear combinations of rows of a complex Hadamard matrix. He asked for a description of (complex) Hadamard matrices with the property that no linear combination of t rows contains more than t zeros; or, failing that, contain no more than $f(t)$ rows where f is a slow-growth function.

* I. Wanless contributed a question informally raised at both meetings: what is the smallest number of nonzero entries in which two Butson-Hadamard matrices of order n can differ? A simple combinatorial argument shows that in the real case this is n; it is conjectured to be the same in the complex case. The Butson-Hadamard case appears to have no specific merit over the general "complex-Hadamard" case, suggesting that the question be asked generally.

  Wanless also posed a puzzle about the largest power of 2 dividing the permanent of a Hadamard matrix of order n, conjecturing that this is also the highest power of 2 dividing $n!$.

* R. Egan asked whether there is a central relative difference set with certain parameters in the dicyclic group of order $8t$. Such a set would imply the Hadamard matrix conjecture. This is a natural place to seek the elusive single, general class of Hadamard matrices in all orders $4t$, which lends itself to study via the nascent algebraic design theory and cocyclic development of designs. Egan provides a lemma suggesting an attack using two $\{\pm 1\}$-sequences with certain properties, and he asks when such pairs can be found beyond those already known, whether recursive constructions can be developed, and whether a probabilistic approach to construction will bear fruit.

* W. Martin asked for new examples of "linking systems" for difference sets in finite abelian groups. A construction discovered by Cameron and Seidel in 1973 suggested that there many be others. In 2014 Davis, Martin and Polhill succeeded in finding linking systems using Galois rings, but the call is for more constructions. Their result suggests the possibility of involving algebraic tools heretofore not brought to bear on the problem.

  Martin also asked for a proof that the existence of more than k mutually unbiased (real) Hadamard matrices of order n implies that $4^k | n$—even just for $k = 3$. Known partial results were given.

Some of these problems—notably those of Craigen, Matolcsi, Życkowski and Wanless—are well-suited for exploration by undergraduate and graduate students; indeed some were posed with that in mind, but simultaneously promise substantial progress on key gaps in our understanding.

39.5 Outcomes of the Meeting

Collaborations were initiated (e.g., between Flannery, Egan, and O Catháin on classifying cocyclic Butson matrices, prompted by K. Życzkowski's remarks about the dearth of libraries of complex Hadamard matrices; cf. [2]). Several preprints are in preparation.

Shortly after the meeting, R. Craigen visited D. Flannery and R. Egan at NUI Galway, Ireland for several months, to pursue foundational questions in algebraic design theory, and the specific problem posed by Egan at the BIRS meeting.

Planning of future conferences in algebraic design theory were initiated. M. Matolcsi undertook to organize the next meeting focused on Hadamard matrices and their generalizations at the Alfréd Rényi Institute of Mathematics, Hungary, in 3 years time.

Participants

Alvarez, Victor (Universidad de Sevilla)
Andrs Armario, Jos (Universidad de Sevilla)
Best, Darcy (Monash University)
Colbourn, Charles (Arizona State University)
Craigen, Robert (University of Manitoba)
Crnkovi?, Dean (University of Rijeka)
Egan, Ronan (National University of Ireland)
Erickson, Jacob (Wright State University)
Flannery, Dane (National University of Ireland, Galway (Ireland))
Frau, Maria (Universidad de Sevilla)
Fujiwara, Yuichiro (California Institute of Technology)
Holzmann, Wolfgang (University of Lethbridge)
Jedwab, Jonathan (Simon Fraser University)
Kharaghani, Hadi (University of Lethbridge)
Lam, Clement (Concordia University)
Martin, William (Worcester Polytechnic Institute)
Matolcsi, Mate (Rnyi Institute)
Munemasa, Akihiro (Tohoku University)
Cathin, Padraig (The University of Queensland)
Olmez, Oktay (Ankara University)
Orrick, William (Indiana University)
Ramp, Hugh (University of Alberta)
Rao, Asha (RMIT University)
Schmidt, Bernhard (Nanyang Technological University)
Suda, Sho (Aichi University of Education)
Szll?si, Ferenc (Tohoku University)
Taghikhani, Rahim (University of Manitoba)
Tan, Ming Ming (Nanyang Technological University)
Tayfeh-Rezaie, Behruz (Institute for Research in Fundamental Sciences (IPM))
Tonchev, Vladimir (Michigan Technological University)
Xiang, Qing (University of Delaware)
Zyczkowski, Karol (Jagiellonian University)

Bibliography

[1] W. Bosma, J. Cannon, and C. Playoust, The Magma algebra system. I. The user language, J. Symbolic Comput. **24** (1997), no. 3-4, 235–265.

[2] W. Bruzda, W. Tadej and K. Życzkowski, `http : //chaos.if.uj.edu.pl/ karol/hadamard/`

[3] W. de Launey and D. L. Flannery, Algebraic design theory, Mathematical Surveys and Monographs vol. 175, American Mathematical Society, Providence, RI, 2011.

[4] K. J. Horadam, Hadamard matrices and their applications, Princeton University Press, Princeton, NJ, 2007.

[5] K.H. Leung and B. Schmidt, New restrictions on possible orders of circulant Hadamard matrices, Designs, Codes and Cryptography (2012), **64**, no. 1-2, 143–151.

[6] B. Schmidt, `http : //www.ntu.edu.sg/home/bernhard/CW/CW.html`

Chapter 40

Recent Advances in Survey Sampling Techniques (14w2202)

July 25 - 27, 2014

Organizer(s): KC Carriere (University of Alberta)

40.1 Overview of the Field

There were six talks by very eminent statisticians: Professor Jon Rao of Carleton University, Professor Wayne Fuller of Iowa State University, Professor Gauri Datta of University of Georgia, Professor Partha Lahiri of University of Maryland, Dr. Torabi of University of Manitoba and Professor Kim of Iowa State University. The main theme of the talks was Small Area Estimation in Survey Sampling. Professor Prasads research in this area is quite well known. In fact, one of the main papers in this area is by Prasad (Prasad and Rao, 1990 JASA) and the main result is known as Prasad-Rao estimator. The talks were discussing the importance of Prasads work in the area, which is still making a significant impact, presenting extensions, nearly 25 years after its publication.

40.2 Presentation Highlights and Scientific Progress Made

The session started with lively introduction by Professor Jon Rao who was the supervisor for Professor Prasad. He presented an overview of the research area of Small Area Estimation. It elucidated the historical development starting with the paper by Fay and Herriot (JASA, 1979). The main unsolved problem in these papers was obtaining the correct uncertainty measure for the prediction of the small area values. Prasad and Rao (1990, JASA) was the first paper that gave an estimator that is still widely used and is very hard to beat even with much more complicated methodologies such as the bootstrap.

It was then continued with presentation by Professor Wayne Fuller who presented a double bootstrap method to estimate prediction error of the small area predictor. One of the main results was how to do double bootstrap in a computationally efficient fashion. The double bootstrap is done using only 1 additional sample, versus B additional samples, at the second stage. It is called the telescopic bootstrap. It was shown by simulations that the telescoping bootstrap works as well, and sometimes better, than the standard double bootstrap procedure.

Professor Gauri Datta discussed how Small Area Estimation is intimately related with the mixed and random effect models. Model selection methods for this class of models are not well developed. One of the issues that needs to be addressed is Are all random effects essential?. The idea is that if good covariates are available for a particular area, one may not use random effect (or, equivalently the random effect has zero variance). The presentation showed how to test for such zero random effects. The method was applied to a data from Massachusetts. It turns out only a few areas really needed the random effects adjustment. The common practice of using of random effects in applied fields may take a note of this issue.

Then, Professor Partha Lahiri presented a penalized likelihood approach (termed here as modified likelihood) to stabilize the estimation of the variance components. The penalty function varies from area or area. Different penalty functions lead to different efficiencies. This works with the Normal mixed model only. Simulations results are encouraging although quite comparable to the bootstrap estimators.

In the second last presentation, Professor Mahmoud Torabi discussed the statistical inference for spatial version of generalized linear mixed models. He generalized Prasad-Rao estimator of prediction error to this case and compared with the bootstrap estimator. The approximation seems to work well.

Lastly, Professor J. K. Kim, Iowa State University gave an applied talk. He applied the techniques of Small Area Estimation to predict election results in Korea. The main contribution was on designing a survey that is accurate but not as expensive as exit polls. They used a survey using smart phones for younger generation and telephone poll for older generation. This improved the non-response rate. It also allowed use of auxiliary information to improve the inference.

40.3 Outcome of the Meeting

We wrapped up our two day workshop on Sunday morning with a round table discussion over coffee. New networks were formed. Promising new research avenues were developed. New friendships were developed. Everyone appreciated the opportunity to be at the workshop in such stunning surroundings, which made doing mathematical and statistical sciences all the more appetizing. It was an exceptional workshop, extremely lively and interactive.

Participants

Carriere, Keumhee (University of Alberta)
Cribben, Ivor (Alberta School of Business)
Datta, Gauri (University of Georgia)
Deng, Bo (Univeristy of Alberta)
Fuller, Wayne (Iowa State University)
Gombay, Edit (University of Alberta)
Heo, Giseon (University of Alberta)
Hooper, Peter (University of Alberta)
Hu, Rui (University of Alberta)
Jiahua Chen, Jiahua (Maryland Population Research Center)
Karunamuni, Rohan (University of Alberta)
Kim, Jae-Kwang (Iowa State University)
Kong, Linglong (University of Alberta)
Lele, Subhash (University of Alberta)
Li, Yin (University of Alberta)
Liu, Box (University of Alberta)
Mizera, Ivan (University of Alberta)
Mohammadi, Farhood (University of Alberta)
Petrov, Pavel (University of Alberta)

Pianzola, Arturo (University of Alberta)
Prasad, NGN (University of Alberta)
Rao, Jon (Carleton University)
Rosychuk, Rhonda (University of Alberta)
Sinha, Sanjoy (Carleton University)
Torabi, Mahmoud (University of Manitoba)
Wiens, Douglas (University of Alberta)
Wong, Weng Kee (University of California, Los Angeles)

Bibliography

[1] NGN Prasad and JNK Rao. The Estimation of the Mean Squared Error of Small-Area Estimators. JASA 1990. Vol. 85, No. 409, pp. 163-171

[2] RE Fay, and RA Herriot. Estimates of Income for Small Places: An Application of James-Stein Procedures to Census Data. JASA 1979.Vol. 74, No. 366. pp. 269-277.

[3] P. Lahiri and JNK Rao. Robust Estimation of Mean Squared Error of Small Area Estimators. JASA 1995. Vol 90, No. 430. pp. 758-566.

[4] Jiming Jiang and P. Lahiri. Estimation of Finite Population Domain Means: A Model-Assisted Empirical Best Prediction Approach. JASA. 2006. Vol 101. No. 473. pp. 301-311.

[5] G. Datta and M. Ghosh. Small area shrinkage estimation. Statistical Science. 2012. Vol. 27. No. 1, pp. 95-114.

Chapter 41

The Fourth International Workshop on the Perspectives on High-dimensional Data Analysis (14w2178)

August 8 -10, 2014

Organizer(s): Ejaz Ahmed (Brock University), Timothy D. Johnson (University of Michigan), Xuewen Lu (University of Calgary), Andrei Volodin (University of Regina)

This workshop went very smooth and was a great success. Besides domestic participants, it had attracted many international participants from USA and Mexico. Many participants at end of the workshop had indicated their interest to take part in a future workshop of a similar type to further discuss research progress in these research areas, and we plan to do so!

The HDDA series has now become a well-established tradition and one of the most visible annual events in North America on cutting edge methodology for high dimensional data and its applications in a broad range of studies, from environmental sciences to cybersecurity to fMRI imaging. The previous annual HDDA workshops were held Toronto, ON (2011), Montreal, QC (2012), and Vancouver, BC (2013). This important workshop series was envisioned and initiated by Professor Ejaz Ahmed.

This workshop has successfully fulfilled the agenda of promoting research activities in the area of high-dimensional data analysis. It has created a rather focused venue for participants to actively discuss and exchange research ideas via presentations and post-presentation informal discussions. The list of speakers at the workshop was really impressive, and most of talks were based on unpublished and on-going work. There are a significant proportion of Canadian speakers, who had been given these opportunities to develop future collaborations among them and with researchers

Twenty five invited talks were presented by influential researchers on various aspects of High-dimensional Data Analysis and were well received by the audience. Most of presentations had followed with insightful comments and interesting discussions. Participants had active exchanges of ideas and in-depth discussion on current research activities and future research directions.

In conclusion, this workshop has achieved the following goals: (1) Presentations have highlighted new methodology development and extensions of existing methods in high-dimensional data analysis, (2) through both presentations and discussions researchers have identified important directions for future research such as algorithmic problems in protein folding, brain imaging and new problems of regularization methods, (3) researchers have made extensive discussion on collaborations and hope to meet again in the next year to exchange results once again, and (4) the workshop has provided a broad range of research problems and up-to-date information for highly qualified personnel who have benefitted in a great deal by meeting and interacting with leading researchers.

We would like to express our thanks to the superb staff and management at BIRS for the encouragement and support in the organization of this workshop. Our special thanks go to Wynne Fong, Chee Chow, Ornela Alquicira, and Linda Jarigina-Sahoo for their time, effort and support.

Participants

Adragni, Kofi (University of Maryland Baltimore County)
Ahmed, Ejaz (Brock University)
Amezziane, Mohamed (Central Michigan University)
Daniels, Michael J. (U of Texas, Austin)
Diao, Guoqing (George Mason University)
Feng, Yang (Columbia University)
Hossain, Shakhawat (U of Winnipeg)
Johnson, Timothy D. (University of Michigan)
Kafadar, Karen (Indiana University)
Khalili, Abbas (McGill University)
Li, James (VisuMap Technologies Inc)
Lu, Xuewen (University of Calgary)
Ma, Shuangge (Yale University)
Michailidis, George (University of Michigan)
Muoz, Maria Pilar (Universitat Politcnica de Catalunya)
Nan, Bin (University of Michigan)
Nathoo, Farouk (University of Victoria)
Raheem, Enayetur (University of Northern Colorado)
Ramirez Ramirez, Lilia Leticia (Instituto Tecnologico Autonomo de Mexico)
Shojaie, Ali (University of Washington)
Singh, Radhey S (University of Waterloo)
Song, Peter (University of Michigan)
Stephens, David A. (McGill University)
Taddy, Matt (University of Chicago Booth School of Business)
Verducci, Joseph S. (The Ohio State University)
Vidyashankar, Anand (George Mason University)
Volodin, Andrei (University of Regina)
Xin, Jack (University of California at Irvine)
Yi, Grace (University of Waterloo)

Chapter 42

Canadian Abstract Harmonic Analysis Symposium (CAHAS) 2014 (14w2200)

August 29 - 31, 2014

Organizer(s): Anthony T.-M. Lau and Volker Runde (both at the University of Alberta)

Abstract Harmonic Analysis.

Abstract harmonic analysis is the area of mathematics that deals with locally compact groups, their representations, and the Banach algebras associated with them. It has had a strong presence in Canada's mathematical community for several decades.

The Conference in Perspective.

The Canadian Abstract Harmonic Analysis Symposium–CAHAS, in short—originated in 1997 with a meeting in Vancouver at the University of British Columbia on the occasion of Edmond Granirer's retirement. Ever since, it has been held on an annual basis at various locations throughout Canada. The moniker Canadian Abstract Harmonic Analysis Symposium probably originated with the 2005 meeting of the series, which was held at the University of Waterloo. Most of these meetings were two days conferences in an "on a shoestring" format. However, some some CAHAS meetings lasted longer. In 2009, for instance, the CAHAS was held in a one week format with almost 80 participants, of whom 15 were plenary speakers, to celebrate the 65th birthday of Anthony To-Ming Lau—one of the organizers of this meeting at BIRS. CAHAS has by now become an established fixture of Canada's mathematical community.

The Conference and the Thematic Program on Abstract Harmonic Analysis, Banach and Operator Algebras at the Fields Institute.

From January to June 2014, there was a Thematic Program held at the Fields Institute organized by the first named organizer of this conference and MATTHIAS NEUFANG of Carleton University and the Université de Lille, I, in France. The conference at BIRS was intended to be a coda to that program with the focus on mostly junior people.

Intentions and Outcome.

As there had been a thematic program at the Fields Institute in the very same area earlier that year, there had—understandbly—been a certain fatigue among more seasoned mathematicians in the area to attend this installment of CAHAS. As we had hoped, this resulted into an unsually high participation of junior mathematicians, i.e., people at the the postdoctoral and graduate student level: of the 25 participants of the meeting, four were at the postdoctoral level, and 13 were graduate students. There were 13 talks given altogether (sadly MICHAEL LAMOUREUX of Calgary had to cancel his participation at the last notice), three of which were given by postdocs and five by PhD students. To be precise:

1. MAHMOOD ALAGHMANDAN (University of Waterloo; postdoc), *Weighted discrete hypergroups and their application to locally compact groups*;
2. MAHYA GHANDEHARI (University of Waterloo; postdoc), *On projections in the group algebra of unimodular groups*;
3. JOSEPH IVERSON (University of Oregon; PhD student), *Translation invariance over an abelian subgroup*;
4. SAFOURA JAFAR-ZADEH (University of Manitoba; PhD student), *Isometric isomorphisms on the annihilator of $C_0(G)$ in $LUC(G)^*$*;
5. MATTHEW MAZOWITA (University of Waterloo; postdoc), *The LUC-compactification and Beurling algebras*;
6. VARVARA SHEPELSKA (University of Manitoba; PhD student), *Weak amenability of weighted group algebras*;
7. NAZANIN TAHMASEBI (University of Alberta; PhD student), *Hypergroups and complementation problems*;
8. MATTHEW WIERSMA (University of Waterloo; PhD student), *L^p-Fourier and Fourier–Stieltjes algebras*.

Outlook for the Area.

As already stated before, eight of the 13 talks presented were delivered by PhD students and postdoctoral fellows. These talks were all of high quality, with respect to both the content and to the style of the delivery. This bodes well for the future of abstract harmonic analysis in Canada. One important fact should not be overlooked: of the 25 participants of the meetings, ten were female, and so were five of the 13 speakers. When it comes to the eight speakers at the postdoctoral or PhD student level, then four of them were female. We are therefore sure that our area will be thriving in the future.

Participans

Alaghmandan, Mahmood (The Fields Institute)
ALDabbas, Eman (University of Alberta)
Bandyopadhyay, Choiti (University of Alberta)
Elgun, Elcim (Lakehead University)
Forrest, Brian (University of Waterloo)
Ghandehari, Mahya (The Fields Institute)
Huang, Qianhong (University of Alberta)
Iverson, Joseph (University of Oregon)
Lau, Anthony To-Ming (University of Alberta)
Loliencar, Prachi (University of Alberta)
Mazowita, Matthew (The Fields Institute)
Neufang, Matthias (Carleton University)

Runde, Volker (University of Alberta)
Salame, Khadime (University of Alberta)
Schlitt, Kyle (University of Alberta)
Shepelska, Varvara (University of Manitoba)
Spronk, Nico (University of Waterloo)
Stokke, Ross (University of Winnipeg)
Tahmasebi, Nazanin (University of Alberta)
Tanko, Zsolt (University of Alberta)
Wang, Ya Shu (National Chung Hsing University)
Wiersma, Matthew (University of Waterloo)
Yasin, Omar (University of Alberta)
Zadeh, Safoura (University of Manitoba)
Zhang, Yong (University of Manitoba)

Chapter 43

Connecting Women in Mathematics Across Canada (14w2196)

October 3 - 5, 2014

Organizer(s): Galia Dafni (Concordia University), Sara Faridi (Dahousie University), Shannon Fitzpatrick (University of Prince Edward Island), Megumi Harada (McMaster University), Malabika Pramanik (University of British Columbia)

43.1 Goals

This is an exciting time for women and visible minorities in the basic sciences. More and more women from diverse backgrounds continue to beat formidable odds and come to the forefront of their professions with spectacular achievements. For the first time in its distinguished history, the Fields medal has been awarded to a woman, Professor Maryam Mirzakhani. The presidents at the helm of the International Mathematical Union (IMU) and the Canadian Mathematical Society (CMS) are two other highly acclaimed female mathematicians, respectively Professors Ingrid Daubechies and Lia Bronsard. For the last decade or so, considerable effort has been invested in researching and ensuring gender equity, and we are beginning to see the gratifying repercussions of this heightened awareness. At the same time, this increase in diversity has not yet resulted in a representation of women and minorities in graduate and postgraduate programs or as university faculty at the rate or proportion one might expect. We are still looking for ways to support this pipeline.

The aim of the 2-day BIRS workshop was to target top female junior mathematicians from across the country, who are close to obtaining a Ph.D. or have just graduated. This is a time when researchers are faced with the challenges of job search in an increasingly tough academic environment. For graduate students, this may involve landing a coveted postdoctoral position. Postdocs on the other hand would be looking for tenure-track and/or instructorship positions after their term. Different job searches come with varying, often non-explicit, criteria. Preparing oneself for a largely unknown hiring process can be stressful. This is especially true for women, who are often a small minority within their respective programs, and hence lack as extensive a support system as men. Also, women role models are much rarer, making it difficult for the junior women researchers to visualize themselves in senior academic roles.

43.2 Activities

The program made an effort to create a valuable experience for the participants within a limited timeframe. The highlights included:

- a collaborative and encouraging environment that facilitated interaction, as well as one-on-one mentorship,
- expert advice, general and personalized, related to research, teaching, giving talks and other facets of academic life,
- the presence of many role models.

We wanted the participating students to leave with the understanding that they are not alone (even though they may be among a mere handful of females in their respective programs), that women are being increasingly successful in challenging and rewarding careers and having a positive impact on their communities.

Given the limited amount of time we had, we broke the program into three parts. We made sure all junior participants were allowed time to present their work to the other attendees, as if they were giving a short job talk. We then had general discussion times built into the program as well as one on one meetings with assigned mentors so that the junior mathematicians could receive feedback on their presentations, as well as general career advice.

Finally, we had three (of the originally planned four) main invited lectures focusing on some major aspects of a mathematical career: Research, University Teaching, and Presenting Research in Conferences. These fantastic talks were interactive, and followed by passionate discussions.

We all came away from the meeting wishing it had been longer! This year we will apply for a 5-day workshop at BIRS which will allow us to cover much more ground.

Participants

Chow, Amenda (University of Waterloo)
DeDieu, Lauren (McMaster University)
Erey, Aysel (Dalhousie University)
Erey, Nursel (Dalhousie University)
Faridi, Sara (Dahousie University)
Fitzpatrick, Shannon (University of Prince Edward Island)
Huntemann, Svenja (Dalhousie University)
Hyndman, Jennifer (University of Northern British Columbia)
Junkins, Caroline (University of Western Ontario)
Karimianpour, Camelia (University of Ottawa)
Kasirzadeh, Atoosa (Ecole Polytechnique de Montreal)
Kuske, Rachel (University of British Columbia)
Matthews, Asia R (Queen's University)
Mynhardt, Kieka (University of Victoria)
Pramanik, Malabika (University of British Columbia, Vancouver)
Pusks, Anna (University of Alberta)
Tahmasebi, Nazanin (University of Alberta)
Teshima, Laura (University of Victoria)
Varughese, Marie Betsy (University of Alberta)
Wang, Shuxin (University of Alberta)
Wodlinger, Jane (University of Victoria)
Yang, Jihyeon Jessie (McMaster University)

Zadeh, Safoura (University of Manitoba)
Zhang, Jing (Concordia University)

Chapter 44

53rd Cascade Topology Seminar (14w2209)

November 7 - 9, 2014

Organizer(s): Kristine Bauer (University of Calgary)

44.1 Overview of the Field

Topology is a pervasive subject, with topological ideas arising in almost all branches of mathematics. As a discipline, topology is divided into several branches, including algebraic topology, geometric topology and differential topology. These branches can be very diffuse, with very little in common between different sub-disciplines, and indeed each branch can be very widely represented amongst many areas of specialization. The goal of the Cascade Topology Seminar is to establish some common ground between topologists in the Cascade region, including the Pacific Northwest United States and Western Canada.

At this particular meeting, there was a focus on algebraic topology. Within this subdiscipline, particular attention was given to the relationship between algebraic topology and K-theory and algebraic geometry, applied topology, and homotopy theory. K**-theory** is an invariant of categories with symmetric monoidal products, and it is in some sense a universal invariant because it is precisely the closest additive approximation of a symmetric monoidal category. K-theory has several incarnations: algebraic and topological K-theory may be the most frequently mentioned types, but K-theory can be widely applied. Indeed, many early applications of K-theory involved connections between topology and number theory, and in recent years more and diverse applications have been developed, especially to motivic cohomology and algebraic geometry. **Applied Topology** can refer to a number of emerging relations between topology and statistics and computer science. One of the most thriving areas of applied topology involves the relationship between topology and the study of data. Topology is the study of shape, and in particular topology is well-suited to study the shape of data. Algebraic invariants of topological spaces can be used to distinguish interesting features of data sets, and this has been a particularly fruitful method of data analysis because topology is well-suited to studying high-dimensional spaces, and algebraic tools are insensitive to small perturbations of data. **Homotopy Theory** is the study of topological spaces up to continuous deformations or homotopies. A central question in this field has been the discovery and computation of homotopy invariants which can determine whether two topological spaces are distinct or not.

44.2 Recent Developments and Open Problems

K-theory and algebraic geometry In the 1990's Voevodsky developed a program which brought together homotopy theory and algebraic geometry. In particular, this involved a program for doing homotopy theory for schemes, as well as developing motivic cohomology, an invariant for schemes. The latter brings algebraic K-theory into the picture, as motivic cohomology was used to prove Minor's conjecture relating the K-theory of a field to its étale cohomology. Voevodsky also proved the Bloch-Kato conjecture, which relates Milnor K-theory to Galois cohomology. Developing this program and related problems (such as computations) is a very active area of research involving many researchers examining different aspects of the program.

Applied Topology The chief tool of topological data analysis is persistent homology, which measures the topological features of simplicial complexes associated to a data set. These complexes vary over time from very course to very fine approximations of data, and persistent homology detects those features which are more important to the data because they persist throughout this process for long periods of time. Applications of persistent homology are emerging almost daily, as this tool is relatively new and ripe enough to be widely used. Medecine, astrophysics, computer science and engineering are a very few of the areas which have benefitted from topological data analysis. Theoretical developments in the field are often driven by applications which demand more features or precision, and extensions of persistent homology and metrics for the associated modules abound.

Homotopy Invariants An important, classical homotopy invariant of spaces is the Lusternik-Schnirelmann- (LS-) category. The LS-category of X is the smallest integer n such that there is an open covering of X by n open sets, each of which is contractible in X. When applied to a manifold, the LS-category gives a bound on the number of critical points of a smooth function on the manifold. In 1971, Ganea conjectured that $cat(X \times S^n) = cat(X) + 1$ for all $n > 0$. Although many cases of this conjectured were demonstrated, in 1998 Iwase provided the first counterexample to Ganea's conjecture. For which spaces Ganea's conjecture holds remains an open question in this area, and bounds on $cat(X)$ in terms of related invariants are still being discovered.

44.3 Presentation Highlights

K-theory and algebraic geometry Four of the six talks were concentrated roughly in this area, though quite disperses within the field, ranging from geometric, to computational, to foundational. **Thritang Tran** offered an explanation of the homological stability of symmetric complements. A sequence of spaces is homologically stable if, eventually, the homology groups $H_i(X_k)$ do not depend on k. In this case, Dr. Tran examined certain explicitly constructed subspaces of symmetric powers of a space M. Dr. Tran explained how this provides a proof of Conjecture F of [9], which in turn is related to motivic stability and the stability in the Grothendieck ring of varieties.

The Farrell-Jones conjecture is the statement that the K- and L-theory of the group ring $R[G]$ is determined by group homology and the K- or L-theory of the group rings $R[V]$, where V varies over the virtually cyclic subgroups of G. The conjecture has been verified for a number of kinds of groups, including [1] and [7]. **Henrik Ruping** gave an overview of the Farrell-Jones conjectures, recent progress and applications.

Rick Jardine gave an overview of two approaches to homotopy theory for presheaves [3]. On the one hand, pro objects of simplicial presheaves is a model for traditional étale homotopy theory. On the other hand, cocycles give an efficient description of the homotopy category of simplicial presheaves. Dr. Jardine gave an overview of both of these approaches, and then gave insight into work in progress relating these two approaches. This subject matter forms part of the foundation of motivic homotopy theory and topological modular forms in stable homotopy theory.

To an audience of homotopy theorists, a *motive* (in the sense of e.g. Voevodsky or Deligne) is something like the stable homotopy category for algebraic geometry. **Jack Morava** offered a philosophy for trying to consolodate the various kinds of motives into a single concept, and explained some of the barriers that have prevented this from happening in the past. In particular, he conjectured the existence of a category which would be the analogue of mixed Tate motives, but built from $K(S^0)$ rather than $K(\mathbb{Z})$, and provided justification for this conjecture. This is inspired by work of Blumberg, Gepner, and Tabuada, who construct categories of non-commutative motives using small stable ∞-categories.

Applied Topology Persistence modules, the time-graded homology modules associated to persistent homology, can be used to classify data. To do so, one needs to measure the distance between two persitence modules. One metric for doing so is the bottleneck metric. **Michael Lesnick** explained how the bottleneck metric can be generalized to incorporate multi-dimensional persistence (a generalization of persistence which measures data using multiple filtrations) by using interleavings. Published results appear in [5] and (now) [6].

Homotopy invariants Don Stanley presented recent progress on work on the LS-category of spaces which are products. It is well-known that $cat(X \times Y) \leq cat(X) + cat(Y)$. An open question is when equality is attained. Taking $Y = S^n$ relates this problem to Ganea's conjecture. Dr. Stanley gave a brief history of counterexamples to Ganea's conjecture and related constructions. In particular, he explained the relationship between counterexamples to Ganea's conjecture, and spaces with the property that $Qcat(X) < cat(X)$, where $Qcat$ is a kind of stablized version of the LS-category. He demonstrated how this leads to the smallest dimensional known counterexample to Ganea's conjecture [8], and Ordóñez and Stanley conjecture that this counterexamples is minimal.

44.4 Outcome of the Meeting

A theme of this meeting is that the majority of the talks included a broad overview of the particular topic or result to be covered. This is in keeping with the goal of the Cascade Topology Seminar, which hopes to build connections amongst the various kinds of topologists. In this meeting, not only were connections made accross the subfields of topology, but also across career stages. The meeting included two graduate students, four post doctoral fellows and eleven faculty members.

Participants

Bauer, Kristine (University of Calgary)
Bleiler, Steven (Portland State University)
Budney, Ryan (University of Victoria)
Cockett, Robin (University of Calgary)
Gerlings, Adam (University of Calgary)
Jardine, Rick (University of Western Ontario)
Kooistra, Remkes (The Kings University)
Koytcheff, Robin (Unviversity of Victoria)
Lesnick, Michael (University of Minnesota)
Luna Pattiarroy, German (University of Calgary)
Morava, Jack (Johns Hopkins University)
Peschke, George (University of Alberta)
Rolfsen, Dale (University of British Columbia)
Rueping, Henrik (University of British Columbia)
Stanley, Donald (University of Regina)
Tran, TriThang (University of Oregon)
Zvengrowski, Peter (University of Calgary)

Bibliography

[1] A. Bartelds, W. Lück, H. Reich and H. Rüping, K- and L-theory of group rings over $GL(n, \mathbb{Z})$, Publications mathematiques de l'IHES, **119**, 2013, 97-125.

[2] A. Blumberg, D. Gepner and G. Tabuada, A universal characterization of higher algebraic K-theory, Geom. Topol., **17**, no. 2, (2013), 733-838.

[3] J. F. Jardine, Cocycles and pro-objects, http://www-home.math.uwo.ca/ jardine/papers/lectures/Calgary.pdf, 2015.

[4] A. Kupers, J. Miller and T. Tran, Homological stability for symmetric complements, Trans. AMS, (2015), to appear.

[5] M. Lesnick, Multidimensional interleavings and applications to topological inference, Ph. D. thesis, Stanford University, 2012.

[6] M. Lesnick, The theory of the interleaving distance on multidimensional persistence modules, Foundations of Computational Mathematics, **15**, no. 3 (2015), 613–650.

[7] H. Rüping, The Farrell-Jones conjecture for S-arithmetic groups, J. Topology, (2013), to appear.

[8] D. Stanley and H. R. Ordóñez, A mimimum dimensional counterexample to Ganea's conjecture, Topology and its Applications, **157**, no. 14 (2010), 2304–2315.

[9] R. Vakil and M. Wood, Discriminants in the Grothendieck ring, Duke Math., **164** (6), (2012), 1139–1185.

Focused Research Group Reports

Chapter 45

Hyperplane Arrangements, Wonderful Compactifications, and Tropicalization (14frg193)

April 20 - 27, 2014

Organizer(s): Graham Denham, June Huh, and Alexander Suciu

One of the main goals for this meeting was to attack long-standing problems about the topology of hyperplane arrangements and their Milnor fibers using methods of toric and tropical geometry. We assembled some experts in tropical geometry and combinatorial algebraic geometry. We started with some interactive discussions about recent progress in the area, then moved on to some intensive group work which, we hope, began some new collaborations as well as furthering ones which were already in progress.

Highlights from the week included the following. Alex Fink outlined the techniques from his joint paper with David Speyer, which interprets the Tutte polynomial of a matroid in terms of a class in K-theory. June Huh explained in detail some ideas from his recently completed thesis involving intersection-theoretic matroid constructions. This included carefully elucidating the key part of the argument in his paper with Eric Katz, which seemed to show the way to strengthening the result. Katz proposed that these two projects could be understood within the same framework, giving a lead for further developments in the area.

Alex Suciu explained his recent work with with Stefan Papadima on the Milnor fibration of a hyperplane arrangement, and the group began a collective effort (as outlined in the proposal) to find a useful compactification of the Milnor fiber using ideas from toric geometry. As we expected, this turned out to be a relatively ambitious project. June Huh suggested using Mumford's notion of a semistable degeneration for this approach, and we attempted to do so explicitly with some small examples, restricting ourselves to a degeneration with toric varieties as fibers.

Michael Falk described work in progress with Eva Feichtner involving the study of resonance varieties for arrangements using tropicalization. The resonance varieties are also relevant to questions about the cohomology of the Milnor fiber, and so we explored as a group possible interplays between compactifications, tropicalization, and the Milnor fibration.

Spending a concentrated and highly intense week in a relatively small group allowed for in-depth and continuing conversations, in particular with new acquaintances. These opportunities (difficult to find at larger meetings) were enhanced by the diversity of backgrounds of the participants. There was general agreement that the focused research group created an effective and stimulating research atmosphere. The work initiated at BIRS is continuing now in several smaller research groups. The intense interactions within the research group gave rise to new projects, which should start bearing fruit in the not too distant future.

List of Participants

1. Graham Denham, University of Western Ontario, Canada.
2. Michael Falk, Northern Arizona University, USA.
3. Eva Maria Feichtner, University of Bremen, Germany.
4. Alex Fink, Queen Mary University, UK.
5. June Huh, University of Michigan, USA.
6. Eric Katz, University of Waterloo, Canada.
7. Hal Schenck, University of Illinois at Urbana-Champaign, USA.
8. Alexander Suciu, Northeastern University, USA.

Organizers

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Chapter 46

Borel complexity and classification of operator systems (14frg204)

August 10 - 17, 2014

Organizer(s): Martin Argerami (University of Regina), Samuel Coskey (Boise State University), Mehrdad Kalantar (Carleton University), Matthew Kennedy (Carleton University), Martino Lupini (York University), Marcin Sabok (McGill University)

The Focused Research Group meeting on "Borel complexity and classification of operator systems" constituted the first systematic attempt to study the complexity of the classification problem for operator systems. (An operator system is a unital, self-adjoint subspace of the space $B(H)$ of bounded linear operators on a Hilbert space.) We sought to find the complexity of the class of all separable operator systems, as well as identify subclasses of operator systems for which the classification problem is tractable.

It is well known that it is hopeless to attempt to obtain any satisfactory classification, in general, of either single operators or operator algebras on an infinite dimensional Hilbert space. Even for the special case of normal operators, which are completely described using the spectral theorem, it is known that no classification is possible with elementary invariants. Specifically, it is shown in [10] that the invariants arising from the spectral theorem are more complex than arbitrary countable structures. More generally, it has been shown that the classification problem for separable C*-algebras has maximal complexity among all the classification problems that admit the orbits of a Polish group action as a complete invariant.

Because of these results, and because even a finitely generated operator system can encode a significant amount of information about the C*-algebra it generates, it was thought that a satisfactory classification of operator systems would be similarly beyond reach. We confirmed this intuition in the case of separable operator systems, showing that the classification problem in this setting has the same complexity as the classification problem for C*-algebras. (The main result of [9] shows that operator systems are classifiable by the orbits of a Polish group action.)

On the other hand we have shown that the class of finitely generated operator systems does in fact admit a satisfactory classification. More precisely, the classification problem for finitely generated operator systems is smooth, which means that they can be explicitly classified using only using real numbers as invariants. (For example, in the particular case of the operator system generated by a unitary operator, a very concrete complete invariant is given by the spectrum of the operator, up to a rigid motion of the circle.) This result generalizes a result of Arveson, [2], who classified finitely represented operator systems.

The result that isomorphism of finitely generated operator systems is smooth is surprising, since no natural and concrete method is known to tell when two finitely generated operator systems are isomorphic. Instead the result is obtained as a consequence of a more general result that applies to any class of proper metric structures that can be axiomatized in the logic for metric structures. (See [3] for a comprehensive introduction.)

Hoping to obtain positive results beyond finitely generated operator systems, we considered the class of approximately finitely represented (AF) operator systems. This is the class of operator systems that can be obtained as a direct limit of operator systems acting on finite dimensional Hilbert spaces. A natural restriction to impose on such direct systems is that the connecting maps are reduced. This guarantees that the direct system is obtained from a corresponding direct system between the C*-envelopes of the building blocks, which allows us to apply the theory of direct limits of C*-algebras. In particular, the C*-envelope of the an AF operator system is an AF C*-algebra. It is natural to conjecture that AF operator systems can be characterized as the operator systems which have AF C*-envelopes. For these operator systems we considered an Arveson–Bratteli invariant that combines the Bratteli diagram of AF C*-algebras from [4] with the invariant for operator systems acting on a finite dimensional Hilbert space introduced by Arveson in [2]. We believe this should provide a complete invariant for the class of AF operator systems, which would generalize both the classification of AF C*-algebras due to Bratteli–Elliott [4, 8] and the classification of finitely represented operator systems due to Arveson [2]. From the perspective of classification, this would imply that these operator systems can be classified by using countable structures as invariants. This result is the best possible, since a result of Camerlo–Gao from [5] implies that the classification problem for AF C*-algebras has maximal complexity among all the classification problems that admit countable structures as complete invariants.

In the future we plan to study the complexity of the classification problem for nest algebras and CSL algebras (CSL stands for "commutative subspace lattice"). Nest algebras are operator algebras introduced by Ringrose as infinite-dimensional generalizations of the algebra of upper triangular matrices [15]. The CSL algebras, which were introduced by Arveson, form a much larger class of operator algebras where the methods of nest algebra theory can still be applied.

A successful classification of nest algebras was obtained by Davidson in [6], building on previous works of Andersen [1] and Larson [12]. However, a similar classification result for CSL algebras is generally believed to be impossible because the perturbation-theoretic arguments at the heart of Davidson's classification theorem do not work for general CSL algebras. We believe that complexity theory can be used to confirm that the classification of CSL algebras is truly harder than the classification of nest algebras.

Finally, a future goal for this collaboration is to obtain a satisfactory classification of "well-behaved" discrete quantum groups, which by duality theory is equivalent to classifying the dual class of compact quantum groups. Compact quantum groups were introduced by Woronowicz in [17, 18] to provide a mathematical foundation for the study of symmetries arising in quantum mechanics. The dual class of discrete quantum groups was subsequently studied in [7, 16]. The theory of discrete and compact quantum groups belong to the theory of locally compact quantum groups, first considered by Kustermans-Vaes [11].

This theory of quantum groups has attracted considerable attention in the recent years. Using a mixture of geometric, algebraic, and functional-analytic techniques, many results for locally compact groups have been generalized to the much broader class of locally compact quantum groups. It would therefore be of great interest to obtain a satisfactory classification for any of several key classes of quantum groups. For example, the full classification of orthogonal easy quantum groups was recently completed in [14], building on previous works of Banica, Bichon, Collins, Curran, Raum, Speicher, and Weber. We plan to consider the class of discrete quantum groups, especially those of Kac type, and show that they admit classification by countable structures. (This is optimal since countable groups already have maximal complexity for countable structures by a result of Mekler [13].) More generally our goal is to study the complexity of the classification problem for quantum groups from the point of view of invariant complexity theory. We believe this will shed new light on the general theory of quantum groups, suggesting which classes of quantum groups are amenable to a satisfactory theory of classification, and which complete invariants may be employed.

Participants

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Bibliography

[1] Niels Toft Andersen, Compact perturbations of reflexive algebras, Journal of Functional Analysis **38** (1980), no. 3, 366–400.

[2] William Arveson, The noncommutative choquet boundary III: operator systems in matrix algebras, Mathematica Scandinavica **106** (2010), no. 2, 196–210.

[3] Itaï Ben Yaacov, Alexander Berenstein, C. Ward Henson, and Alexander Usvyatsov, Model theory for metric structures, Model theory with applications to algebra and analysis. Vol. 2, London Mathematical Society Lecture Note Series, vol. 350, Cambridge University Press, 2008, p. 315–427.

[4] Ola Bratteli, Inductive limits of finite dimensional C*-algebras, Transactions of the American Mathematical Society **171** (1972), 195–234.

[5] Riccardo Camerlo and Su Gao, The completeness of the isomorphism relation for countable boolean algebras, Transactions of the American Mathematical Society **353** (2001), no. 2, 491–518.

[6] Kenneth R. Davidson, Similarity and compact perturbations of nest algebras., Journal für die reine und angewandte Mathematik **1984** (1984), no. 348, 72–87.

[7] Edward G. Effros and Zhong-Jin Ruan, Discrete quantum groups I: the Haar measure, International Journal of Mathematics **05** (1994), no. 05, 681–723 (en).

[8] George A Elliott, On the classification of inductive limits of sequences of semisimple finite-dimensional algebras, Journal of Algebra **38** (1976), no. 1, 29–44.

[9] George A. Elliott, Ilijas Farah, Vern Paulsen, Christian Rosendal, Andrew S. Toms, and Asger Törnquist, The isomorphism relation for separable C*-algebras, Mathematical Research Letters **20** (2013), no. 6, 1071–1080.

[10] Alexander S. Kechris and Nikolaos E. Sofronidis, A strong generic ergodicity property of unitary and self-adjoint operators, Ergodic Theory and Dynamical Systems **21** (2001), no. 5, 1459–1479.

[11] Johan Kustermans and Stefaan Vaes, Locally compact quantum groups, Annales Scientifiques de l'École Normale Supérieure **33** (2000), no. 6, 837–934.

[12] David R. Larson, Nest algebras and similarity transformations, Annals of Mathematics **121** (1985), no. 2, 409–427.

[13] Alan H. Mekler, Stability of nilpotent groups of class 2 and prime exponent, The Journal of Symbolic Logic **46** (1981), no. 4, 781–788.

[14] Sven Raum and Moritz Weber, The full classification of orthogonal easy quantum groups, arXiv:1312.3857 (2013).

[15] J. R. Ringrose, On some algebras of operators, Proceedings of the London Mathematical Society **s3-15** (1965), no. 1, 61–83.

[16] A. Van Daele, Discrete quantum groups, Journal of Algebra **180** (1996), no. 2, 431–444.

[17] S. L. Woronowicz, Compact matrix pseudogroups, Communications in Mathematical Physics **111** (1987), no. 4, 613–665 (EN).

[18] S. L. Woronowicz, Compact quantum groups. Symétries quantiques, (Les Houches, 1995), North-Holland, Amsterdam (1998), 845–884.

Chapter 47

Geometric aspects of p-adic automorphic forms (14frg207)

October 26 - November 2, 2014

Organizer(s): Ana Caraiani (Princeton University), Ellen Eischen (University of North Carolina at Chapel Hill), Elena Mantovan (California Institute of Technology)

47.1 Overview of the field

The Langlands program is a vast network of conjectures, meant to provide a bridge between seemingly different areas of mathematics, such as representation theory, harmonic analysis and number theory. At its heart lies the conjectural correspondence between Galois representations and automorphic forms. Over the past two decades, there has been a spectacular amount of progress in the Langlands program, leading to the resolution of major open questions such as Fermat's Last Theorem, the Sato-Tate conjecture and Serre's conjecture. In addition, there have been recent breakthroughs, such as the work of Harris-Lan-Taylor-Thorne and Scholze associating Galois representations to classes in the cohomology of locally symmetric spaces for GL_n [5, 7]. All of these developments have depended crucially on the p-adic interpolation of automorphic forms. Further studying p-adic and mod p automorphic forms is likely to lead to new advances in the field.

47.2 Recent developments and open problems

The Betti cohomology of locally symmetric spaces for GL_n with $\mathbb{Q}_p$ coefficients can be related to automorphic forms on GL_n, by work of Franke. Therefore, the mod p cohomology of the same locally symmetric spaces can naturally be thought of as a space of mod p automorphic forms. Recently, Scholze constructed Galois representations attached to these mod p classes [7]. These Galois representations are characterized by matching Frobenius eigenvalues and Satake parameters at unramified places. For applications, for example in order to prove new automorphy lifting theorems as Calegari and Geraghty propose [2], one often needs to know more subtle information about these Galois representations. One crucial missing piece of information would be that they satisfy local-global compatibility at places above p. When combined with the Calegari-Geraghty method, such a result could have striking consequences, such as modularity or even the Sato-Tate conjecture for elliptic curves over imaginary quadratic fields. (We remark that local-global compatibility at ramified places not dividing p is the subject of Varma's dissertation [8], and that she is currently working on the case $l = p$ in the context of [5].)

47.3 Scientific progress made

During this meeting, we focused on investigating a specific instance of local-global compatibility at places above p for torsion classes, namely the ordinary case. Our ultimate goal is to understand systems of Hecke eigenvalues occurring in the ordinary part of completed cohomology of locally symmetric spaces for GL_n (as defined below) and prove that their associated Galois representations are ordinary at p. For a precise statement, see, for example, Conjecture 6.27 of [6].

This question turns out to be closely related to a natural question about p-adic automorphic forms on unitary (or symplectic) Shimura varieties. For simplicity, say that we are considering a unitary Shimura variety S for the group $G := U(n,n)$ defined over $\mathbb{Q}$. This example is extremely relevant to us as the cohomology of locally symmetric spaces for GL_n over an imaginary quadratic field contributes to the boundary cohomology of a unitary Shimura variety of this type.

As starting point, we note that (regular algebraic) classical automorphic forms can be thought of either as sections of automorphic vector bundles over S or as systems of Hecke eigenvalues occurring in the Betti cohomology of S. The two notions can be compared in this generality via Faltings' BGG spectral sequence (for elliptic modular forms this is just the classical Eichler-Shimura theory).

In the coherent setting, Hida showes that p-adic automorphic forms can also be realized as certain global sections over the Igusa tower $\mathcal{T}$ (by construction $\mathcal{T}$ is the universal space trivializing automorphic vector bundles over an open dense set of S, namely the ordinary locus). On the other hand, when working with Betti or étale cohomology, there is a natural definition of p-adic automorphic forms as classes which occur in the completed cohomology of locally symmetric spaces:

$$\tilde{H}^*(\mathbb{Z}_p) := \varprojlim_n (\tilde{H}^*(\mathbb{Z}/p^n)), \text{ for } \tilde{H}^*(\mathbb{Z}/p^n) := \varinjlim_{K_p} H^*(\mathcal{S}_{K^pK_p}, \mathbb{Z}/p^n),$$

where the direct limit is over all open compact subgroups $K_p \subseteq G(\mathbb{Q}_p)$.

One of the key ingredients in Scholze's construction of Galois representation is a p-adic comparison (almost) isomorphism between étale and coherent cohomologies of perfectoid spaces. In our context, say for simplicity with mod p coefficients, it relates $\tilde{H}^*(\mathbb{F}_p)$, thought of as the mod p étale cohomology of the perfectoid Shimura variety $\mathcal{S}_{K^p}$, to the mod p coherent cohomology of $\mathcal{S}_{K^p}$. A natural question is whether the two notions of ordinary classes (on the étale and on the coherent side) can be matched under this comparison.

More precisely, we investigated the following question. Let $\mathcal{S}_{K^p,1}$ be the $\Gamma_1(p^\infty)$-tower of Shimura varieties, and $H^{i,\mathrm{ord}}(\mathcal{S}_{K^p,1}, \mathbb{F}_p)$ denote the part of its cohomology where the U_p operator acts invertibly (we refer to this space as the ordinary part of its cohomology). Also let $H^{0,\mathrm{ord}}(\mathcal{T}, \mathcal{O}_\mathcal{T})$ denote the part of the space of global sections over the Igusa tower $\mathcal{T}$ where the U_p operator acts invertibly.

Conjecture 47.3.1 *Every system of Hecke eigenvalues which occurs in the space $H^{i,\mathrm{ord}}(\mathcal{S}_{K^p,1}, \mathbb{F}_p)$ is the reduction modulo p of a system of Hecke eigenvalues occurring in $H^{0,\mathrm{ord}}(\mathcal{T}, \mathcal{O}_\mathcal{T})$.*

We note that Hida proves that the systems of Hecke eigenvalues which occur in $H^{0,\mathrm{ord}}(\mathcal{T}, \mathcal{O}_\mathcal{T})$ correspond to classical automorphic forms on $U(n,n)$ which are ordinary at p. Their associated Galois representations are known to satisfy local-global compatibility at $l = p$ by work of Caraiani [3]. Conjecture 47.3.1 is therefore closely related to our main goal. As further motivation, we also remark that Conjecture 47.3.1 could be a first step towards a general overconvergent Eichler-Shimura theory.

In the case of modular curves, related results have been proven by Cais [1] and Wake [9]. Both their works heavily rely on the study of the geometry of integral models. Since integral models are harder to work with in the higher-dimensional setting when there is bad reduction, we instead approached this question by reformulating it in terms of the perfectoid Shimura variety $\mathcal{S}_{K^p}$ and its associated Hodge-Tate period domain $\mathcal{F}\ell_G$. During our focused research group, we understood a number of ingredients which should play a key part in the proof of Conjecture 47.3.1.

47.3.1 The ordinary part of completed cohomology

In order to relate Hida's ordinary cohomology $H^{i,\mathrm{ord}}(\mathcal{S}_{K^p,1}, \mathbb{F}_p)$ to the mod p étale cohomology of the perfectoid Shimura variety $\mathcal{S}_{K^p}$ we used Emerton's theory of ordinary parts [4]. We checked that Emerton's ordinary parts functor, when applied to the completed cohomology $\tilde{H}^*(\mathbb{F}_p)$ recovers precisely the spaces $H^{*,\mathrm{ord}}(\mathcal{S}_{K^p,1}, \mathbb{F}_p)$. For a general Shimura variety, the relationship is via the Hochschild-Serre spectral sequence; this means we can reinterpret the spaces we are interested in as the equivariant cohomology of $\mathcal{S}_{K^p}$.

47.3.2 The geometry of the Hodge-Tate period domain

The Hodge cocharacter μ defining the Shimura variety S determines a parabolic subgroup $P_\mu \subseteq G$. The perfectoid Shimura variety $\mathcal{S}_{K^p}$ is equipped with a map of adic spaces

$$\pi_{HT} : \mathcal{S}_{K^p} \to \mathcal{F}\ell_G,$$

where $\mathcal{F}\ell_G$ is the adic space associated to the variety G/P_μ. (The fact that any Shimura variety of Hodge type admits such a period morphism is forthcoming joint work of Caraiani and Scholze.) The idea is that $\mathcal{S}_{K^pK_p}$ is a moduli space of abelian varieties equipped with extra structures; this map is induced by the Hodge-Tate filtration on the p-adic étale cohomology of the family of abelian varieties pulled back to $\mathcal{S}_{K^p}$. We call $\mathcal{F}\ell_G$ the Hodge-Tate period domain. A key property is that the map π_{HT} is equivariant for the natural action of $G(\mathbb{Q}_p)$ on both spaces.

To understand the ordinary part of completed cohomology, we studied an analogue of the U_p-operator acting on the equivariant cohomology of $\mathcal{F}\ell_G$. We showed that this operator contracts a large open subset of $\mathcal{F}\ell_G$ to the anticanonical locus - a subset of the ordinary locus which is particularly well-behaved. Moreover, certain preliminary computations lead us to expect that our U_p acts topologically nilpotently on the complement of this large open subset. These two observations together imply that ordinary systems of Hecke eigenvalues only contribute to the cohomology of the anticanonical locus.

47.3.3 The anticanonical tower and the Igusa tower

Both the anticanonical tower and the Igusa tower $\mathcal{T}$ live over the ordinary locus of the integral model of our Shimura variety S with hyperspecial level at p. Using the moduli-theoretic description of both spaces, we checked that the anticanonical tower can be identified with the perfection of the Igusa tower. This means that we can trace systems of Hecke eigenvalues which occur as global sections over the anticanonical tower to systems of Hecke eigenvalues corresponding to ordinary (classical) automorphic forms.

47.3.4 Logistics

In order to bring everyone up to speed with the various aspects of the questions described above, we scheduled a number of expository talks in the beginning of the meeting. The topics were Hida's theory of ordinary cohomology, Emerton's theory of ordinary parts, Scholze's theory of perfectoid spaces, his construction of the anticanonical tower over the ordinary locus of Siegel modular varieties, the Hodge-Tate period map and p-adic comparison theorems. In addition, as we made progress on various topics, we assembled a set of working notes, to which we all have access via an online repository and which we intend to refine in the coming months.

47.4 Outcome of the meeting

We are hopeful that the ideas outlined above should play a key part in the proof of Conjecture 47.3.1. We are writing a joint paper exploring this topic as well as the related question of local-global compatibility at $l = p$ for ordinary torsion classes.

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Bibliography

[1] B. Cais, The Geometry of Hida Families I: Lambda-adic de Rham cohomology, (2014), preprint arXiv:1407.5707.

[2] F. Calegari and D. Geraghty, Modularity Lifting Theorems beyond the Taylor-Wiles Method. II, (2012), preprint arXiv:1209.6293.

[3] A. Caraiani, Monodromy and local-global compatibility for $l = p$, Algebra Number Theory, **8** (2014), 1597–1646.

[4] M. Emerton, Ordinary parts of admissible representations of p-adic reductive groups I. Definition and first properties, Astérisque, **331** (2010), 355–402.

[5] M. Harris and K.-W. Lan and R. Taylor and J. A. Thorne, On the Rigid Cohomology of Certain Shimura Varieties, (2013), preprint.

[6] C. Khare and J. A. Thorne, Potential automorphy and the Leopoldt conjecture, (2014), preprint arXiv:1409.7007.

[7] P. Scholze, On torsion in the cohomology of locally symmetric varieties, (2013), preprint arXiv:1306.2070.

[8] I. Varma, Local-global compatibility for regualr algebraic cuspidal automorphic representations when $\ell \neq p$, (2014), preprint arXiv:1411.2520.

[9] P. Wake, The Lambda-adic Eichler-Shimura isomorphism and p-adic etale cohomology, (2013), preprint arXiv:1303.0406.

Research in Teams Reports

Chapter 48

Operator limits of random matrices (14rit187)

March 2 - 9, 2014

Organizer(s): Benedek Valkó, (University of Wisconsin – Madison), Bálint Virág (University of Toronto)

The main objective of the workshop was to complete a joint project of the two participants on operator limits of certain random matrices.

48.1 Background and Motivation

Wigner introduced the Gaussian ensembles in the 1950s to model large atomic nuclei, whose energy levels were eigenvalues of such a complex system that it may as well be taken to be random. They exhibited repulsion, unlike independent random points. Dyson found that their joint density is given by

$$\frac{1}{Z_{n,\beta}}\, e^{-\frac{\beta}{4}\sum_{k=1}^{n}\lambda_k^2} \prod_{1\le j<k\le n} |\lambda_j-\lambda_k|^\beta, \tag{48.1.1}$$

where $\beta = 1, 2, 4$ correspond to real symmetric and complex Hermitian, and self-dual quaternion Gaussian matrices. In order to distill an essential random eigenvalue process, one takes a limit as $n \to \infty$. For $\beta = 1, 2, 4$, the Gaudin-Mehta theorem (see e.g. [6]) shows that in the bulk there is a point process limit. While the finite n distribution dates back to 1962, the general beta point process limit was first shown in the participants' paper [11]; these are the Sine_β processes.

These point processes (especially in the $\beta = 2$ case) show up as limits in various places in mathematics. One of the most famous examples is the Montgomery-Dyson conjecture [7], which states that y-coordinates of the critical zeros of the Riemann ζ-function, i.e. the set $\mathcal{Z} = \{y : \zeta(1/2 + iy) = 0\}$, 'looks like' the Sine_2 process. To be more precise: if U is uniform on $[0, 1]$ then $(\mathcal{Z} - t \cdot U)\log t$ is supposed to converge in distribution to the point process Sine_2.

The Hilbert-Pólya conjecture is an approach to proving the Riemann hypothesis – the goal is to find a self-adjoint operator whose zero set is the same as that of $\mathcal{Z}$. The natural random matrix version of the question (attributed to Sarnak) is whether there is a natural random self-adjoint operator whose zero set is the Sine_2 process.

The study of the general Gaussian β-ensembles got a big boost from the work of Dumitriu and Edelman [1] who introduced a random tridiagonal matrix model with joint eigenvalue density given by (48.1.1). Their paper provided a tridiagonal representation for another related beta-ensemble, and similar representations appeared in [3] for beta generalizations of other classical random matrix ensembles. Edelman and Sutton [10], [2] conjectured that in the appropriate scaling limit these tridiagonal matrix models converge to certain random differential operators, and the point process limits of the beta ensembles are given by the spectra of these operators.

These predictions were confirmed rigorously for the so-called soft edge and hard edge limit scaling limits in [9] and [8] . In both cases one can show that the appropriate scaling limits of the tridiagonal random matrix models are given by certain second order differential operators with random potential and these operators have an a.s. discrete spectrum (which give the limiting point processes).

The starting point for our research project was to find a similar representation for the Sine_β processes (the bulk scaling limits), for the $\beta = 2$ case this would resolve the question posed by Sarnak.

48.2 Recent Developments and Open Problems

Recently we managed to find an random operator representation for the Sine_β process. The operator in question is a first order two-dimensional differential operator, it fits into the general framework of the classical Dirac operators. In order to define it, one first needs the hyperbolic Brownian motion $\mathcal{B}$ satisfying the SDE

$$d\mathcal{B} = (1 - |\mathcal{B}|^2)dZ, \qquad \mathcal{B}_0 = 0,$$

where $Z = Z_1 + iZ_2$ with independent real standard Brownian motions Z_1, Z_2. Let

$$X_t = \frac{1}{\sqrt{1 - |\mathcal{B}_t|^2}} \begin{pmatrix} 1 & \mathcal{B}_t \\ \overline{\mathcal{B}_t} & 1 \end{pmatrix}, \qquad J = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}, \qquad \tau(t) = -\beta^{-1} \log(1 - t).$$

Then the differential operator

$$2JX^2_{\tau(t)}\, \partial_t,$$

acting on functions $[0, 1] \to \mathbb{C}^2$ with appropriate boundary and L_2 conditions has an a.s. discrete spectrum which is distributed as the Sine_β process. (Note that the β dependence only appears via the time change function τ.)

The goal of the workshop was to explore various other random matrix models to see whether similar Dirac operator representations appear in other places. We also wanted to study how the found random operator could be used to prove limit theorems for the finite beta ensembles. Finally, we hoped to unify the descriptions of the soft edge, hard edge and bulk limits of β-ensembles.

48.3 Scientific Progress Made

We found the workshop to be extremely fruitful, and we have made significant progress in our project. Here is a partial list of the results of the meeting.

- We understood the connection between the so-called carousel description of the Sine_β process given in [11] and the oscillation theory of Dirac operators. This also allowed us to give an alternative description of the hard edge limit operator given in [8] as a random Dirac operator, unifying the descriptions of the hard edge and bulk cases.

- We set up the framework for a robust method for proving operator level scaling limits for random tridiagonal and random CMV matrices. It relies on the observation that the inverse of Dirac operators are Hilbert-Schmidt integral operators, and for many of the finite models one can recover a discrete approximation of the limiting integral operator in the finite systems. We apply the method to study the operator level convergence for the

Gaussian β-ensemble given in (48.1.1), the circular β-ensemble (for which the point process limit was proved in [4]) and for a family of random discrete Schrödinger operators studied in [5]. As a consequence we gave a proof for the fact that the limit of the circular β-ensembles and the bulk limit of the Gaussian β-ensembles are the same.

- We described how the soft edge limiting operator appears as a limit of the hard edge operators (this is the so-called hard-to-soft transition).

48.4 Outcome of the Meeting

We are currently in the process of writing up our results. One of the participants (Virág) is an invited speaker at the 2014 International Congress of Mathematics. Some of the results of the workshop will also appear in his contribution to the Proceedings of ICM [12].

Participants

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Bibliography

[1] I. Dumitriu and A. Edelman. Matrix models for beta ensembles. J. Math. Phys., 43(11): 5830–5847, 2002.

[2] A. Edelman and B. D. Sutton. From random matrices to stochastic operators. J. Stat. Phys., 127: 1121–1165, 2007.

[3] R. Killip and I. Nenciu CMV: the unitary analogue of Jacobi matrices Comm. Pure Appl. Math., 60(8): 1148–1188, 2007.

[4] R. Killip and M. Stoiciu. Eigenvalue statistics for CMV matrices: from Poisson to clock via random matrix ensembles. Duke Math. J., 146(3):361–399, 2009.

[5] E. Kritchevski, B. Valkó, and B. Virág. The scaling limit of the critical one-dimensional random Schrödinger operator. Comm. Math. Phys., 314(3):775–806, 2012.

[6] M. L. Mehta. Random matrices, volume 142 of Pure and Applied Mathematics (Amsterdam). Elsevier/Academic Press, Amsterdam, third edition, 2004.

[7] H. L. Montgomery. Distribution of the zeros of the Riemann zeta function. In Proceedings of the International Congress of Mathematicians (Vancouver, B. C., 1974), Vol. 1, 379–381, 1975

[8] J. A. Ramírez and B. Rider. Diffusion at the random matrix hard edge. Communications in Mathematical Physics, 288(3):887–906, 2009.

[9] J. A. Ramírez, B. Rider, and B. Virág. Beta ensembles, stochastic Airy spectrum, and a diffusion. J. Amer. Math. Soc., 24(4):919–944, 2011.

[10] B. D. Sutton, The stochastic operator approach to random matrix theory, Thesis (Ph.D.)–Massachusetts Institute of Technology, 2005

[11] B. Valkó and B. Virág. Continuum limits of random matrices and the Brownian carousel. Inventiones Math., 177:463–508, 2009.

[12] B. Virág. Operator limits of random matrices. To appear in the Proceedings of ICM 2014, Seoul

Chapter 49

On a System of Hyperbolic Balance Laws Arising from Chemotaxis (14rit198)

March 30 - April 6, 2014

Organizer(s): Dong Li (University of British Columbia), Kun Zhao (Tulane University)

1. Background and Motivation.

In contrast to random diffusion without orientation, chemotaxis is the biased movement of cells/particles toward the region that contains higher concentration of beneficial or lower concentration of unfavorable chemicals. The former often refers to the attractive chemotaxis and latter to the repulsive chemotaxis. Well-known examples of biological species experiencing chemotaxis include the slime mold amoebae *Dictyostelium discoideum*, the flagellated bacteria *Escherichia coli* and *Salmonella typhimurium*, and the human endothelial cells (cf. [16]). Chemotaxis has been advocated as a leading mechanism to account for the morphogenesis and self-organization of a variety of biological coherent structures such as aggregates, fruiting bodies, clusters, spirals, spots, rings, labyrinthine patterns and stripes, which have been observed in experiments (cf. [4, 5, 7, 8, 16]). In the last 30-35 years, among several works investigating taxes, chemotaxis research shows a significantly high ratio (>95%). Between the year 1975 and 2006, more than 22,000 papers in the scientific and medical literature were devoted to this phenomenon (PubMed), with the frequency of publication continuing to increase, which points to the underlined importance of chemotaxis research both in biology and medicine.

In a 1966 article published in *Science* (cf. [1]), Adler reported an important experimental result regarding the traveling bands of motile *Escherichia coli*. In the experiment, bands of *Escherichia coli* were observed to travel at constant speed when the bacteria were placed in one end of a capillary tube containing oxygen and an energy source. Four years later, in a series of seminal works (cf. [11, 12, 13]), Keller and Segel developed an effective mathematical model which nowadays is known as the Keller-Segel Chemotaxis Model (KSCM), and successfully reproduced the experimental result of Adler from a rigorous mathematical aspect. In its general form, the KSCM reads

$$\begin{cases} \partial_t u = D\Delta u - \nabla \cdot (\chi u \nabla \phi(v)), \\ \partial_t v = \varepsilon \Delta v + g(u, v), \end{cases} \tag{0.1}$$

where u and v denote the cell density and chemical concentration, respectively; $D > 0$ and $\varepsilon \geq 0$ are cell and chemical diffusion coefficients, respectively; and χ is the chemotactic sensitivity coefficient. The chemotaxis is called to be attractive if $\chi > 0$ and repulsive if $\chi < 0$, where $|\chi|$ measures the strength of the chemical signal. Here $\phi(v)$ is referred to as the chemotactic sensitivity (CS) function describing the signal detection mechanism and $g(u, v)$ is a function characterizing the chemical growth and degradation. In [11, 12, 13], based on a phenomenological observation, the authors chose the CS function to be the *logarithmic* function: $\phi(v) = \log(v)$, which reflects the fact that bacteria are sensitive to very small change in oxygen if the concentration of oxygen is also very small. The logarithmic sensitivity also indicates that cell chemotactic response to the chemical signal follows the

Weber-Fechner law which has prominent applications in biological modelings (cf. [2, 3, 6, 13]). Also in [11, 12, 13], the chemical production function was chosen as $g(u, v) = uv^m (0 \le m < 1)$ to entail that the chemical signal grows algebraically. By using these functions, the authors provided sufficient conditions under which traveling wave solutions to the KSCM exist and are stable. The results were consistent with the experimental observations reported in [1]. Since then, the KSCM has provided a cornerstone for many of works in chemotaxis research, its success being a consequence of its intuitive simplicity, analytical tractability and capability to model the basic dynamics of chemotactic populations. An extensive body of literature is devoted to the mathematical analysis of such model, see e.g. the survey papers [9, 10] and the references therein.

Since the initiation of the KSCM, researchers gradually recognized that many biological systems can be more accurately modeled by random walkers that deposit non-diffusible chemical signals that modify the local environment for succeeding passages. This phenomenon corresponds to one of the limiting cases of the KSCM, that is, when the diffusion of chemical substance is so small that it is negligible, i.e., $\varepsilon \to 0$. The resulting system of equations is of *hybrid* (PDE-ODE) type:

$$\begin{cases} \partial_t u = D\Delta u - \nabla \cdot (\chi u \nabla \phi(v)), \\ \partial_t v = g(u, v). \end{cases} \tag{0.2}$$

Twenty-seven years later since the pioneering work of Keller and Segel, Othmer and Stevens [17] proposed a version of (0.2) by taking $\phi(v) = \log(v)$, $g(u, v) = uv - \mu v$. The resulting equations then take the form:

$$\begin{cases} \partial_t u = D\Delta u - \nabla \cdot (\chi u \nabla \log(v)), \\ \partial_t v = uv - \mu v, \end{cases} \tag{0.3}$$

where $\mu \ge 0$ is a constant describing the natural degradation rate of the chemical signal. Direct applications of (0.3) include modeling of haptotaxis and initiation of angiogenesis.

Although the hybrid model looks similar to the KSCM, the two models differ significantly from each other. From the biological point of view, the chemical signal in the hybrid model is non-diffusive and grows exponentially instead of algebraically, which suggests that finite-time blowup may occur (cf. [17]). From the mathematical perspective, because the chemical diffusion coefficient of the hybrid model is zero and its chemical production function corresponds to a limiting case of the KSCM ($g(u, v) = uv^m$, $0 \le m < 1$ for KSCM, $m = 1$ for hybrid model), many existing methods for handling the KSCM do not work for the hybrid model. In spite of the widely appreciated magnitude of research conducted on the classic KSCM, there has been little work in the literature investigating the analytical and biological aspects of the hybrid model. A comprehensive analysis of such a nonlinear/degenerate system under general conditions is important for understanding fundamental phenomena in chemotaxis. Immediately after the hybrid model was developed, Levine and Sleeman [14] provided a comprehensive qualitative and numerical analysis for the model. In particular, explicit solutions describing aggregation and blow up of attractive chemotaxis and collapse of repulsive chemotaxis were constructed in one-dimensional space by choosing special initial data. The result was subsequently generalized in [18, 19]. Such evidence has led researchers in the field to appreciate that the hybrid model is capable of describing fundamental phenomena in chemotaxis.

However, the aforementioned research ceased when facing the challenge of validating the results obtained in [14] under *general conditions* on initial data, due to the lack of effective technical devices for handling the degeneracy of the system. This leaves the questions of global existence, finite-time blowup and long-time behavior of smooth solutions of the hybrid model widely open.

2. Recent Development and Open Problems.

From the biological point of view, when the spatial domain is large or the size of objectives considered (like bacteria) is small, the Cauchy problem of (0.3) becomes particularly relevant. Recently in [15], by developing a novel technique, we obtained the following results for the Cauchy problem of (0.3) in multi-dimensional spaces:

- local well-posedness and a blowup criteria of large smooth solutions in $\mathbb{R}^n, \ \forall\, n \in \mathbb{N}$,
- global well-posedness of small smooth solutions in $\mathbb{R}^n, \ n = 1, 2, 3$,
- a novel explicit (*frequency-by-frequency stretched-exponential*) decay rate of small smooth solutions in $\mathbb{R}^n, \ n \geq 4$.

The results have been widely appreciated by researchers and inspired many related work in the field. However, none of those results gives a definite answer to the question of *global well-posedness and long-time behavior of large smooth solutions* of (0.3), even in $\mathbb{R}^1$. The question is directly related to validating the results obtained in [14] under general conditions on initial data. Furthermore, the frequency-by-frequency time decay rate of small smooth solutions is restricted to the case in which the spatial dimension is greater than three which is unrealistic from the biological point of view.

3. Scientific Progress Made.

We have made significant progress during the one-week workshop at BIRS. Here is a list of results obtained during the meeting.

- We developed a novel energy method and proved the global well-posedness and long-time behavior of *large* smooth solutions of the Cauchy problem of (0.3) in $\mathbb{R}^1$. The results showed that constant ground states of the Cauchy problem is *globally stable*. It thus rigorously demonstrated the phenomenon of collapse in chemotactic repulsive problems with non-diffusible signal and logarithmic sensitivity under general conditions. The result is consistent with the explicit and numerical solutions constructed in [14].

- We identified the algebraic time decay rate of of one-dimensional smooth solutions towards constant ground states under very mild conditions on initial data, based on the global well-posedness result and by using weighted energy method.
- We re-developed our Fourier method (cf. [15]) and established a frequency-by-frequency stretched-exponential decay rate of small smooth solutions in $\mathbb{R}^1$ which makes the result biologically meaningful.
- We proved the global well-posedness of *almost large* smooth solutions in $\mathbb{R}^n$, $n = 2, 3$ under very mild conditions on initial data, which improved our previous result obtained in [15].
- The analytic techniques we developed during the workshop are of independent interest and can be applied to a family of chemotaxis models and models in other scientific research areas. Furthermore, they are expected to generate positive outcome in the investigation of the global stability of one-dimensional traveling wave solutions of (0.3) which is an important biological problem and a significant mathematical challenge.

4. Outcome of the Meeting.

Our results obtained for the one-dimensional Cauchy problem have been submitted to a peer-reviewed journal for publication. We are currently in the process of writing up the multi-dimensional results. One of the participants (K. Zhao) presented the one-dimensional results at the SIAM Conference on the Life Sciences which was held in Charlotte, North Carolina, USA, on August 4 - 7, 2014. K. Zhao is also an invited speaker at the 2015 International Congress on Industrial and Applied Mathematics which will be held in Beijing, China. The results obtained during the workshop will be reported at the conference.

Participants

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References

[1] J. Adler. Chemotaxis in Bacteria. *Science* **153** (1966): 708–716.

[2] W. Alt and D. Lauffenburger. Transient behavior of a chemotaxis system modeling certain types of tissue inflammation. *J. Math. Biol.* **24** (1987): 691–722.

[3] D. Balding and D.L. McElwain. A mathematical model of tumour-induced capillary growth. *J. Theor. Biol.* **114** (1985): 53–73.

[4] E. Budrene and H. Berg. Complex patterns formed by motile cells of Escherichia coli. *Nature* **349** (1991): 630–633.

[5] E. Budrene and H. Berg. Dynamics of formation of symmetrical patterns by chemotactic bacteria. *Nature* **376** (1995): 49–53.

[6] F. W. Dahlquist, P. Lovely, and D. E. Jr Koshland. Qualitative analysis of bacterial migration in chemotaxis. *Nature, New Biol.* **236** (1972): 120–123.

[7] R.M. Ford and D.A. Lauffenburger. Measurement of bacterial random motility and chemotaxis coefficients: II. application of single cell based mathematical model. *Biotechnol. Bioeng.* **37** (1991): 661–672.

[8] R.M. Ford, B.R. Phillips, J.A. Quinn and D.A. Lauffenburger. Measurement of bacterial random motility and chemotaxis coefficients: I. stopped-flow diffusion chamber assay. *Biotechnol. Bioeng.* **37** (1991): 647–660.

[9] T. Hillen and K. Painter. A user's guide to PDE models for chemotaxis. *J. Math. Biol.* **58** (2009): 183–217.

[10] D. Horstmann. From 1970 until present: the Keller-Segel model in chemotaxis and its consequences: I. *Jahresber. Deutsch. Math.-Verein* **105** (2003): 103–165.

[11] E.F. Keller and L.A. Segel. Initiation of slime mold aggregation viewed as an instability. *J. Theor. Biol.* **26** (1970): 399–415.

[12] E.F. Keller and L.A. Segel. Model for chemotaxis. *J. Theor. Biol.* **30** (1971): 225–234.

[13] E.F. Keller and L.A. Segel. Traveling bands of chemotactic bacteria: a theoretical analysis. *J. Theor. Biol.* **26** (1971): 235–248.

[14] H. Levine and B. Sleeman. A system of reaction diffusion equations arising in the theory of reinforced random walks. *SIAM J. Appl. Math.* **57** (1997): 683–730.

[15] D. Li, T. Li and K. Zhao. On a hyperbolic-parabolic system modeling repulsive chemotaxis. *Math. Models Methods Appl. Sci.* **21** (2011): 1631–1650.

[16] J.D. Murray. *Mathematical Biology I: An Introduction.* Springer, Berlin, 3rd edition, 2002.

[17] H. Othmer and A. Stevens. Aggregation, blowup and collapse: The ABC's of taxis in reinforced random walks. *SIAM J. Appl. Math.* **57** (1997): 1044–1081.

[18] Y. Yang, H. Chen, and W. Liu. On existence of global solutions and blow-up to a system of the reaction-diffusion equations modeling chemotaxis. *SIAM J. Math. Anal.* **33** (2001): 763–785.

[19] Y. Yang, H. Chen, W. Liu and B. Sleeman. The solvability of some chemotaxis systems. *J. Differential Equations* **212** (2005): 432–451.

Chapter 50

Effective Field Theory Outside the Horizon (14rit184)

April 27 - May 4, 2014

Organizer(s): C.P. Burgess (McMaster University, Perimeter Institute and CERN), R. Holman (Carnegie-Mellon University), G. Tasinato (Portsmouth University), M. Williams (McMaster University)

Our goal in getting together at BIRS was to complete our research program to identify the Effective Field Theory that describes the physics outside the Hubble horizon during inflation. Although we did not complete all of the work in the one week, we did clear up the majority of conceptual issues and cleared the way for completing a paper on the topic during the summer. It was posted to the ArXiV in late august (see http://arxiv.org/abs/1408.5002) [1].

50.1 Overview of the Field and Open Problems

It has long been known that Nature comes to us with an enormous variety of scales, and each can be understood largely on its own terms without needing to understand them all at once. One of the triumphs of 20th Century physics was the discovery that the mathematics with which we describe Nature — quantum field theory — shares this property. That is, in quantum field theory the details of short-distance physics tend to be largely irrelevant for the understanding of long-distance physics (a property called 'decoupling').

For example, not much need be known about the details of nuclei in order to understand the vast majority of the properties of atoms, and indeed this property was important for being able to unravel how atoms work. Ultimately this decoupling property — that states that each layer of structure can be understood on its own — is what allows progress in science.

Skillfully exploiting the decoupling property forces one to display the relevant scales in a problem and using the decoupling of one scale from another is often the difference between an untractable problem and a successful analysis. The tool for doing so is called an Effective Field Theory (EFT), which captures the long-distance dynamics together with the few ways it can depend on shorter-distance structure [2].

50.1.1 Implications for cosmology

This general observation has implications for cosmology which, as the science of the Universe as a whole, is the science of the longest scales of all. Cosmology is presently in a 'golden age' in which detailed measurements (such as of the Cosmic Microwave Background, or CMB) are for the first time allowing precision inferences about the overall contents and evolution of the Universe.

In particular, evidence has long been building that the Universe once passed through a very early epoch of accelerated Universal expansion, often called an inflationary phase [3]. Part of the evidence for this arises because correlations are observed in the sky (such as the temperature of the CMB as seen in different directions) that relate regions that have never been in causal contact (inasmuch as signals would have had to have traveled faster than light to do so) throughout the history of the universe (if this history is extrapolated to the past without an epoch of accelerated expansion).

The regions between which correlations are difficult to understand lie outside the Hubble scale of the spacetime describing the cosmology and what happens during inflation to make understanding easier is that the Universe expands faster than does the Hubble length. This allows physical correlations to be established at small scales where causal processes can act, and then to be stretch out to become 'outside the horizon' or longer than the Hubble scale.

Since scales outside the horizon are the longest ones about which we have direct evidence, a long-standing question asks what the EFT is for physics outside the horizon.

50.2 Scientific Progress Made

We believed we knew what this EFT would be and used the workshop to try to decide if we were right. It turns out that we were, and so we were able to use our time to identify its features and check that it reproduces things people know about the extra-Hubble regime in inflationary cosmology.

Our proposal was that the EFT for extra-Hubble physics should be of the same form as the EFT that describes particles moving through a medium, like light or electrons through water or neutrinos through the Sun. These theories are a bit different from ordinary EFTs inasmuch as they allow information exchange between the degrees of freedom being followed (eg the particles) and those of their environment that are not being measured in detail (eg the fluid). As a result the appropriate description of these systems is a Lindblad equation [4], describing the evolution of the quantum density matrix of the system being measured.

In the inflationary application the system being followed (the 'particles') consists of all field modes that have wavelengths larger than the Hubble length, and those not being followed (the 'fluid') are those field modes with wavelengths shorter than the Hubble scale. By applying the Lindblad equation to this system we were able to show that the leading description turns out to agree with Starobinsky's Stochastic Theory of Inflation [5], which essentially treats the evolution of extra-Hubble modes as a random walk. We could show that the Lindblad equation reduces for the diagonal elements of the density matrix to the Fokker-Planck equation governing the probabilities of Starobinsky's random walk.

But we also found additional information. In principle we should be able to compute the systematic corrections to Starobinsky's formulation, in a way that has not yet been possible to do. We also found that all of the off-diagonal elements of the density matrix rapidly go to zero (in a field basis) and this has the physical interpretation of describing the de-coherence of initially quantum fluctuations (that are believed to give rise to primordial fluctuations in inflation) into classical fluctuations (as assumed in analyzing the implications of primordial fluctuations for observations on the CMB). We think this fills in an important conceptual missing step in the standard description of primordial fluctuations.

Our results were posted in the ArXiV listing given above, and will be submitted for publication to a journal soon. Our ideas have (so far) been well received at talks given at various meetings in North America and Europe over the summer.

Participants

Burgess, Cliff (Perimeter Institute)
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Williams, Matthew (McMaster University)

Bibliography

[1] C.P. Burgess, R. Holman, G. Tasinato and M. Williams, EFT Beyond the Horizon: Stochastic Inflation and How Primordial Quantum Fluctuations Go Classical, arXiv:1408.5002.

[2] For some reviews aimed at gravity formulated as an EFT see:

C. P. Burgess, "Quantum gravity in everyday life: General relativity as an effective field theory," Living Rev. Rel. **7** (2004) 5 [gr-qc/0311082];

W. D. Goldberger, "Les Houches lectures on effective field theories and gravitational radiation," hep-ph/0701129;

J. F. Donoghue, "The effective field theory treatment of quantum gravity," AIP Conf. Proc. **1483** (2012) 73 [arXiv:1209.3511 [gr-qc]].

[3] A. D. Linde, "The Inflationary Universe," Rept. Prog. Phys. **47**, 925 (1984).

[4] C. Cohen-Tannoudji, J. Dupont-Roc and G. Grynberg, *Atom Photon Interactions*, Wiley, New York, 1992;

V.F. Sears, *Neutron Optics*, Oxford University Press, 1989;

H. Haken, The Semiclassical and Quantum Theory of the Laser, in *Quantum Optics: Proceedings of the Tenth Session of the Scottish Universities Summer School in Physics, 1969* ed. by S. M. Kay and A. Maitland, and references therein.

[5] A. A. Starobinsky, Stochastic de Sitter (inflationary) stage in the early universe, *In *De Vega, H.j. (Ed.), Sanchez, N. (Ed.): Field Theory, Quantum Gravity and Strings*, 107-126*

Chapter 51

Alexandrov Geometry (14rit188)

May 4 - 11, 2014

Organizer(s): S. Alexander (University of Illinois at Urbana-Champaign), V. Kapovitch (University of Toronto), A. Petrunin (Penn State University)

51.1 Overview of the Field

Alexandrov Geometry has been much developed in the last 20 years. Perelman's solution of the Poincaré conjecture has drawn wide attention to the theory of spaces with lower curvature bounds. Spaces with upper curvature bounds have turned out to interact extensively with other branches of mathematics such as geometric analysis and geometric group theory, as well as having applications to such varied fields as dynamical systems in mechanics, and robotics.

51.2 Overview of the Project

The purpose of our research stay was to work on our book "Alexandrov Geometry". Our book is a comprehensive text and reference work on the fields of curvature bounded below and curvature bounded above. Although these two fields developed quite independently, they have many similar guiding intuitions and technical tools. Our approach is novel in its attention to the interrelatedness of the two fields, and its emphasis on the way each illuminates the other.

We should emphasize that this is truly a research project. The book will contain a lot of new material. In addition, almost every theorem will appear in an improved form and in the correct generality.

In addition to all the basic material in both fields, the book includes all the important advanced material on spaces of curvature bounded below. This material is unavailable in any book, and not all of it is in the literature. For spaces of curvature bounded above, we are emphasizing topics and proofs inspired by considering the two contexts simultaneously, and again include material not in the literature.

51.3 Progress Made

At present, our draft is about 368 pages; more than half available online. The final version should be about 500 pages. As a result of our workshop, three new chapters now available online there were also number of improvements in all the parts of the book.

We were working on the book for more than half a year without face-to-face contact. During this time, a number of issues accumulated. We were able to get through the complete list of them and make very substantial progress in just one week at Banff.

Since the last meeting we were mostly working on the chapter on volume (currently chapter 30). This was one of the hardest chapters to write. It is used a lot everywhere in the book and it took us quite some time to make a comprehensive presentation sutable for all chapters in the book. The main part of the chapter is written and checked carefully by all of us.

An outline and timetable were drawn up for remaining topics in curvature bounded above.

There were countless corrections and improvements made, even in chapters written a while ago. A number of proofs became more transparent. These findings improve the book's coherence and elegance.

Participants

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Chapter 52

Dirichlet spaces and de Branges–Rovnyak spaces (14rit183)

June 15 - 22, 2014

Organizer(s): Omar El-Fallah (Université Mohammed V, Rabat), Karim Kellay (Université Bordeaux 1), Javad Mashreghi (Université Laval), Thomas Ransford (Université Laval)

52.1 Overview of the Field

The spaces mentioned in the title are two interesting families of Hilbert spaces of holomorphic functions, both contained inside H^2, the classical Hardy space on the unit disk $\mathbb{D}$.

52.1.1 Weighted Dirichlet spaces

Given a non-negative function $\omega \in L^1(\mathbb{D}, dA)$ and $f \in H^2$, we define the weighted Dirichlet integral

$$\mathcal{D}_\omega(f) := \frac{1}{\pi}\int_{\mathbb{D}} |f'(z)|^2\,\omega(z)\,dA(z).$$

The weighted Dirichlet space $\mathcal{D}_\omega$ is the set of $f \in H^2$ such that $\mathcal{D}_\omega(f) < \infty$. It is a Hilbert space with respect to the norm $\|\cdot\|_{\mathcal{D}_\omega}$ defined by $\|f\|^2_{\mathcal{D}_\omega} := \|f\|^2_{H^2} + \mathcal{D}_\omega(f)$.

The case of primary interest is where ω is a positive superharmonic function on $\mathbb{D}$. In this case, there is a unique positive finite measure μ on $\overline{\mathbb{D}}$ such that

$$\omega(z) = \int_{\mathbb{D}} \log\Big|\frac{1-\overline{\zeta}z}{\zeta - z}\Big|\frac{1}{1-|\zeta|^2}\,d\mu(\zeta) + \int_{\mathbb{T}} \frac{1-|z|^2}{|\zeta - z|^2}\,d\mu(\zeta) \qquad (z \in \mathbb{D}).$$

We then write $\mathcal{D}_\mu$ for $\mathcal{D}_\omega$. It can be shown that, if $f \in \mathcal{D}_\mu$, then f has radial limits μ-a.e. on $\mathbb{T}$, and

$$\mathcal{D}_\mu(f) = \int_{\overline{\mathbb{D}}}\int_{\mathbb{T}} \Big|\frac{f(\lambda) - f(\zeta)}{\lambda - \zeta}\Big|^2\,\frac{|d\lambda|}{2\pi}\,d\mu(\zeta). \qquad (52.1.1)$$

The classical Dirichlet space is obtained by taking μ to be normalized Lebesgue measure on $\mathbb{T}$. When μ is a general measure on $\mathbb{T}$, we obtain the harmonically weighted Dirichlet spaces, first introduced by Richter [9] as part of his analysis of closed shift-invariant subspaces of the classical Dirichlet space, and subsequently studied by Richter and Sundberg in [10] (see also [6, Chapter 7]). The study of general superharmonic weights was initiated by Aleman [1]. They have the advantage of including both the harmonic weights and the important family of radial weights $\omega(z) = (1-|z|^2)^\alpha$ for $0<\alpha<1$.

52.1.2 De Branges–Rovnyak spaces

Let b be a holomorphic function on $\mathbb{D}$ such that $|b|\le 1$. The de Branges–Rovnyak space $\mathcal{H}_b$ is the Hilbert space of holomorphic functions on $\mathbb{D}$ with reproducing kernel $(1-\overline{b}(w)b(z))/(1-\overline{w}z)$.

If b is an inner function, then $\mathcal{H}_b = H^2 \ominus bH^2$, a closed subspace of H^2 often called a model subspace.

In this project, we are interested exclusively in the 'opposite' case, namely when $\log(1-|b|^2)\in L^1(\mathbb{T})$. This condition is equivalent to b being a non-extreme point of the unit ball of H^∞. It is also equivalent to $\mathcal{H}_b$ containing the polynomials. Henceforth, we always assume that b satisfies this condition.

Under this hypothesis on b, there is a unique outer function a such that $a(0)>0$ and $|a|^2+|b|^2=1$ a.e. on $\mathbb{T}$. It can be shown that $f\in\mathcal{H}_b$ iff $T_{\overline{b}}f\in T_{\overline{a}}(H^2)$, where $T_{\overline{a}}, T_{\overline{b}}$ denote the Toeplitz operators associated to $\overline{a},\overline{b}$ respectively. In this case there is a unique function $f^+\in H^2$ such that $T_{\overline{b}}f = T_{\overline{a}}(f^+)$, and

$$\|f\|^2_{\mathcal{H}_b} = \|f\|^2_{H^2} + \|f^+\|^2_{H^2}. \tag{52.1.2}$$

We write $\phi := b/a$. Note that $\phi\in\mathcal{N}^+$, the Smirnov class. Conversely, every $\phi\in\mathcal{N}^+$ is of the form $\phi=b/a$ for a unique pair (b,a) as above. Thus, specifying ϕ is equivalent to specifying b, and it is often more convenient to work in terms of ϕ.

The spaces $\mathcal{H}_b$ were introduced by de Branges and Rovnyak in the appendix of [4] and further studied in [5]. The initial motivation was to provide canonical model spaces for certain types of contractions on Hilbert spaces. Subsequently it was realized that these spaces have numerous connections with other topics in complex analysis and operator theory, in particular through Toeplitz operators. For further information on this topic, we refer to the books of de Branges and Rovnyak [5], Sarason [11], and the forthcoming monograph of Fricain and Mashreghi [7].

52.2 Recent Developments and Open Problems

Sarason [12] discovered a strong connection between certain Dirichlet spaces and de Branges–Rovnyak spaces. He showed that, if μ is the Dirac mass at a point $\zeta\in\mathbb{T}$, then the Dirichlet space $\mathcal{D}_\mu$ is isometrically equal to the de Branges–Rovnyak space $\mathcal{H}_b$, where b corresponds to the function $\phi(z):=z/(1-\overline{\zeta}z)$. For this choice of ϕ, it is quite easy to see that dilation is a contraction on $\mathcal{H}_b$, in other words $\|f_r\|_{\mathcal{H}_b}\le\|f\|_{\mathcal{H}_b}$, where $f_r(z):=f(rz)$. Sarason used this to deduce that dilation is also a contraction on $\mathcal{D}_\mu$.

The authors of [2] obtained a converse to Sarason's result: the only measures μ on $\mathbb{T}$ for which $\mathcal{D}_\mu$ is isometrically equal to some $\mathcal{H}_b$ are point masses. The proof made use of a formula expressing the norm of certain functions in $\mathcal{H}_b$ in terms of their Taylor coefficients and those of ϕ: if f is holomorphic in a neighbourhood of $\overline{\mathbb{D}}$, then $\sum_{j\ge0}\widehat{f}(j+k)\overline{\widehat{\phi}(j)}$ converges absolutely for each k, and

$$\|f\|^2_{\mathcal{H}_b} = \sum_{k\ge0}|\widehat{f}(k)|^2 + \sum_{k\ge0}\Big|\sum_{j\ge0}\widehat{f}(j+k)\overline{\widehat{\phi}(j)}\Big|^2. \tag{52.2.1}$$

It was left open whether this same formula is valid for all $f\in\mathcal{H}_b$.

It was also shown in [2] that, for certain b, dilation is no longer a contraction on $\mathcal{H}_b$, and even that $\limsup_{r\to1}\|f_r\|_{\mathcal{H}_b}=\infty$ for some $f\in\mathcal{H}_b$. It was left open whether $\limsup$ can be replaced by $\liminf$. This was of interest because the only proofs that polynomials are dense in $\mathcal{H}_b$ were non-constructive, and knowing that we always have $\liminf_{r\to1}\|f_r\|_{\mathcal{H}_b}<\infty$ would open the door to the construction of polynomial approximants to f.

The question of when $\mathcal{D}_\mu$ is isomorphically equal to $\mathcal{H}_b$ (as opposed to isometrically equal) was raised in [2] and studied in [3] for the case of measures μ on $\mathbb{T}$. It was shown that, in order for $\mathcal{D}_\mu$ to be isomorphically equal to some $\mathcal{H}_b$, it is necessary that μ be singular with respect to Lebesgue measure on $\mathbb{T}$, and sufficient that μ have finite support. It was left open whether there are any examples of μ with infinite support.

In the classical Dirichlet space, it is known that every function has tangential limits at almost every point of the unit circle, where the tangential approach region at ζ is of the form $|z-\zeta| = O(|\log(1-|z|)|)$ (see [8]). It is still an open problem to determine the optimal approach region for $\mathcal{D}_\mu$ for general μ.

52.3 Scientific Progress Made

52.3.1 Dilation in $\mathcal{H}_b$

We solved affirmatively the problem of whether $\limsup$ can be replaced by $\liminf$.

Theorem 52.3.1 *There exist b and $f \in \mathcal{H}_b$ such that $\|f_r\|_{\mathcal{H}_b} \to \infty$ as $r \to 1$.*

The proof actually gives a little more, namely an example such that $|(f_r)^+(0)| \to \infty$ as $r \to 1$. From this, it is a simple matter to deduce that formula (52.2.1) does **not** hold for general $f \in \mathcal{H}_b$. Indeed:

Corollary 52.3.2 *There exist b and $f \in \mathcal{H}_b$ such that $\sum_{j\geq 0} \widehat{f}(j)\overline{\widehat{\phi}(j)}$ diverges.*

52.3.2 Polynomial approximation in $\mathcal{H}_b$

Though the preceding theorem kills off the possibility of obtaining polynomial approximants in $\mathcal{H}_b$ via dilations, we did find another method for constructing such approximants, based on the following result.

Theorem 52.3.3 *Let (ψ_n) be a sequence in H^∞ such that $\|\psi_n\|_{H^\infty} \to 1$ and $\psi_n(0) \to 1$. Then, for all $f \in \mathcal{H}_b$, we have $\|T_{\overline{\psi}_n} f - f\|_{\mathcal{H}_b} \to 0$.*

If p is a polynomial, then so is $T_{\overline{\psi}_n} p$. If, in addition, $\psi_n \in aH^\infty$, then $T_{\overline{\psi}_n}$ is a bounded operator from H^2 into $\mathcal{H}_b$ with norm at most $\|\psi_n/a\|_{H^\infty}$. Combined with the theorem, this leads to a constructive proof of

Corollary 52.3.4 *Polynomials are dense in $\mathcal{H}_b$.*

52.3.3 Isometric equality between $\mathcal{D}_\mu$ and $\mathcal{H}_b$

We extended the results of [12] and [2] from harmonic weights to superharmonic weights.

Theorem 52.3.5 *Let μ be a finite positive measure on $\overline{\mathbb{D}}$ and let $\phi \in \mathcal{N}^+$ (with corresponding b). Then $\mathcal{D}_\mu = \mathcal{H}_b$ with equality of norms if and only if there exist $\zeta \in \overline{\mathbb{D}}$ and $\alpha \in \mathbb{C}$ such that*

$$\mu = |\alpha|^2\delta_\zeta \qquad \textit{and} \qquad \phi(z) = \alpha z/(1-\overline{\zeta}z).$$

The 'if' part of the theorem leads quickly to the following corollary.

Corollary 52.3.6 *If μ is a finite positive measure on $\overline{\mathbb{D}}$, then*

$$\mathcal{D}_\mu(f_r) \leq \frac{2r}{1+r}\mathcal{D}_\mu(f) \qquad (0 < r < 1).$$

52.3.4 Isomorphic equality between $\mathcal{D}_\mu$ and $\mathcal{H}_b$

With the ultimate aim of constructing new examples of pairs (μ, b) with $\mathcal{D}_\mu = \mathcal{H}_b$ isomorphically, we studied a family of examples of $\mathcal{H}_b$-spaces for which it is possible to compute the norm exactly.

Theorem 52.3.7 *Let ν be a complex measure on $\overline{\mathbb{D}}$, and let $\phi(z) := z \int (1 - \overline{\zeta} z)^{-1} \, d\nu(\zeta)$ $(z \in \mathbb{D})$. Then, for all f holomorphic in a neighborhood of $\overline{\mathbb{D}}$, we have*

$$\|f\|^2_{\mathcal{H}_b} = \|f\|^2_{H^2} + \int_{\mathbb{T}} \Big| \int_{\overline{\mathbb{D}}} \frac{f(\lambda) - f(\zeta)}{\lambda - \zeta} \, d\nu(\zeta) \Big|^2 \frac{|d\lambda|}{2\pi}.$$

If, in addition, $\nu \ll \mu$ and $d\nu/d\mu \in L^2(\mu)$, then $\mathcal{D}_\mu \subset \mathcal{H}_b$.

52.3.5 Tangential approach regions for $\mathcal{D}_\mu$

We had just enough time for a summary discussion of this problem. It seems likely that the optimal approach region should be expressed in terms of the reproducing kernel of $\mathcal{D}_\mu$. Although there is no explicit expression for this kernel, there are now precise estimates for its norm. We intend to return to this problem.

52.4 Outcome of the Meeting

The results obtained have now been written up as a detailed report with a view to eventual publication. It is a pleasure to thank BIRS for the opportunity to advance our work in such a pleasant setting. We also acknowledge with thanks financial support from the UMI-CRM.

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Bibliography

[1] A. Aleman, The multiplication operator on Hilbert spaces of analytic functions, Habilitationsschrift, Fern Universität, Hagen, 1993.

[2] N. Chevrot, D. Guillot and T. Ransford, De Branges–Rovnyak spaces and Dirichlet spaces, J. Funct. Anal. **259** (2010), 2366–2383.

[3] C. Costara and T. Ransford, Which de Branges–Rovnyak spaces are Dirichlet spaces (and vice versa)?, J. Funct. Anal. **265** (2013), 3204–3218.

[4] L. de Branges and J. Rovnyak, Canonical models in quantum scattering theory, in: Perturbation Theory and its Applications in Quantum Mechanics, Wiley, New York, 1966, 295–392.

[5] L. de Branges and J. Rovnyak, Square Summable Power Series, Holt, Rinehart and Winston, New York, 1966.

[6] O. El-Fallah, K. Kellay, J. Mashreghi, T. Ransford, A Primer on the Dirichlet Space, Cambridge University Press, Cambridge, 2014.

[7] E. Fricain, J. Mashreghi, Theory of $\mathcal{H}(b)$ Spaces, Vol. I, New Monographs in Mathematics 20, Cambridge University Press, Cambridge, 2014.

[8] A. Nagel, W. Rudin and J. Shapiro, Tangential boundary behavior of functions in Dirichlet-type spaces, Ann. of Math. (2) **116** (1982), 331–360.

[9] S. Richter, A representation theorem for cyclic analytic two-isometries, Trans. Amer. Math. Soc. 328 (1991), 325–349.

[10] S. Richter, C. Sundberg, A formula for the local Dirichlet integral, Michigan Math. J., 38 (1991), 355–379.

[11] D. Sarason, Sub-Hardy Hilbert Spaces in the Unit Disk, John Wiley & Sons Inc., New York, 1994.

[12] D. Sarason, Local Dirichlet spaces as de Branges-Rovnyak spaces, Proc. Amer. Math. Soc. **125** (1997), 2133–2139.

Chapter 53

Spectrum Asymptotics of Operator Pencils (14rit182)

July 20 - 27, 2014

Organizer(s): Birgit Jacob (University of Wuppertal), Kirsten Morris (University of Waterloo)

53.1 Motivation

Consider the system of equations on a Hilbert space $\mathcal{Z}$

$$\begin{aligned} \dot{x}(t) &= Ax(t) + Bu(t) \\ y(t) &= Cx(t). \end{aligned}$$

where A is a closed densely defined operator that generates a strongly continuous semigroup. Also, B and C are bounded operators and u, y are scalar-valued so for some b, $c \in \mathcal{Z}$, $Bu = bu$, $Cx = \langle c, x \rangle$. This is a general framework that includes systems modeled by partial differential or delay-differential equations. In the control system configuration, u is an external control variable and y is an observation. The simplest control law for a system is a constant gain,

$$u(t) = -ky(t) + v(t),$$

where $k > 0$ is real and $v(t)$ is an external signal.

Thus, the spectrum of $A - kBC$ as $k \to \infty$ is of interest in analyzing the dynamics of the controlled system. A plot of these eigenvalues as $k \to \infty$ is known as a root locus plot. More generally, the question of how the spectrum of an operator $A_k = A - kD$ for some fixed operators A, D varies with a parameter k can also be formulated in terms of a root locus. The behavior of the spectrum as $k \to \infty$ is particularly difficult to analyze. Since the behaviour of the root locus, particularly at infinity, can be quite different from that of finite-dimensional approximations, such as finite elements, there are practical applications to theoretical analysis.

53.2 Overview

Zeros have the same importance in control that eigenvalues do for dynamics.

Definition 53.2.1 *The invariant zeros of $\Sigma(A, B, C)$ are the set of all λ such that*

$$\begin{bmatrix} \lambda I - A & -B \\ C & 0 \end{bmatrix} \begin{bmatrix} x \\ u \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{53.2.1}$$

has a solution for some scalar u and non-zero $x \in D(A)$.

The invariant zeros are the solution to a generalized eigenvalue problem involving an operator pencil.

Extension of the nature of the zeros and of the root locus, well-known for finite-dimensional systems, to infinite-dimensions has been elusive. In [1] the root locus is considered for the case where A is self-adjoint with compact resolvent on a Hilbert space $\mathcal{Z}$, B is a linear bounded operator from $\mathbb{C}^p$ to $\mathcal{Z}$, and $C : D(C) \to \mathbb{C}^p$ where $D(A) \subset D(C)$ is A-bounded. A complete analysis of collocated boundary control of parabolic systems on an interval was provided in [2]. The analysis in that paper uses results from differential equations theory and is difficult to extend to more general classes. In [4] high-gain output feedback of infinite-dimensional systems in the case where A generates an analytic semigroup and $B = C^*$ was studied. The zeros of the system are given as the eigenvalues of an operator and a nonlinear stabilizing feedback law is constructed. Zeros of systems where A is self-adjoint and $B = C^*$ are shown to be real and be bounded by α if $A + A^* \leq 2\alpha I$ on $D(A)$ in [9]. If moreover, the system transfer function can be written in spectral form, and additional technical conditions are satisfied, the poles and the zeros interlace on the real axis.

The problem of defining and analyzing the root locus of infinite-dimensional systems can be formulated as determining the asymptotic spectrum of a class of operator pencils. Unfortunately, these theoretical problems have not been well-studied. We have been working on this problem for a few years and have made some significant progress. We have shown that the root locus for infinite-dimensional systems is well-defined. If no invariant zeros are in the spectrum of A each eigenvalue of A defines a branch of the root locus and these curves are smooth and non-intersecting. Moreover, if any branch converges to a point, that point is a zero of the system. Conversely, each zero is the terminus of a branch of the root locus. If A is self-adjoint and the system is collocated ($b = c$) then the zero interlace with the eigenvalues on the real axis. On an infinite-dimensional space, there are no asymptotes: every branch converges to a zero. (On a finite-dimensional space there is a single asymptote along the negative real axis.) However, large distance from our respective universities and our other duties has made it difficult to obtain a length of uninterrupted time to work on the remaining, difficult, problems. The week at the Banff Centre was amazingly helpful in terms of finding answers to some open problems, and also in discovering some unexpected avenues of future research.

53.3 Outcome of the Meeting

We have now shown that if A is skew-symmetric and the system is collocated, then all the zeros of the system are imaginary and interlace with the eigenvalues. As the index number increases, the zeros (under certain conditions) become arbitrarily close to the eigenvalues. Also, the entire negative real axis is in the root locus and is an asymptote. Note that the asymptotic behavior of the root locus is very different self-adjoint and skew-adjoint systems.

An unexpected avenue that appeared was the importance of the pseudo-spectrum.

Definition 53.3.1 *[8] For any $\varepsilon > 0$ the ε-pseudospectrum of an operator $A : D(A) \subset \mathcal{Z} \to \mathcal{Z}$ is*

$$\sigma_\varepsilon(A) = \{s \in \mathbb{C} \mid \|sz - Az\| < \varepsilon \text{ for some } z \in D(A), \|z\| = 1\}.$$

In general, the pseudospectrum of an operator can be quite different from its spectrum. However, for normal operators the ε-pseudospectrum equals the union of ε-balls around the spectrum of A.

Theorem 53.3.1 *[8] If A is normal,*

$$\sigma_\varepsilon(A) = \bigcup_n B(\lambda_n, \varepsilon)$$

where $B(\lambda,\varepsilon) := \{s \in \mathbb{C} \mid |s-\lambda| < \varepsilon\}$.

Theorem 53.3.2 *[6, Thm. 2.3] Suppose that* $\Sigma(A,B,C)$ *is a system with* $\langle b,c\rangle \neq 0$. *Define*

$$Kz = \frac{\langle Az, c\rangle}{\langle b,c\rangle}, \quad A_\infty z = Az - bKz, \quad z \in D(A_\infty) = D(K) = D(A). \tag{53.3.1}$$

Then, indicating the kernel of C *by* $c^\perp := \{x \in X \mid \langle x,c\rangle = 0\}$, $(A+bK)(c^\perp \cap D(A)) \subset c^\perp$ *and the invariant zeros of* $\Sigma(A,B,C)$ *are eigenvalues of* $A_\infty|_{c^\perp}$. *Moreover, denoting by* $\{\mu_n\}$ *the invariant zeros of* $\Sigma(A,B,C)$, *the corresponding eigenfunctions of* $A_\infty|_{c^\perp}$ *are given by* $\{(\mu_n I - A)^{-1} b\}$.

Theorem 53.3.2 generalizes to systems for which $\langle b,c\rangle = 0$ [6, 7].

The following theorem shows that under certain assumptions, the zeros are asymptotically close to the pseudospectrum of A. A sequence $\{\phi_n\}$ in $\mathcal{Z}$ is called a Riesz system in $\mathcal{Z}$ if there exists an isomorphism $S \in L(\mathcal{Z})$ such that $\{S\phi_n\}$ is an orthonormal system in $\mathcal{Z}$.

Theorem 53.3.3 *Suppose that* $\Sigma(A,B,C)$ *is a system with* $\langle b,c\rangle \neq 0$, *the eigenfunctions of* A_∞, *see (53.3.1), corresponding to the invariant zeros of* $\Sigma(A,B,C)$ *form a Riesz system, and* $c \in D(A^*)$. *Write the invariant zeros of* $\Sigma(A,B,C)$ *as* $\{\mu_1,\mu_2,\ldots\}$ *(repeated according to multiplicity) and indicate the corresponding eigenfunctions of* A_∞ *by* $\{z_1,z_2,\ldots\}$. *Recall that the eigenvalues of* A *are indicated by* $\{\lambda_n\}$. *Then for any* $\varepsilon > 0$ *there is* N *so that for all* $n > N$

$$\|Az_n - \mu_n z_n\| < \varepsilon,$$

that is, $\mu_n \in \sigma_\varepsilon(A)$.

This is used to show that in many cases the zeros become asymptotically close to the eigenvalues. The results described briefly here have been submitted to a major journal [3] and we plan we present our work at a large conference next year.

53.4 Future Research Directions

The application of the pseudo-spectrum to the analysis of zeros is new. It now appears that the pseudo-spectrum can be very useful in analyzing the stability of control systems. Unfortunately, little is known about the pseudo-spectrum for operators. Do operators with a Riesz basis have pseudo-spectrum equal to ε-spectrum balls? Is the root locus is in the ε-spectrum balls around the eigenvalues?

Also, consider a more general spectral problem than (53.2.1):

$$\beta \begin{bmatrix} I & 0 \\ 0 & 0 \end{bmatrix} z = \alpha \begin{bmatrix} A & -B \\ C & 0 \end{bmatrix} z$$

For $\beta \neq 0$, $\lambda = \frac{\alpha}{\beta}$ is the invariant zeros. But $\beta = 0$ (or $\lambda = \infty$) is also an eigenvalue. The root locus of delay, self-adjoint and skew-adjoint cases have totally different behavior at infinity. Does pseudo-spectrum of this pencil provide any insight into the asymptotic behavior of the spectrum of operator pencils?

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Bibliography

[1] S. Pohjolainen, Computation of transmission zeros for distributed parameter systems, Int. J. Control, vol. 33, no. 2, pp. 199–212, 1981.

[2] C. I. Byrnes, D. Gilliam, and J. He, Root-locus and boundary feedback design for a class of distributed parameter systems, SIAM Jour. on Control and Optimization, vol. 32, no. 5, pp. 1364–1427, 1994.

[3] B. J. Jacob and K. A. Morris, Root Locus for Infinite-dimensional systems, IEEE Trans. on Automatic Control, submitted.

[4] T. Kobayashi, Zeros and design of control systems for distributed parameter systems, Int. J. Systems Science, vol. 23, no. 9, pp. 1507–1515, 1992.

[5] B. Kouvaritakis and A. G. J. MacFarlane, Geometric approach to analysis and synthesis of system zeros. I. Square systems, Internat. J. Control, vol. 23, no. 2, pp. 149–166, 1976.

[6] K. Morris and R. E. Rebarber, Feedback invariance of siso infinite-dimensional systems, Mathematics of Control, Signals and Systems, vol. 19, pp. 313–335, 2007.

[7] ——, Zeros of siso infinite-dimensional systems, International Journal of Control, vol. 83, no. 12, pp. 2573–2579, 2010.

[8] L. Trefethen and M. Embree, Spectra and pseudospectra. Princeton University Press, Princeton, NJ, 2005

[9] H. Zwart and M. B. Hof, Zeros of infinite-dimensional systems,IMA Journal of Mathematical Control and Information, vol. 14, pp. 85–94, 1997.

Chapter 54

Statistical Predictions for Chain Ladder Data (14rit206)

August 24 - 31, 2014

Organizer(s): I. Mizera (University of Alberta, Edmonton), M. Maciak (Czech University of Life Sciences, Prague), M. Pešta (Charles University, Prague)

The main purpose of our participation was to work out our idea of a new prediction proposal, which was experimentally showed to perform better than classical methods used in the actuarial science nowadays.

The objective of the BIRS "research in teams" proposal was to meet all three of us together to communicate recent developments in the area of chain ladder data prediction arising in the actuarial science and to make substantial progress towards finishing our common research in this topic, including a collaborative paper preparation.

We can undoubtedly say now that this objective was met. We found the BIRS environment very inspirational and beneficial for all of us: we were able to resolve most of our theoretical as well as practical issues involved, we set an ambitious course for our future collaboration and we did most of the work to finalize our paper and to submit it for publishing soon.

First of all, there was an acute demand to supply the new estimation proposal with some theoretical background that was still missing. There was also a need to verify the method via some simulation and real data results and we also wanted to provide a full scale comparison of all available methods. Moreover, we wanted to discuss and establish some common approaches for further developments as we can see a great potential for this type of statistical analysis in different areas, not just the actuarial science itself.

We believed our prediction proposal can perform significantly better than classical estimation procedures commonly used these days. We had some initial simulation results indicating such expectations however, no theoretical results were available mainly due to some highly technical issues involved in proofs. Although, we did not finish all the theoretical work we intended, it turned out our stay in Banff was very inspirational indeed - not only we showed our proposal can perform much better when using traditional goodness-of-fit measures but we also came up with a different understanding of the model background and we tried a new algorithm concept which even outperforms our own proposal while it requires much simpler and more straightforward theoretical calculations in general.

We also had many useful and bearing discussions together on possible extensions and improvements taking an advantage of some popular topics in statistics, like atomic pursuit methods, convex optimization or empirical processes, all of which can be further pursued and investigated in future.

54.1 Overview of the Field

The chain ladder data are common in the actuarial science: data comes in a triangular shape which arises in predicting reserves that insurance companies are required to keep to comply with regulatory statutes. There are several methods focusing on chain ladder data predictions proposed and even implemented in the statistical software environment R.

Development factors models are generally based on weighted linear regression models, e.g., chain ladder method [6]. These types of methods are very sensitive to the most recent claim amounts [9, Chapter 4], i.e., small changes in the last diagonal of the observed triangle produce large disturbances in the predictions. Moreover, these models are not robust against outliers [9, Chapter 2].

Bayesian methods in claims reserving combine expert knowledge or existing prior information with observations, e.g., Bornhuetter-Ferguson method [2], Cape-Cod method [3]. All of these classes of models require very disputable so-called expert judgement, which can be very influential and questionable as well in order what kind of expert knowledge should be take into account. Generalized linear models (GLM) in non-life insurance [4] suffer from the fact that the input data are in a triangular fashion, not a complete rectangular table. In many GLM reserving methods, there are too many parameters comparing to the number of observations and the number of parameters also depends on the number of observations. This fact yields very volatile parameter estimates together with not very robust prediction.

Several authors have already investigated copula modeling approach in chain ladder data, e.g., [8]. Generally, the mean square error (MSE) is widely used as one of the most important valuation criteria in the insurance business [5].

54.2 Scientific Progress Made in BIRS

Given the recent financial crisis and common corporate insurance policies the main emphasis in the chain ladder prediction is not only posed on overall precision in prediction but the final amount of reserves plays a key role as well and the lowest reserve possibly predicted is preferred.

While several methods, even implementations in the statistical software environment R, already exist, we were able to propose a new approach that outperforms all of them in both aspects above: better mean square error precision as well as smaller overall amount of reserves required. Our idea is motivated by the Delaigle and Hall (2013) paper but the theoretical background is however, different. Our prediction proposal is based on the ”nearest” foregoing period (two various proposals at the end depending on two different interpretation of the word ”nearest”) with a complete information rather than using a classical mean based approach, which seems to be quite unreliable and very non-robust mainly due to a very low amount of data (usually as low as 1 up to 10) used for prediction.

During our collaboration in BIRS, we were able to resolve some important theoretical issues we were dealing with as we set down the main principles for the methodological background of our proposal however, some technical proofs are quite challenging and we were not able to finish all necessary work in just one week.

On the other hand, while trying to solve some technical problems of the original proposal we pointed at another possible understanding of the principle behind and it turned out we could even outperform our original proposal while, in addition, having a great advantage of much simpler theoretical background and more straightforward technical proofs in hand with the alternative concept.

Thus, in BIRS we mutually compared both our proposals with standard chain ladder prediction approaches using over 300 real data scenarios - complete chain ladder data provided by different insurance companies where the upper triangle part of data is used for the prediction itself and the lower data triangle part was used to validate the prediction at the end.

Last but not least, we investigated the potential of the proposed methodology in some other areas of statistics and real life situations: specifically, we were provided with online newspaper data recording a post (article) specific amount of readers arising in time where the main interest was to predict further development in order to apply more targeted commercials for example. Another area with a similar data arising principle is the biometric theory of the so-called growth curves in Biology. Even though, there are some obvious dissimilarities and different theoretical background assumptions one has to account for, there is a great potential for the chain ladder prediction methods in statistics and there is no need one should be closely focused on actuarial science and actuarial data only.

54.3 Outcome of the Meeting

During the week at BIRS we had a great opportunity to meet together and to investigate and brainstorm all topics of our common interest, which we greatly appreciate. We proposed two variants for the chain ladder prediction method where both of them outperform classical approaches used nowadays, when evaluating the precision by the mean squared error (the only standard goodness-of-fit measure—sometimes even required by law—to be used by insurance companies).

While at BIRS, we were able to canvass and clear up most of major problems related to theoretical or practical issues and using a few hundreds of real data scenarios we were able to perform quite complex and overall comparison of classical methods with both our proposals, where both of them outperformed classical approaches significantly. We are now about to finish a paper on this topic concluding all important facts we learned together at BIRS. The paper will be submitted for publication in relevant scientific journal.

Additionally, we had a great chance to strengthen our collaboration as we can see far more potential for these methods in statistics and real life situations now. There are of course whole new problems and challenges arising but we believe we can bridge them over and exploit all hidden potential of our proposals and all their advantages. We all intend to continue with our collaboration in future and not only in the area of chain ladder prediction. This gives us confidence in possibly many more papers we could work on together.

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Bibliography

[1] A. Delaigle and P. Hall, Classification using censored functional data, JASA, **108**, 1269–1283, (2013).

[2] R. L. Bornhuetter and R. E. Ferguson, The actuary and IBNR, Proceedings of the Casualty Actuarial Society, **LIX**, 181–195, (1972).

[3] H. Bühlmann, Estimation of IBNR reserves by the methods chain ladder, Cape Cod and complementary loss ratio, International Summer School 1983 (unpublished), (1983).

[4] P. D. England and R. J. Verrall, Stochastic claims reserving in general insurance (with discussion), British Actuarial Journal, **8**(3), 443–518, (2002).

[5] Š. Hudecová and M. Pešta, Modeling dependencies in claims reserving with GEE, Insurance: Mathematics and Economics, **53**(1), 786–794, (2013).

[6] T. Mack, Distribution-free calculation of the standard error of chain ladder reserve estimates, ASTIN Bulletin, **23**(2), 213–225, (1993).

[7] M. Pešta and Š. Hudecová, Asymptotic consistency and inconsistency of the chain ladder, Insurance: Mathematics and Economics, **51**(2), 472–479, (2012).

[8] M. Pešta and O. Okhrin, Conditional least squares and copulae in claims reserving for a single line of business, Insurance: Mathematics and Economics, **56**, 28–37, (2014).

[9] M. V. Wüthrich and M. Merz, Stochastic claims reserving methods in insurance, Wiley, (2008).