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Contents

Five-day Workshop Reports

Chapter 1

Representation Theory Connections to (q,t)-Combinatorics (19w5131)

January 20 - 25, 2019

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In 2007, a workshop was held at the Banff research station entitled *Applications of Macdonald polynomials*[1]. The focus of that meeting was related to a number of mathematical problems that arose in the roughly 20 years prior.

That workshop served to highlight some of the directions of research related to the following discoveries.

- In 1988, Macdonald [Mac88] introduced a family of symmetric functions $P_\lambda(X; q, t)$ that depended on parameters q and t and a family of non-symmetric polynomials $E_\alpha(X; q, t)$ which are a basis for the polynomial ring. An open problem remains to find a combinatorial interpretation for the transition coefficients $K_{\lambda\mu}(q, t)$ from the Macdonald symmetric functions to a Schur basis.

- In 1994, Garsia, Haiman [Hai94, GarHai96] stated a series of conjectures related to a symmetric group representation known as the diagonal harmonics which is the quotient ring of polynomials in two sets of variables of size n by the ideal generated by the ideal generated by the symmetric group invariants.

- One of the conjectures stated that this space was of dimension $(n + 1)^{n-1}$ (and this was resolved in 2001 by Haiman [Hai99, Hai01, Hai02, Hai02b]), but further investigation into the combinatorics of parking functions by Haglund, Haiman, Loehr, Remmel and Ulyanov [HHLRU05] lead them to 'the shuffle conjecture' in 2004, a q, t-combinatorial formula for the graded Frobenius character of the module.

In the last eleven and a half years since that conference, there have been a number of remarkable breakthroughs related to these and the other research problems highlighted at that conference. A number of exciting connections have arisen over the last few years between Macdonald polynomials and invariants of torus knots and torus links [Gor13, GN15, GORS14, Hag16].

These new connections lead to the development of extensions of the shuffle conjecture to labeled paths that lie above the diagonal of an $m \times n$ rectangle [ALW14, GORS14, GMV16, GM16, BGLX16, GLXW15].

In addition, many new questions in this area arose out of the operator realization of the elliptic Hall algebra of Burban, Schiffman and Vasserot [5, SV13] that left many open questions and connections to the representation theory and knot invariants left to be explored [MS, Ber16].

[1] `https://www.math.upenn.edu/~jhaglund/conf/finalreportbirs07.pdf`

In 2015, Carlsson and Mellit [CM15] proved the shuffle conjecture and shortly after Mellit [Mel16] proved the rational shuffle conjecture. This progress resolved a major open problem in the area and caused a shift of research in this area.

In 2016, Haglund, Remmel and Wilson [HRW15] discovered a conjecture which proposed a combinatorial model for the symmetric function expression $\Delta_{e_k}(e_n)$ and called this 'the Delta conjecture.' In the case that $k = n$, the Delta conjecture reduces to the shuffle conjecture, but it currently remains unresolved.

We saw the workshop "Representation Theory Connections to (q, t)-Combinatorics" at BIRS as an opportunity to re-visit some of the remaining open problems and re-assess what are the most interesting open questions in this area. The focus of research in the field has shifted in the last decade given that the research leading up to the proof of the shuffle conjecture uncovered many new connections between representation theory, the elliptic Hall algebra and knot invariants.

Three of the objectives that were listed in the proposal of this workshop are summarized in the following bullet points:

1. to connect some of the combinatorial and algebraic methods recently developed with quasi-symmetric functions. [ELW10, HLMvW11a, BBSSZ14, As15, AsSer16, Rob14]

2. consider positivity of symmetric function expressions arising in this context from the perspective of representation theoretical constructions [HRW15, GORS14, HRS1, HRS2, Rho16, GHRY]

3. make connections between symmetric functions, combinatorial formulae, the elliptic Hall algebra and torus knot invariants. [Ber16, 5, Gor13, GN15, Hik14, LW08, MS, MMR14, Mel16, Neg13, Neg14, Sch12, SV13]

We chose to have a small number of presentations and give participants ample time to discuss ideas. The following is a list of the presentations that we will discuss in summary below.

1. Speaker: **François Bergeron**
   Title : *Multivariate modules for (m, n)-rectangular combinatorics I and II*

2. Speaker: **Adriano Garsia**
   Title: *Some Conjectures with Surprising Consequences*

3. Speaker: **Matthew Hogancamp**
   Title: *How to compute superpolynomials*

4. Speaker: **Lauren Williams**
   Title: *From multiline queues to Macdonald polynomials via the exclusion process*

5. Speaker: **Sami Assaf**
   Title: *Nonsymmetric Macdonald polynomials and Demazure characters*

6. Speaker: **Brendon Rhoades**
   Title: *Spanning configurations*

7. Speaker: **Gabriel Frieden**
   Title: *Kostka–Foulkes polynomials at $q = -1$*

8. Speaker: **Luc Lapointe**
   Title: *m-symmetric Macdonald polynomials*

9. Speaker: **Hugh Morton**
   Title: *A skein-theoretic model for the double affine Hecke algebras*

We mentioned that the Macdonald polynomials was one of the discoveries that motivated this area of research and was one of the topics highlighted in in the workshop in 2007. They reappeared in several of the talks in this workshop. The talk by Sami Assaf was on non-symmetric Macdonald polynomials and their expansion into Demazure characters using a crystal structure. The talk by Luc Lapointe showed a new approach to the problem of finding a combinatorial interpretation for the Macdonald q, t-Kostka coefficients using larger algebras to lift their structure. The talk by Lauren Williams showed how Macdonald polynomials arise in two combinatorial models, one called multi-line queues and another was the multispecies asymmetric simple exclusion process.

The talks by Matthew Hogencamp and Hugh Morton explained connections between knot invariants and q, t-combinatorics and connections with representation theory. In particular, the talk on "how to compute super-polynomials" discussed a combinatorial technique for Khovanov-Rozansky homology which has led to the computation of the rational q, t-Catalan.

A number of the other talks focused on the connections of representation theory and their connections to q, t-combinatorics. The extension of the shuffle conjecture known as the Delta conjecture appeared tangentially in a number of the talks. We mention that one of the basic open problems related to the Delta conjecture was to find a plausible candidate for a module of the symmetric group S_n whose bigraded Frobenius characteristic is given by the symmetric function side of the Delta conjecture. As luck would have it, organizer M. Zabrocki found such a candidate (see (1.0.1) and [Zab19]) the day before the conference, and shared it with the conference attendees, which led to a lot of interesting discussions and further conjectures. The presentation of Adriano Garsia discussed the phenomenon (outlined in [Ber16]) of replacing q with $q + 1$ in a Schur positive symmetric function arising from q, t-combinatorics and the expression is very often positive when expanded in the e-basis. He presented a growing list of expressions where this phenomenon can be proven. François Bergeron presented a number of results and broad conjectures about symmetric functions which encode the $Gl_k \times S_n$ character of multidiagonal harmonics. In particular he proposed explicit modules for which the aforementioned symmetric functions appear as characters,. This gives a entirely new representation theoretic foundation for the result established by Mellit and Carlsson which ties together the $m \times n$-rectangular path combinatorics and the elliptic Hall algebra based formulas appearing in the rectangular compositional shuffle formula (see [BGLX16, HMZ12, Hic14]). Not only do these new symmetric functions open the way to a broad program of research, but they tie together most of the previous areas of research in the domain, including the Delta conjecture, and suggest many natural generalization. In the final discussion, it was realized that they also merge nicely with the candidate proposed for the Delta conjecture by Mike Zabrocki, as well as suggesting generalizations to both the multivariate case and the $m \times n$-rectangular one.

In addition, on the Thursday of the workshop meeting, the afternoon session was devoted to asking participants to submit a summary of the major open problems in this area. The participants also submitted a written summary after the meeting which was published on the webpage. While a longer more detailed versions of these problems appears in the summary on the web page, we provide a summary below that gives a flavor of the mathematics discussed at this conference.

Presenter: **François Bergeron**
Outline: The probability that a monomial positive symmetric function is actually Schur positive is

$$\frac{1}{\prod_{\mu \vdash n} \sum_{\lambda \vdash n} K_{\lambda\mu}} .$$

"Consider the q-analogue of these formulae obtained by replacing the Kostka numbers by the q-Kostka polynomials (or even (q, t)), can we give a natural interpretation of this as a probability of some sort?"

Presenter: **Lauren Williams**
Outline: Given a matrix $M = (m_{ij})$ with entries are symmetric polynomials. M is totally Schur positive if each square sub-matrix has Schur positive determinant. An example of this are the Jacobi-Trudi matrices, but are there others?

Presenter: **Hugh Morton**
Outline: Is it possible to create a non-degenerate bilinear form on braids in the torus that can be used to determine linear independence? What is the HOMFLY skein in this case?

Presenter: **Brendan Pawlowski**
Define Stanley symmetric functions, affine Stanley symmetric functions, involutive Stanley symmetric functions and (finally) affine involutive Stanley symmetric functions. It can be shown that the affine involutive Stanley symmetric functions have positive coefficients when expanded in the affine Stanley Schur functions, but what other properties do they have?

Presenter: **Peter Samuelson**
Outline: The elliptic Hall algebra $E_{q,t}$ is an algebra over $\mathbb{C}(q,t)$ which was defined by Burban and Schiffmann as a "universal Hall algebra of elliptic curves over finite fields." There is an action of $E^+_{q,t=q}$ action on Sym. Question: Does the action of $E_{q,t=q}$ on $Sym \otimes Sym$ extend to generic t?. The "vertical subalgebra" (generated by the $u_{0,n}$) acts on Sym (essentially) by Macdonald operators, which are diagonalized by Macdonald polynomials. The module $Sym \otimes Sym$ has a basis $s_{\lambda,\mu}$ of "double Schur functions," and this diagonalizes the "vertical subalgebra" of the skein algebra. A positive answer to this question would (presumably) lead to "double" Macdonald polynomials, which would be indexed by pairs of Young diagrams, so a followup question is "how much of Macdonald theory carries through to double Macdonald polynomials"?

Presenter: **Marino Romero**
Outline: In the 1990's Bergeron and Garsia presented a sequence of conjectures that they labelled Science Fiction [BG99]. For α a partition, let M_α be the Garsia-Haiman module. One approach to proving the $n!$ conjecture is to understand why for partitions α and β each found by removing a single cell from a larger partition μ, then

$$\dim(M_\alpha \bigwedge M_\beta) = n!/2\ .$$

More generally, the Frobenius image is given by

$$Frob_{qt}\left(M_\alpha \bigwedge M_\beta\right) = \frac{T_\beta \tilde{H}_\alpha - T_\alpha \tilde{H}_\beta}{T_\beta - T_\alpha} = \left(\frac{1}{1 - T_\alpha/T_\beta}\right)\tilde{H}_\alpha + \left(\frac{1}{1 - T_\beta/T_\alpha}\right)\tilde{H}_\beta$$

where $\tilde{H}_\beta$ is the Macdonald symmetric function where $T_\mu = \prod_{(i,j)\in\mu} q^i t^j$. These conjectures extend to larger collections of partitions.

Presenter: **Mikhail Mazin**
Outline: Take m and n relatively prime. There is a bijection between lattice paths which lie below the diagonal in an $n \times m$ rectangle and partitions which are simultaneously m and n cores. There are q, t- countings of both sides which agree. That is, on the left hand side you have a q, t counting of paths below the diagonal in an $m \times n$ rectangle and this is equal to a right hand side of a q, t counting of the partitions which are simultaneously m and n cores.

Consider again the m and n relatively prime and let $(M, N) = (dm, dn)$. The q, t-counting can be naturally generalized both for lattice paths that stay below the diagonal in an $M \times N$ rectangle and for the simultaneous M, N-core partitions. However, they are not equal anymore. In fact, the set of simultaneous M, N-core partitions is infinite in the non relatively prime case, and the resulting generating function is not a polynomial, but rather a power series (a rational function with denominator $(1-q)^{d-1}$). Both counts are related to some deep and interesting mathematics. The paths under the diagonal appear in the compositional Shuffle theorem by Erik Carlsson and Anton Mellit [CM15], and simultaneous cores correspond to invariants of torus links.

The open question is what is the precise relation between these two q, t-countings in the non relatively prime case.

Presenter: **Gabriel Frieden**
Outline: Haglund, Haiman, and Loehr gave a combinatorial formula for the monomial expansion [HHL05] One appealing approach to finding the Schur expansion would be to define a crystal structure on the set of fillings of μ that preserves the statistics maj and inv; the Schur expansion would then be given by the weights of the highest

elements in the crystal structure. In the case where μ has two columns, Haglund-Haiman-Loehr defined a suitable crystal structure on the fillings [HHL05].

In the case where μ has three columns, Blasiak [2] recently proved a conjectured rule of Haglund [Hag04] for the Schur expansion. We propose the problem of finding a maj- and inv-preserving crystal structure on fillings of partitions with three columns.

Presenter: **François Bergeron**
Outline: For any operator $F_{m,n}$, on symmetric functions coming from the elliptic Hall algebra. Define the operation $\hat{F}_{m,n} := F_{m,n}|_{t=1}$. There is an identity that is simple to state, but begs for a proof:

$$\hat{F}_{m,n} \cdot f = f \cdot (\hat{F}_{m,n} \cdot 1).$$

In other words, $\hat{F}_{m,n}$ is simply a multiplication operator. This is certainly not the case (in general) for $F_{m,n}$.

Presenter: **Mike Zabrocki**
Outline: Let

$$\mathbb{Q}[X_n, Y_n; \Theta_n] := \mathbb{Q}[x_1, x_2, \ldots, x_n, y_1, y_2, \ldots, y_n; \theta_1, \theta_2, \ldots, \theta_n]$$

be the polynomial ring in three sets of variables, the first two are commuting and the third one is anti-commuting (and the variables of different flavors commute). The invariants of this polynomial ring (here denoted by Sym, with Sym^+ standing for those that are constant term free) are generated by analogues of the power sums

$$p_{r,s} = \sum_{i=1}^{n} x_i^r y_i^s \text{ and } \tilde{p}_{r',s'} = \sum_{i=1}^{n} \theta_i x_i^{r'} y_i^{s'}$$

for $0 < r + s \leq n$ and $0 \leq r' + s' < n$. Define the analogue of the diagonal harmonics as

$$\mathrm{SDCoinv}_n := \mathbb{Q}[X_n, Y_n; \Theta_n] / \langle p_{r,s}, \tilde{p}_{r',s'} | 0 < r + s \leq n, 0 \leq r' + s' < n \rangle \ .$$

Based on computational evidence of the Frobenius series, $n \geq 1$,

$$\mathrm{Frob}_{qtz}(\mathrm{SDCoinv}_n) = \Delta'_{e_{n-1}[X - \varepsilon z]}(e_n), \tag{1.0.1}$$

where $e_{n-1}[X - \varepsilon z] = e_{n-1} + z e_{n-2} + z^2 e_{n-3} + \cdots + z^{n-1}$ and $\Delta'_f(\tilde{H}_\mu[X; q, t]) = f[B_\mu - 1]\tilde{H}_\mu[X; q, t]$.

We can make the following interesting further conjecture. Let $\mathcal{E}_n[Q; Z] = \sum_\mu a_\mu[Q] s_\mu[Z]$ be the symmetric functions described in François Bergeron's talk on Monday and Tuesday as a symmetric function expression for the multivariate analogue of the diagonal harmonics, then let

$$\mathrm{Coinv}_n^{k,k'} := \mathbb{Q}[X_n^{(1)}, \ldots, X_n^{(k)}; \Theta_n^{(1)}, \ldots, \Theta_n^{(k')}] / \langle \mathrm{Sym}^+ \rangle$$

be the coinvariant space in k sets of commuting variables and k' sets of anti-commuting variables (such that the anticommuting variables also anticommute among themselves).

Let Q_k represent the alphabet $q_1, q_2, \ldots, q_k$ to keep track of the degrees in the $X_n^{(i)}$ variables and $T_{k'}$ represent the alphabet $t_1, t_2, \ldots, t_{k'}$ as variables which keep track of the degrees in the $\Theta_n^{(i)}$ variables, then we conjecture that

$$\mathrm{Frob}_{Q_k, T_{k'}}(\mathrm{Coinv}_n^{k,k'}) = \mathcal{E}_n[Q_k - \varepsilon T_{k'}; Z]$$

for $k + k' > 0$.

Overview

In 1988 I. G. Macdonald [Mac88] introduced a family of symmetric functions with parameters q and t to unify the treatment of both Hall-Littlewood and Jack symmetric functions. These functions and the operators for which they are eigenfunctions have since been shown to have deep connections with diverse areas of mathematics including: algebra, representation theory, and algebraic geometry; as well as mathematical physics.

In 2007, a workshop was held at the Banff research station entitled *Applications of Macdonald polynomials*. The presentations at that time covered the main motivating questions and research on the subject that were then relevant. Nearly a decade later, research in this area has seen a significant expansion and, while some of the previously open questions have now been resolved, new and even broader questions have risen.

One of the original motivating open questions about Macdonald's functions was to find a combinatorial interpretation for the q, t-polynomial coefficients when expanded in the Schur basis. To approach this problem Garsia and Haiman [GarHai93] conjectured a bi-graded representation theoretical model for Macdonald symmetric functions. Haiman [Hai94] discovered the space of diagonal harmonics as a closely related bi-graded symmetric group representation. These constructions allowed Haiman to connect Macdonald symmetric functions to the Hilbert Scheme of n points in a plane [Hai99] and eventually prove [Hai01, Hai02, Hai02b] the Schur positivity of both the Macdonald symmetric functions and a formula for the bi-graded Frobenius characteristic for the diagonal harmonics. This progress left many beautiful and fascinating algebraic and combinatorial conjectures that still remain to be resolved (see for instance [BG99, BGHT99]), and others that followed in the years after up to very recently (e.g. [HHLRU05, LW08, HMZ12, Ber13, GN15, HRW15, BGLX16]). In short, this original motivating quest for a combinatorial formula for the Schur expansion of the Macdonald symmetric functions and the Frobenius characteristic of the diagonal harmonics is still very much open, and it has been expanded in several significant directions.

One focus of the meeting in 2007 was on the lattice combinatorics which arise in symmetric function expressions involving the operator ∇ [BG99, BGHT99]. At the time of that meeting, the Shuffle Conjecture [HHLRU05] was proposed as a conjectural combinatorial expression for the monomial expansion of the Frobenius characteristic of the diagonal harmonics in terms of labeled Dyck paths (alternatively, ∇ acting on an elementary symmetric function). In 2015 this conjecture was proven [CM15] and this has caused a shift in the questions that researchers will next try to answer. This proposal for a meeting dedicated to this subject is timely because the questions that are now prioritized as being the most important to solve have changed. A number of exciting connections have arisen over the last few years between Macdonald polynomials and invariants of torus knots and torus links. In a recent preprint Mellit [Mel16], building on results in his proof of the Shuffle Conjecture with Carlsson, posted a proof of the Rational Compositional Shuffle Conjecture of Bergeron, Garsia, Leven, and Xin [BGLX16]. This contains the Shuffle Conjecture as a special case, and also implies a number of nice combinatorial formulas which have been sought after by other researchers. For example, it implies a conjecture of Gorsky, Oblomkov, Rasmussen, and Shende [GORS14] giving a purely combinatorial formula, in terms of (q, t)-weighted Dyck paths, for the superpolyniomial of the (m, n) torus knot.

Our intention is to bring together researchers to focus on three main aspects of q, t-combinatorics and representation theory: connections to knot invariants, techniques to obtain Schur positive expansions from quasi-symmetric function expansions, and the development of representation theoretical models of the q, t-polynomial expressions. Many new questions have appeared, some of which are outlined in [Ber16], coming from interesting connections with an operator realization of the elliptic Hall algebra introduced by Schifmann, Burban, and Vasserot [SV13].

The following bibliography gives significant indications of the impact of the Banff meeting from 2007, and of the growth of the community of researchers in this area since then. The wide-ranging expertise now present in this community contributes to show that this subject would benefit from a focused meeting. Many of the participants of the previous meeting went on to make important discoveries in the intervening decade. Now that many new applications and connections have arisen, a new meeting should have even more impact.

Statement of the objectives of the workshop: ——————————————

Objectives

The main questions in this area of research are often twofold, one more combinatorial and the other more algebraic. The combinatorial part aims at finding interesting combinatorial interpretations for Schur expansions of symmetric functions that are calculated in terms of Macdonald polynomials, or of operators for which they are eigenfunctions. The algebraic counterpart aims to link these combinatorial considerations to representation theoretical interpretations, with irreducible representations of the symmetric group encoded as Schur functions. Symmetric function theory serves as a bridge between combinatorics and representation theory.

A first focus of this meeting will be to connect some of the combinatorial and algebraic methods recently developed with quasi-symmetric functions. Quasi-symmetric expansions are known for Macdonald symmetric functions and expressions related to the Shuffle Conjecture and its generalizations. Successful methods exist for transforming quasi-symmetric expansions to Schur expansions [ELW10, As15], but they have not produced an effective combinatorial interpretation for the Schur coefficients in these expressions. Another approach has lead to the development of two analogues of the Schur functions in the context of quasi-symmetric functions. One of these arises from the quasi-symmetric functions constructed from Demazure atoms [HLMvW11b] and another comes from a generalization of the Jacobi-Trudi expansion of Schur functions [BBSSZ14]. Quasi-symmetric function expansions in either of these bases have the potential of giving the desired Schur expansions. We expect that these techniques will have wide ranging applications to many other positivity questions related to symmetric functions [St99, Ber16].

A second focus will be to consider positivity of symmetric function expressions arising in this context from the perspective of representation theoretical constructions. Notable historical examples are the Garsia-Haiman modules and the module of diagonal harmonics. This whole portion of the subject has moved into a brand new direction with recent work on two fronts: combinatorics and knot theory, with the elliptic Hall algebra serving as a link between the two. The combinatorial perspective corresponds a generalization to the (m, n)-lattice context of the classical combinatorial setup (which corresponds to $m = n + 1$). A parallel compelling topic of current interest in knot invariants is the study of colored Khovanov homology for (m, n)-torus knots. Both subjects have been shown to have strong connections to Macdonald polynomial theory, and related operators.

Largely through Haiman's work connecting Macdonald polynomials to the Hilbert scheme [Hai01], a large number of bigraded character formulas have recently emerged from math physics, expressed as sums of Macdonald polynomials with rational coefficients. The goal is to start with these sums and obtain positive Schur expansions whose coefficients have a nice combinatorial description. In general this program is quite challenging, but we have already been able to make partial progress, such as obtaining positive monomial expansions similar to those occurring in the Shuffle Conjecture.

From the mathematical physics side, when the bigraded character formulas are restricted to hook shapes, we often obtain a formula for a polynomial knot invariant. For example, E. Gorsky has noticed that the expression

$$< \nabla e_n, \sum_{k=0}^{n} e_{n-k} h_k a^k > \tag{1.0.2}$$

is equal to the superpolynomial knot invariant for the $(n + 1, n)$ torus knot. By [Hag04], this polynomial is a (q, t)-analog of the Schröder number, and can be expressed as a sum over (q, t)-weighted Schröder paths. More generally, if in (1.0.2) we replace ∇e_n by $Q_{m,n}(-1)^n$, where m, n are relatively prime and the $Q_{m,n}$ operators are generators for the Eliptic Hall Algebra as discussed in [BGLX14], [BGLX16], then the right-hand-side of (1.0.2) becomes the superpolynomial of the (m, n) torus knot.

Several other related results and conjectures have followed. For example, Elias and Hogancamp have a new recurrence from which they obtain results on the homology of the (n, n) torus link, conjecturally connecting this to ∇p_{1^n} through work of Gorsky and Negut. In a preprint on the arXiv, A. Wilson [W15] has extended some of their ideas, giving a conjectured combinatorial model for ∇p_{1^n} in terms of labelled Dyck paths. In addition, a student of Gorsky has a (q, t)-Fibonacci number which conjecturally models aspects of knot homology, while Arthamonov and Shakirov have developed q, t-Macdonald formulas associated to torus knots in genus two. We hope to bring together researchers in knot homology and algebraic combinatorics to exploit these exciting connections.

With all these developments as a background it seems very timely to have a meeting in which all these original approaches will be allowed to interplay. It is reasonable to expect that significant advances in the subject will follow. This assertion is strongly supported by the eminent success that followed our previous meeting of 10 years ago.

Participants

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Chapter 2

Optimal Transport Methods in Density Functional Theory (19w5035)

January 27 - February 1, 2019

Organizer(s): Mathieu Lewin (CNRS and Université Paris Dauphine), Paola Gori-Giorgi (Vrije Universiteit Amsterdam), Brendan Pass (University of Alberta)

What is Density Functional Theory?

An approximation of Schrödinger's first eigenvalue

Quantum mechanics is a very impressive theory, developed in the beginning of the XX century to describe the microscopic world. One of its most important achievements is the Schrödinger equation, which allows, in principle, to predict properties of materials and chemical compounds, including the outcome of chemical reactions. Central to computational chemistry, solid state physics and materials science is the lowest eigenvalue E_0 (a.k.a. ground-state energy) of the N-electron hamiltonian H_{el} for given positions X_i of the M nuclei with charges Z_i (Born-Oppenheimer approximation),

$$H_{el} = \underbrace{-\frac{\hbar^2}{2}\sum_{i=1}^{N}\Delta_{x_i}}_{=\hbar^2\, T} + \underbrace{\sum_{1\leq i<j\leq N}\frac{1}{|x_i-x_j|}}_{=V_{ee}} + \sum_{i=1}^{N} v(x_i), \qquad v(x) = -\sum_{\alpha=1}^{M}\frac{Z_\alpha}{|x-X_\alpha|}, \tag{2.0.1}$$

with $x_i, X_i \in \mathbb{R}^3$ and

$$E_0 = \inf_{\Psi\in\mathcal{A}_N}\langle\Psi, H_{el}\Psi\rangle, \qquad \mathcal{A}_N = \left\{\Psi \in H^1((\mathbb{R}^3\times\{\uparrow,\downarrow\})^N;\mathbb{C}) \ : \ \Psi \text{ antisymmetric}, \ ||\Psi||_{L^2}=1\right\}. \tag{2.0.2}$$

Unfortunately, the apparent simplicity of Eq. (2.0.1) is an illusion. Even if this one-line operator is believed to describe the richness of the microscopic world, it has no known analytical eigenvalue for more than one electron and one nucleus, and the numerical cost involved to compute approximate solutions for realistic materials and chemical compounds grows extremely fast with the number of particles in the system. Physicists and chemists are obliged to turn to approximations, relying partly on empirical considerations.

Density functional theory (DFT), by virtue of its excellent compromise between computational efficiency and accuracy, is the method of choice for the electronic structure calculations in computational chemistry and solid-state physics. Invented in the early days of quantum mechanics, DFT uses the one-electron density $\rho(x)$ (marginal) as key variable,

$$\rho(x) = N \sum_{s_1,\cdots,s_N\in\{\uparrow,\downarrow\}} \int_{\mathbb{R}^{3(N-1)}} |\Psi(x,s_1,x_2,s_2,\cdots,x_N,s_N)|^2 dx_2\cdots dx_N, \tag{2.0.3}$$

to rewrite the infimum in Eq. (2.0.2) as

$$E_0 = \inf_{\rho\in\mathcal{R}_N} \left\{ F_\hbar^{\mathrm{LL}}[\rho] + \int_{\mathbb{R}^3} v(x)\rho(x)dx \right\}, \tag{2.0.4}$$

with the set of N-representable densities

$$\mathcal{R}_N = \left\{ \rho \geq 0,\ \int_{\mathbb{R}^3} \rho = N,\ \sqrt{\rho} \in H^1(\mathbb{R}^3) \right\},$$

and where the (universal) Levy-Lieb universal functional $F_\hbar^{\mathrm{LL}}[\rho]$ is defined as

$$F_\hbar^{\mathrm{LL}}[\rho] = \inf_{\substack{\Psi\in\mathcal{A}_N\\ \rho_\Psi=\rho}} \left\langle \Psi, (\hbar^2 T + V_{ee})\Psi \right\rangle. \tag{2.0.5}$$

DFT only became popular in the 70's in solid-state physics thanks to the Kohn-Sham (KS) formalism, in which the functional $F_\hbar^{\mathrm{LL}}[\rho]$ is decomposed as

$$F_\hbar^{\mathrm{LL}}[\rho] = \hbar^2 T_s[\rho] + U[\rho] + E_{xc}[\rho]$$

where

$$U[\rho] = \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\rho(x)\rho(y)}{|x-y|} dxdy$$

is the classical Coulomb energy of the density ρ and

$$T_s[\rho] = \min\left\{ \frac{1}{2}\sum_{i=1}^N \int_{\mathbb{R}^3} |\nabla\phi_i|^2\ :\ \sum_{i=1}^N |\phi_i|^2 = \rho,\ \langle\phi_i,\phi_j\rangle = \delta_{ij},\ \phi_i \in H^1(\mathbb{R}^3\times\{\uparrow,\downarrow\}) \right\},$$

is the lowest kinetic energy that can be achieved with N independent electrons having the prescribed density ρ. Since $T_s[\rho]$ is a somewhat better understood functional, in this form only the exchange-correlation functional $E_{xc}[\rho]$ needs to be approximated. The mother of all models for $E_{xc}[\rho]$ is the so-called Local Density Approximation (LDA) where the exchange-correlation energy is taken to be the average over all $x \in \mathbb{R}^3$ of the lowest energy per unit volume $e_{\mathrm{xc}}^{\mathrm{HEG}}\big(\rho(x)\big)$ of an infinite electron gas having the constant density $\rho(x)$ at this point $x \in \mathbb{R}^3$:

$$E_{xc}[\rho] \simeq \int_{\mathbb{R}^3} e_{\mathrm{xc}}^{\mathrm{HEG}}\big[\rho(x)\big]\, dx. \tag{2.0.6}$$

For a general mathematical presentation of DFT, we refer for instance to [34, 5].

Kohn-Sham DFT became very popular in the 90's in chemistry with the introduction of empirical approximations for $E_{xc}[\rho]$ beyond the local-density approximation (2.0.6). One central idea is to introduce gradient corrections, taking into account the fact that ρ is indeed not constant locally. But other improvements have played an important role, like for hybrids models using a bit of the exact exchange energy in Hartree-Fock theory.

Despite its enormous success, the predictive power of Kohn-Sham DFT is still hampered by inadequate approximations for near-degenerate and strongly-correlated systems. Crucial examples are transition metal complexes (key for catalysis), stretched chemical bonds (key to predict chemical reactions), technologically advanced functional materials, and man-made nanostructures.

On the other hand, DFT is a source of difficult mathematical problems, whose resolution requires top-level mathematical research. This research, in turn, has the potential to influence real applications in Chemistry and Physics.

The use of Optimal Transport methods in DFT

The purpose of the BIRS workshop held in January 2019 was to bring together physicists, chemists and applied mathematicians working on the **use of Optimal Transport (OT) methods in DFT**. This very fruitful line of research has emerged very recently and a new community is currently exploring its ability to improve our understanding of correlations in Coulomb systems [41].

Over the last 30 years, the theory of optimal transportation has grown into a fertile mathematical field. It has many applications, both within and beyond Mathematics, in such diverse fields as economics, meteorology, geometry, statistics, fluid mechanics, design problems and engineering. An overview of this theory can be found in the monograph written by the fields medalist Cédric Villani [45].

It was only realized recently by mathematicians [9, 4, 16, 11] that the central problem of finding the lowest Coulomb energy of N-particle probabilities at given first marginal (a.k.a. the charge density) $\rho(x)$, appearing as the $\hbar \to 0$ limit of $F_\hbar^{\mathrm{LL}}[\rho]$,

$$F^{\mathrm{LL}}_{\hbar\to 0}[\rho] = V_{ee}^{\mathrm{SCE}}[\rho] + O(\hbar), \qquad V_{ee}^{\mathrm{SCE}}[\rho] = \inf_{\substack{\Psi\in\mathcal{A}_N \\ \rho_\Psi=\rho}} \langle \Psi, V_{ee}\Psi\rangle \tag{2.0.7}$$

is a multi-marginal optimal transport problem. The infimum on the right side is always attained if the set of anti-symmetric Ψ's is enlarged to N-particle symmetric probability measures, having the prescribed marginal ρ. Methods in the spirit of optimal transport had however been used before in Physics and Chemistry, in particular in the seminal works of Seidl [40] and his collaborators [43, 42, 22, 39] on the strictly-correlated electrons (SCE) model, as well as in the older work of Lieb-Oxford [35] who derived a lower bound on this energy.

In order to address the full complexity of this new field and make significant progress, it seems mandatory to use an interdisciplinary approach. From the point of view of Chemistry and Physics, it is important to have a good knowledge of the mathematical properties of the problem, in order to develop new efficient and reliable approximations. DFT is a quantum theory in which a large part of the quantum effects are well captured by the Kohn-Sham formalism. Its semi-classical (strongly correlated) limit provides new information on the effects that are missed by Kohn-Sham DFT. The understanding of this limit is thus essential to develop approximate functionals that can address strongly-correlated systems. From the point of view of mass transportation theory, the Coulomb problem in DFT poses new challenges which have the potential to impact other applications. The fact that there are N prescribed marginals in the Coulomb DFT problem, contrary to the standard OT case $N = 2$, poses new mathematical difficulties, which have not yet been completely understood.

This BIRS workshop allowed for very fruitful interactions between different communities: chemists and physicsts working on DFT and on the quantum many-body problem, mathematicians from optimal transport, mathematical physics, probability theory, and numerical methods.

The first challenge in this kind of interdisciplinary workshops is to set a common language. For this reason, we had scheduled a series of review/introductory talks from experts of the various disciplines. This was extremely helpful, and was very much appreciated by all the participants. At the end of the workshop we have also organized a round table, where several perspectives or general strategies have been discussed. Overall, the workshop was a real success.

Some Highlights and Open Problems

In this section we discuss some important points raised during the workshop, as well as open problems.

Monge or not Monge?

An important question, which has been mentioned several times during the workshop, is to understand when there are Monge-type N-particle minimizers of the Kantorovich multi-marginal optimal transport problem (2.0.7). Monge states indeed can be parametrized by much less variables, leading to a dramatic decrease of complexity in practical computations. In addition, Monge states have a clearer physical interpretation in terms of "strictly correlated systems". This is because in a Monge state the positions $x_2, ..., x_N$ of $N-1$ electrons are completely determined by the position x_1 of the remaining electron. The corresponding probability measure is therefore typically supported over a space of very low dimension.

The standard method for establishing the existence of Monge solutions for optimal transport problems, which consists of showing that any Kantorovich solution has Monge structure, fails for multi-marginal problems with repulsive costs. One issue is symmetry; for $N = 3$ or more electrons, there is no mapping $\mathbb{R}^3 \to \mathbb{R}^{3(N-1)}$ other than the diagonal $x \mapsto (x, x, ..., x)$ (which is clearly not optimal) whose graph is symmetric under all permutations, and so the direct Monge ansatz cannot allow for all solutions. Even allowing for symmetrized Monge states does not capture all solutions, however, as competing interactions can lead to solutions degenerating onto higher dimensional submanifolds. Therefore, existence of (symmetrized) Monge solutions remains a challenging open problem.

In his review talk, Luca Nenna has given several numerical examples taken from [2] where minimizers are Monge or not. No clear intuition of what property of ρ implies the existence of Monge minimizers has emerged yet. On the other hand, Gero Friesecke has proposed in his review talk the concept of quasi-Monge states [17] which still imply a big decrease of complexity. Those have been proved to be minimizers in a toy model with discrete marginals but more investigation is required for general marginals.

More generally, it seems important to improve our understanding of the structure, regularity and sparsity properties of optimal plans for multi-marginal transport problems. Results in this direction for certain cost functions include [18, 21, 27, 38, 36], but repulsive costs, including the Coulomb cost arising in DFT, are much more challenging. This was explained at length by Liugi De Pascale in his review talk about the theory of multi-marginal optimal transport.

The challenging semi-classical limit $\hbar \to 0$

The second-order asymptotic in $\hbar$ of the limit in (2.0.7) has been predicted in [24]. It is only recently that the first order could be fully justified mathematically [9, 3, 31, 10]. It has been mentioned several times in the workshop that establishing the second-order rigorously is an important open problem. This essentially reduces to a semi-classical limit at fixed density, a very original setting which has never been considered in the mathematical literature, to our knowledge.

In the same direction, it has been predicted in [23, 24, 25] that the fermionic nature of the electrons should only affect the $\hbar$ expansion by an exponentially small error. Providing a proof of this fact is a very challenging open problem.

Towards a more solid mathematical foundation of DFT

During his review talk, Éric Cancès has summarized our mathematical knowledge about the foundations of Density Functional Theory. Several important questions remain. This includes for instance the understanding of when the Kohn-Sham nonlinear eigenvalues satisfy the aufbau principle (that is, are the N first eigenvalues of the corresponding mean-field operator). This problem has already been mentioned ten years ago in [6] and no real progress has been made in this direction.

The Hohenberg-Kohn theorem is the main mathematical result in DFT. Until recently, it was however plagued with a missing unique continuation principle for many-particle Schrödinger operators. This problem has been solved recently by Louis Garrigue in [19, 20] and announced at the conference, but the assumptions on the potentials are not yet optimal. In addition, the magnetic field case and current density functional theories need to be better understood [28], as was largely discussed by Andre Laestadius in his talk.

Finally, Jonas Lampart has discussed in his talk the difficulties of giving a mathematical basis to time-dependent DFT [15]. It was indeed mentioned several times during the conference that extending the OT limit of DFT to time-dependent problems is an interesting problem. In particular one should focus on understanding exact properties of adiabatic kernels. First results in this direction have already appeared in [29, 8].

Local Density Approximation and the Homogeneous Electron Gas

We have mentioned above in (2.0.6) the Local Density Approximation which consists in assuming that ρ is essentially constant locally (in boxes of volume dx) and to replace the local energy per unit volume by that of an infinite gas having the constant density $\rho(x)$ in the whole space. Understanding the regime in which the approximation is valid was the object of several discussions during the workshop. Kieron Burke has mentioned in his review talk several possible regimes in which he thinks that the LDA must be right. In the classical case $\hbar = 0$, a result of this kind was recently proved and reported during the conference [33, 13], for densities rescaled in the manner $\rho(x/N^{1/3})$. Extending these results to the quantum case is an important question.

In Physics and Chemistry, the Homogeneous Electron Gas is always identified with another system, sometimes called Jellium, where the density is not assumed to be constant over the whole space, but the electrons are instead submitted to an external positively-charged compensating uniform background. The link between Jellium and the Homogeneous Electron Gas is uncertain mathematically, especially after it was recently remarked that the usual proof does not work [32] for the Coulomb potential. In her talk, Codina Cotar has announced the recent theorem [12] that only the Coulomb potential poses some problems. For any potential in the form $|x|^{-s}$ with $s > 1$, Jellium and the Homogeneous Electron Gas have the same ground state energy in infinite volume. During the round table, Kieron Burke has however insisted on the remark that the values of the densities which matter in real systems are all above the solid-fluid phase transition of Jellium, hence are in the regime where Jellium necessarily coincides with the HEG.

A somewhat related question is to better understand the optimal constants in the Lieb-Oxford inequality [35, 32, 44], which provides exact constraints on the functional $F_{\hbar}^{\rm LL}[\rho]$. The optimal constant is sometimes believed to be the low-density limit of the uniform electron gas energy. In his talk, Simone Di Marino has reviewed the situation and started to explain a work in preparation about the 1D case, which can be fully understood using optimal transport methods.

Numerical challenges in Kohn-Sham(-SCE)

In his review talk Jianfeng Lu has introduced the Kohn-Sham density functional theory and he has especially focused on the self-consistent iteration in order to find a fixed point of the Kohn-Sham map. He has also presented the state of the art concerning the development of fast numerical solvers to solve these very high-dimensional problems. Concerning some recent developments which have been presented during the workshop we mention the one by Z. Musslimani [7] who numerically solve KS fixed point equation by mean of a spectral renormalization method and the preconditioning approach by A. Levitt [30].

Numerics for multi-marginal optimal transport

In his review talk Luca Nenna has presented the three main approaches to solve optimal transport problems and then he focused on the entropic regularization of Optimal Transport and the Sinkhorn algorithm [1, 37]. However this kind of approach presents some limitations in the case of multi marginal optimal transport with Coulomb cost since the computational cost increases exponentially in the number of marginal. This problem can be partially avoided by a multi-scale approach as the one introduced in [2]. Another kind of promising approaches (which seems to overcome the computational cost of the number of marginals) has been presented during the session on the numerical method for multi-marginal optimal transport: the one by L. Ying [26] and the one based on an approximation of the OT problem via marginals constraints moment by R. Coyaud [14].

Outcome of the Meeting

We expect that the cross-fertilization initiated by bringing together researchers in mathematical physics, optimal transport, physics and chemistry will have a significant impact on the field moving forward, contributing in particular to the resolution of many of the open problems described above. Informal discussion with the participants indicate that one important impact of the workshop will be the integration of the cultures of the various communities involved. We expect in particular that mathematicians, through their discussions with physicists and chemists, will consider problems holding increased physical or chemical relevance.

Participants

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Chapter 3

Frontiers in Single-cell Technology, Application and Data Analysis (19w5032)

Feb 24 - March 1, 2019

Organizer(s): Quan Long (University of Calgary), Jie Peng (University of California), Pei Wang (Icahn School of Medicine at Mount Sinai)

Overview

The last few years have seen an explosion of high throughput single-cell technologies for quantifying genetic, epigenetic, and RNA expression levels within individual cells, with the technologies for single-cell RNA sequencing comparatively the most mature. These breakthroughs pave the way for exploring biological systems at an unprecedented level of details. They allow us to look into inter-cellular variations and interactions and intra-tissue heterogeneity in biological samples, thus enabling the investigation of many fundamental biological questions far beyond those that could be tackled by traditional bulk tissue experiments. Single-cell technologies have led to the developments of novel computational and statistical methods that encompass data preprocessing, modeling and inference. Despite the progress, there is still much work to be done to meet the challenges and make use of the opportunities posed by the new data type.

Although there are sessions in statistical and computational biology conferences focusing on single-cell data analysis, researchers from these fields as well practitioners of these technologies would greatly benefit from a focused workshop, where it will be possible to exchange ideas, raise new questions and build future collaborations. Through this workshop, we aim to disseminate cutting-edge technological and computational advancements, to identify new challenges in data analysis and modeling, to provide a platform for interdisciplinary dialogue and to help shape future directions for this burgeoning field. The workshop was organized around the following topics:

- Single-cell technology: Experimental techniques and challenges.
- Biology applications based on single-cell technologies.
- Single-cell data analysis.
  - Computational and bioinformatics tools for data processing, integration, and visualization.
  - Statistical modeling to handle confounding effects, cell-to-cell variations, and intra-tissue heterogeneity.

During the workshop, we brought together both researchers who developed computational and statistical tools, as well as those who applied computational tools within their own domain, to identify key remaining challenges in these tools and develop collaborations to solve them. The workshop provided a unique opportunity for biologists, biotechnologists, statisticians and bioinformaticians to communicate, collaborate and work together to further advance this important research field.

Single-Cell Technologies

In the past decade, diverse technologies of single-cell experiments have been invented, including single-cell sequencing, single-cell transcriptomics, single-cell epigenomics and single-cell proteomics. Different types of experiments involve different technologies/platforms. Specifically, single-cell sequencing and transcriptomics are both based on the latest high-throughput sequencing technologies. In single-cell epigenomics experiments, sequencing techniques are further integrated with other physical/chemical/molecular approaches to monitor cytosine modification, protein-DNA interaction, chromatin structure, and three dimensional DNA organization. Moreover, single-cell mass cytometry instruments integrate mass spectrometry and cytometry technologies and enable real time monitoring of multi-protein targets.

Broad Biological Applications Based on Single-Cell Technologies

These diverse single-cell technologies have profoundly advanced single-cell biology research, from bench to clinic. In basic biology, all events at the single-cell level are stochastic, and single-cell experiments allow scientists to quantify and model this stochasticity, and from these models, draw inferences on the relationships between genes as well as the relationship between a gene and its epigenetic environment. Single-cell experiments allow much higher resolution in the study of transcriptional regulation. At the tissue level, single-cell experiments allow the discovery of new cell types and the characterization of known cell types and their relationships to each other. In clinical practice, single-cell experiments have direct applications, for example, to the quantification of intra-tumor heterogeneity in oncology and to the tracking of immune cell development in immunology.

Germline genomics and single-cell analysis of brain tumors
Brain cancer is one of the deadliest cancers, for example, GBM has poor clinic outcomes (i.e., with a survival of 1-2 years), low-grade glioma (LGG) with IHD1 wild-type (wt) has poor clinic outcomes as well, however, LGG with IDH1 mutations (mut) has good survival (i.e., with a survival of 5-6 years). It has been debated for years whether the LGG is the precursor of the GMB. Dr. Edwin Wang from University of Calgary conducted single-cell genomic analysis of LGG-IDH (wt), LGG-IDH (mut) tumors and GBM and developed methods to conduct the analysis. At the same time, Dr. Wang and team members analyzed the germline genomes of the patients. Their analysis showed that GMB with IDH (wt) and LGG with IDH (wt) have independent origins. Furthermore, they showed that nature killer (NK) cells play an important role in cancer progression and metastasis. The number of germline inherited variants affecting NK cell defects are negatively correlated with patient survival. A person who has high mummer of NK cell genetic defects has much higher chance to get brain tumors.

Single-cell RNA-sequencing of differentiating iPS cells reveals dynamic genetic effects on gene expression
Genetic variation affects human traits and disease risk via myriad pathways, including through changes in gene expression. Expression quantitative trait locus (eQTL) mapping is a widely-used approach to elucidate such effects. Dr. Daniel Seaton from The European Bioinformatics Institute leveraged a population-scale human induced pluripotent stem cell (iPSC) bank to study, in vitro, the effect of genetic variation on gene expression during human development. By combining single-cell transcriptome sequencing with a pooled experimental design of 125 cell lines, they assay gene expression variability across iPSC differentiation to two different fates: definitive endoderm and dopaminergic neurons. This allowed discovery of 1,000s of eQTLs in distinct developmental stages and cell types. Dr. Seaton and collaborators developed an allele-specific expression-based approach to identify eQTLs that are sensitive to differentiation and other cellular processes. For example, 800 eQTL effects were dynamic

across differentiation to endoderm, and these dynamics were generally uncorrelated with overall changes in gene expression. In sum, their data and methods illustrate the power of combining pooled iPSC lines with scRNA-seq to simultaneously discover and characterise genetic variants affecting gene expression in differentiating cells.

Effectively comparing publicly available single cell datasets: a case study in glioblastoma multiforme

Glioblastoma multiforme (GBM) is an aggressive form of brain cancer, accounting for 17% of all brain tumours and it has a poor prognosis. Despite this, the minority of GBMs with isocitrate dehydrogenase gene mutations have relatively good prognostic outcomes. Microglia and macrophage content of GBMs is widely described as up to one-third of all the total cells within the tumor. Flow cytometry of IDH-mutant and wild type show more pro-inflammatory markers in IDH-mutant tumours, but macrophages and microglia cannot be reliably distinguished with protein markers. To determine the distinct roles of microglia and macrophages, GBM and GBM-IDH mutant single cell datasets from publicly available on GEO were analyzed, revealing that the immune phenotype of the good prognosis IDH-mutant GBMs is driven by pro-inflammatory microglia. Challenges in quality control, normalizing, clustering, cell-type labelling and visualizing disparate datasets were addressed in this analysis, as well the labelling of spectra of behaviour like pro- vs anti-inflammatory.

Understanding gene regulation using single cell RNA-seq data

Single-cell analytics offers tremendous opportunity for studying different levels of gene regulation at single-cell resolution. Dr. Liu briefly introduced some of their preliminary results for designing computational methods in understanding cell type-specific polyadenylation, miRNA regulation, as well as cancer drug response prediction.

Single cell transcriptomics and fate mapping of ependymal cells reveals an absence of neural stem cell function

Ependymal cells are multi-ciliated cells that form the brain's ventricular epithelium and a niche for neural stem cells (NSCs) in the ventricular-subventricular zone (V-SVZ). In addition, ependymal cells are suggested to be latent NSCs with a capacity to acquire neurogenic function. This remains highly controversial due to a lack of prospective in vivo labeling techniques that can effectively distinguish ependymal cells from neighboring V-SVZ NSCs. Dr. Stratton described a transgenic system that allows for targeted labeling of ependymal cells within the V-SVZ. Single-cell RNA-seq revealed that ependymal cells are enriched for cilia-related genes and share several stem-cell-associated genes with neural stem or progenitors. Under in vivo and in vitroneural-stem- or progenitor-stimulating environments, ependymal cells failed to demonstrate any suggestion of latent neural-stem-cell function. These findings suggest remarkable stability of ependymal cell function and provide fundamental insights into the molecular signature of the V-SVZ niche.

Characterizing cell type-specific responses to stimuli using single cell RNA sequencing

Single cell RNA sequencing (scRNA-seq) technologies are quickly advancing our ability to characterize the transcriptional heterogeneity of biological samples, given their ability to identify novel cell types and characterize precise transcriptional changes during previously difficult-to-observe processes such as differentiation and cellular reprogramming. An emerging challenge in scRNA-seq analysis is the characterization of cell type-specific transcriptional responses to stimuli, when the similar collections of cells are assayed under two or more conditions, such as in control/treatment or cross-organism studies.

Dr. Quon has presented a novel computational strategy for identifying cell type specific responses using deep neural networks to perform unsupervised domain adaptation. Compared to other existing approaches, ours does not require identification of all cell types before alignment, and can align more than two conditions simultaneously. He has discussed on-going applications oftheirmodel to two problem domains: characterizing hematopoietic progenitor populations and their response to inflammatory challenges (LPS), in which their have identified putative subpopulations of long term HSCs that differentially respond to the challenge, and characterizing the malaria cell cycle process, in which they identify transcriptional changes associated with sexual commitment.

Single Cell Assessment of Tumor Heterogeneity

Each tumor is composed of multiple cell types, characterized by different genomic and transcriptomic profiles. Many methods have been proposed for the classification of tumor samples into different subtypes based on bulk tumor data. For this classification, a common practice is to utilize existing gene signatures that are expected to be upregulated in a particular subtype. A challenge when dealing with single cell transcriptomic data is due the high frequency of missing values. In fact, key markers specific to a particular subtype might be missing in most of the cells. Another challenge is that most of the existing gene signatures were experimentally validated using bulk tumor data; and therefore might not be appropriate for single cell transcriptomic data analysis. Dr. Petralia reviewed current methods utilized to classify single cells into different subtypes. In addition, Dr. Petralia propose a new method, which can classify cells into different subtypes while dealing with the sparse nature of the data. Different methods are compared based on single cell sequencing transcriptomic profiles of breast cancer data.

Single-Cell Data Analysis: Challenges and Opportunities

Single-cell data is complex and noisy, and presents new challenges arising from both the technical noise in the experiments as well the stochastic nature of single-cell biology. Some of the main technical issues with single-cell RNA sequencing arise from the experimental biases introduced within each cell in the RNA extraction, reverse transcription, and amplification steps. Cell size and cell cycle differences are also new sources of biological variation that needs to be modeled and accounted for. Moreover, the data is very sparse, with many zeros, due both to the technical issue of experimental dropout as well as the biological phenomenon of transcriptional bursting. How these various sources of noise impact downstream analyses, and how best to remove them, still remains under much debate. Yet, addressing these technical issues is necessary for reliable conclusions to be drawn from single-cell experiments.

The computational tools for analysis of single-cell profiles are still in their infancy. Both the sparsity and lower total read counts characteristic of single-cell profiles make tools previously developed for even the most basic analyses ill-suited for direct application to single-cells. As a result, in the past few years there has been an explosion in terms of new bioinformatics tools for performing tasks in common with bulk sample analysis and furthermore tools to analyze data for entirely new problems are now being developed (e.g. for ordering of single-cells along a differentiation trajectory, detecting bifurcating points in those trajectories, or identifying new cell types in collections of single-cells).

Transfer Learning in Single Cell Transcriptomics

Cells are the basic biological units of multicellular organisms. The development of single-cell RNA sequencing (scRNA-seq) technologies have enabled us to study the diversity of cell types in tissue and to elucidate the roles of individual cell types in disease. Yet, scRNA-seq data are noisy and sparse, with only a small proportion of the transcripts that are present in each cell represented in the final data matrix. Dr. Zhang proposed a transfer learning framework to borrow information across related single cell data sets for de-noising and expression recovery. The goal is to leverage the expanding resources of publicly available scRNA-seq data, for example, the Human Cell Atlas which aims to be a comprehensive map of cell types in the human body. Dr. Zhang's method is based on a Bayesian hierarchical model coupled to a deep autoencoder, the latter trained to extract transferable gene expression features across studies coming from different labs, generated by different technologies, and/or obtained from different species. Through this framework, Dr. Zhang and collaborators explore the limits of data sharing: How much can be learned across cell types, tissues, and species? How useful are data from other technologies and labs in improving the estimates from your own study? She has also discuss the implications of technical batch artifacts in the joint analysis of multiple data sets, and propose strategies for alignment of data across batch.

Impact of Misspecified Dependence on Clustering of RNA-seq Gene Expression Profiles

Clustering RNA-seq data is used to characterize environment-induced (e.g., treatment) differences in gene expression profiles by separating genes into clusters based on their expression patterns. Wang et al. (2013, Briefings in Bioinformatics) recently adopted the bi-Poisson distribution, obtained via the trivariate reduction method, as a model for clustering bivariate RNA-seq data. Dr. Leon discussed discuss the inadequacy of the bi-Poisson distribution in modelling the correlation between dependent Poisson counts, and its impact on clustering such data. Dr. Leon introduced the bi-Poisson Gaussian copula distribution as an alternative copula-based model that incorporates a flexible dependence structure for the counts. Dr. Leon then reported simulation results to investigate the impact on clustering of Poisson counts of misspecified dependence structures. Their simulations indicate that the clustering performance of the bi-Poisson distribution suffers when the cluster-specific correlations are negative, as the bi-Poisson distribution allows only positive correlations. Dr. Leon also found that although large positive values are also not admissible under the bi-Poisson distribution, their effect is minimal, especially when clusters are well separated. Dr. Leon illustrate their methodology on a lung cancer RNA-seq data.

Penalized Latent Dirichlet Allocation Model in Single Cell RNA Sequencing

Single cell RNA sequencing (scRNA-seq) data are counts of RNA transcripts of all genes in species' genome. Viewing the genes as building blocks of the genetic language, Dr. Wu and collaborators adapt the Latent Dirichlet Allocation (LDA) model, a generative probabilistic model originated in natural language processing(NLP), to scRNA-seq experiments. Dr. Wu and collaborators considered the DNA as nature's language using a four-letter alphabet, and the genome of a species defines its dictionary. The active transcriptome of a single cell is a document composed of different copies of various words, and the analogy of topics are biological functions a cell is performing. The observed transcript counts are a result of transcripts generated from a mixture of biological processes, each with a different gene usage frequency. She proposed a penalized version of LDA to reflect the sparsity expected in biological data. Dr. Wu and collaborators demonstrate that inferred biological topic frequency is a meaningful dimension reduced representation of the single cell transcriptomes and delivers improved accuracy in cell type clustering/classification.

Integrative Differential Expression Analysis and Gene Set Enrichment Analysis in Single Cell RNAseq Studies

Single cell RNA sequencing (scRNAseq) has been widely applied for transcriptomics analysis. One important analytic task in scRNAseq is to identify genes that are differentially expression (DE) between different cell types or cellular states and to perform subsequent gene set enrichment analysis (GSEA) to detect biological pathways that are enriched in the identified DE genes. These two types of analytic tasks – DE analysis and GSEA – are often treated as two sequential steps in commonly used analytic pipelines. However, these two tasks are intermingled with each other: while DE results are indispensable for detecting enriched gene sets and pathways, the detected enriched gene sets and pathways also contain invaluable information that can in turn improve the power of DE analysis. Therefore, integrating GSEA and DE analysis into a joint statistical framework can potentially improve the power of both. In the workshop, Dr. Zhou described a Bayesian hierarchical model (iDEA) to integrate GSEA and DE analysis. With simulations, Dr. Zhou show that, by integrating GSEA with DE, their method dramatically improves the power of DE analysis and the accuracy of GSEA over commonly used existing approaches. Dr. Zhou also illustrate the benefits of their new method with applications to two published scRNAseq data sets.

Fast and accurate alignment of single-cell RNA-seq samples using kernel density matching

With technologies improved dramatically over recent years, single cell RNA-seq (scRNA-seq) has been transformative in studies of gene regulation, cellular differentiation, and cellular diversity. As the number of scRNA-seq datasets increases, a major challenge will be the standardization of measurements from multiple different scRNA-seq experiments enabling integrative and comparative analyses. However, scRNA-seq data can be confounded by severe batch effects and technical artifact. In addition, scRNA-seq experiments generally capture multiple cell-types with only partial overlaps across experiments making comparison and integration particularly challenging. To overcome these problems, Dr. Chen and collaborators have developed a method, dmatch, which can both remove unwanted technical variation and assign the same cell(s) from one scRNA-seq dataset to their corresponding cell(s) in another dataset. By design, their approach can overcome compositional heterogeneity and partial overlap of cell types in scRNA-seq data. Dr. Chen further showed that this method can align scRNA-seq data accurately across tissues biopsies.

A statistical simulator scDesign for rational scRNA-seq experimental design

Single-cell RNA-sequencing (scRNA-seq) has revolutionized biological sciences by revealing genome-wide gene expression levels within an individual cell. However, a critical challenge faced by researchers is how to optimize the choices of sequencing platforms, sequencing depths, and cell numbers in designing scRNA-seq experiments, so as to balance the exploration of the depth and breadth of transcriptome information. In the workshop, Dr. Li present a flexible and robust simulator, scDesign, the first statistical framework for researchers to quantitatively assess practical scRNA-seq experimental design in the context of differential gene expression analysis. In addition to experimental design, scDesign also assists computational method development by generating high-quality synthetic scRNA-seq datasets under customized experimental settings. In an evaluation based on 17 cell types and six different protocols, scDesign outperformed four state-of-the-art scRNA-seq simulation methods and led to rational experimental design.

Reconstructing gene regulatory dynamics along pseudotemporal trajectories using single-cell RNA-seq

Single-cell RNA-seq (scRNA-seq) provides a powerful technology for analyzing gene expression landscape of individual cells in a heterogeneous cell population. Ordering cells along a pseudotemporal trajectory based on cells' progressively changing transcriptome is a useful way to elucidate cells' developmental lineages and decode dynamic gene expression programs along developmental processes. Today, scRNA-seq is the most widely used high-throughput single-cell functional genomic technology. However, this technology only measures transcriptome and does not directly provide information on cis-regulatory element (CRE) activities. Building upon previous work on predicting chromatin accessibility using RNA-seq in bulk samples, Dr. Ji developed a new method for predicting CRE activities in single cells using scRNA-seq. In the workshop, Dr. Ji introduced their new tool that uses scRNA-seq to construct cells' pseudotemporal trajectories and infer CREs' dynamic activities along pseudotime. Using this method, one can conduct pseudotime analysis of transcriptome and regulome simultaneously using only scRNA-seq data. Analyses of the Human Cell Atlas data demonstrate that this method is capable of reconstructing cells' gene regulatory programs along developmental processes.

Reconstructing haplotypes from bulk-sequencing data

Pooled sequencing (Pool-seq) is a next-generation sequencing (NGS) strategy where the genomes of several individuals from a population are grouped together and bulk-sequenced. Pool-seq provides an efficient and cost-effective alternative to genome sequencing of individuals or single cells, especially in contexts where pathogen genomes are inherently mixed. To determine the frequencies of individual-level polymorphisms and linkage disequilibrium (LD) from a population, the aggregated variation data must be de-convoluted in silico, an even more difficult task when haplotypes are not previously known and must be assembled de novo. Dr. Long has proposed a program, PoolHap, approximates the genotypic resolution of single-cell sequencing using only Pool-seq data by integrating population genetics models with genomics algorithms to reconstruct haplotypes.

Missing Imputation in Single-Cell RNA Sequencing Data

Single-cell RNA-sequencing (ScRNA-seq) technology is widely used to obtain genome-wide gene expression data at single-cell level. Often ScRNA-seq data contains large number of missing values or zero gene expression levels, which could be either biologically driven or technically driven due to the low capture efficiency of the sequencing technology. This imposes a great challenge to the downstream analysis as many (advanced) data analysis tools/models can not deal with missing values. Dr. Chowdhury from Icahn School of Medicine at Mount Sinai and team members developed a novel imputation method: DreamAI which is a consensus imputation algorithm based on multiple imputation strategies involving prediction-based imputation algorithms, machine learning algorithms, nearest neighbor clustering and low rank matrix approximation algorithms. Dr. Chowdhury apply DreamAI on ScRNA-seq data to impute the missing values and compare its performance with some existing methods.

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Chapter 4

Isogeometric Splines: Theory and Applications (19w5196)

February 24 - March 1, 2019

Organizer(s): John Evans (University of Colorado Boulder), Bert Jüttler (Johannes Kepler University, Linz), Giancarlo Sangalli (University of Pavia)

Overview of the Field

The allure of simulation-based engineering is that once a model of an engineering system is constructed, its design can be optimized for performance. Unfortunately, this promise of optimal system has still largely not been realized for complex systems. One of the largest challenges preventing this realization is the so-called design-through-analysis bottleneck.

The design-through-analysis bottleneck results from the fact that different geometric representations of engineering systems are utilized in design (geometric modeling) and analysis (numerical simulation). In design, geometric primitives such as Non-Uniform Rational B-Splines (NURBS) are employed to represent a geometry of interest, while in analysis, polygonal meshes are typically utilized to represent the same geometry. Consequently, design optimization requires not only changing the design representation and creating a new analysis mesh at each design iteration, but doing so in a way that is both automatic and tightly integrated (since it must be done repeatedly until convergence) and differentiable (since efficient and scalable optimization methods require gradients of simulation outputs with respect to design parameters).

The framework of Isogeometric Analysis (IGA), introduced in 2005 by Thomas J.R. Hughes and co-authors, has emerged as a very attractive approach to simulation-based engineering [1, 2]. IGA bridges the gap between design and analysis by employing a uniform representation for the geometry of engineering objects and for the physical quantities defined on it. This eliminates the need for slow and error-prone conversion processes between designed geometry and simulation models, and it enables the possibility of widespread use of design optimization tools in simulation-based engineering.

Given its potential to reshape simulation-based engineering, IGA has recently been the subject of a substantial amount of research activity at a global scale. In particular, there has been a near-exponential growth of publications. According to SCOPUS, there were 12 IGA-related papers published in refereed journal proceedings in 2008, 63 in 2011, 110 in 2014, and 360 in 2018.

Recent Developments and Open Problems

Despite the growth and popularity of IGA, it still suffers from a severe flaw. Namely, state-of-the-art techniques in geometric modeling (i.e., Bernstein-Bezier representations, Trimmed B-splines/NURBS, and Boundary Representations (BREPS)) are generally unable to be directly employed in analysis, especially for complex three-dimensional geometries of arbitrary topology. Consequently, the vision for this workshop was to develop a unified geometric modeling framework, which we refer to as isogeometric splines, that satisfies both the needs of design and analysis *a priori*. In particular, we seek a geometric modeling framework that can:

(i) Represent objects in arbitrary spatial dimension,

(ii) Represent objects of arbitrary topology or genus in a watertight manner,

(iii) Represent canonical objects such as conic sections exactly,

(iv) Represent localized features with minimal disruption and meaningful design parameters,

(v) Represent not just one geometry but rather families of geometries for design space exploration, optimization, and uncertainty quantification,

(vi) Easily incorporate geometric and topological operations and editing, and

(vii) Easily generate volume parameterizations from surface parameterizations.

Moreover, to meet the needs of analysis, the underlying basis should exhibit optimal approximation and conditioning properties and possess fast algorithms for basis evaluation, differentiation, and integration.

It should be noted that we are not looking to reinvent the wheel with isogeometric splines but instead seek to unify existing approaches and extend them. With this in mind, there exist several emerging technologies which we expect isogeometric splines to leverage, including subdivision surfaces [3], T-splines [4, 5], and hierarchical B-splines [6].

Presentation Highlights

During the workshop, each of the 21 participants had a 45-minute time slot to present his or her work. All presentations were of high quality and led to inspiring discussions. The following presentations were among the highlights of the week:

- Artem Korobenko (Canada) presented his results about "Isogeometric analysis for fluids, structures and fluid-structure interaction". He showed an impressive picture of the potential of the isogeometric simulation technology for demanding engineering applications arising in the aerospace, marine, and energy sectors.
- Carla Manni (Italy) presented her work on "Sharp error estimates for spline appoximation", focusing on a priori error estimates in L^2 with explicit constants for approximation by splines of maximal smoothness. This contribution showed that the advent of IGA inspired new research on classical topics in approximation theory.
- Nelly Villamizar (UK), who talked about the "Dimension of spline spaces and fat points ideals", clearly demonstrated that results from advanced algebraic geometry are highly significant for the construction of smooth isogeometric spline discretizations.
- Derek Thomas (United States), presenting "U-splines: Splines over unstructured meshes", showed how a start-up company has begun to transform the latest mathematical results from the IGA community into a commercial product that may change the traditional way of performing numerical simulation in industry.

See also Section 6 for further information about the talks at this workshop.

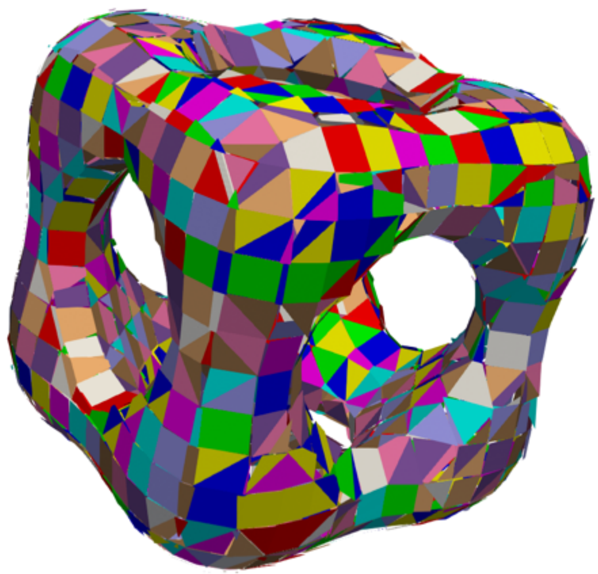

Figure 4.1: Linearization of a 3D object defined by trimming

Scientific Progress Made

Several talks during the workshop highlighted recent research advances that may aid in the development of a unified geometric modeling framework, namely isogeometric splines, that satisfies both the needs of geometry and analysis *a priori*, and several talks also identified deficiencies in state-of-the-art geometric modeling approaches toward the realization of a geometric modeling framework. In particular:

(i) Both the state-of-the-art and emerging approaches for geometric modeling in IGA were identified. We specifically mention the talks by Derek Thomas and Jessica Zhang on unstructured spline and T-spline representations.

(ii) The most pressing needs of geometry and analysis were identified. In particular, how to deal with trimmed representations (cf. Fig. 4.1) is currently one of the main issues facing the IGA community, and this topic was discussed by several participants, including René Hiemstra and Bert Jüttler.

(iii) The workshop also identified needs that are not met by current approaches and challenges the IGA community faces in meeting these needs. Besides trimming, the construction and analysis of globally smooth representations on multi-patch domains is needed for the discretization of high-order problems (e.g., Kirchhoff-Love plates and shells [7], the Cahn-Hilliard equation [8], the Navier-Stokes-Korteweg equations [9], etc.) on complex geometries.

(iv) Several promising approaches, including those originating outside of the computational geometry and numerical analysis communities, were presented. For instance, complementary approaches for addressing the problem of globally smooth representations were presented by Jorg Peters via techniques from classical geometric modeling, by Thomas Takacs based on numerical analysis, and by Nelly Villamizar with the help of results from algebraic geometry.

Outcome of the Meeting

Though the workshop did not produce any immediate results, we are convinced that its long-term impact cannot be understated. Design space exploration, optimization, and uncertainty quantification have the potential to dramatically improve the performance, efficiency, and reliability of engineering systems, though these tools have largely been limited to the academic sector. IGA harbors the potential to enable design space exploration, optimization, and uncertainty quantification in engineering practice. Nonetheless, the lack of a unifying mathematical framework which simultaneously addresses the competing needs of geometry and analysis have so far prevented the widespread adoption of IGA. Thus, the primary purpose of the workshop was to focus the vision of the IGA community and unify it toward a set of common goals. The workshop certainly fulfilled this purpose, as the participants identified the most pressing needs of geometry and analysis, the needs which are not met by state-of-the-art approaches, and the challenges the IGA community faces in meeting these needs. In addition, the workshop helped to establish new interdisciplinary collaborations between not only mathematicians and engineers but also between mathematicians across subfields (e.g., between numerical analysts and algebraists).

At the end of the workshop, it was clear that there remain several research advances that must be made before the workshop's vision for isogeometric splines can be realized. First, the problem of trimming must be resolved in a satisfactory manner, for instance, by the removal of trimming curves entirely or by the introduction of robust analysis procedures capable of handling trimmed objects. Second, the problem of constructing globally smooth representations of objects of arbitrary topology must be fully addressed, especially in the three-dimensional setting. Third, the problem of surface-to-volume parameterization remains largely unsolved, even though high quality volume parameterizations are required for the analysis of fluid flow and wave propagation. Fourth, while many new geometric modeling technologies have been introduced to address both the needs of design and analysis, most of these technologies are not able to incorporate topological operations that are common in solid modeling. Finally, virtually none of the geometric modeling technologies that have been introduced directly or naturally allow for the specification of geometric variability, and such a specification is required for the purposes of design space exploration, optimization, and uncertainty quantification.

It should be finally mentioned that the realization of isogeometric splines will not only impact simulation-based engineering but also rapid prototyping. Three-dimensional printing and additive layer manufacturing technology require watertight, three-dimensional input designs in order to produce reliable manufactured geometries. Given the rapid growth of rapid prototyping techniques, there is a pressing need for a change in paradigm to allow for watertight, three-dimensional geometric modeling, and the workshop's vision for isogeometric splines meets this need.

Abstracts

For completeness, the abstracts associated with each of the presentations of the workshop are included below.

The impact of parametrization on numerical approximation for isogeometric finite elements
John Evans

High-order finite element methods, including isogeometric finite element methods, harbor the potential to deliver improved accuracy per degree-of-freedom versus low-order methods. Their success, however, hinges upon the use of a curvilinear mesh of not only sufficiently high accuracy but also sufficiently high quality.

In this talk, theoretical results are presented quantifying the impact of mesh parameterization on the accuracy of a high-order finite element approximation, and a formal definition of shape regularity is introduced for curvilinear meshes based on these results. This formal definition of shape regularity in turn inspires a new set of quality metrics for curvilinear finite elements. Computable bounds are established for these quality metrics using the Bernstein-Bézier form, and a new curvilinear mesh optimization procedure is proposed based on these bounds. Numerical results confirming the importance of shape regularity in the context of high-order finite element methods are presented, and numerical results demonstrating the promise of the proposed curvilinear mesh optimization procedure are also provided.

The theoretical results presented in this talk apply to any piecewise-polynomial or piecewise-rational finite element method posed on a mesh of polynomial or rational mapped simplices and hypercubes. As such, they apply not only to classical continuous Galerkin finite element methods but also to discontinuous Galerkin finite element methods and even isogeometric methods based on NURBS, T-splines, or hierarchical B-splines.

This is joint work with Luke Engvall.

Untrimmed splines: Analysis suitable CAD

René Hiemstra

Current CAD technologies describe geometry by means of the boundary representation or simply B-rep. Boolean operations, ubiquitous in computer aided design, use a process called trimming that leads to a non-conforming description of geometry that is un-editable and incompatible with all downstream applications, thereby inhibiting true interoperability across the design-through-analysis process.

We propose a modeling paradigm in which designers are given the tools to create watertight, editable and conforming descriptions of geometry with interactive control over the boundary surface parameterization.

The methodology is based on recent advances in topological vector field design and processing. First, a smooth frame field is computed, by minimizing an appropriate energy functional on a background mesh of the initial B-rep, that is compatible with sparse or dense input constraints on alignment and size. Frame-field singularities, which together satisfy the topological invariant known as the Poincaré-Hopf theorem, are automatically placed and can be modified by the user. The frame field is used as a guide for the reparameterization of the initial B-rep into a conforming watertight and editable spline description.

In line with the main rationale of isogeometric analysis, the meshing and reparameterization techniques are applied within CAD as part of the design process, instead of as a post-processing step. The modeling tools actively support the design, analysis and manufacturing process as a whole, enabling true interoperability across these different disciplines and thereby support efficient product development.

This is joint work with Kendrick Shepherd and Thomas Hughes.

Quadrature rules for trimmed domains

Bert Jüttler

A common representation of a Computer-Aided Design (CAD) model is a boundary representation (B-rep), which typically consists of trimmed tensor-product NURBS patches. A trimmed surface patch consists of a tensor-product surface and a set of trimming curves on the surface that specify the boundary of the actual surface. Therefore, it represents only a part of the full tensor-product surface.

Computing integrals over trimmed domains both efficiently and accurately remains a challenging problem, notably for use in the frame of isogeometric analysis (IgA). In this talk, we present a specialized quadrature rule for trimmed domains, where the trimming curve is given implicitly by a real-valued function on the whole domain.

We follow an error correction approach: In a first step, we obtain an adaptive subdivision of the domain in such a way that each cell falls in a predefined base case. We then extend the classical approach of linear approximation of the trimming curve by adding an error correction term based on a Taylor expansion of the blending between the linearized implicit trimming curve and the original one.

This approach leads to an accurate method which improves the convergence of the quadrature error by one order compared to piecewise linear approximation of the trimming curve. It is at the same time efficient, since essentially the computation of one extra one-dimensional integral on each trimmed cell is required. Finally, the method is easy to implement, since it only involves one additional line integral and refrains from any point inversion or optimization operations. The convergence is analyzed theoretically and numerical experiments confirm that the accuracy is improved without compromising the computational complexity. Finally, we show that the method can be extended to trimmed trivariate representations, paving the way to isogeometric simulations on trimmed domains in 3D.

This is joint work with Felix Scholz and Angelos Mantzaflaris.

Multi-patch isogeometric analysis with C^2-smooth functions
Mario Kapl

We present a framework for the construction of a globally C^2-smooth isogeometric spline space over a specific class of planar multi-patch geometries, called bilinear-like G^2 multi-patch geometries. This class of geometries includes the subclass of bilinear multi-patch parameterizations and is characterized by the property to have the same kinds of connectivity functions along the patch interfaces as the bilinear parameterizations. The C^2-smooth isogeometric space is generated as the linear span of three different types of basis functions called patch, edge and vertex functions corresponding to the single patches, edges and vertices of the multi-patch domain. The construction of the single functions is simple, works uniformly for all possible multi-patch configurations and leads to basis functions with small local supports.

The potential of the constructed C^2-smooth space for applications in isogeometric analysis is demonstrated on the basis of several examples. Amongst others, we present a framework for solving the triharmonic equation, a sixth order partial differential equation, over planar multi-patch geometries. This problem requires the use of a C^2-smooth space as discretization space for the corresponding partial differential equation. Moreover, we perform isogeometric collocation to obtain a C^2-smooth solution of Poisson's equation over a planar multi-patch domain. Finally, we numerically show by means of L^2-approximation that the considered space of globally C^2-smooth isogeometric functions possesses optimal approximation properties, and that the generated C^2-smooth basis functions are well-conditioned.

This is joint work with Vito Vitrih.

Isogeometric analysis for fluids, structures and fluid-structure interaction
Artem Korobenko

This talk focuses on application of isogeometric analysis in various problems of computational mechanics. We first start with turbulent flows. The fluid mechanics is governed by incompressible Navier-Stokes equations posed on a moving domain using ALE framework. The equations are discretized in space using quadratic NURBS. The Variational Multiscale (VMS) method is used for turbulence modeling with mesh relaxation on a boundary. It is shown that higher order continuity basis functions provide better turbulence statistics. Also, the complex geometries can be modeled more accurately. The benefits of using IGA is presented on several examples, including atmospheric flow modeling over Bollund hill and Perdigao terrain.

Next, the NURBS-based IGA is applied to the damage modeling in composite structures. The higher order continuity of quadratic NURBS basis function allows the application of thin-shell theory such as Kirchhoff-Love, where your functions should be at least C^1-continuous. This also improves the stress representation which relax the strain localization. The numerical framework is applied to model progressive damage in UAV under extreme flight conditions and fatigue damage in wind turbine blades.

Finally, the computational FSI framework is presented with non-matching discretization on a boundary. The system of non-linear equations are solved iteratively using Newton-Raphson method with the block iterative coupling. The linearized system of equations is solved using GMRES. The framework is applied to simulate wind turbines at full scale under realistic operational conditions.

The show that FSI framework with IGA provides accurate solutions for various challenging problems, providing the data-of-interests that is not readily available or hard to acquire during the experiments.

B-spline-based monotone multigrid methods for the valuation of American options
Angela Kunoth

The valuation of an American option with Heston's stochastic volatility model leads to a free boundary problem in terms of a two-dimensional parabolic partial differential equation with a diffusion, convection and reaction term depending on the price of the underlying asset and its volatility.

We formulate this problem as a parabolic variational inequality on a closed convex set. To determine optimal risk strategies, one is not only interested in the solution of the variational inequality but specifically in the pointwise derivatives of the solution up to order two in space, the so-called Greeks. Initial conditions are commonly given as piecewise linear continuous functions which we approximate with B-splines with coinciding knots at the points where the initial condition is not differentiable. Furthermore, an improvement of the approximations of the spatial derivatives in the initial time steps is achieved by employing Rannacher timestepping. For solving the nonsymmetric discretised variational inequality in each time step and determining the derivative of the solution, we develop a monotone multigrid method for high order B-splines (with possibly coinciding knots) together with a projected iterative scheme. To do so, we construct restriction operators and monotone coarse grid approximations for tensor product B-splines of arbitrary order.

We demonstrate in the numerical experiments that we achieve fast convergence rates of the monotone multigrid method and highly accurate approximations of the Greeks.

This is joint work with Sandra Boschert.

Sharp error estimates for spline approximation
Carla Manni

The emerging field of isogeometric analysis (IGA) triggered a renewed interest in the topic of spline approximation and related error estimates. In particular, isogeometric Galerkin methods aim to approximate solutions of variational formulations of differential problems by using spline spaces of possibly high degree and maximal smoothness.

In this talk we focus on a priori error estimates in L^2 with explicit constants for approximation by splines of maximal smoothness defined on arbitrary knot sequences. We provide accurate estimates, which are sharp or very close to sharp in several interesting cases. These a priori estimates are actually good enough to cover convergence to eigenfunctions of classical differential operators under k-refinement.

The key tools to get these results are the theory of Kolmogorov L^2 n-widths, and related optimal spaces, and the representation of the considered Sobolev spaces in terms of integral operators described by suitable kernels.

This is joint work with Espen Sande and Hendrik Speleers.

Exploring geometrically continuous isogeometric functions in 3D
Angelos Mantzaflaris

One advantage of the framework of isogeometric analysis is that it allows for discretization spaces providing high order smoothness. Using these spaces can be beneficial when solving high order partial differential equations, including the Cahn-Hilliard equation, the Navier-Stokes-Korteweg equation and Kirchhoff-Love shells.

In addition, multi-patch parameterizations are required when considering more complex geometries, and the construction of globally smooth spline functions is a non-trivial problem. This has motivated research on the coupling of isogeometric multi-patch spline spaces across interfaces.

On the one hand, the coupling constraints can be enforced weakly, using variational methods or Lagrangian multiplier-based approaches. On the other hand, the smoothness constraints can be imposed strongly. It turns out that this is particularly well suited for generating C^0–smooth isogeometric splines on multi-patch domains. Furthermore, the construction of multipatch isogeometric discretizations possessing higher order smoothness has attracted lately the attention of several research groups, and has revived the interest of classical works in computer-aided design. Virtually all existing studies refer to the case of two variables, addressing properties such as dimension, suitable discretization bases, approximation and conditioning, etc.

The generalization to the trivariate case of these results is known to be more involved, both from a theoretical and practical viewpoint. In our work we follow a computational approach to discover the first formulas for the dimension of trivariate C^1–smooth isogeometric splines on two-patch domains. We obtain certified results by using exact rational computations on the corresponding linear algebra problem. Moreover, we observe recurring patterns in the nullspace of a collocation matrix expressing the C^1–conditions and we reduce the global problem to local, independent computations of compactly supported basis functions. Preliminary studies of the approximation power of the resulting spaces and discretization bases are encouraging. Nevertheless, we have just scratched the surface of the trivatiate case, since the treatment of domains with more general topology as well as rigorous mathematical theories remain open.

This is joint work with Katharina Berner and Bert Juettler.

Isogeometric analysis for compressible flows in complex industrial geometries
Matthias Möller

In this talk, we describe our IGA framework for the numerical analysis of rotary positive displacement pumps and, in particular, twin-screw compressors. Our approach is based on the overall philosophy that an efficient simulation and, at a later stage, optimization requires the co-design of all components involved in the pipeline, that is, the geometry model and the simulation tools. We present a fully automated algorithm for generating time sequences of analysis-suitable multi-patch parameterizations of counterrotating twin-screw rotor profiles that do not involve topology changes over time and fully exploit the computational potential of modern high-performance computing platforms. The algorithm is based on elliptic grid generation principles and adopts a mixed variational formulation that makes it possible to handle multi-patch parameterizations and parameterizations with C^0 spline basis functions directly. The second part of the talk describes our isogeometric flow solver which, following our co-design philosophy, makes use of auto-generated compute kernels to achieve optimal computational efficiency for each individual patch. The convective term of the Galerkin discretization is stabilized by flux-correction techniques that have been generalized to high-order B-splines in order to suppress the generation of unphysical oscillations in the vicinity of shocks and discontinuities. We finally address the curse of round-off errors which start to become a severe issue for high-order methods. In fact, round-off errors dominate the overall error already for moderate problem sizes if the approximation order is sufficiently large, rendering classical grid convergence studies impractical. We propose a novel a posteriori approach for predicting the optimal mesh width $h_{opt}^{(p)}$ as a function of the approximation order p and perform so-called $h_{opt}^{(p)}p$-refinement to reduce the total error effectively.

Geometrically smooth splines on meshes
Bernard Mourrain

In CAGD, a standard representation of shapes is a boundary representation using parametrized surfaces based on tensor product B-spline functions, which are the basis of the space of piecewise polynomial functions on a grid with a given regularity and degree. However, the complete description of a complex shape by tensor product B-spline patches may require to intersect and trim them, resulting in a geometric model, which is inaccurate or difficult to manipulate or to deform. To circumvent these difficulties, one can consider geometric models composed of quadrangular patches, glued together in a smooth way along their common boundary.

A first objective is to analyze the space of spline functions attached to such constructions. Given a topological complex $\mathcal{M}$ with glueing data along edges shared by adjacent faces, we study the associated space of geometrically smooth spline functions that satisfy differentiability properties across shared edges. We describe algebraic techniques, which involve the analysis of the module of syzygies of the glueing data, to determine the dimension formula of these spaces, for high enough degree. Dimension formula for polynomial patches and B-spline patches are provided. We present a general and algorithmic method for computing the basis. The construction yields basis functions naturally attached respectively to vertices, edges and faces.

The second objective is to construct efficiently geometrically smooth splines on meshes. We present a new subdivision scheme for computing geometrically smooth spline surfaces from a coarse quadrangular mesh. The resulting surface is G^1 everywhere and C^2 except at extraordinary vertices. Each face of the quadrangular mesh is associated to a bi-quintic spline patch. The Catmull-Clark subdivision scheme is used to compute the control points of B-spline patches associated to the faces of the quadrangular mesh. The nearest geometrically smooth biquintic spline surface is then explicitly computed by projection on the space of G^1 splines.

This is joint work with Ahmed Blidia, Nelly Villamizar, and Gang Xu.

Splines on irregular meshes
Jorg Peters

Splines elegantly connect the discrete and continuous computational world via control nets. Their extension to irregular meshes where the tensor-structure breaks down is essential and provides a rich source of mathematical insights. This talk emphasizes the role of splines over irregular meshes in the context of joining geometric design and engineering analysis in the spirit of iso-geometric analysis.

After a brief review of the rich literature since 1984 on using regular splines both for geometry and analysis, the talk presents a classification of techniques for irregular patch layout. Among the smooth surface constructions, the main distinction is between singular constructions (subdivision surfaces, polar layout surfaces, vertex-singular surfaces and rational Gregory surfaces) and regular parameterizations (geometrically smooth, transfinite and generalized barycentric constructions).

With focus on quad meshes and computing on surfaces, the talk discusses in detail: geometrically smooth constructions with T-junctions; subdivision stabilized by guide surfaces and made nearly finite by acceleration; and the class of vertex-singular surface constructions that can be generalized to volumetric hexahedral complexes with irregular edges and points.

Quadrature schemes based on spline quasi-interpolation for Galerkin IgA-BEM
Maria Lucia Sampoli

Boundary Element Method (BEM) is a numerical method to solve PDEs, in which the original problem is reformulated as a system of integral equations defined only on the boundary of the domain. The main advantages of the method are a reduced dimension of the computational domain and the simplicity to solve external problems. One of the important challenges in this topic is to accurately and efficiently solve singular integrals that arise from the boundary integral equations so formulated. Therefore, designing suitable quadrature schemes is one of the main active research topic in BEM. Recently new quasi-interpolation (QI) based quadrature rules have been introduced specifically for IgA-BEM setting. Such quadrature schemes are tailored for B-splines that are the considered basis functions. Quasi-interpolation allows to take advantage of the local support of the basis functions and to provide an approximation using the desired polynomial degree, keeping low the computational costs. The developed quadrature rules, hence provide very good accuracy and optimal convergence rate. Weakly, strongly and hyper-singular kernels related to the 2D integral formulation of the Laplace equation with different types of boundary conditions have been studied giving promising results especially when compared to standard and newest approaches applied in an isogeometric Galerkin BEM context. Moreover local refinability of the approximated solution of the problem is achieved by using hierarchical B-spline spaces.

Bernstein-Bézier techniques for continuous multivariate piecewise harmonic polynomials on simplicial partitions
Tatyana Sorokina

Since the only smooth harmonic splines are polynomials, continuous harmonic splines deserve special attention as possible subspaces for solving PDEs, and modeling harmonic functions. Bernstein-Bézier techniques for analyzing continuous harmonic splines in n variables are developed. Dimension and a minimal determining set for special splits are obtained using the new techniques. We show that both dimension and bases strongly depend on the geometry of the underlying partition. In particular, the angles in the triangulation play an important role. Due to a very small dimension of harmonic polynomials (as opposed to full polynomials), it is impossible to construct harmonic FEMs on unrefined simplicial partitions. We construct quadratic harmonic conforming FEMs on Clough-Tocher refinements and other special partitions.

Construction of smooth B-splines on Powell-Sabin triangulations
Hendrik Speleers

In this talk we will discuss the construction of a suitable B-spline representation for smooth splines on general triangulations. The considered splines have smoothness r and degree $d \geq 3r-1$, and are defined over a special refinement of the given triangulations. In such a refinement, called Powell-Sabin refinement, every triangle of the triangulation is split into six subtriangles. The B-spline construction can be geometrically interpreted as determining a set of triangles that must contain a specific set of points. The B-spline functions possess several interesting properties:

- local support,
- linear independence,
- nonnegative partition of unity.

This B-spline representation exhibits a natural definition of control points and an intuitive control structure in terms of local triangular nets. These triangular nets locally mimic the shape of the spline surface, and hence they can be used in the geometric design of smooth surfaces. On the other hand, such representation also presents interesting properties for engineering analysis. In particular, the representation allows for:

- stable evaluation and differentiation,
- efficient triangular Bézier extraction,
- optimal approximation and convergence,
- adaptive local mesh refinement.

Overlapping multi-patch domains in IGA
Thomas Takacs

In isogeometric analysis the domain of interest is usually represented by B-spline or NURBS patches, as they are present in standard CAD models. In order to avoid trimming, complicated domains can be represented as a union of simple overlapping subdomains, parameterized by single spline patches. Numerical simulation on such complicated domains is a serious challenge in IGA.

In this talk, we present a non-iterative, robust and efficient method. The computational domain is represented as a collection of B-spline based geometries with overlaps. Consequently, the problem is divided into several sub-problems, which are coupled in an appropriate way. The resulting system can be solved directly in a single step. We compare the proposed method with iterative Schwarz domain decomposition approaches and explore the advantages of our method, especially when handling subdomains with small overlaps.

We will show that the problems can be solved on overlapping patches by a simple non-iterative method, without using trimming. Summing up, our method significantly simplifies the domain parameterization problem. The performance of the proposed method is demonstrated by several numerical experiments in two and three dimensions.

This is joint work with Somayeh Kargaran, Bert Juettler, Stefan Kleiss, and Angelos Mantzaflaris.

Efficient preconditioners for *k*-refined isogeometric analysis
Mattia Tani

In this talk we discuss preconditioning strategies suited for isogeometric analysis, that are robust with respect to the spline degree p and to the mesh size h. Starting with the Poisson problem, we discuss a preconditioner that represents the same problem discretized on the reference domain. The preconditioner can be applied in a very efficient way thanks to the Fast Diagonalization method, that exploits the tensor structure of the basis functions. We then consider the heat equation, and consider a space-time discretization where smooth splines are used both in space and in time. We develop two numerical formulations for this problem, a symmetric high-order least squares formulation, and a nonsymmetric low-order Galerkin formulation. For both approaches, we develop robust preconditioners that can be applied efficiently thanks to a variant to the Fast Diagonalization method. We finally highlight advantages and drawbacks of the two formulations.

This is joint work with Gabriele Loli, Monica Montardini, Mauro Negri, and Giancarlo Sangalli.

U-splines: Splines over unstructured meshes
Derek Thomas

Isogeometric design and analysis is a growing area of research in computational engineering. In an isogeometric approach, the exact CAD representation is adopted as the basis for analysis. To unlock the full potential of isogeometric analysis depends strongly upon the analysis-suitable nature of the underlying geometry. Analysis-suitable geometry possesses a basis that is rich enough for both shape and solution representation. The exact analysis-suitable representation of smooth geometry is essential for correct solution behavior across many application domains. In this talk, we will present motivation and results for algorithms to construct unstructured spline basis functions over unstructured quad meshes (i.e., U-splines) that allow for the presence of T-junctions between mesh faces. We focus particularly on the requirements generality and linear independence of the basis functions. Our construction relaxes the analysis-suitability constraints that have been established for T-splines. We also consider the inclusion of extraordinary points in the mesh.

This is joint work with Luke Engvall, Steven Schmidt, Kevin Tew, and Michael Scott.

Polynomial splines of non-uniform bi-degree on T-meshes: Combinatorial bounds on the dimension
Deepesh Toshniwal

Polynomial splines on triangulations and quadrangulations have myriad applications and are ubiquitous, especially in the fields of computer aided design, computer graphics and computational analysis. Here, focusing on polynomial splines on T-meshes, we study the problem of computation or estimation of the spline space dimension. The general case of splines with polynomial pieces of differing bi-degrees is considered. In particular, using tools from homological algebra, introduced in the context of splines by Billera in 1988, we generalize the approach presented in Mourrain in 2014 and present combinatorial lower and upper bounds on the dimension. We also present sufficient conditions for the lower and upper bounds to coincide. Several examples are provided to illustrate application of the theory developed.

This is joint work with Bernard Mourrain and Thomas Hughes.

Recent developments for isogeometric methods with hierarchical splines
Rafael Vazquez

In this talk I will present several recent results towards the efficient use of hierarchical splines. I will first present a coarsening algorithm for the construction of admissible meshes, and show its advantages in the solution of the transient heat equation with a moving heat source. I will also present the construction of an additive multilevel preconditioner, based on admissible meshes, in such a way that the condition number is bounded and independent of the number of levels. In the last part of the talk I will show results on the construction of hierarchical C^1 basis functions on geometries constructed with two patches.

Dimension of spline spaces and fat points ideals
Nelly Villamizar

In this talk we will address the problem of proving a general formula for the dimension of spline spaces defined on polytopal partitions, particularly triangulations and tetrahedral complexes. We will show the connection between this problem and the study of the Hilbert series of fat points ideals in projective space. Combinatorial upper and lower bounds on the dimension will be presented to illustrate the advances and open problems in spline theory.

A practical unstructured spline modeling platform for isogeometric analysis applications
Jessica Zhang

As a new advancement of traditional finite element method, isogeometric analysis (IGA) adopts the same set of basis functions to represent both the geometry and the solution space, integrating design with analysis seamlessly. In this talk, I will present a practical unstructured spline modeling platform that allows IGA to be incorporated into existing commercial software such as Abaqus and LS-DYNA, heading one step further to bridge the gap between design and analysis. The platform includes all the necessary modules of the design-through-analysis pipeline: pre-processing, surface and volumetric spline construction, analysis and post-processing. Taking IGES files from commercial computer aided design packages, Rhino specific files or mesh data, the platform provides several control mesh generation techniques, such as converting any unstructured quadrilateral/hexahedral meshes to T-meshes, frame field based quadrilateral meshing, and polycube method. Truncated T-splines, hierarchical B-splines and subdivision basis functions are developed, supporting efficient local refinement and sharp feature preservation. To ensure analysis suitability, partition of unity, linear independence and optimal convergence rate of these basis functions are studied in our research.

IGA has very broad engineering applications like the finite element method, and specific application requirements always bring us new research problems and drive the future research directions. At the end of this talk, I will present several practical application problems to demonstrate the capability of our software platform. In addition to mechanics characterization for Navy, NAVAIR and Honda applications, in recent years we also developed novel image registration techniques using truncated hierarchical B-splines, an IGA solver to simulate material transport in complex neuron trees, and a new SimuLearn system to combine finite element method with machine learning for 4D printing.

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Chapter 5

Asymptotic algebraic combinatorics (19w5220)

March 10 - 15, 2019

Organizer(s): Alejandro Morales (University of Massachussetts at Amherst), Igor Pak (University of California, Los Angeles), Greta Panova (University of Southern California), Dan Romik (University of California, Davis), Nathan Williams (University of Texas at Dallas)

Introduction

Algebraic Combinatorics is an area of mathematics that employs methods of abstract algebra, notably group theory and representation theory, in various combinatorial contexts and, conversely, applies combinatorial techniques to problems in algebra and representation theory. Many of its problems arise from the need of quantitative and explicit understanding of algebraic phenomena like group representations and decompositions into irreducible representations, dimension formulae for modules, intersection numbers in geometry etc.

An important topic relates to Young tableaux, which carry the representation theory for the symmetric and general linear groups. The representation theory of S_n and GL_n is also carried with some structure to the ring of symmetric functions, which can also be interpreted as refined generating functions for discrete objects like Young Tableaux, plane partitions etc.

Initially Algebraic Combinatorics focused on the enumerative properties of these algebraic objects and then their combinatorial understanding. Notably such a result was the famous Hook-Length formula of Frame-Robbinson-Thrall, which gives the dimension of the irreducible representation $\mathbb{S}_\lambda$ of S_n, equivalently the number f^λ of Standard Young Tableaux of shape λ, as a product formula over the boxes in the Young diagram of λ:

$$f^\lambda = \dim \mathbb{S}_\lambda = \frac{n!}{\prod_{u\in\lambda} h_u}\,. \tag{5.0.1}$$

Besides its inherent beauty, this formula is useful in Asymptotic Representation Theory and Probability to determine the "typical" shape λ of a random standard Young Tableaux in the Plancherel distribution, a classical result of Vershik–Kerov [32] (see also the book [26] and the survey [29]).

Other such remarkable formulas include the enumeration of reduced decompositions of some permutations (see [4]), the hook-content formula for the number of semi-standard Young Tableaux (see e.g. [14, 28]). When no formula is possible, a concise combinatorial interpretation is also a solution like the rule for computing the

Littlewood-Richardson coefficients $c^{\lambda}_{\mu\nu}$, the multiplicities in the tensor product decompositions of GL_n irreducibles, giving them as the number of integer points in a polytope.

However, more often than not, formulas like (5.0.1) and interpretations like the Littlewood-Richardson rule are a miracle rather than a property. No explicit product formula is known for the number of plane partitions of general shapes λ, nor for the number of skew SYTs and skew SSYTs nor for the number of reduced words of a permutation, nor for the number of monomials of a Schubert polynomial. No positive formula, nor any form of discrete interpretation (#P formula) is known for the Kronecker coefficients (the analogues of Littlewood–Richardson coefficients for the decomposition of tensor products of irreducible representations of the symmetric group), nor for the Gromov–Witten invariants for the cohomology of the Grassmannian (whose combinatorics study is yet another major subfield of Algebraic Combinatorics), or alternatively the multiplicative structure constants of Schubert polynomials.

Yet discrete objects of algebraic origins like Schur functions, SYTs and plane partitions are also related to integrable models of particle or dimer configurations within Statistical Mechanics. These objects are also central to Asymptotic Representation Theory. In these fields, and, more generally, in Probability, the problems are about understanding the large scale limit or asymptotic behavior rather than having explicit exact formulas and descriptions. Other problems, coming from Geometric Complexity Theory (GCT) and the distinction of permanent vs determinant as a "P vs NP" approach, involve the comparison of various representation-theoretic multiplicities related to the Littlewood-Richardson, plethysm and Kronecker coefficients.

Algebraic Combinatorics has long since reached the boundary of the universe of explicit exact formulas. Yet major problems from Statistical Mechanics to GCT remain unsolved as they don't fall into the special world of objects enumerated by exact product formulas. Hence we need to find asymptotic formulas for the main objects of Algebraic Combinatorics and study the emerging field of **Asymptotic Algebraic Combinatorics**.

Previous advances in such directions came from Asymptotic Representation Theory originated by Vershik–Kerov, Kirillov, Okounkov, Borodin–Gorin–Rains, Biane et al. and continued recently in light of Integrable Probability and the analysis of interacting particle systems through interlacing arrays corresponding in the discrete world to SSYTs. Such results were largely possible thanks to the presence of "nice" formulas like product formulas, finite determinants, Selberg-type integrals etc, see [11, 12, 17].

Faced with the lack of such formulas for objects like skew SSYTs and Littlewood–Richardson coefficients, we now aim to study the asymptotics of these quantities using algebraic combinatorics, bijections, analytic combinatorics, and computer simulations. The workshop gathered specialists in Algebraic Combinatorics, Probability, Representation Theory with the aim of studying various available techniques for such analysis beyond the settings of integrable probability or classical analytic combinatorics.

Outstanding open problems

The main goal of the workshop was to bring together people from all the relevant areas, which are naturally very disjoint—Algebraic Combinatorics, Analytic Combinatorics, Probability, and Representation Theory, to share results and methods and establish the **asymptotic study of objects and quantities in Algebraic Combinatorics**. As mentioned in the introduction, the asymptotic analysis is the next step after exhausting the possibilities for nice product formulas. Yet, it is also necessary for the applications into Statistical Mechanics, Asymptotic Representation Theory, Geometric Complexity Theory and Algebraic Geometry.

Below we include a list of some concrete problems and applications that we were hoping we might address and make progress on during and as a result of the workshop. It is worth noting that, between the time we made our plans for the workshop and its actual occurrence, several of the problems were solved; this illustrates the fast-paced and dynamic nature of the field.

- Determine the asymptotic expansion of $f^{\lambda/\mu}$ as $\lambda/\mu \to \alpha/\gamma$, a region in the plane between two curves α, γ. By [18] we have $\log f^{\lambda/\mu} = \frac{1}{2} n \log n + O(n)$, where recent work of Morales-Pak-Tassy show that the next term of the expansion is $cn + o(n)$ for some constant c. Determine its dependence on the limit shape.

- Study the asymptotic behavior of $f^{\lambda/\mu}$ when λ, μ approach some limit curves. The question for what limit curves of λ/μ with $|\mu| = c|\lambda|$ and $c > 0$ a fixed constant is the dimension $f^{\lambda/\mu}$ asymptotically maximal has been recently answered in [24].
- Determine the asymptotic growth of the Littlewood–Richardson coefficients $c^{\lambda}_{\mu\nu}$, when λ, μ, ν approach certain limit curves as before, under the right rescaling.
- Stanley showed in [28, supp. exc. 79(c)] that for the Littlewood–Richardson coefficients we have $\log_2 \max_{\lambda,\mu,\nu,\lambda\vdash n} c^{\lambda}_{\mu\, nu} \sim \frac{n}{2}$. Find the limit shapes of the partitions λ, μ, ν where this maximum is achieved, and determine the asymptotic behavior when $\updownarrow, \mu, \nu$ approximate given curves. The conjecture of Stanley claims that both λ, μ and ν have to be Plancherel for the maximum to be achieved (personal communication), and was partially resolved in [24].
- For the Kronecker coefficients $g(\lambda, \mu, \nu)$ what is $\log_2 \max_{\lambda,\mu,\nu\vdash n} g(\lambda, \mu, \nu)$, and what is the general asymptotic behavior when λ, μ, ν approach given curves. The maximum is achieved when λ, μ, ν are all Plancherel [24].
- For the plethysm coefficients $a_\lambda(d[n])$, relevant to GCT, determine their growth as a function of n, d, λ.
- Determine $\mathfrak{S}_w(1^n)$, the evaluation of the Schubert polynomial at $(1, \ldots)$, asymptotically as a function of n and certain characteristics of w like occurrence of 231 patterns, see [15, 30, 33].
- Determine the number R_w of reduced words of w asymptotically as a function of certain characteristics of w like occurrence of 231 patterns.
- Determine the typical permutations at the equator of the weak Bruhat order. This problem is equivalent to the "great circle conjecture" in the random sorting networks of [2], and was solved in an exciting recent paper by Duncan Dauvergne (who presented his results at the workshop; see Section 3 below).
- Study the asymptotic expansion as a function of the variables x of the normalized skew Schur function

  $$\frac{s_{\lambda/\mu}(x_1, \ldots, x_k, 1^{n-k})}{s_{\lambda/\mu}(1^n)}$$

  as λ/μ approaches a limit profile. Alternatively, analyze lozenge tilings in "skew" domains, i.e. left and right boundaries given by μ, λ respectively, as opposed to the only studied case when one boundary is flat.
- Study the asymptotics of S_n normalized characters (after the breakthrough results by Biane, see [3], and Feray–Śniady, [6])
- Study the asymptotic limit surface of the distribution of monomials of Hilbert series in diagonal harmonics, proposed and christened "Marco Polo surface" by A. Garsia (cf. the proof of the shuffle conjecture in [5]).

Selected advances in the theory presented at the workshop

Twenty-two speakers presented their work during the workshop. We include below a short list of the theoretical advances presented in a few of the talks.

1. **Hook formulas for enumeration and asymptotics of skew tableaux**. Many analyses of the asymptotic behavior of Young tableaux are based on the classic hook-length product formula of Frame, Robinson and Thrall [7] for tableau of partition shape. However, this approach is limited in that it does not make it possible to answer questions about limit shapes except in a few simple cases (rectangular and staircase-shape tableaux) or derive asymptotics for tableaux of skew shapes, a regime where no product formula is known. Alejandro Morales (University of Massachussetts, Amherst) presented a novel enumerative and

asymptotic analysis for skew shapes relying on a new beatiful class of formulas to count skew tableaux by Naruse [20, 21] (announced in 2014) and Okounkov–Olshanski (1998) [23] that are positive sums of products of hooks. This talk summarized several of his recent papers, coauthored with Pak and Panova, studying the combinatorics and asymptotics of Naruse's formula and an upcoming paper with Zhu on the Okounkov–Olshanski formula.

2. **The Archimedean limit of random sorting networks.** Duncan Dauvergne from the University of Toronto presented his recent proof of the 2006 random sorting networks conjecture made by Angel, Holroyd, Romik and Virág [2]. This exciting result is the culmination of a sequence of papers by the authors of the 2006 paper, Gorin, Mustazee, and others, and constitutes a major advance in the field. The methods developed to attack the problem will surely play a role in future work on offshoots and analogues of the original problem.

3. **Limit shapes of Young tableaux.** Svante Linusson (KTH Royal Institute of Technology, Stockholm) presented his recent joint work with Robin Sulzberger and Samu Potka on the limit shape of shifted staircase standard Young tableaux, with applications to 132-avoiding sorting networks. The results are an application of the calculus of variations methods used to analyze limit shapes of random Young tableaux, as developed in earlier work by Vershik-Kerov, Logan-Shepp and Pittel-Romik, and discussed in the book [26].

4. **Generalized Pólya urn models and Young tableaux.** Cyril Banderier (Université Paris-Nord) presented additional results on limit distributions for random staircase shape Young tableaux derived in his recent work with Marchal and Wallner. These results are based on an innovative technique that relates the questions on these tableaux to a class of generalized Pólya urns. The related questions on Pólya urns can in turn be answered using sophisticated methods of analytic combinatorics.

5. **Evaluation of determinants.** Many problems in asymptotic algebraic combinatorics lead to algebraic quantities such as determinants, which we often wish to evaluate precisely and/or asymptotically. This leads to difficult questions about evaluation of determinants. Christian Krattenthaler (University of Vienna) gave a survey talk in which he illustrated with a few examples how determinants with interesting evaluations can arise in applications, and how one can formulate conjectures about the evaluations of such determinants and eventually prove those conjectures through a series of artful manipulations, inspired generalizations, experimental calculations, and a carefully honed intuition.

Selected open problems presented at the workshop

In addition to presentations by speakers of recent advances in the theory and survey talks about established methods and directions, we held a session in which participants could present some exciting open problems they are thinking about. In this section we discuss just a few of the problems presented. A full list of problems was compiled by Nathan Williams, one of the workshop participants, and made available to all the participants. We hope that this will stimulate future research and collaboration efforts.

Constants in asymptotic expansions of tilings (presented by Vadim Gorin, MIT)

The number of tilings of a hexagonal domain Ω by lozenges was given by MacMahon as

$$\#\text{tilings of } \Omega = \prod_{i=1}^{A}\prod_{j=1}^{B}\prod_{k=1}^{C} \frac{i+j+k-1}{i+j+k-2}.$$

The number of tilings of more general domains by lozenges don't usually have such nice formulas, but we can still ask about the following asymptotic expansion:

$$\ln\big(\#\text{tilings of } L\cdot\Omega\big) = L^2\gamma_1 + (L\ln L)\gamma_2 + L\gamma_3 + \cdots. \tag{5.0.2}$$

It is known that the first constant γ_1 in Equation 5.0.2 can be written for any domain as

$$\gamma_1 = \iint_\Omega S(\nabla h)dxdy.$$

The second constant γ_2 is believed to be "somewhat universal," mostly not dependent on the shape of the domain.

Problem 5.0.1. *What is the third constant in Equation 5.0.2? Vadim thinks it should be able to be written as*

$$\gamma_3 = \oint_\psi f(\textit{tangent})d\ell,$$

where f is some "mysterious" function.

Limit properties of tableau tuples (presented by Jang Soo Kim, Sungkyunkwan University)
Let A be a fixed standard Young tableau (SYT) of size r. We say that an SYT T contains A if A is equal to the tableau obtained from T by removing all cells containing integers greater than r.

Conjecture 5.0.2. *[29, Conjecture 6.1]*

$$\lim_{n\to\infty} \Pr \begin{pmatrix} \textit{a random } m\textit{-tuple } (T_1,\dots,T_m) \textit{ of} \\ \textit{SYT of size } n\textit{, all the same shape} \\ \textit{with each } T_i \textit{ containing } A \end{pmatrix}$$
$$= \lim_{n\to\infty} \Pr \begin{pmatrix} \textit{a random } m\textit{-tuple } (T_1,\dots,T_m) \textit{ of} \\ \textit{SYT of size } n\textit{,} \\ \textit{with each } T_i \textit{ containing } A \end{pmatrix}.$$

This conjecture may seem intuitively obvious by the following argument. The only difference between the two limits is the condition that $T_1, \dots, T_m$ must have the same shape. Since there is a limit shape of a standard Young tableau of size n when n tends to infinity, even if we choose $T_1, \dots, T_n$ independently, the shapes of $T_1, \dots, T_m$ should be almost the same. Therefore, the additional condition should not change the probability, and we should obtain (**??**).

But this "intuitive proof" is incorrect because we haven't used any properties of tableau containment: if it were correct, it would hold for any property of tableaux. More generally, let p : SYT $\to \{\mathrm{True}, \mathrm{False}\}$ be a tableau property and define

$$P_n = \Pr \begin{pmatrix} \text{a random } m\text{-tuple } (T_1,\dots,T_m) \text{ of} \\ \text{SYT of size } n\text{, all the same shape} \\ p(T_i) \text{ for } 1 \le i \le m \end{pmatrix} \text{ and}$$
$$Q_n = \Pr \begin{pmatrix} \text{a random } m\text{-tuple } (T_1,\dots,T_m) \text{ of} \\ \text{SYT of size } n\text{,} \\ p(T_i) \text{ for } 1 \le i \le m \end{pmatrix}.$$

For example, when $p(T)$ is the statement that the number of rows of T is greater than the number of columns of T then

$$\frac{1}{2} = \lim_{n\to\infty} P_n \neq \lim_{n\to\infty} Q_n = \frac{1}{2^m}.$$

Problem 5.0.3. *Find the statements $p(T)$ for which $\lim_{n\to\infty} P_n = \lim_{n\to\infty} Q_n$.*

Note. *Fedor Petrov sketched the idea of a proof of Conjecture 5.0.2.*

Problems related to hook formulas for d-complete posets (presented by Soichi Okada, Nagoya University)

Theorem 5.0.4. *(Naruse–Okada [21]) Let P be a connected d-complete poset and F an order filter of P. Then the multivariate generating function of $(P \setminus F)$-partitions is given by*

$$\sum_{\pi \in \mathcal{A}(P \setminus F)} \boldsymbol{z}^\pi = \sum_{D \in \mathcal{E}_P(F)} \frac{\prod_{v \in B(D)} \boldsymbol{z}[H_P(v)]}{\prod_{v \in P \setminus D}(1 - \boldsymbol{z}[H_P(v)])},$$

where D runs over all excited diagrams of F in P.

Problem 5.0.5. *Find a combinatorial (bijective) proof. More explicitly, find a decomposition*

$$\mathcal{A}(P \setminus F) = \bigsqcup_{D \in \mathcal{E}_P(F)} \mathcal{A}(P \setminus F)_D$$

such that

$$\sum_{\pi \in \mathcal{A}(P \setminus F)_D} \boldsymbol{z}^\pi = \frac{\prod_{v \in B(D)} \boldsymbol{z}[H_P(v)]}{\prod_{v \in P \setminus D}(1 - \boldsymbol{z}[H_P(v)])}.$$

Note. *This is proven in the famous paper [16] for skew shapes using the Hillman-Grassl algorithm.*

Conjecture 5.0.6. *(Okada [22]) If P is a connected d-complete poset, then*

$$\sum_{\sigma \in \mathcal{A}(P)} W_P(\sigma; q, t) \boldsymbol{z}^\sigma = \prod_{v \in P} \frac{(t\boldsymbol{z}[H_P(v)]; q)_\infty}{(\boldsymbol{z}[H_P(v)]; q)_\infty}.$$

Known Results : The conjecture holds

- if $q = t$ (Peterson–Proctor's hook product formula),
- if P is a rooted tree (use the binomial theorem and induction),
- if $P = D(\lambda)$ is a shape (= Young diagram) (Okada),
- if $P = S(\lambda)$ is a shifted shape (= shifted Young diagram) (Okada),
- if P is a bird (Ishikawa).

Asymptotics of oscillating tableaux (presented by Sam Hopkins, University of Minnesota)

In his nice survey "The Ubiquitous Young Tableau" [27], Sagan highlights three classes of tableaux: ordinary Standard Young Tableaux, shifted Standard Young Tableaux, and oscillating tableaux. Many people have studied asymptotics of both ordinary and shifted SYTs—what about oscillating tableaux?

An SYT of shape λ is a walk in Young's lattice of partitions from the empty shape $\varnothing$ to λ that only goes upwards. An oscillating tableau of shape λ is a walk in Young's lattice of partitions from the empty shape $\varnothing$ to λ that can use both upwards and downwards steps. More formally, an oscillating tableau of shape λ and length ℓ is a sequence $(\varnothing = \lambda^0, \lambda^1, \ldots, \lambda^\ell = \lambda)$ of partitions such that λ^i and λ^{i+1} differ in exactly one box for all i.

(Oscillating tableaux play roughly the same role for the symplectic group that SYT play for the general linear group.)

Problem 5.0.7. *Study asymptotics of oscillating tableaux. We can take either $\ell \to \infty$ or $|\lambda| \to \infty$ or both. In terms of what we "observe" from a random oscillating tableau $T = (\lambda^0, \lambda^1, \ldots, \lambda^\ell)$, there are various options, including:*

- *observe the Young diagram $\lambda^{\lfloor c\ell \rfloor}$ for some $0 < c < 1$ (which hopefully limits to a limit curve with the right normalization);*

- *write i at a box u if u belongs to exactly i of the λ^j, and observe these heights as a surface (which hopefully limits to a limit surface with the right normalization).*

Why could we hope for nice asymptotics? Because there are equally good product formulas for oscillating tableaux as for SYT! Set $\mathrm{OT}(\lambda, \ell)$ to be the set of oscillating tableaux of shape λ and length ℓ.

Theorem 5.0.8 (Sundaram [31]). *Let $|\lambda| = k$. Then*

$$\#\mathrm{OT}(\lambda, k+2n) = \binom{k+2n}{k} \cdot (2n-1)!! \cdot f^\lambda,$$

where $f^\lambda := \#\mathrm{SYT}(\lambda)$ is given by the usual hook-length formula.

There are also weights one can apply to oscillating tableaux (which don't make sense for SYTs) and which still give product formulas:

Theorem 5.0.9 (Hopkins-Zhang [9]). *Let $|\lambda| = k$. Then*

$$\sum_{T \in \mathrm{OT}(\lambda, k+2n)} \mathrm{wt}(T) = \#\mathrm{OT}(\lambda, k+2n) \cdot (k+2n+1) \cdot \frac{3k+2n}{6},$$

where $\mathrm{wt}(\lambda^0, \ldots, \lambda^\ell) := \sum_{i=0}^{\ell} |\lambda^i|$.

Theorem 5.0.10 (Han-Xiong [8]). *Let $|\lambda| = k$. Then*

$$\sum_{T \in \mathrm{OT}(\lambda, k+2n)} \mathrm{wt}_P(T) = \#\mathrm{OT}(\lambda, k+2n) \cdot (k+2n+1) \cdot Q(k, 2n+k),$$

where $\mathrm{wt}_P(\lambda^0, \ldots, \lambda^\ell) := \sum_{i=0}^{\ell} P(|\lambda^i|, i)$ for any fixed bivariate polynomial $P(x,y)$, and $Q(x,y)$ is another bivariate polynomial depending on P (in a recursive way).

It would also be interesting to study random oscillating tableaux according to these weights (e.g., can clearly obtain Plancherel measure with $\lambda = \varnothing$ in this way).

Nonstandard longest increasing subsequences (presented by Robin Pemantle, University of Pennsylvania)
It is well-known [26, 32] that the expected length of the longest increasing subsequence (LIS) of a random permutation of length n is $2\sqrt{n}$. Consider instead the expected length of the LIS of a simple random walk (i.e., steps of ± 1, each with probability $1/2$). By [1, Theorem 2], this expectation is at least $(1/1000)\sqrt{n}\log_2 n$.

The Ultra-fat tailed random walk is defined in [25, Section 2.2]. For a fixed number of steps, the following easier construction will do. Let π be a random permutation on $[N]$ and let $\{Y_i\}$ be IID ± 1 fair coin flips. For $k \leq N$, let

$$S_k = \sum_{j=1}^{k} Y_j 10^{\pi(j)}.$$

Problem 5.0.11. *Determine the length of the LIS in $S_1, S_2, \ldots, S_N$.*

It is shown in [25] that the mean and median are bounded between two powers of N, determined by recursions, and in particular it is at least $N^{0.69}$ and at most $N^{0.82}$. Neither recursion can yield a sharp bound. Simulations show it is around $N^{0.71}$.

Stanley's Schubert shenanigans (presented by Greta Panova, University of Southern California)
This problem originates with Richard Stanley. Each permutation $w \in S_n$ has a corresponding Schubert polynomial $\mathfrak{S}_w(x_1, x_2 \ldots, x_n)$. Define

$$\gamma_n = \max_{w \in S_n} \mathfrak{S}_w(1, 1, \ldots, 1).$$

Using well-known formulas for Schubert polynomials, γ_n can be rephrased in terms of reduced words, or in terms of pipe dreams.

Conjecture 5.0.12 ([30, Section 5])**.**

1. *Show that the limit* $\lim_{n \to \infty} n^{-2} \log_2 \gamma_n$ *exists.*
2. *Compute the value* c *of this limit.*
3. *Find the permutation(s)* w *achieving* γ_n*.*

It is known that

$$2^{n^2/4} < \gamma_n < 2^{\binom{n}{2}}.$$

Moreover, if c exists, then $0.2932362762 < c < 0.46$; the lower bound is obtained by considering a family of "layered permutations" [19], while the upper bound follows from a "rigorous heuristic argument" due to due to Damir Yeliussizov and Igor Pak (unpublished) for the corresponding $\limsup$. In [15], Merzon and Smirnov conjectured (on the basis of numerical evidence for $n \leq 10$) that this family realizing the lower bound also realizes the upper bound:

Conjecture 5.0.13 ([15, Conjecture 5.7])**.** *Every permutation* $w \in S_n$ *with* $\mathfrak{S}_w(1, 1, \ldots, 1) = \gamma_n$ *is a layered permutation.*

A panel discussion on the future of the field

This workshop has been the first attempt by the organizers to gather together experts from multiple areas with the goal of catalyzing new research and a fruitful exchange of ideas in asymptotic algebraic combinatorics. We feel that the area of the workshop is undergoing tremendous growth and becoming established as an important area of research. To help inform our and the participants' thinking about future directions, we held a panel session in which the future of asymptotic algebraic combinatorics (and more generally algebraic combinatorics), was discussed. The panelists were Igor Pak and Dan Romik, and the panel was moderated by Greta Panova. Many others among the workshop participants expressed opinions about future directions for the field, both in the mathematical sense and in terms of how activities should be organized, how we can better support the progress of graduate students and early-career researchers, and so on. This was a thought-provoking experience.

Participants

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Chapter 6

Mathematical Criminology and Security (19w5101)

March 17 - 22, 2019

Organizer(s): Theodore Kolokolnikov (Dalhousie University), David J.B. Lloyd (University of Surrey), Martin Short (Georgia Institute of Technology)

Overview of the Field

Mathematical criminology and security is an emerging field that combines quantitative and qualitative criminology theories with mathematical analysis and methods to provide new tools for understanding and predicting criminal behavior. These tools may then be employed by law enforcement practitioners to provide evidence-based policing strategies to aid in efficient resource allocation.

Mathematical criminology to date has focused on two main areas: predictive policing and understanding crime hotspot formation. Predictive policing emerged from the seminal work of Mohler [14] where they modelled burglary crime via a self-exciting point process in order to capture the repeat victimisation temporal dynamics. This approach is very different to multi-level modelling and statistical analysis commonly done in criminology which usually only attempts to model explanatory variables or static count models; see [18] for a review of current quantitative criminology. The self-exciting point-process model has proven to be the key basis for all subsequent work in the field due to is simplicity and versatility.

One of the key observations from the predictive policing is that urban crime clusters in space. Developing an understanding of the reasons for why hotspots form and how they will react to police intervention has been a major area for the field [28, 1, 26, 2, 30, 10, 9] The modelling of crime hotspot formation starting from agent-based models has produced an Dynamical systems and partial differential equation analysis has helped to show that there are two types of hotspots (supercritical and subcritical) and these are either displaced or completely eliminated by hotspot policing.

Along side the mathematical work, there has been a considerable amount of quantitative and qualitative criminology research. However as pointed out by Prof. P. Jeffrey Brantingham in his talk at the workshop, despite all the research no significant improvement in the prediction of crime as been achieved using multi-level modelling. This leads to the key question in the field: have we reached the limits of predictive crime models or are we missing something in the models?

Recent Developments and Open Problems

We focus on developments made by mathematicians working in criminology who are using a variety of statistical, modelling, and dynamical systems/partial differential equations techniques.

Recent advances have been in uncertainty quantification and data assimilation techniques for criminology/policing applications such as inferring network structures e.g., social networks, or links between crimes []. There has also been a considerable amount of work on analysing the statistical link between road networks and crime [ref].

- Prediction and inference:
  - inferring network structure: roads, social
  - inferring crime linkage
- Modelling:
  - urban crime/burglary PDE models
  - Coordination games
  - age-structured models

Presentation Highlights

- P. Jeffrey Brantingham: The Structure of Criminological Theory

  Prof. Brantingham opened up the workshop on the structure of criminological theory where he highlighted a possible ‘crises’ in explaining crime in that there have been no major improvements in multi-level statistical models commonly used in quantitative criminology. In his talk, Prof. Brantingham outlined the key problem in trying to explain variability in crime across space, time and individuals.

- Patricia Brantingham: Patterns in Crime: An Overview

  Prof. Brantingham gave an overview of core concepts in patterns in crime such as activity space, awareness space, push and pull in cities. Understanding the underlying structure of a city is very important in trying to uncover crime patterns. A key concept that was introduced was that of ‘Directionality’ to a crime location for individual criminals leading to ‘Directionality boundaries’ where crime is observed to be maximal. Open problems presented include how to combine mobility data and models to improve crime prediction, modelling fear-of-crime, and what topology can say about

- Jonathan Ward: Agent-based models and data assimilation

  Dr. Ward presented various mathematical tools to analyse and combine data with agent-based models (known as ABMs). ABMs are commonly used on computational sociology to model individuals as agents and their actions/interactions. Mathematically, these models are very hard to analyse and combine with data and there is an immediate need to develop new mathematical techniques for AMBs. Dr. Ward presented various techniques such as bayesian model selection, data assimilation, and equation-free methods.

- Craig Gilmour: Self-Exciting Point Processes for Crime

  Mr. Gilmour presented his work looking at using the Hawkes process for predicting crime space and time locations. He looked at Chicago and highlighted that a constant background crime rate does not fit the data. It is suggest that an anisotropic background crime rate with an isotropic excitation rate.

- Baichuan Yuan: An Efficient Algorithm for Spatiotemporal Multivariate Hawkes Process and Network Reconstruction

Mr. Yuan presented his work on developing uncertainty quantification methods to infer a hidden network structure based on event count data using a Hawkes process model. The key challenge here is that to infer a large networks requires a large amount of data and computationally efficient methods. Mr. Yuan presented a novel approach to the problem and demonstrated his method on a real social network application. It is clear that there are some interesting future directions for research in this area from both a statistical and modelling perspective.

- Michael Porter: Spatial event hotspot prediction using multivariate Hawkes features

  Prof. Porter talked about how one might determine if two crimes are linked together using a combination of a Hawkes process to determine the probability that one crime is linked/caused by another and linkage using a logistic regression model. Open problems presented here were

  – Can the self-exciting models help estimate linkage probabilities?

  – Can we use linkage to help inform self-exciting models?

- Yao Xie: Scanning statistics for crime linkage detection

  Prof. Xie talked about their work on change point detection to detect anomalies and how to develop data driven police patrol zones optimally. For the change point detection a generalised likelihood ratio detection statistic was developed. Open problems in this area include developing good spatio-temporal-textual point processes and developing a reinforcement learning approach.

- Naratip Santitissadeekorn: Approximate filtering of intensity process for Poisson count data

  Dr. Santitissadeekorn presented his recent work on developing sequential data assimilation (filtering) techniques for the discrete-time Hawkes process on a lattice. The objective is to develop efficient tracking methods rather than reconstruction of the past. Open problems in this area including developing efficient filters for crime linkage detection and network problems.

- George Mohler: Predicting crime is easy, using crime predictions is hard

  In this talk, an overview of crime prediction algorithms was presented and the problems associated with trying to using crime prediction software in practice. Practical problems such as how to increase officer buy-in or how to get the public or other groups more involved in using crime models were discussed. It was also discussed how one can introduce ‘fairness’ into the system to deal with bias in the data. Open problems such as should models be regulated and how to make use of probabilistic predictions were discussed.

- Hao Li: Uncertainty Quantification for Semi-Supervised Multi-class Classification in Ego-Motion Analysis of Body-Worn Videos

  Mr. Li presented his work on how to perform classification of body-worn police videos with a small amount of annotated training data. The main problem is that a massive amount of video data is collected without labelling and it is a problem how to make efficient use of human labelling (triage)? For this problem he developed a novel uncertainty quantification algorithm to carry out the labelling efficiently and highlight where human labelling is required. This was then demonstrated on real data.

- Nancy Rodriguez-Bunn: Modelling Riot Dynamics

  Prof. Rodriguez-Bunn presented her work on modelling the 2005 French riots using a non-homogeneous Poisson process and a Susceptible-Infected-Recovered model. Open problems in this area are how to effectively model and forecast riot activity.

- Chunyi Gai: Existence and stability of spike solution in SIRS model with diffusion

  This talk looked at a variant of the Susceptible-Infected-Recovered model from epidemiology with spatial diffusion that can lead to stationary spatial spikes in the infected population. A stability analysis of the spikes was carried out. An open problem is to analyse spatio-temporal spikes.

- Toby Davies: Street networks and their role in crime modelling

  This talk looked the link of the street network and burglary crime. Several challenges were highlighted such as how 'Directionality' can be reconciled with the street network, community structure and analyse of immunity when crime does not happen despite being predicted. It was also discussed how to link a network-based models to continuous continuum models.

- Wen-Hao Chiang: Multi-armed bandit problem on rescue resource allocation

  This talk presented the problem of how to use hot-spot prediction for early resource allocation leading to the problem of exploration versus exploitation. The key challenge is how to develop efficient algorithms to solve this problem.

- Ian Brunton-Smith: Collective efficacy and crime in London: The importance of neighbourhood consensus

  In this talk, the criminology theory for collective efficacy was presented and new opportunities for mathematical modelling of collective efficacy was suggested. For instance, can mechanistic models help understand the formation/dynamics of spatio-temporal consensus of collective efficacy? can we understand the impact of external events like terror attacks?

- Maria R D'Orsogna: Santa Monica, the train and proposition 47

  In this talk an analyse of violent crime in Santa Monica and the possible reasons for the recent increase (a new train line or proposition 47 law change) were investigated. Open problems here are in trying to determine the key causes of violent crime patterns to change.

Scientific Progress Made

The workshop ran several discussion groups to focus on key areas of interest.

- Bias - boundaries of patrols: too little police on boundaries, too much police (worry about incidental arrests reinforcing crime hotspots) could mathematically model
- Networks and neighbourhood/community effects: this session discussed how one might model various physical transportation networks and link this with social networks.
- Directionality: mobility $\rightarrow$ direction of crime to travel paths, what is a boundary and porosity of boundaries. Geographic profiling. Predictive incorporating into self-exciting models, mobility data.
- Prevention and Intervention - prevention is defined as long-term and intervention as short-term. Open problem to look at age-structured models to predict 40year crime waves and to investigate intervention strategies e.g. at what age should society intervene? Main challenge is to overcome the low probabilities of events and either saying intervene on everyone or no one.

Outcome of the Meeting

The meeting highlighted two main interesting directions for the future of mathematical criminology:

- The first area for future work is in prediction and inference where recent developments in uncertainty quantification and data assimilation could be combined with network models to help improve explaining the variability in crime.

- The second area for future work highlighted is in modelling and mathematical analysis of other types of criminology (Learning) theories such as social disorganisation, differential association, control theory, ANOMIE, conflict theory, labelling theory etc. The aim of the models would be to combine various qualitative theories to see if they can explain
- Build a community and organise workshops to develop the field of mathematical criminology.

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Chapter 7

New and Evolving Roles of Shrinkage in Large-Scale Prediction and Inference (19w5188)

7 - 12 April, 2019

Organizer(s): Edward George (University of Pennsylvania), Eric Marchand (University of Sherbrooke), Gourab Mukherjee (University of Southern California), Debashis Paul (University of California, Davis)

Overview of the Field

The BIRS workshop "New and Evolving Roles of Shrinkage in Large-Scale Prediction and Inference" brought in thirty-six experts in statistical theory, methods and related applied fields to assess the latest developments and explore new directions in the field of shrinkage methodology and algorithm development for large-scale prediction and statistical inference. There were twenty-six talks and two discussion sessions during the workshop focusing on both the current and future state of this rapidly evolving field. The talks were divided into the following themes:

- Empirical Bayes and optimal shrinkage under heterogeneity and asymmetry,
- Shrinkage priors for Bayesian prediction and inference,
- Spectral shrinkage and inferences under unknown covariances,
- Non-linear shrinkage and penalization methods for structured estimation,
- Efficient and scalable shrinkage algorithms for Big Data Analytics.

Overall there was general consensus that shrinkage methods are now omnipresent in modern data science. The traditional roles of shrinkage have been massively revolutionized as complex shrinkage penalties pertinent to modern data structures are used for large-scale predictive modeling. Historically, the elegant mathematical statistics theory developed following the celebrated works of [87, 86, 9] guided and popularized the usage shrinkage perspective in varied applications as a tool to calibrate bias-variance trade-off. Over the past decades, there has been enormous growth of new applied shrinkage methods. The foundational decision theoretic perspectives now needs to be extended to complex high-dimensional framework to be useful for evaluating efficacy of modern methods. The recent developments in shrinkage theory and methods that were presented in this workshop illustrate the conjoint evolution of field in theory and methods. There has been increasing emphasis on non-linear shrinkage methods that can adapt to latent structure in the data generation process. Lasso-type methods in the Frequentist domain and local-global shrinkage prior based methods in the Bayesian domain have been very successful in variable selection applications. Though contemporary Frequentist and Bayesian approaches to structured shrinkage modeling involves different computational tools, the corresponding estimators are often proved to enjoy similar decision theoretic optimality properties. Shape constraint estimation has been a vibrant area in the recent years yielding pragmatic robust methods based on non-parametric maximum likelihood methodology. The workshop also displayed shape-constrained estimation in the Bayesian domain where novel approaches to set-up constrained MCMC samplers are being used. The workshop had talks involving inference in domains where the covariance structure is unknown and needs to be estimated from the data. These recent works involve new mathematical statistics ideas particularly those involving the spectrum of large matrices and yielded powerful methodologies that can be applied to inventory management, weather forecasting, health-care and environmental sciences. The workshop also illustrated recent developments in predictive density estimation. High-dimensional predictive density estimates adapting to various constrains has been developed and they can be used for probability forecasting in a host of modern applications. The power of predictive density estimation methods were displayed by showing their superior risk properties compared to estimative plug-in approaches. The participants agreed that there is a growing need for a confluence of modern theory and large-scale shrinkage applications. This confluence is extremely important for disciplined growth of the subject by understanding the operating characteristics and working principles of innumerable different penalties proposed by practitioners and data enthusiasts.

Recent Developments and Open Problems

The workshop brought to fore the latest usage of shrinkage methodology along with their associated theoretical support and guarantees. Perhaps, the Gaussian sequence model [48] is the simplest framework to explicitly study the role of different kinds of linear and non-linear shrinkage [95, 10, 9, 19]. The optimal direction and magnitude of shrinkage has been well-studied in this set-up [14, 32, 33] and these traditional results have lead to an elegant mathematical theory for risk analysis and decision theory in models where the number of parameters increases along with sample size and equals to the number of observations. These form the foundations for shrinkage theory in modern complex models though closed form estimators and exact tractable analysis is not available here. An intrinsic challenge in shrinkage methods is accurate estimation of the shrinkage hyper-parameters so that the resultant algorithm is tuned for optimal estimative or predictive performance. Most of these traditional results dealing with optimal shrinkage consider a parametric family of estimators indexed by shrinkage hyper-parameters that are then optimally tuned [22, 23, 11, 21, 68]. In real-world applications, these parametric families of estimators often have limited usage and there is need to consider flexible non-parametric counter-parts. Conducting optimal non-parametric shrinkage estimators is difficult [13] and very recently powerful theory and methods in that direction have been proposed [46, 47, 53, 54, 85, 18] by using *Non-parametric Maximum likelihood* (NPMLE) based techniques. This workshop had four talks demonstrating the applicability of NPMLE in constructing potent non-parametric shrinkage estimators. These recent works shows that incorporating shape constraints such as monotonicity improves these estimation frameworks and the resultant estimators are robust and adaptive. A convenient aspect of these estimators is that they can be computed using convex optimization solvers. In this context, the recent R package REBayes of [52] has seen popular usage for implementing these methods.

In complex models that are typically used in contemporary data analysis, the empirical Bayes (EB) perspective [79, 80, 96, 1] is used as an efficient interface for conducting shrinkage by pooling information through a hierarchical set-up. Hierarchical modeling has become an increasingly important statistical method in modeling large and complex datasets as it provides an effective tool for combining information and achieving partial pooling of inference [89, 57, 6]. The applications of hierarchical models involve simultaneous inference on different parameters of interest that are related through a higher level similarity and are often well modeled by a second-level prior. The workshop showcased recent developments in optimal selection of shrinkage magnitude and directions in hierarchical models and applications of hierarchical random effects modeling in mortality rate estimation and individualized prediction [37].

In many contemporary applications [42] auxiliary information regarding the second level structures (such as correlation patterns) is available and can only be suitably incorporated in the hierarchical framework through nonexchangeable priors. Recent work of [5] presented in this workshop develops a generic predictive program for constructing efficient shrinkage rules in a non-exchangeable Gaussian model with with an unknown spiked covariance structure. Shrinkage is facilitated through a family of commutative priors for the mean parameter that are governed by a power hyper-parameter which varies over perfect independence to highly dependent scenarios. Bayes predictive rules in such as set-up involve quadratic forms in functionals of the unknown population covariance. Random matrix theory results [75, 74, 49]are used to correctly estimate the shrinkage estimator in such a Bayesian hierarchical model. Recent Bayesian and Frequentist methods for inducing shrinkage in models with unknown covariance is also covered. Consistent boootstrap based programs for estimation of several spectral statistics have been developed [62, 50]. Recently works have lead to several new methods for estimating the spectral distribution such as by empirical tilting. Novel asymptotic estimation of the distributions of eigen vectors of high-dimensional structured random matrices are developed in [25] for applications in network inference. In spatial statistics, statistical computations for large datasets are a challenge, as it is extremely difficult to store a large covariance or an inverse covariance matrix, and compute its inverse, determinant or Cholesky decomposition. In this domain, scalable matrix-free conditional samplings algorithms are being developed for estimation in spatial mixed models [20].

The workshop documented recent progress in predictive density estimation. The goal in *Predictive Density Estimation* (prde) is to use past data to choose a probability distribution that will be good in predicting the behavior of future samples. The problem of predictive density estimation is one of the most fundamental problems in statistical prediction analysis (See [3, 30, 29]). Traditionally, prediction analysis has dealt with extracting as much information as possible from a small data set. However, over the last decade high-dimensional prde has recieved much attention. Recently, decision theoretic parallels have been established between the predictive density estimation and the multivariate normal mean estimation problem [34, 38, 35, 12, 55, 51, 93, 39, 64]. Connections between the two estimation regimes under parametric constraints have been explored by [92], [26], [60], [70] and [69]. Here, recent development in structured predictive density estimation in varied parametric models were discussed. The resultant density estimates possess optimal predictive log-likelihood properties and can be used in a host of modern applications where data sets with large numbers of predictors are increasingly being collected.

While most of these developments in prde are in the sequence models, the workshop covered regression techniques in high-dimensional model with many more covariates than observations. Here, variable selection is important for constructing good estimators of the unknown parameters [2]. Recent developments in this domain has lead to scalable Bayesian shrinkage priors with desirable posterior concentration [7, 8, 61, 91]. Some of the most popular Bayesian variable selection techniques [67, 36, 44] are built on the “spike and slab” prior distribution. Spike and slab approaches and their computationally tractable extensions have recently been very successfully applied in selecting variables in high-dimensional sparse regression models (See [73, 7, 83, 81, 82, 43] and the references therein).Of particular note is the wide usage of continuous spike-and-slab methods exemplified by horse-shoe priors based methods [76, 77, 91, 61]. Bayesian inference methods for adaptation to shape constraints and approximate Bayesian computations reinvigorating traditional MCMC methods for large scale Bayesian shrinkage are vibrant areas of modern research in this stream of works.

The workshop also covered new directions where empirical Bayes and related shrinkage ideas are beginning to be employed for improving existing inference methodologies. The role of shrinkage in testing hypothesis related to functional data [17] as well as empirical Bayes methods for matrix completion [66] and modern causal inference problems were discussed.

Open Problems

One of the generic themes of the presentations in the workshop was the importance of extending inferential paradigms from point or interval estimation to predictive inference. Here is a brief list of topics that fit into this research agenda.

1. Predictive density estimation has traditionally focused on usage of the Kullback-Leibler loss. However, new phenomena have begun to emerge in the context of statistical models involving high-dimensional parameters with the utilization of a wider variety of losses that include chi-square, total variation and Wasserstein metrics. One broad class of research problems is to conduct systematic studies to develop understanding and effective strategies for predictive inference for various classical models such as Gaussian sequence model, Poisson regression model, linear regression models and various models for longitudinal data under such loss functions.

2. High-dimensional inference poses a multitude of challenges and opportunities. While usage of shrinkage strategies in high-dimensional problems has a long history, the literature on predictive inference for these problems is still relatively limited. Some relevant open problems include (a) choice of appropriate sparse and dense priors for linear models with unknown covariance; and (b) choice of priors for optimal predictive inference for low-dimensional functionals of high-dimensional parameters.

3. Graphical models have emerged as a powerful modeling paradigm for complex multivariate data. The question of predictive inference for such models has been largely unexplored. One of the challenges here is to come up with appropriate models for describing probabilistic structures on graph spaces that are both analytically and computationally tractable.

Presentation Highlights

The workshop demonstrated fascinating progress in *predictive density estimation* (prde). Prde has traditionally been one of the most fundamental problems in statistical inference [31, 3]. Over the past decade, tractable decision theoretic progress regarding efficacies of Bayesian and Frequentist approaches to prde has been made. Éric Marchand summarized these recent results across different loss functions and varied useful parametric set-ups [26, 60, 59, 58, 63]. Bill Strawderman showed that under Kullback-Leibler divergence in spherically symmetric distributions, there exists alluring parallels between point prediction and predictive density estimation and minimum risk equivariant densities can be dominated by Harmonic priors [27]. Iain Johnstone showed that in high dimensional predictive density estimation under sparsity constraints there exists decision theoretic contrasts with minimax sparse location estimation results [69]. These contrasts can be explained by analyzing minimax optimal sparse discrete priors [72]. The minimax risk of popular spike-and-slab prdes were also obtained. Fumiyasu Komaki demonstrated the recent progress made in prde in discrete Poisson models. Prediction in discrete models differs in fundamental aspects from prediction in continuous models [56]. In particular, Fumiyasu Komaki proposed shrinkage priors so that its associated non-parametric Bayesian prde under Kullback-Leibler loss. Keisuke Yano presented optimal tuning and usage of prde in poisson models under sparsity constraints[94]. Sparsity in count data implies situations where there exists an overabundance of zeros or near-zero counts and these sparsity constrained framework relates to zero-inflated models. All of the above developments are built in models with known covariances. Takeru Matsuda [65] showed that in models with unknown covariance, predictive density estimates based on singular value shrinkage prior have efficient prediction properties.

Bill Strawderman and Eric Marchand connected frequentist risk in predictive density estimation with the shrinkage location estimators in Gaussian sequence models. Selection of optimal shrinkage parameters in sequence models is a vibrant area of research. Yuzo Maruyama presented ensemble minimaxity [16] of James-Stein type [45] estimators in heteroskedastic sequence set-ups. Roger Koenker presented a non-parametric estimation framework for modeling binary response by single-index models with random coefficients [40]. A new approach for computing the Nonparametric maximum likelihood estimation (NPMLE) that significantly increases computational tractability was developed. Aditya Guntuboyina discussed empirical Bayes estimation of multivariate normal means [85] using NPMLE and extended NPMLE based shrinkage estimation to mixture of regression set-ups. Jiaying Gu demonstrated the applicability of Nonparametric empirical Bayes methods in econometric applications dealing with heterogeneity in both the location and scale parameters. She investigated the performance of NPMLE based ranking methods for studying several compound decision problems in teacher quality evaluation using administrative data. The talk illustrated the importance of empirical Bayes ideas in providing elegant interfaces and interpretative robust estimators for dealing with delicate policy questions. It led to much excitement and considerable discussions among the audience. It was highlighted that unlike most state-of-the -art black-box modeling approaches, the rigorous nature of empirical Bayes rules provide the much needed assurances needed for framing data-driven policy in sensitive applications such as evaluations based incentives, remunerative penalties and terminations.

The workshop had several talks on non-linear shrinkage in Bayesian regression models. Edward George demonstrated the powerful role of continuous shrinkage priors in sparsity constrained high-dimensional models [83]. Malay Ghosh showed that in high-dimensional multivariate regression model, horse-shoe [77, 76] priors can be used for efficient Bayesian estimation [91, 61]. Anirban Bhattacharya presented recent efforts to scale up Bayesian computation in high- dimensional and shape-constrained regression problems. The transition kernel of an exact MCMC algorithm was perturbed to ease the computational cost per step while maintaining accuracy. Debdeep Pati showed that in Bayesian shape constrained estimation, commonly used priors are not suitable and proposed a novel alternative strategy based on shrinking the coordinates using a multiplicative scale parameter. The proposed shrinkage prior [78] guards against the mass shifting phenomenon while retaining computational efficiency.

Another interesting attribute in this workshop was research talks on statistical methods to deal with unknown covariances. Feng Liang presented the problem of estimating a high-dimensional sparse precision matrix in a Bayesian framework. She showed that adaptation in shrinkage and sparsity levels can be induced by a mixture of Laplace priors [28]. Miles Lopes showed that several spectral statistics can be non-parametrically well estimated in high-dimensional set-ups by using bootstrap based methods [62]. Sanjay Chaudhuri presented the problem of estimating the spectral distribution of large covariance matrices by exponential titling in regimes where sample size as well as the dimension increases proportionately. Debashis Mondal presented modern Bayesian and Frequentists approaches to deal with large covariance matrices in saptial mixed models. Tractable shrinkage estimation using matrix-free conditional samplings algorithms was demonstrated [20]. Yingying Fan showed that asymptotic distributions of eigen vectors in large random matrices can be adequately estimated and used for large-scale network inference [25]. Gourab Mukherjee extended the emprical Bayes framework in Gaussian sequence model [89, 90] and considered prediction under unknown covariance in a hierarchical framework guided by a flexible family of non-cummutative priors. Under spiked structure, the resultant Bayes predictors can be well evaluated in such non-exchangeable flexible models [5].

There were several other fascinating attributes of shrinkage methods that were also displayed in the workshop. Xinyi Xu demonstrated the potential of Bayes factors in Bayesian hypothesis testing and model comparisons. Jinchi Lv presented an interesting methodology in high-dimensional nonparametric inference where distance correlation is used for inference pertaining to attributes related to a pair of large random matrices. Holger Dette showed that hypothesis of practical relevance in functional data analysis often can not be tested by existing methodologies and developed a new bootstrap based test for conducting accurate two-sample tests for those purposes [17]. Jialiang Li presented a model averaging method for constructing a prediction function [88]. Several semi-parametric models are weighted for prediction of the mean response. The non-parametric regression models are marginally approximated by spline basis functions and fitted by Bayesian MCMC algorithm. Syed Ejaz Ahmed demonstrated the role of shrinkage in removing implicit bias in Big data applications. He showed how shrinkage rules can be re-calibrated to remove post selection bias in complex regression models. Qingyuan Zhao discussed the potential of using an empirical Bayes perspective [95, 96] in modern usage of causal inference in medical and heath care applications.

Scientific Progress Made

There were two discussion sessions during the workshop in which the participants summarized the progress made during the meetings by connecting the dots among the rigorous scientific talks. Several new perspectives in regards to modern applications of shrinkage in big-data applications came up in the discussions. These discussions led to a bigger picture on the current themes of research on shrinkage methods as well as on potential application areas. In large-scale predictive modeling in biology, economics, finance, healthcare, management and marketing sciences, it is now commonplace to use some notions of shrinkage to construct robust algorithms [24, 84, 71, 15, 4].

An interesting attribute of this workshop was the assimilation of mathematical theory with statistical methods used in modern applications. Another feature was the increasing involvement of sophisticated Bayesian computational procedures to implement shrinkage strategies involving complex hierarchical models [78, 7, 83, 81, 82, 91]. A further significant development has been in terms successful demonstration of Bayesian shrinkage strategies in "non-standard" problems motivated by modern applications [65, 66]. Finally, there were several talks on novel shrinkage strategies for shape-restricted inference and high-dimensional inference [85, 62, 41], topics that are becoming increasingly important in modern statistics.

Outcome of the Meeting

The workshop showcased the latest advances in the domain of predictive inference and shrinkage procedures in statistics. Some of the key areas of development in contemporary statistics have been (i) inference for high-dimensional data; (ii) sparse parameterization of complex models; (iii) inference under geometric constraints; (iv) computational developments for large volumes of data, and (v) enhanced Bayesian methodologies for nonparametric and semiparametric problems. This meeting has been successful in bringing together experts from each of these fields, and thereby providing a platform for an informative exchange of ideas across these related disciplines. Several collaborative research efforts, including new research proposals and exchange visits by various scholars, have been taking shape as a direct consequence of the academic exchanges during this workshop.

One of the notable features of the workshop was the participation of a large number of young researchers in the field. The key member of the organizing committee, Dr. Gourab Mukherjee, is Assistant Professor of Data Sciences and Operations in the University of Southern California. Among the participants, quite a few were either Assistant Professor or Postdoctoral Scholars in various reputed universities. This workshop therefore allowed these young researchers to showcase their exciting research to the some of the most highly respected senior researchers in the field. At the same time the workshop provided a nice networking opportunity to these young researchers, many of them are expected to be leaders in their respective fields of research.

Participants in the workshop also laid out a number of open problems in the areas of predictive inference and shrinkage-based statistical procedure. It is expected that this meeting will work as a catalyst in bringing together researchers across disciplines to solve the mathematical and computational challenges associated with these exciting questions.

Participants

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Dette, Holger (Ruhr-Universität Bochum)
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Fan, Yingying (University of Southern California)
Gangopadhyay, Ujan (University of Southern California)
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Ghosh, Malay (University of Florida)
Gu, Jiaying (University of Toronto)
Guntuboyina, Aditya (University of California, Berkeley)
Johnstone, Iain (Stanford University)
Koenker, Roger (University College London)
Komaki, Fumiyasu (The University of Tokyo)
Li, Jialiang (Associate Professor)
Liang, Feng (University of Illinois at Urbana Champaign)
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Lv, Jinchi (University of Southern California)
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Pati, Debdeep (Texas A&M University)
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Xu, Xinyi (Ohio State University)
Yano, Keisuke (University of Tokyo)
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Chapter 8

Modelling of thin liquid films - asymptotic approach vs. gradient dynamics (19w5148)

April 28 - May 3, 2019

Organizer(s): Uwe Thiele (Westfälische Wilhelms-Universität), Neil Balmforth (University of British Columbia), Andrew Hazel (University of Manchester), Chun Liu (Illinois Institute of Technology)

Overview of the Field

Thin films and shallow droplets of simple liquids on solid substrates have for many years been described quite successfully by thin-film evolution equations (often called lubrication or long-wave equations) derived from the basic transport equations of physico-chemical hydrodynamics employing a long-wave approximation [13, 2]. In the more recent years the approach has been extended to complex liquids. The wide variety of systems that are considered include relatively simple nonvolatile molecular liquids, volatile liquids, liquids with insoluble and soluble surfactants, mixtures of simple liquids, particle suspensions, liquid crystals and a number of non-Newtonian liquids. Film and drop dynamics is described for a number of distinct physical systems where the system either approaches equilibrium states or may remain in out-of-equilibrium states that are driven by persistent fluxes. Examples include the dewetting dynamics of thin films on horizontal or structured solid substrates, the behaviour of drops and films inside (rimming flow) and outside (coating flow) of a rotating cylinder, the spreading of surfactant solutions, the transfer of liquid from a bath onto a moving plate, particle-laden liquid films flowing down an incline, morphological transitions of individual sliding drops and the behaviour of their ensembles, and osmotically spreading biofilms. Additional influences may be included, e.g., thermal effects resulting in thermal Marangoni flows, chemical or topographical substrate heterogeneities, slip of the liquid at the solid substrate, phase transitions as evaporation/condensation, dissolution or deposition, and the dynamics of the surrounding phases.

Recent Developments and Open Problems

In most cases, thin-film models are derived by employing a consistent asymptotic procedure, i.e., a small parameter ε is introduced that corresponds to the ratio of typical length scales orthogonal and parallel to the substrate (e.g., equilibrium contact angle, plate inclination, ratio of film thickness and cylinder radius) and governing equations and boundary conditions are expanded in ε to derive evolution equations to different order for the local film height, h, and other adequate order parameter fields (e.g., concentration fields). These are normally 4th order partial differential equations. In the case of a simple nonvolatile dewetting liquid on a smooth solid substrate under the sole influence of capillarity and wettability the equation reads

$$\partial_t h \;=\; -\nabla\cdot\left[\frac{h^3}{3\eta}\nabla(\gamma\Delta h + \Pi(h))\right]$$

where η and γ stand for the dynamic viscosity and surface tension of the liquid and $\Pi(h) = -df(h)/dh$ is the Derjaguin (or disjoining) pressure that encodes the wettability of the substrate and is related to the wetting potential $f(h)$ [18]. It was noted early on by Oron & Rosenau as well as by Mitlin [14, 11, 19] that such equations can often be written as gradient dynamics for the conserved order parameter field h, namely, as

$$\partial_t h \;=\; \nabla\cdot\left[Q(h)\nabla\frac{\delta F}{\delta h}\right]$$

where $Q(h) = h^3/3\eta$ is a mobility function and $F[h]$ is the free energy functional (at the same time a Lyapunov functional)

$$F[h] \;=\; \int\left[\frac{\gamma}{2}(\nabla h)^2 + f(h)\right]dx\,dy$$

that consists of contributions of surface energy (in long-wave or small-gradient approximation) and wetting energy (in Mitlin's case [11, 19]). The latter formulation brings the thin-film equation into the wide class of gradient dynamics models (for conserved fields) that also includes the Cahn-Hilliard equation, phase-field crystal equations, models for epitaxial growth [6, 19] and models for membrane dynamics — implying that addressing important general questions for one of these models will affect our knowledge regarding the others. These models can often be directly derived based on deeper thermodynamic principles such as Onsager's variational principle [4, 5].

However, although over the years quite a number of thin-film models have been derived employing asymptotic methods for various liquids in relaxational settings (i.e., without flow of energy or mass across the system boundaries) [13, 2, 12] gradient dynamics forms have been discussed for a few models only and these studies are typically more recent. Most involve several coupled fields; examples include dewetting two-layer films [15, 9], films of mixtures [1, 21, 24] and surfactant covered films [20]. In the course of discussions at previous international workshops and between colleagues it became clear that beyond the simple case given above where asymptotic and gradient dynamics approaches are identical, frequently asymptotically derived models differ in important details from the gradient dynamics form. For instance, there exist correctly derived asymptotic models that can not be brought into a gradient dynamics form. As an example, appendix A of [20] reflects on such a discussion that came up during the Programme *Mathematical Modelling and Analysis of Complex Fluids and Active Media in Evolving Domains* at the Isaac Newton Institute for Mathematical Sciences (Cambridge, May–Aug 2013). Further, there exist many *ad-hoc* amendments to thin-film models (in this way incorporating additional physical effects) that can influence the gradient dynamics structure.

One such improvement to the lubrication approximation proposed in [7] and later by [17] consists of using the full curvature (as opposed to its linearised form) of the free surface (i.e., Laplace pressure term) which at first view one might discard as being in conflict with the standard lubrication approach. However, in a gradient dynamics context one may interpret this approach as employing a better approximation for the surface energy while not touching the approximation of the dynamics. This provides an interpretation of why it is a successful approach. At present, comparisons of full Stokes flow calculations with lubrication models of different order on the one hand and a gradient dynamics model on the other hand are underway for the dynamics of a film outside a rotating cylinder. They show that the latter more faithfully captures the correct dynamics and even qualitative behaviour over a wider range of control parameters [23]. This development in approximated hydrodynamic models for free surface flows is in itself quite intriguing, however, at the same time it parallels a tendency in general Soft Matter Science to consider dynamical models that can be derived with Onsager's variational principle [16, 4]. One aim of our workshop has been to discuss these approaches between the different communities.

A second aim has been related to the question concerning the origin of mesoscale and macroscale quantities employed in asymptotic and gradient dynamics models in the case of simple and complex liquids. For instance, the gradient dynamics approach places a large weight on the underlying energy functional $F[h]$. However, in many cases the energies themselves are approximations that are only valid for part of the thickness range in which they are employed in practical calculations. For instance, most employed Derjaguin (or disjoining) pressures diverge for vanishing film height implying that a microscopic precursor film exists everywhere outside a macroscopic drop of partially wetting liquid on a solid substrate. Early on, it was discussed that a cut-off should be introduced [3], but this is infeasible in most thin-film models. Another more modern approach is to obtain the necessary parameters and functional dependencies directly from appropriate microscopic approaches as Molecular Dynamics simulations [10, 22] or classical Density Functional Theories [8]. This is, however, not yet realised beyond the case of simple liquids. The workshop has aimed at highlighting the importance of a seamless connection of microscale, mesoscale and macroscale models that should be reached in the future and at discussing pathways towards this aim.

Realisation of the workshop

During the workshop we have considered the two related questions that one has to resolve when establishing new thin film models: (i) Which modelling strategy should one follow, i.e., is it more important that a model is asymptotically correct or that it corresponds (in the appropriate limits) to a gradient dynamics on a physically reasonable energy functional? (ii) The second question is how one obtains the energetic and dynamic ingredients of a thin-film model in a consistent manner?

This aim we have pursued on the one hand with a classical workshop programme consisting of scheduled talks of the individual scientists that spoke about particular projects in areas closely related to thin films and drops on substrates; see the final list of participants in the appendix. Each speaker had been asked to relate their particular considered questions, methodology and results to the theme and to the main questions of the workshop. Each 20min talk was accompanied by 5min general discussion. This has worked out quite well as most participants related their work to the general question and the discussions picked up on these relations. We report on the scheduled talks in section 8 below.

On the other hand our programme contained ample time for discussion: informal ones during coffee and lunch breaks, dinner time and during the free afternoon, and more formal ones in the scheduled well-attended discussion sessions on Thursday afternoon and Friday morning. We reflect on these discussions in section 8 below.

Presentation Highlights

Each morning started with the talk contribution of one of the organisers. In particular, the Monday was opened by an overview talk by U. Thiele on gradient dynamics approaches for thin liquid films; on Tuesday C. Liu spoke about general diffusion and dynamic boundary conditions; N. Balmforth presented on Wednesday, describing thin-film models for viscoplastic fluid; on Thursday, A. Hazel gave a direct comparison of asymptotic and gradient dynamics approaches to coating and rimming flows discussing their advantages and disadvantages. In this way he directly compared the two main approaches for improvements that are discussed in the literature, namely going to asymptotic models of higher order or establishing gradient dynamics models with a focus on an improved description of the energetic aspects.

Overall, about half of the talks discussed specific thin-film models for relevant hydrodynamic systems that are employed for the analysis of different physical systems related to modern experiments and applications. Examples include the talks by C. Falcon, Y. Stokes, T.-S. Lin, M. Chugunova, V. Ajaev, S. Kumar, S. Wilson, I. Hewitt, R. Cimpeanu, T. Witelski and J.J. Feng. In the course of these talks it was discussed how to improve and apply these models, e.g., when either stretching the parameter region where they are applied or when adapting them to novel experimental situations or new materials. For instance it was pointed out that one may introduce thin-film models for suspensions first in the dilute limit and then to expand them to higher solute concentrations by improving the underlying energy functional of the gradient dynamics formulation of the hydrodynamic model.

This was further elaborated in the discussion sessions. It was pointed out that individual *ad-hoc* amendments of diffusion constants, Marangoni forces, and Derjaguin pressures often result in inconsistent models. Examples of simple liquids in more complex situations were presented by M. Sellier (optimal pancake control), A.G. Gonzalez (breakup of liquid grids into regular drop patterns) and M. Fontelos López (discrete self-similarity in thin-film rupture). The general mathematical structure of thin-film model was discussed by R. Krechetnikov.

In a number of presentations state-of-the-art models were presented for rather complex fluids and (biological) soft matter. A. Rey discussed the dynamics of soft anisotropic media as liquid crystals and hierarchically structured biomolecules, while K. John presented biofilm models that consists of a gradient dynamics for biomass in the film, biosurfactants and water with nutrients that is supplemented by bioactive terms. Y.-N. Young spoke about long-wave dynamics of a lubrication layer under an inextensible elastic membrane and S. Gurevich reported on spatio-temporal patterns in dynamic self-assembly systems based on surfactant, and the control of such systems. Control was also the subject of the contribution of A. Thompson on falling films. Deposition patterns of colloidal particles were reported by O. Manor — relating also to the talk of X. Man and U. Thiele. The talks of R. Cuerno and O. Pierre-Louis showed that also the evolution of solid surfaces (irradiated by an energetic ion beam or dissolving into a solution) is governed by equations of the same class and should therefore be seen in the same context of thin-film equations. There the existence and form of gradient dynamics formulations is not yet clear. M. Shearer and S. Li discussed aspects of flow and instabilities in Hele-Shaw cell.

The different approaches were also brought into the context of the wider recent development in Soft Matter Science to consider models for complex media that can be derived with Onsager's variational principle, i.e., based on variations of the Rayleighian, which consists of the rate of change of a free energy functional and a dissipation functional, with respect to rates/fluxes. X. Man discussed how this approach is used to study the drying of liquid droplets based on a few macroscopic degrees of freedom and D. Peschka presented a description of drop and contact line dynamics via generalised gradient flows.

Thin-film models are often mesoscopic or macroscopic models that rely on input from the microscale. While the procedure is well established for quantities as surface tension, only a few approaches are pursued for other quantities such as wetting potential and Derjaguin pressure that encode wettability or indeed transport coefficients. Approaches for complex liquids are still rather scarce. During the workshop, M. Müller described how to connect particle-based simulations to continuum models employing examples from simple and multicomponent polymer liquids, S. Hendy discussed MD simulations of droplets on tilted superhydrophobic and SLIPS surfaces and irradiation by an energetic ion beam. A. Archer reported on hybrid thin-film kinetic Monte Carlo modelling of droplets evaporating, coalescing and sliding on surfaces.

Discussion Highlights

During the talks, a number of relevant and fundamental questions were raised that required perspectives broader than those of a single speaker to answer. Among those, the participants selected the three main themes below for discussion by all participants in separate sessions. While these discussions rarely provide immediate answers, they are important to identify themes and future research directions for the research community.

Discussion on fundamental assumptions and choice of dissipation in gradient flows

Short contributions on the board by: D. Peschka (abstract gradient flows); U. Thiele (mesoscopic models); X. Man (Onsager's variational principle and Rayleighian).

Introduction: Energetic variational principles are a cornerstone of modern modelling approaches in complex physical systems and are related to many important concepts from fluid dynamics, chemistry, thermodynamics, and soft condensed matter systems. While being a general abstract framework, the importance of this concept justifies itself through the many particular examples presented during the workshop. While in many systems equilibrium theory makes the proper choice of the driving thermodynamic potential easy to understand, the concept of dissipation appears sometimes more elusive. Therefore, this discussion was aimed at providing different viewpoints for this concept and to provide a few examples.

Discussion: The first part of the discussion focussed on the general gradient flow formalism. Different points of view for the general construction were presented by different participants of the workshop. Ranging from more abstract mathematical approaches to specific finite-dimensional examples and despite slight technical differences, the experts from different fields unanimously agree on the general structure. In this part, the discussion mainly aimed at understanding the restrictions of gradient based models, understanding the restrictions that one has when adding terms to the dissipation, and discussing different aspects of the benefit one has when recasting a known partial differential equation in the form of a gradient dynamics model. While it seemed rather difficult to address all the different aspects that were interesting to the audience, the importance of different dissipation mechanisms became clear for everyone. Aspects of modelling correction terms for dissipative effects were also briefly discussed. Specific examples that had been mentioned during the workshop include diffusion & convection, conserved and non-conserved order parameters (Cahn-Hilliard and Allen-Cahn equations), thin liquid films, Stokes flow with free boundaries, reactions/evaporation/condensation/drying/solidifications, dynamic contact angles, flows with heat, biological systems (tear film and cellular systems), interface energies, pattern formation and deposition, higher order energies (full curvature), nematics, non-Newtonian rheology, porous medium and Hele-Shaw flows.

Questions that have been addressed in particular are

1. What is the theoretical foundation (Onsager, Rayleigh, Helmholtz, ...)?
2. What are possible extensions, e.g., to inertial effects, higher order terms, complex fluids, non-Newtonian rheology, hysteresis and memory, ... ?
3. What are limitations / what is the validity range of such structures?
4. What is the role of boundary conditions or kinetic boundary equations?
5. How does one deal with degeneracy in the dissipation?

Discussion of linking MD simulations and continuum mechanics with and without inclusion of fluctuations
Short contributions by: Lou Kondic (jumping droplets), Andrew Archer (kinetic Monte-Carlo and continuum equations), Marcus Müller (model hierarchy, sequence of approximations)

Introduction: While molecular dynamics (MD) is widely considered a first-principles approach, but it is computationally very expensive even for mesoscopic length and time scales. On diffusive and hydrodynamic time scales, it is prohibitively so. Hybrid approaches combining mesoscopic continuum models and microscopic MD or kinetic Monte-Carlo (KMC) models offer a viable alternative to speed-up simulations. But continuum models also benefit from the input of molecular dynamics simulations, which can provide much needed material-specific parameters and behaviours (e.g. constitutive laws) as input data.

Discussion: To motivate the discussion, a set of MD simulation videos showing droplets bouncing from a substrate and corresponding continuum simulations where shown and short contributions summarised some main aspects. Then possible ways of how the different modelling approaches can benefit from each other where discussed. Additionally, approaches that include fluctuations in continuum models were of interest to the participants, but were only briefly discussed.

After the discussion all participants could appreciate the way in which microscopic models can benefit meso- and macroscopic modelling, either by parameter passing or by hybridisation, e.g., by “dragging a MD simulation along via a mesoscale simulation” or via microlevel timesteps with continuum time integration. However, it also became clear that the coarse-grained MD and KMC simulations also contain a number of assumptions and tricky details that themselves need connection to and derivation from more precise models on smaller scales as, e.g., force fields obtained in atomistic MD simulations or electronic (quantum) Density Functional Theory (DFT); e.g., there

is no simple toolbox where one can just input the material(s) (e.g., some alcane, water, polystyrene, DNA) whose dynamics one wants to study, and run MD simulations to obtain precise quantitative predictions.
Other mentioned issues relate to the use of thermostats and assumption of certain thermodynamic ensembles in the MD simulations. Some participants mentioned Phase-Field-Crystal methods, but this was not further elucidated.

Questions that have been addressed in particular are

1. What can continuum models learn from microscopic MD/DFT models?
2. Which macroscopic parameters are needed to set the parameters of MD/DFT models?
3. What are the relevant timescales?
4. How can the ability to quantitatively predict system behaviour be improved?

Discussion of disjoining pressures, particularly in "complex" situations
Short contributions at the board by: U. Thiele (overview); L. Kondic (spinodal dewetting); M. Sellier (reconstruction of disjoining pressure from traveling waves).

Introduction: There is a general agreement on some general properties of the disjoining pressure. For example, the energetic minimum defines the contact angle, which is a macroscopic measurable quantity. The thickness corresponding to the location of the minimum can be interpreted as a precursor or adsorption layer liquid film thickness and has been observed in some experiments on the nanometer scale.

The general form of long-range interaction form that is often used is suggested by the classical theory of Derjaguin & Lifshitz for van der Waals forces. However, in particular the values and the form for concrete complex physical systems (mixtures, particle suspensions, multilayer, polymers) are often chosen in a seemingly heuristic manner. In this discussion different approaches to choose and measure disjoining pressures and the importance of these different choices were discussed.

Discussion: In a short presentation, the standard form of the disjoining pressure for thin-films was presented and different variants, i.e., dependence on concentration, dependence on position on the substrate, oscillatory behaviour (multiple minima of the wetting energy), higher order terms, and the algebraic form of the potential were discussed. It was stressed that choices of wetting energies, in particular, for complex liquids have implications for the resulting gradient flow dynamics (consistency). For instance, employing a concentration- and film height-dependent wetting energy will result in a concentration- and film height-dependent disjoining pressure and other contributions that are vaguely similar to Marangoni fluxes (Korteweg fluxes).

Besides ample evidence for long-ranged interactions, the discussion again showed that there is still some deficit in the use of the calculated values for theoretical predictions. This is related to the above discussion of the relation of microscopic and mesoscopic models.

Another line of argument concerned the form of the wetting energy/disjoining pressure as a function of film height, as this implicitly assumes there is a closed film of constant density and well defined free surface. However, instead of as "film height", alternatively, the independent variable can be interpreted as "adsorption", i.e., the excess number of molecules per area where the gas density at coexistence provides the reference value. This is a more general concept as it does not imply a constant liquid density throughout the layer. For thick liquid films the two measures are proportional to each other, but for very thin films adsorption is more general as it also captures sub-monolayers of diffusing molecules or densities close to a hydrophobic solid that are lower then the gas density (negative adsorption).

Questions that have been addressed in particular are

1. What are the generally accepted theoretical foundations?
2. Are there any particular systems for which fine details of disjoining pressure plays a role?

3. How does one measure the disjoining pressure in a convincing way across all film heights and for all wetting properties?

4. How does one implement the disjoining pressure into a gradient flow dynamics consistently?

5. What are realistic disjoining pressures: rough surfaces, oscillations in height and lateral direction, line tension, impact of ions/electrical fields?

6. Does the slope of the interface have to be taken into account?

Outcome of the Meeting

All participants agreed that the workshop was very instructive and resulted in many interesting discussions between participants of various scientific backgrounds that will influence the future direction of their research. The combination of individual presentations and discussion sessions allowed us to work out the problems many people are concerned with. In this way it became clear that there is a number of important questions, like the coupling of microscopic and mesoscopic models where competing approaches develop and many questions still remain open.

These questions are being right now increasingly discussed in a number of contexts and the participants believe that the ongoing “miniaturisation” of soft matter and fluidic systems considered by the scientific community will result in an ever increasing importance to solve the discussed problems. The workshop has already helped the scientists from the different communities to further develop a common understanding of the challenges in the development of meso- and macroscale thin-film models for complex liquids and of their self-consistency and consistency with neighbouring microscopic approaches.

We believe that during the workshop the participating scientists have established the basis for new stable working collaborations.

Participants

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Chapter 9

Nonlinear Geometric PDE's (19w5065)

6 -10 May, 2019

Organizer(s): Pierpaolo Esposito (Universitá di Roma Tre), Monica Musso (University of Bath), Angela Pistoia (Universitá di Roma La Sapienza)

Overview of the Field

The study of geometric PDEs has been fundamental to solve very classical problems in geometry, and has given rise to new challenging ones. This area of mathematics mixes together different ideas and tools coming from geometry and from analysis. On one side, the geometric structure of these PDEs often translates into technical difficulties related to the presence of some intrinsic geometric invariance of the problem, like conformal invariance, gauge invariance, etc, that is reflected in a possible lack of compactness of the functional embeddings for the natural spaces of functions associated with the problems. Technical tools coming from analysis are often crucial to overcome this type of difficulties, among others related to regularity or a priori estimates on solutions. On the other hand, the geometric intuition of the problem always contributes to the identification for the natural quantities to keep track of, and suggests the correct result to pursue. This two-fold aspect of the study of geometric PDEs makes it both challenging and complex, and require the use of several refined techniques to overcome the major difficulties encountered. These are the main reasons why Geometric PDEs are a field of research which is currently very active.

The use of nonlinear PDEs arguments in geometric problems has progressed very rapidly in recent years. Thus it is timely to have a new BIRS workshop on Nonlinear Geometric PDEs which covers different topics of the field. Actually, a periodic workshop on these themes would be expected after a couple of years, to see much further developments, with a lot of interesting new results and directions to discuss.

Outcome of the meeting

The workshop gathered international researchers in the areas of geometric analysis and geometric and nonlinear partial differential equations (PDEs).

In particular the following topics have been addressed.

1. Local and non-local elliptic equations from conformal geometry.

The general aim is to deform the metric of a given manifold in a conformal way so that the new one possesses special properties. Classical examples are the uniformization problem of two dimensional surfaces and the Yamabe problem in dimension greater or equal to three. In particular, the problem of prescribing the Q-curvature discovered by Branson has been intensely studied by analysts as a generalization of scalar curvature in Yamabe-type problems. The sigma(k)-Yamabe problem is a generalization of the Yamabe problem introduced by Viaclovsky and it has spawned vast activity and progress in the analysis of fully nonlinear partial differential equations.

The classical example of the Yamabe problem in dimension greater or equal to three has a variational structure and it can be expressed in the form of a non-linear PDEs on the ambient manifold for the conformal factor. Existence and qualitative properties of positive solutions to such equations are by now considerably well understood. Much less is known on the existence of sign-changing solutions.

Some of the results presented in the conference are:

- **Juan Carlos Fernández** Supercritical problems on the round sphere and the Yamabe problem in projective spaces. Given an isoparametric function f on the round sphere and considering the space of functions $w \circ f$, the Yamabe-type problem can be reduced to

$$(1) \qquad -\Delta_{g_0} + \lambda u = \lambda |u|^{p-1} u \text{ on } S^n$$

with $\lambda > 0$ and $p > 1$, into a second order singular ODE of the form

$$w'' + \frac{h(r)}{\sin r} w' + \lambda \left(|w|^{p-1} w - w \right) = 0,$$

with boundary conditions $w'(0) = 0$ and $w'(\pi) = 0$, and where h is a monotone function with exactly one zero on $[0, \pi]$. Using a double shooting method, for any $k \in N$, if $n_1 \leq n_2$ are the dimensions of the focal submanifolds determined by f and if $p \in \left(1, \frac{n-n_1+2}{n-n_1-2}\right)$, this problem admits a nodal solution having at least k zeroes. This yields a solution to problem (1) having as nodal set a disjoint union of at least k connected isoparametric hypersurfaces. As an application and using that the Hopf fibrations are Riemannian submersions with minimal fibers, we give a multiplicity result of nodal solutions to the Yamabe problem on CP^m and on HP^m, the complex and quaternionic projective spaces respectively, with m odd.

- **Bruno Premoselli** Compactness of sign-changing solutions to scalar curvature-type equations with bounded negative part.
Given the equation $\triangle_g u + hu = |u|^{2^*-2} u$ in a closed Riemannian manifold (M, g), where h is some Holder continuous function in M and $2^* = \frac{2n}{n-2}$, $n := dimM$, he is interested in a sharp compactness result on the sets of sign-changing solutions whose negative part is a priori bounded. The result is obtained under the conditions that $n \geq 7$ and $h < (n-2)/(4(n-1)) S_g$ in M, where S_g is the Scalar curvature of the manifold. These conditions are optimal by constructing examples of blowing-up solutions, with arbitrarily large energy, in the case of the round sphere with a constant potential function h.

- **Jérôme Vétois** Influence of the scalar curvature and the mass on blowing-up solutions to low-dimensional conformally invariant equations.
A result of Olivier Druet provides necessary conditions for the existence of blowing-up solutions to a class of conformally invariant elliptic equations of second order on a closed Riemannian manifold whose energy is a priori bounded. Essentially, these conditions say that for such solutions to exist, the potential function in the limit equation must coincide, up to a constant factor, at least at one point, with the scalar curvature of the manifold and moreover, in low dimensions, the weak limit of the solutions must be identically zero. New existence results show the optimality of these conditions, in particular in the case of low dimensions.

A new recent notion of fractional curvature leads to a non-local Yamabe problem, namely the existence of a metric, conformally equivalent to the given one, whose fractional scalar curvature is constant.

- **Maria del Mar Gonzalez** Nonlocal ODE, conformal geometry and applications.
  We study radially symmetric solutions for a semilinear equation with fractional Laplacian. Contrary to the local case, where we can give a solution to an ODE by simply looking at its phase portrait, in the nonlocal case we develop several new methods. We will give some applications, in particular to the existence of solutions of the singular fractional Yamabe problem, and the uniqueness of steady states of aggregation-diffusion equations.

- **Seunghyeok Kim** A compactness theorem of the fractional Yamabe problem.
  Since Schoen raised the question of compactness of the full set of solutions of the Yamabe problem in the C^0 topology (in 1988), it had been generally expected that the solution set must be C^0-compact unless the underlying manifold is conformally equivalent to the standard sphere. In 2008-09, Khuri, Marques, Schoen himself and Brendle gave the surprising answer that the expectation holds whenever the dimension of the manifold is less than 25 (under the validity of the positive mass theorem whose proof is recently announced by Schoen and Yau) but does not if the dimension is 25 or greater. On the other hand, concerning the fractional Yamabe problem on a conformal infinity of an asymptotically hyperbolic manifold, Kim, Musso, and Wei considered an analogous question and constructed manifolds of high dimensions whose solution sets are C^0-noncompact (in 2017). In this talk, we show that the solution set is C^0-compact if the conformal infinity is non-umbilic and its dimension is 7 or greater. Our proof provides a general scheme toward other possible compactness theorems for the fractional Yamabe problem.

Some related problems has been studied by

- **Gabriella Tarantello** Minimal immersions of closed surfaces in hyperbolic 3- manifold.
  Motivated by the the work of K. Uhlenbeck, we discuss minimal immersions of closed surfaces of genus larger than 1 on hyperbolic 3-manifold. In this respect we establish multiple existence for the Gauss-Codazzi equations and describe the asymptotic behaviour of the solutions in terms of the prescribed conformal structure and holomorphic quadratic differential whose real part identifies the corresponding second fundamental form.

- **Pierpaolo Esposito** Log-determinants in conformal geometry.
  I will report on a recent result concerning a four-dimensional PDE of Liouville type arising in the theory of log-determinants in conformal geometry. The differential operator combines a linear fourth-order part with a quasi-linear second-order one. Since both have the same scaling behavior, compactness issues are very delicate and even the "linear theory" is problematic. For the log-determinant of the conformal laplacian and of the spin laplacian we succeed to show existence and logarithmic behavior of fundamental solutions, quantization property for non-compact solutions and existence results via critical point theory.

- **Andrea Malchiodi** On the Sobolev quotient in sub-Riemannian geometry.
  We consider a class of three-dimensional "CR manifolds" which are modelled on the Heisenberg group. We introduce a natural concept of "mass" and prove its positivity under the conditions that the Webster curvature is positive and in relation to their (holomorphic) embeddability properties. We apply this result to the CR Yamabe problem, and we discuss the properties of Sobolev-type quotients, giving some counterexamples to the existence of minimisers for "Rossi spheres", in sharp contrast to the Riemannian case.

2. Properties of solutions to PDE's on manifolds.

The goal is to investigate some properties, such as rigidity, regularity, stability, of solutions of nonlinear PDEs on manifolds.

- **Virginia Agostiniani** Monotonicity formulas in linear and nonlinear potential theory.
  In this talk, we first recall how some monotonicity formulas can be derived along the level set flow of the

capacitary potential associated with a given bounded domain Ω. A careful analysis is required in order to preserve the monotonicity across the singular times, leading in turn to a new quantitative version of the Willmore inequality. Remarkably, such analysis can be carried out without any a priori knowledge of the size of the singular set. Hence, the same order of ideas applies to the p-capacitary potential of Ω, whose critical set, for $p \neq 2$, is not necessarily negligible. In this context, a generalised version of the Minkowski inequality is deduced.

- **Giovanni Catino** Some canonical Riemannian metrics: rigidity and existence.
  In this talk, which is the second part of a joint seminar with P. Mastrolia (Università degli Studi di Milano), I will present some results concerning rigidity and existence of canonical metrics on closed (compact without boundary) four manifolds. In particular I will consider Einstein metrics, Harmonic Weyl metrics and some generalizations.

- **Paolo Mastrolia** Generalizations of some canonical Riemannian metrics.
  In this talk, which is the first part of a joint seminar with G. Catino (Politecnico di Milano), I will introduce some generalization of certain canonical Riemannian metrics, presenting two possible approaches (curvature conditions with potential and critical metrics of Riemannian functionals). The main result is related to the existence of a new canonical metric, which generalizes the condition of harmonic Weyl curvature, on every 4-dimensional closed manifold.

- **Lorenzo Mazzieri** Sharp Geometric Inequalities on manifolds with nonnegative Ricci curvature.
  Given a complete Riemannian manifold with nonnegative Ricci curvature and Euclidean volume growth, we characterize the Asymptotic Volume Ratio as the infimum of the Willmore Energy over smooth closed hypersurfaces. An optimal version of Huisken's Isoperimetric Inequality for 3-manifolds is obtained as a consequence of this result.

- **Dario Monticelli** The Poisson equation on Riemannian manifolds with a weighted Poincaré inequality at infinity.
  We prove an existence result for the Poisson equation on non-compact Riemannian manifolds satisfying a weighted Poincaré inequality outside a compact set. Our result applies to a large class of manifolds including, for instance, all non-parabolic manifolds with minimal positive Green's function vanishing at infinity. On the source function we assume a sharp pointwise decay depending on the weight appearing in the Poincaré inequality and on the behavior of the Ricci curvature at infinity. We do not require any curvature or spectral assumptions on the manifold.

- **Roger Moser** On a type of second order variational problem in L-infinity.
  Let K be an elliptic (not necessarily linear) second order differential operator. Suppose that we want to minimise the L-infinity norm of K(u) for functions u satisfying suitable boundary conditions. Here K may represent, e.g., the curvature of a curve in the plane or the scalar curvature of a Riemannian manifold in a fixed conformal class, but the problem is not restricted to questions with a geometric background. If the operator and the boundary conditions are such that the equation K(u) = 0 has a solution, then the problem is of course trivial. But since this is a second order variational problem, it may be appropriate to prescribe u as well as its first derivative on the boundary of its domain, which in general rules out this situation. In the cases studied so far, the solution, while not trivial, still has a nice structure, and one feature is that —K(u)— is always constant. The sign of K(u) may jump, but we have a characterisation of the jump set in terms of a linear PDE. Furthermore, in some cases we have a unique solution, even though the underlying functional is not strictly convex.

- **Susanna Terracini** Liouville type theorems and local behaviour of solutions to degenerate or singular problems.

We consider an equation in divergence form with a singular/degenerate weight

$$-\mathrm{div}(|y|^a A(x,y)\nabla u) = |y|^a f(x,y) \quad \text{or } \mathrm{div}(|y|^a F(x,y))\ ,$$

Under suitable regularity assumptions for the matrix A and f (resp. F) we prove Hölder continuity of solutions and possibly of their derivatives up to order two or more (Schauder estimates). In addition, we show stability of the $C^{0,\alpha}$ and $C^{1,\alpha}$ a priori bounds for approximating problems in the form

$$-\mathrm{div}((\varepsilon^2+y^2)^a A(x,y)\nabla u) = (\varepsilon^2+y^2)^a f(x,y) \quad \text{or } \mathrm{div}((\varepsilon^2+y^2)^a F(x,y))$$

as $\varepsilon \to 0$. Finally, we derive $C^{0,\alpha}$ and $C^{1,\alpha}$ bounds for inhomogenous Neumann boundary problems as well. Our method is based upon blow-up and appropriate Liouville type theorems.

3. Geometric evolution equations

Many geometric variational problems can be approached via evolutionary methods. The Yamabe flow in conformal geometry and the mean curvature flow are two examples with connections to problems in differential geometry and mathematical physics.

Results on the analysis of possible blow-up phenomena for several non-linear flows have been presented.

- **Monica Musso** Singularity formation in critical parabolic equations.
  In this talk I will discuss some recent constructions of blow-up solutions for a Fujita type problem for powers p related to the critical Sobolev exponent. Both finite type blow-up (of type II) and infinite time blow-up are considered.

- **Mariel Saez** On the uniqueness of graphical mean curvature flow.
  In this talk I will discuss on sufficient conditions to prove uniqueness of complete graphs evolving by mean curvature flow. It is interesting to remark that the behaviour of solutions to mean curvature flow differs from the heat equation, where non-uniqueness may occur even for smooth initial conditions if the behaviour at infinity is not prescribed for all times.

- **Juan Davila** Helicoidal vortex filaments in the 3-dimensional Ginzburg-Landau equation.
  We construct a family of entire solutions of the 3D Ginzburg-Landau equation with vortex lines given by interacting helices, with degree one around each filament and total degree an arbitrary positive integer. Existence of these solutions was conjectured by del Pino and Kowalczyk (2008), and answers negatively a question of Brezis analogous to the the Gibbons conjecture for the Allen-Cahn equation.

- **Manuel del Pino** Singularity for the Keller-Segel system in R^2.
  We construct solutions of the Keller-Segel system which blow-up in infinite time in the form of asymptotic aggregation in the critical mass case, with a method that does not rely on radial symmetry, and applies to establish stability of the phenomenon.

4. Concentration phenomena in local and non-local problems.

The geometric invariances often lead to the existence of solutions which blows-up at single points or at higher dimensional sets. The localization of the blowing-up sets strongly depends on the geometric properties of the problem. It is an active field in nonlinear analysis to constructs solutions to PDEs exhibiting this kind of phenomena.

Problems in 2D have been treated in

- **Weiwei Ao** On the bubbling solutions of the Maxwell-Chern-Simons model on flat torus
  We consider the periodic solutions of a nonlinear elliptic system derived from the Maxwell-Chern-Simons model on a flat torus Ω:

$$\begin{cases} \Delta u = \mu(\lambda e^u - N) + 4\pi \sum_{i=1}^n m_i \delta_{p_i}, \\ \Delta N = \mu(\mu + \lambda e^u)N - \lambda\mu(\lambda + \mu)e^u \end{cases} \text{in } \Omega,$$

where $\lambda, \mu > 0$ are positive parameters. We obtain a Brezis-Merle type classification result for this system when $\lambda, \mu \to \infty$ and $\lambda << \mu$. We also construct blow up solutions to this system.

- **Luca Battaglia** A double mean field approach for a curvature prescription problem.
  I will consider a double mean field-type Liouville PDE on a compact surface with boundary, with a nonlinear Neumann condition. This equation is related to the problem of prescribing both the Gaussian curvature and the geodesic curvature on the boundary. I will discuss blow-up analysis, a sharp Moser-Trudinger inequality for the energy functional, existence of minmax solution when the energy functional is not coercive.

- **Teresa D'Aprile** Non simple blow-up phenomena for the singular Liouville equation.
  Let Ω be a smooth bounded domain in R^2 containing the origin. We are concerned with the following Liouville equation with Dirac mass measure

  $$-\Delta u = \lambda e^u - 4\pi N_\lambda \delta_0 \quad \text{in} \quad \Omega,$$

  with $u = 0$ on $\partial\Omega$. Here λ is a positive small parameter, δ_0 denotes Dirac mass supported at 0 and N_λ is a positive number close to an integer N ($N \geq 2$) from the right side. We assume that Ω is $(N + 1)$-symmetric and the regular part of the Green's function satisfies a nondegeneracy condition (both assumptions are verified if Ω is the unit ball) and we provide an example of non-simple blow-up as $\lambda \to 0^+$ exhibiting a non-symmetric scenario. More precisely we construct a family of solutions split in a combination of $N + 1$ bubbles concentrating at 0 arranged on a tiny polygonal configuration centered at 0.

- **Massimo Grossi** Non-uniqueness of blowing-up solutions to the Gelfand problem.
  I will consider blowing-up solution for the Gelfand problem on planar domains. It is well known that blow up at a single point must occur at a critical point x of a "reduced functional" F, whereas uniqueness of blowing up families has been recently shown provided x is a non-degenerate critical point of F. We showed that, if x is a degenerate critical point of F and satisfies some additional generic condition, then one may have two solutions blowing up at the same point. Solutions are constructed using a Lyapunov-Schmidt reduction.

- **Gabriele Mancini** Bubbling nodal solutions for a large perturbation of the Moser-Trudinger equation on planar domains.
  I will discuss some results obtained in collaboration with Massimo Grossi, Angela Pistoia and Daisuke Naimen concerning the existence of nodal solutions for the problem $-\Delta u = \lambda u e^{u^2+|u|^p}$ in Ω, $u = 0$ on $\partial\Omega$, where $\Omega \subseteq R^2$ is a bounded smooth domain and $p \to 1^+$. If Ω is ball, it is known that the case $p = 1$ defines a critical threshold between the existence and the non-existence of radially symmetric sign-changing solutions with λ close to 0. In our work we construct a blowing-up family of nodal solutions to such problem as $p \to 1^+$, when Ω is an arbitrary domain and λ is small enough. To our knowledge this is the first construction of sign-changing solutions for a Moser-Trudinger type critical equation on a non-symmetric domain.

- **Luca Martinazzi** Topological and variational methods for the supercritical Moser-Trudinger equation.
  We discuss the existence of critical points of the Moser-Trudinger functional in dimension 2 with arbitrarily prescribed Dirichlet energy using degree theory. If time permits, we will also sketch an approach on Riemann surfaces using a min-max method á la Djadli-Malchiodi.

- **Aleks Jevnikar** Uniqueness and non-degeneracy of bubbling solutions for Liouville equations.
  We prove uniqueness and non-degeneracy of solutions for the mean field equation blowing-up on a non-degenerate blow-up set. Analogous results are derived for the Gelfand equation. The argument is based on sharp estimates for bubbling solutions and suitably defined Pohozaev-type identities.

A non-local version of these kind of problems has been studied in

- **Azahara DelaTorre** The non-local mean-field equation on an interval.
  We study the quantization properties for a non-local mean-field equation and give a necessary and sufficient condition for the existence of solution for a "Mean Field"-type equation in an interval with Dirichlet-type boundary condition. We restrict the study to the 1-dimensional case and consider the fractional mean-field equation on the interval $I = (-1, 1)$
  $$(-\Delta)^{\frac{1}{2}} u = \rho \frac{e^u}{\int_I e^u dx},$$
  subject to Dirichlet boundary conditions. As in the $2-$dimensional case, it is expected that for a sequence of solutions to our equation, either we get a $\mathcal{C}^\infty$ limiting solution or, after a suitable rescaling, we obtain convergence to the Liouville equation. Then, we can reduce the problem to the study of the non-local Liouville's equation. One of the key points here is to find an appropriate Pohozaev identity. We prove that existence holds if and only if $\rho < 2\pi$. This requires the study of blowing-up sequences of solutions. In particular, we provide a series of tools which can be used (and extended) to higher-order mean field equations of non-local type. We provide a completely non-local method for this study, since we do not use the localization through the extension method. Instead, we use the study of blowing-up sequences of solutions.

A related problem

- **Michal Kowalczyk** New multiple end solutions in the Allen-Cahn and the generalized second Painlevé equation.
  In this talk I will discuss two new constructions of the multiple end solutions. In the case of the Allen-Cahn equation the ends are asymptotic to the Simons cone in R^8. The case of the generalized second Painlevé equation in R^2 is somehow different since there is no apparent underlying geometric problem. Yet we can interpret the behavior of the solution as being asymptotic along the axis to: two one dimensional Hastings-McLeod solution, the heteroclinic solution of the Allen-Cahn equation and the trivial solution.

- **Bob Jerrard** Some Ginzburg-Landau problems for vector fields on manifolds.
  Motivated in part by problems arising in micromagnetics, we study several variational models of Ginzburg-Landau type, depending on a small parameter $\varepsilon > 0$, for (tangent) vector fields on a 2-dimensional compact Riemannian surface. As $\varepsilon \to 0$, the vector fields tend to be of unit length and develop singular points of a (non-zero) index, called vortices. Our main result determines the interaction energy between these vortices as $\varepsilon \to 0$, allowing us to characterize the asymptotic behaviour of minimizing sequence.

Critical problems in higher dimension where a concentration phenomena naturally appears.

- **Thomas Bartsch** A spinorial analogue of the Brezis-Nirenberg theorem.
  Let (M, g, σ) be a compact Riemannian spin manifold of dimension $m \geq 2$, let $S(M)$ denote the spinor bundle on M, and let D be the Atiyah-Singer Dirac operator acting on spinors $\Psi : M \to S(M)$. We present recent results on the existence of solutions of the nonlinear Dirac equation with critical exponent
  $$D\Psi = \lambda\Psi + f(|\Psi|)\Psi + |\Psi|^{\frac{2}{m-1}}\Psi$$
  where $\lambda \in R$ and $f(|\Psi|)\Psi$ is a subcritical nonlinearity in the sense that $f(s) = o\left(s^{\frac{2}{m-1}}\right)$ as $s \to \infty$.

- **Riccardo Molle** Nonexistence results for elliptic problems in contractible domains.
  In this talk I will consider nonlinear elliptic equations involving the Laplace or the p-Laplace operator and nonlinearities with supercritical growth, from the viewpoint of the Sobolev embedding. I'll present some new nonexistence results in contractible and non starshaped domains. The domains that are considered can be arbitrarily close to non contractible domains and their geometry can be very complex.

- **Frédéric Robert** Hardy-Sobolev critical equation with boundary singularity: multiplicity and stability of the Pohozaev obstruction.
  Let Ω be a smooth bounded domain in R^n $(n \geq 3)$ such that $0 \in \partial\Omega$. In this talk, we consider issues of non-existence, existence, and multiplicity of variational solutions for the borderline Dirichlet problem,

$$\left\{ \begin{array}{rcll} -\Delta u - \gamma \frac{u}{|x|^2} - h(x)u & = & \frac{|u|^{2^\star(s)-2}u}{|x|^s} & \text{in } \Omega, \\ u & = & 0 & \text{on } \partial\Omega, \end{array} \right. \qquad (E)$$

  where $0 < s < 2$, $2^\star(s) := \frac{2(n-s)}{n-2}$, $\gamma \in R$ and $h \in C^0(\overline{\Omega})$. We use sharp blow-up analysis on –possibly high energy– solutions of corresponding subcritical problems to establish, for example, that if $\gamma < \frac{n^2}{4} - 1$ and the principal curvatures of $\partial\Omega$ at 0 are non-positive but not all of them vanishing, then Equation (E) has an infinite number of (possibly sign-changing) solutions. This complements results of the first and third authors, who showed in that if $\gamma \leq \frac{n^2}{4} - \frac{1}{4}$ and the mean curvature of $\partial\Omega$ at 0 is negative, then (E) has a positive solution. On the other hand, our blow-up analysis also allows us to prove that if the mean curvature at 0 is positive, then there is a surprising stability of regimes where there are no variational positive solutions under C^1-perturbations of the potential h. In particular, we show non-existence of such solutions for (E) whenever Ω is star-shaped and h is close to 0, which include situations not covered by the classical Pohozaev obstruction.

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Chapter 10

Geometry of Real Polynomials, Convexity and Optimization (19w5180)

May 27 - 31, 2019

Organizer(s): Grigoriy Blekherman (Georgia Institute of Technology), Daniel Plaumann (TU Dortmund University), Levent Tunçel (University of Waterloo), Cynthia Vinzant (North Carolina State University)

Overview of the Field

The workshop was focussed on recent interactions among the areas of real algebraic geometry, the geometry of polynomials, and convex and polynomial optimization. A common thread is the study of two important classes of real polynomials, namely hyperbolic and nonnegative polynomials. These two themes are interacting deeply with optimization as well as theoretical computer science. This interaction recently led to solutions of several important open problems, new breakthroughs and applications.

The study of hyperbolic polynomials originated in PDE theory, with researchers like Petrovksy laying the foundations in the 1930s. This was further developed by Gårding [1959], Atiyah, Bott and Gårding [1972, 1973], as well as Hörmander. Interest and active research in the area was renewed in the early 1990s in connection with optimization. Since then, there has been an amazing amount of activity allowing the subject to branch into and have a significant impact on a wide range of fields, including systems and control theory, convex analysis, interior-point methods, discrete optimization and combinatorics, semidefinite programming, matrix theory, operator algebras, and theoretical computer science.

The other main focus of the workshop was the closely related study of nonnegative polynomials and polynomial optimization. A systematic study of nonnegative polynomials already appeared in Minkowski's early work in the 19th century. Then, Hilbert, in his famous address at the International Congress of Mathematicians in 1900, asked for characterizations of nonnegative polynomials, including this question in his research agenda setting list of foundational problems.

Since the 1990s, this has become closely related to polynomial optimization, i.e., the optimization of polynomials subject to polynomial constraints. This very general class of optimization problems subsumes many others. For example, many combinatorial optimization problems (e.g. MAXCUT) can be formulated as optimization of a quadratic objective on the discrete hypercube $\{0,1\}^n$, which is defined by quadratic equations $x_i(x_i-1)=0$. By duality, understanding polynomials nonnegative on a given the set is equivalent to optimization over that set. A natural way to approximate nonnegative polynomials is using sums of squares. Such approximations are tractable because testing whether a polynomial is a sum-of-squares can be done with semidefinite programming. The resulting sum-of-squares relaxations (also known as Lasserre relaxations) have gained prominence both for practical use and for theoretical considerations. For instance, one of the consequence of the Unique Games Conjecture is that the simplest sum-of-squares relaxation for MAXCUT (the famous Goemans-Williamson relaxation) gives the optimal approximation factor among all the polynomial time algorithms. On the practical side, sum of squares relaxations have also been used for computing Lyapunov functions and for certified control in robotics. While sum-of-squares relaxations often perform well in practice, the reason for this behavior is not well-understood and is of prime interest both theoretically and practically.

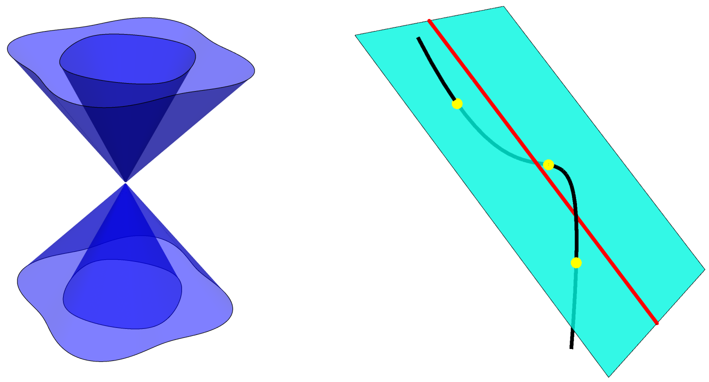

Figure 10.1: A hyperbolic hypersurface and hyperbolic space curve

Recent Developments and Open Problems

The areas of nonnegative polynomials, hyperbolic polynomials, mathematical optimization and theoretical computer science in collaboration and in interaction with each other have been producing many ground-breaking and surprisingly powerful results with far-reaching applications.

The theory of hyperbolic polynomials provides a very natural domain to formulate deep, far reaching yet elegant research problems. Because hyperbolicity appears in so many contexts, structural results about hyperbolic polynomials and their hyperbolicity cones can reverberate and have tremendous impact in several areas. For example, the works of Brändén, Gurvits, Helton-Vinnikov, Renegar together establish fundamental tools for understanding hyperbolicity cones, operations preserving hyperbolicity, determinantal polynomials, and inequalities appearing in coefficients. This increased facility with hyperbolic polynomials has helped enable a number of recent breakthroughs, including work of Gurvits on generalizations of Van der Waerden's conjecture and Bapat's conjecture as well as the recent proof of the Kadison-Singer conjecture by Marcus, Spielman and Srivastava. Recently these techniques have also been extended to a more general class of polynomials called Lorentzian or completely log-concave polynomials [1, 6]. Many properties of hyperbolic polynomials extend to this more general class, such as matroidal support and closure under derivatives, and have led to resolutions of open problems in matroid theory, including Mason's conjecture on the number of independent sets [2, 5] and the Mihail-Vazirani conjecture on the mixing time of certain Markov chains [1]. The analogues of many pieces of the well-developed theory of hyperbolic polynomials remain unresolved. Such generalizations would be desirable in their own right, as well as for applications to problems in combinatorial optimization and approximation theory.

Problem 10.0.1. *Extend the theory of hyperbolic polynomials (e.g. hyperbolicity cones, hyperbolic programming, characterization of operations preserving hyperbolicity) to the class of completely log-concave polynomials.*

Among the fundamental research problems in the area stands the "Generalized Lax Conjecture" relating hyperbolic and semidefinite programming. Several strict versions of this conjecture have been disproved, but the most general is still open.

Generalized Lax Conjecture. *Every hyperbolicity cone is a spectrahedron (i.e. linear section of the cone of positive semidefinite matrices).*

Work of Kummer on determinantal representations in [11] provides perhaps the strongest evidence for the conjecture, but there is a crucial positivity condition missing. Recent work by James Saunderson provides a necessary condition on the size of a spectrahedral representation based on the length of chains of faces of these cones [16]. A somewhat related question posed by Nemirovskii during the 2006 International Congress of Mathematicians, later conjectured by Helton and Nie, was disproved by Scheiderer in December 2016.

Theorem 10.0.2 (Scheiderer [17])**.** *Not every convex semialgebraic set is the projection of a spectrahedron.*

Scheiderer's construction is closely related related to the complexity of sums-of-squares representations mentioned below, and the ramifications of this work are still being developed and understood.

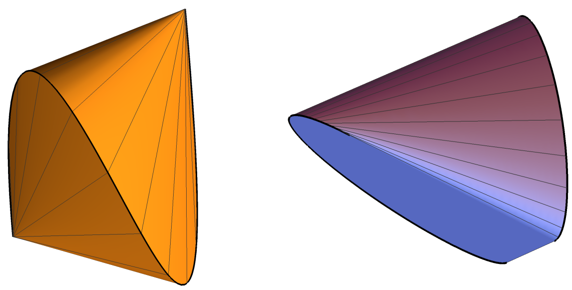

Figure 10.2: The spectrahedron of trigonometric moments given by the convex hull of the curve parametrized by $(\cos(\theta), \cos(3\theta), \cos(3\theta))$ and the dual cone of nonnegative trigonometric functions.

Part of the recent development in the theoretical understanding of sums-of-squares relaxations has come from connections with classical algebraic geometry. There seems to be a deep intrinsic connection between the quality of low-degree sum-of-squares relaxations and the classical properties of the algebraic set (e.g. Castelnuovo-Mumford regularity). Blekherman, Sinn, Smith, and Velasco have developed many of these connections [4], but several open questions remain. For example, one fundamental open question is the Pythagoras number of the d-th Veronese embedding of $\mathbb{P}^n$, which is related to is the number of squares needed to achieve all sums of squares of a fixed degree.

Question. *What is the lowest number $N(n, d)$ such that any sum of squares in $\mathbb{R}[x_0, \ldots, x_n]_{2d}$ is a sum of $N(n, d)$ squares?*

Even for $n = 2$, this is still open for $d \geq 4$, where it is known that $d + 1 \leq N(2, d) \leq d + 2$.

Another way that the sum of squares method is used is to certify graph density inequalities in extremal combinatorics (these are called Turán problems). Here, squaring takes place inside the *gluing algebra* of partially labelled graphs. Unlike in Hilbert's 17th problem, it was shown by Hatami and Norine in [8] that there exist graph density inequalities that cannot be certified using sums of squares of rational functions, but no explicit examples are known.

Question. *Find an explicit graph density inequality that cannot be written as a sum of squares of rational functions in the gluing algebra.*

This question may also be of interest in theoretical computer science, where sum of squares hierarchy is considered one of the most powerful methods of addressing combinatorial problems. Finding strong obstructions to sums of squares representability would shed more light on the power of the hierarchy. For recent progress on sums of squares for graph densities see Rekha Thomas' talk and [3].

On the one hand, each of these open problems and conjectures is interesting for the research areas of real algebraic geometry, operator theory, the geometry of polynomials, convex and polynomial optimization, as well as theory of computing and theoretical computer science. On the other hand, when we focus on a more detailed view from one of these research areas, many other variants of these open problems emerge.

For example, in the context of the Generalized Lax Conjecture above and Scheiderer's Theorem from December 2016, a convex and polynomial optimization viewpoint leads to a related open problem:

Question. *Is every hyperbolicity cone a spectrahedral shadow? (I.e., can we express every hyperbolicity cone as a projection of a spectrahedral cone?)*

If the Generalized Lax Conjecture is true, then the answer to the above question is trivially "yes". Interest in this version of the open problem partly stems from the fact that the set of linear optimization problems over extended formulations (or lifted formulations) essentially includes the set of linear optimization problems over the shadow (or the projection) as a special case.

When we consider Generalized Lax Conjecture and its variants from the viewpoint of computational complexity of solving the underlying convex optimization problems, further variants of these open problems emerge:

- Suppose K is a hyperbolicity cone that is spectrahedral. Based on the minimal defining hyperbolic polynomial of K, what is the smallest dimensional positive semidefinite cone which expresses K as a linear slice?
- Suppose K is a hyperbolicity cone that is spectrahedral shadow. Based on the minimal defining hyperbolic polynomial of K, what is the smallest dimensional positive semidefinite cone which expresses K as a projection (shadow) of a linear slice?

For recent progress in this direction, see [14] and Saunderson's talk.

Presentation Highlights

This workshop brought together established experts and young researchers from the areas of real algebraic geometry, the geometry of polynomials, and convex and polynomial optimization, to review the most recent significant discoveries and strive to forge new connections.

Each day of the workshop started with a one-hour talk that in addition to reporting on recent developments also gave an accessible overview of the background.

The workshop started with Victor Vinnikov's talk the first half of which gave a splendid introduction to the general area of stable polynomials and hyperbolic polynomials. Then in the second half Vinnikov focused on recent results on determinantal representations of hyperbolic polynomials. Vinnikov's talk made a connection to another BIRS workshop from 2010 when another participant, Petter Brándén had solved a major open problem in the field, leading to what is now called the Generalized Lax Conjecture.

The theme of determinantal representations of hyperbolic polynomials and stable polynomials continued throughout the workshop. Mario Kummer's talk addressed the representability question by focusing on convex cones constructed from algebraic curves by taking their convex hull.

Many talks served a bridging property between real algebraic geometry and convex optimization, convex geometry and convex analysis. Renegar presented a very general framework for subgradient methods. One of the most interesting cases being those optimization problems that are expressible as the intersection of a hyperbolicity cone and an affine space (hyperbolic programming problems). James Saunderson connected expressive power (via extended or lifted formulations) of classes of convex cones to the beautiful geometric measure of boundary structure of cones known as longest chain of faces. Jiawang Nie considered the classical saddle point problem in continuous optimization when the given functions are polynomials. Utilization of duality theory and Lasserre hierarchy and, exploiting the algebraic structure of the setup and that of Lagrange multipliers were highlighted. Simone Naldi considered the convex feasibility problem together with the theory of infeasibility certificates in the conic setup and brought the language and power of projective geometry to bear on the subject.

Didier Henrion attacked the classical problem of solving nonlinear PDEs using the Lasserre hierarchy. Jean-Bernard Lasserre proposed tractable semi-algebraic approximations employing the Christoffel-Darboux Kernel.

Rainer Sinn presented recent results on the joint numerical range of Hermitian matrices, which tie in with a general study of duality for hyperbolicity cones.

The theory of moment problems was treated in several talks, and some of these also dealt with the infinite dimensional generalizations. Maria Infusino considered extensions of tools for finite-dimensional moment problems to infinite dimensional settings in an hour-long overview. Salma Kuhlmann discussed the generalization of the theory of moments to the setting of symmetric algebras (algebra of symmetric tensors).

The theory and applications of completely log-concave polynomials or equivalently Lorentzian polynomials were featured in several of the talks. This class of polynomials strictly generalizes hyperbolic polynomials, yet they admit characterizations involving the Lorentzian signature (of the quadratic derivatives). Shayan Oveis Gharan gave an overview of how hyperbolic and completely log-concave polynomials can be used to approximate NP-hard counting problems using both deterministic and probabilistic algorithms. Nima Amari's talk followed up on this survey by focussing on log-concave polynomials coming from combinatorial structures called matroids. In particular, Amari talked about approximating the number of bases of a matroid by approximating the evaluation of a particular log-concave polynomial. Petter Brändén's hour-long survey completed the development of the theory of connections between hyperbolic polynomials, Lorentzian polynomials and discrete convexity.

Bachir El Khadir showed that all convex forms in 4 variables and of degree 4 are sums of squares. El Khadir also showed an attractive generalization of the Cauchy-Schwarz inequality. Rekha Thomas gave a survey talk on using sums of squares method to prove graph density inequalities and highlighted new results on the limitations of the sum of squares method, answering problems posed by Lovász. The number of squares used in a sum of squares decomposition is also an interesting quantity, useful in applications, such as Euclidean distance realization. Greg Smith's talk examined the number of squares needed to write any sum of squares on a projective variety (called Pythagoras number of the variety). He introduced a new algebraic invariant of the variety, called quadratic persistence, which is useful is giving lower bounds on the Pythagoras number.

Nonnegativity certificates given by sums of nonnegative circuit polynomials (Mareike Dressler) and sums of arithmetic-geometric mean exponentials (Riley Murray) were also studied.

The noncommutative theory of sums of squares and matrix inequalities, that ties in with functional analysis, was featured in two talks, by Igor Klep and by Jaka Cimpric.

The theme of complexity in real algebraic geometry was also central to a number of talks. Saugata Basu and Cordian Riener reported on joint work concerning the computation of the Betti numbers of semialgebraic sets that are invariant under the symmetric group.

Marie-Françoise Roy spoke about a new proof of the fundamental theorem of algebra from the intermediate value theorem for real polynomials. This forms part of a long-term project to find resp. improve complexity bounds for the real nullstellensatz. Mohab Safey El Din explained a novel approach for computing resp. approximating the volume of a semialgebraic set, significantly improving the previously known complexity bounds.

Eli Shamovich presented a modern extension of the classical Hermite method for counting the roots of a complex polynomial in the upper half plane to quadrature domains. Mihai Putinar tied in the geometry of polynomials with Hermitian sums of squares and demonstrated a more precise version of a classical Lemma due to Laguerre, developed in joint work with the late Serguei Shimorin.

List of speakers and the titles of their talks (in the order of appearance in the workshop)

1. Victor Vinnikov (Hyperbolicity, stability, and determinantal representations)
2. Mario Kummer (When is the conic hull of a curve a hyperbolicity cone?)
3. James Saunderson (Limitations on the expressive power of convex cones without long chains of faces)
4. Igor Klep (Noncommutative polynomials describing convex sets)
5. Saugata Basu (Vandermonde varieties, mirrored spaces, and cohomology of symmetric semi-algebraic sets)
6. Gregory Smith (Sums of squares and quadratic persistence)
7. Rainer Sinn (Kippenhahn's Theorem for the joint numerical range)
8. Shayan Oveis Gharan (From Counting to Optimization and Back using Geometry of Polynomials)
9. Nima Anari (Computing Log-Concave Polynomials)
10. James Renegar (A framework for applying subgradient methods)
11. Cordian Riener (Algorithms to compute topological invariants of symmetric semi algebraic sets)
12. Bachir El Khadir (On sum of squares representation of convex forms and generalized Cauchy-Schwarz inequalities)
13. Jiawang Nie (The Saddle Point Problem of Polynomials)
14. Simone Naldi (Conic programming: infeasibility certificates and projective geometry)
15. Rekha Thomas (Graph Density Inequalities and Sums of Squares)
16. Didier Henrion (Solving non-linear PDEs with the Lasserre hierarchy)
17. Jean-Bernard Lasserre (Tractable semi-algebraic approximation using Christoffel-Darboux kernel)
18. Maria Infusino (From finite to infinite dimensional moment problems)
19. Salma Kuhlmann (The moment problem for the algebra of symmetric tensors)
20. Mihai Putinar (Positive integral kernels for polar derivatives)
21. Marie-Francoise Roy (Quantative Fundamental Theorem of Algebra)
22. Mohab Safey El Din (On the computation of volumes of semi-algebraic sets)
23. Eli Shamovich (Counting the number of zeroes of polynomials in quadrature domains)
24. Jakob Cimpric (Some non-commutative nullstellensaetze)
25. Petter Brändén (Stable polynomials, Lorentzian polynomials and discrete convexity)
26. Mareike Dressler (Optimization over the Hypercube via Sums of Nonnegative Circuit Polynomials)
27. Riley Murray (SAGE certificates for signomial and polynomial nonnegativity)

Scientific Progress Made

While it is too early to determine the long term impact of a week long conference, we are convinced that it successfully provided exposure of researchers from a diverse set of fields to each other's research and ideas.

One precedent for such success was the 2010 Banff meeting on "Convex Algebraic Geometry". This workshop had a significant overlap in participants with the current one. Over the intervening nine year, connections have developed into fully fledged research areas.

One such example of this fruition is the connection of matroids, stable polynomials, and determinantal representations that was made by Petter Brändén at the 2010 meeting, at which he disproved one version of the "generalized Lax conjecture" using tools from matroid theory. These connections between determinants, stable polynomials, and matroids led to papers by several of the participants of the current workshop and to the recent theory of Lorentzian and completely log-concave polynomials, which have resolved several long-standing open questions ranging in matroid theory (Mason's conjecture) and Markov-chains (Mihail-Vazirani conjecture). The three workshop talks on these recent developments introduced this material to several researchers in the field.

Outcome of the Meeting

For this workshop, we intentionally invited researchers from several different fields, ranging from real algebraic geometry, operator theory, convex optimization, and theoretical computer science. Both the morning introductory talks and the long lunch-breaks were designed to encourage participants to learn new material from each other. We received positive feedback from several participants about how many new people they were able to meet and that the conference had a greater exchange of ideas than usual. There are also several on going collaborations among the participants of the program coming from different countries and the opportunity to meet and exchange ideas in person is invaluable.

One of the other impact of the 2010 meeting at Banff was the development of a strong community of young researchers in the field. In fact, three of the the current organizers were junior participants at this conference. In order to continue this positive momentum, there were several (at least seven) excellent talks by young participants. This workshop introduced them to the experts in the field and we hope that they will develop to be leaders of the field.

Participants

Anari, Nima (Stanford University)
Basu, Saugata (Purdue University)
Blekherman, Greg (Georgia Tech)
Branden, Petter (KTH Royal Institute of Technology)
Cimpric, Jaka (University of Ljubljana)
Dressler, Mareike (UC San Diego)
El Khadir, Bachir (Princeton University)
Helton, Bill (UC San Diego)
Henrion, Didier (University of Toulouse)
Infusino, Maria (University of Konstanz)
Klep, Igor (The University of Auckland)
Kuhlmann, Salma (Universität Konstanz)
Kummer, Mario (TU Berlin Germany)
Lasserre, Jean-Bernard (LAAS-CNRS 7, Toulouse)
Manevich, Dimitri (TU Dortmund University Germany)
Murray, Riley (CalTech)
Naldi, Simone (Université de Limoges)

Nie, Jiawang (University of California San Diego)
Piontek, Roland (TU Dortmund University Germany)
Plaumann, Daniel (TU Dortmund University)
Putinar, Mihai (UCSB)
Renegar, James (Cornell University)
Riener, Cordian (UiT - The Arctic University of Norway)
Roshchina, Vera (University of New South Wales)
Roy, Marie-Francoise (Universite de Rennes 1)
Safey El Din, Mohab (Sorbonne University)
Saunderson, James (Monash University)
Scheiderer, Claus (Univ-Konstanz Germany)
Scholten, Georgy (NCSU)
Shamovich, Eli (University of Waterloo)
Sinn, Rainer (Freie Universitaet Berlin)
Smith, Gregory G. (Queen's University)
Tetali, Prasad (Georgia Institute of Technology)
Thomas, Rekha (University of Washington)
Tunçel, Levent (University of Waterloo)
Vinnikov, Victor (Ben Gurion University of the Negev)
Vinzant, Cynthia (University of Washington)

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Chapter 11

Toward a Comprehensive, Integrated Framework for Advanced Statistical Analyses of Observational Studies (19w5198)

June 2-7, 2019

Organizer(s): Michal Abrahamowicz (McGill University, Montreal, Canada, Contact Organizer), Marianne Huebner (Michigan State University, East Lansing, MI, USA), Willi Sauerbrei (Medical Center, University of Freiburg, Freiburg, Germany)

The STRATOS initiative — motivation, mission, structure and main aims

The overall objective of the 19w5m198 BIRS Workshop was to further boost and consolidate the research activities of the international initiative for STRengthening Analytical Thinking for Observational Studies (STRATOS) (www.stratos-initiative.org). Therefore, to facilitate understanding of the rather unique character and goals of the Workshop, we begin this Report with a short overview of the STRATOS initiative, including its *raison d'être*, overall mission, internal structure and main objectives.

Lack of statistical expertise is now recognized as a significant brake on scientific progress across a wide range of empirical sciences. For instance, an influential article in The Economist (19/10/2013), 'Unreliable research: Trouble at the lab.' commented: *"Scientists' grasp of statistics has not kept pace with the development of complex mathematical techniques for crunching data. Some scientists use inappropriate techniques because those are the ones they feel comfortable with; others latch on to new ones without understanding their subtleties. Some just rely on the methods built into their software, even if they don't understand them."*

According to the general paradigm of modern sciences, statistical analysis methods are key to translate raw empirical data into new insights in, and deeper understanding of, complex processes affecting human health, the economy, environment, and many other phenomena studied in different branches of science. Yet, the complexity of such processes, and of the observable data they generate, create numerous analytical challenges. In the 21st century, parallel progress in the theory of mathematical statistics and computational resources and technology led to dynamic developments in statistical methodology, resulting in a large number of increasingly complex, ever more flexible, statistical techniques and models that allow researchers to account for several complexities frequently encountered in analyzing real-life data. Unfortunately, many of these important developments are ignored in every-day practice of data analysis, including analyses reported in influential publications in high-impact medical or social sciences journals. Consequently, the design and analysis of recent, often complex and costly, observational studies of human health and welfare often exhibit serious weaknesses. This leads to misleading inferences, which may, in turn, adversely affect the effective- ness or safety of different treatments, social or economic policy programs etc.

Formulating and overcoming these formidable challenges requires a well structured, highly interactive collaboration between a large, international group of statistical experts, whose research combines development of new methodology with collaborative research on real-life applications and whose joint, complementary expertise covers different sub-areas of statistical research. Indeed, such need arises due to a combination of (i) ever increasing complexity and variety of analytical challenges encountered in the majority of important observational studies, together with (ii) the increasing trend for narrow specialization, necessary to achieve cutting-edge novel developments in modern statistics. Together, these two trends imply that no single university-based (bio-)statistics department and no team of (bio-)statisticians (working in even the largest private or public research institutes or, e.g., pharmaceutical companies) is able to ensure state-of-the-art expertise regarding even a reasonable fraction of analytical challenges encountered in real-life applications. At present, particular challenges are being addressed by leading authorities in different areas of statistical research, but little effort is invested in combining the results of these separate developments and ensuring their material impact on the practice of data analysis. This situation provided the motivation for, and the driving vision behind, the STRengthening Analytical Thinking for Observational Studies (STRATOS) initiative. The STRATOS Initiative was launched in 2013 at the 34th conference of the International Society of Clinical Biostatistics (ISCB). It is connected to this society and had dedicated invited sessions or mini-symposia at almost all ISCB annual meetings in 2013–19 (with the only exception in 2017). After an Invited STRATOS session at the bi-annual meeting of the International Biometric Society (IBS) in 2016, the STRATOS initiative was invited to publish a series of short papers in the Biometric Bulletin, the official newsletter of IBS.

The initiative brings together leading, internationally recognized, methodological experts in several areas of statistics essential for the analyses of observational studies, who — at present — are grouped in nine Topic Groups (TGs), each focusing on a different, highly relevant area of statistical research (see Table 1 below). The experts' joint, largely complementary, knowledge allows the initiative to address complex analytical challenges in the design and analysis of observational studies, by developing, validating and comparing state-of-the-art methods for various topics. To increase the impact of our endeavors on empirical research, individual topic groups are working to summarize our findings by developing practical guidance regarding 'best practice' to address a particular set of analytical challenges (e.g. handling of measurement error or dealing with right-censored time-to-event data). The guidance covers such practical issues as e.g. the awareness of potential pitfalls due to inappropriate use of 'conventional' methods, the choice of appropriate, validated analytical methods able to overcome specific challenges, and software that can be used to implement these advanced methods.

We are entering the era of 'big data' with automated collection of very large amounts of data and the paradigm of empirical sciences shifting toward 'data science'. However, 'big data' will not help answering such essential prognostic or etiology questions if researchers use designs and statistical methods which are unsuitable, e.g. by being unable to account for the complexity of the underlying dynamic multi-factorial processes. Therefore, it is of central importance to gain knowledge about advantages and disadvantages of alternative statistical approaches, and their dependence on the data structure. Equally important is to develop, validate and explain to end-users state-of-the-art methods that can address frequent limitations (e.g. missing data, measurement errors, unmeasured confounding) and complexities of the data (e.g. non-linear relationships of continuous variable with the outcome, time-varying effects, mediation).

One of the fundamental objectives of the STRATOS approach is to develop guidance for data analysts and

Table 1. STRATOS Topic Groups and co-Chairs

	Topic Groups	Co-Chairs
TG1	Missing Data	James Carpenter, Kate Lee
TG2	Selection of variables and functional forms in multivariable analysis	Georg Heinze*, Aris Perperoglou*, Willi Sauerbrei*
TG3	Initial Data Analysis	Marianne Huebner*, Saskia le Cessie*, Werner Vach*
TG4	Measurement Error and Misclassification	Laurence Freedman*, Victor Kipnis*
TG5	Study Design	Suzanne Cadarette*, Mitchell Gail*
TG6	Evaluating Diagnostic Tests and Prediction Models	Ewout Steyerberg*, Ben van Calster*
TG7	Causal Inference	Els Goetghebeur*, Ingeborg Waernbaum
TG8	Survival Analysis	Michal Abrahamowicz*, Per Kragh Andersen*, Terry Therneau*
TG9	High dimensional Data Analysis	Lisa McShane*, Joerg Rahnenfuehrer*

* Indicates Participants of the BIRS 19w5198 Workshop.

researchers with different levels of statistical training, skills and experience. Specifically, we have identified three levels of statistical knowledge, each of which would require a somewhat different type of targeted guidance, and we have outlined the main criteria to be used when developing guidance aimed at the analysts at each level. Initially, we are working to derive guidance for experienced statisticians ('level 2'), which requires work on state-of-the-art methodology for each specific topic group. For each topic considered (see next section) several analytical strategies have been proposed in the statistical literature, but knowledge about their properties and relative strengths and weaknesses is often insufficient, as meaningful comparisons are rare and evidence-based guidance are lacking. For more details see Sauerbrei *et al*, (*Statistics in Medicine*, 2014, 33, 5413–5432), the STRATOS website http://www.stratos-initiative.org/ and short articles in the *Biometric Bulletin* (available on the STRATOS website).

Objectives of the Workshop

Overall Objectives:
The two, closely inter-related, overarching objectives of the 19w5m198 BIRS Workshop were to (i) further boost and consolidate the research activities of the STRATOS Topic Groups, and to (ii) identify and initiate new interdisciplinary collaborations between experts in different areas of statistical methodology, regrouped in different Topic Groups. (Both goals built on the earlier success of the 2016 BIRS Workshop 16w5091 that provided the first opportunity for a large group of 38 STRATOS members, and seven research trainees, to meet in-person, exchange ideas, jump-start several joint articles writing and develop an operational plan for further development and internal homogenization of the scientific and knowledge translation endeavors.)

In particular, during the 2019 Workshop, regarding objective (i), individual Topic Groups proposed recommendations to address the main analytical challenges within their area of expertise. Then, regarding objective (ii), based on these recommendations, we have started designing comprehensive strategies to deal *simultaneously* with several problems likely to be encountered in real-life empirical studies. By providing a unique opportunity for in-person discussions between experts from 14 countries on 3 continents, the Workshop was essential to initiate and largely facilitate such inter-disciplinary discussions and developments.

Specific Goals:
The 4 inter-related specific goals of the workshop were:

1. To provide an overview of the methods, related to the area of expertise of individual Topic Groups, applied

in the current empirical studies and identify the priorities for improving the methodological quality of such studies;

2. To identify methodological challenges, within the area of expertise of Topic Group, that require further validation or comparison of new or existing methods, and outline the analytical work or simulation studies necessary to provide reliable evidence supporting specific approaches and demonstrating the limitations of other methods, in the spirit of 'neutral comparison studies' (see the following article https://doi.org/10.1002/bimj.201700129);

3. To identify analytical challenges at the cross-roads of the interests of various Topic Groups, and to initiate new between-Groups collaborations on the new developments necessary to address such complex challenges in order to approximate the complexity of large real-life empirical observational studies, as well as comprehensive simulations necessary to assess and validate the resulting new methods;

4. To develop the uniform format, criteria, and general content for the integrated STRATOS-based guidance documents.

Overview of the Workshop participants and activities

Participants

Despite a few late cancellations we had no problems to fill all the 42 available places at BIRS. With 42 participants from 14 countries, spread over 3 continents, the meeting had truly a global character. Five research trainees, including 4 PhD students and 1 post-doc fellow, attended, in addition to one Research Associate. Among the 42 participants, 15 (36%) were women. Because of private reasons, the two co-chairs of Topic Group 1 (Missing data) could not attend and, therefore, this topic played only a marginal role in the 2019 Workshop.

Overview of the presentations and discussions

On Monday morning, we started with a summary of the recent developments of the STRATOS Initiative. During the week, we had several keynote talks by internationally recognized authorities. Frank Harrell (TG2) and Per Kragh Andersen (TG8) spoke about issues which were not directly related to the current work of any topic group, but which could be relevant for the future of STRATOS. Mitchell Gail, one of the chairs of the Design group (TG5) spoke about potential collaborations of the Design group with several other TGs. This talk was highly relevant for jump-starting several new inter-TG collaborations, one of the main aims of the Workshop. The Measurement Errors topic group (TG4) had recently made much progress and we decided dedicating a 90-minute plenary session to presentations from TG4. In four talks, Laurence Freedman, Victor Kipnis, Ruth Keogh and Pam Shaw summarized the results from the last year and presented directions for new research. During the first two days of the Workshop, each of 7 other TGs represented at the Workshop summarized their progress and plans for future in 45-minute plenary presentations. TG presentations also included thoughts about potential collaborations with other TGs, which created the basis for further discussions that initiated several joint efforts between topic groups (more details below in section 5 on new inter-TG collaborations). We had also more detailed presentations from two panels (talks from Lisa McShane and Saskia le Cessie from the Simulation Panel and Mark Baillie presented ideas of the new Visualization Panel).

Progress of the Glossary Panel was outlined in video presentation from Martin Boeker (Freiburg, Germany), an expert in medical informatics. In addition, we had shorter presentations from the Data Set and the Knowledge Translation panels.

To allow more detailed discussions and time for outlining the content of future manuscripts within TGs, as well as discussions between members of different TGs and/or panels, we also decided dedicate a substantial amount of time to separate meetings in smaller groups. These discussions often continued in the evenings. Results of these small groups discussions were presented and discussed on Friday morning, in two general sessions that summarized the conclusions of the BIRS meeting and provided an outlook for main activities planned for the next two years.

Summary of progress and plans by Topic Groups

Overview

Over the course of several plenary meetings, spread across the 5 days of the BIRS Workshop, each of the eight Topic Groups (TGs) represented at the Workshop, and selected cross-cutting Panels, presented their recent progress in the research activities leading toward the ultimate goal of developing the guidance regarding the choice, evaluation and implementation of state-of-the-art statistical methods relevant for addressing analytical challenges frequently encountered in their specific areas of interest. (Please see Table 1 above for the overview of the topics being the main focus of different TGs). (The exception was TG1 'Missing data', that – because of a number of conflicting responsibilities by its members – was represented only by a single member, and a PhD student who gave a talk on missing data). These presentations and updates helped inform and learn not only about the successes obtained so far, but also about the outstanding challenges, and the potential solutions that need to be evaluated to provide rigorous evidence regarding which methods may work, and under what conditions. All members benefitted immensely from face-to-face meetings, made possible by the BIRS grant. This was vital for establishing new long-term research collaborations, both within individual TGs, and – especially – between members of different TGs who have identified a number of the complex analytical challenges that will require combining the expertise developed within particular groups (outlined in more detail below). Such in-person meetings will also largely facilitate future continuation of these new collaborations, which – for the next two years - will rely almost exclusively on email and teleconferences.

Progress and Future Plans of individual Topic Groups

TG2: Selection of variables and functional forms in multivariable analysis

Discussions and interactions

All three co-chairs and six members of the topic group were present, as well as 2 trainees (1 post-doctoral fellow and 1 PhD student). This excellent representation led to productive conversations and initiation of several future projects and manuscripts (see below). Frank Harrell delivered a plenary talk on *"Controversies in Predictive Modeling, Machine Learning, and Validation."*

Research: current

The meeting allowed the plans of the group to be consolidated as follows:

- State-of-the-art paper on variable selection has been completed. It was decided to upload a copy at arxiv.org and the paper was submitted for publication in *Diagnostic and Prognostic Research.*

- Geraldine Rauch presented the current status of the manuscript on *'Systematic review of statistical series in medical journals'*. Following the BIRS meeting, a protocol has been finalized in a collaboration between Geraldine Rauch and Georg Heinze, and associates and was submitted as publication to a medical journal.

- Marie-Eve Beauchamp and Michal Abrahamowicz presented the current status of the collaborative paper, involving several TG2 members, on *'Systematic review of methods used for modeling of continuous variables and variables selection in medical and epidemiological journals'*. The protocol and evaluation criteria have been finalized, and currently data are independently extracted by two reviewers, one in Oxford, UK and one at McGill, in Canada.

Research: future

- A Topic Group meeting, to start a new collaboration on systematic evaluation and comparison of various spline-based approaches for selecting functional forms, will take place in Bonn, Germany on November 21-22, 2019. Presentations at the STRATOS-oriented Invited Sessions at ISCB 2020 (Krakow, Poland) and IBC 2020 (Seoul, South Korea) by TG2 members are planned.

- The group has identified a set of seven important open problems in their "State-of-the-art" paper. Members are expected to express their interested in leading relevant work. Further discussions will take place in the meeting in Bonn.

- Variable selection: Georg Heinze would lead on a new TG2 paper on variable selection, that will partly build on his previous work. Protocol for a simulation study is currently in preparation.

- Splines: Aris Perperoglou to lead a follow-up paper, building on the published TG2 paper on the review of spline packages in R.

- Procedures for variable & functional form selection: Willi Sauerbrei will take the lead for the new collaborative TG2 paper that will address both challenges simultaneously.

- Post-selection shrinkage: There is some preliminary work by Michael Kammer (Georg Heinze's student). Results will be included in Michael Kammer's PhD thesis.

- 'What is an appropriate stability measure?' Daniela Dunkler has submitted a session proposal for CEN2020 conference in Berlin on 'Variable selection and model instability', including contributions from Ewout Steyerberg (TG6), and Georg Heinze (TG2), Riccardo de Bin (TG9), Christine Wallisch.

- A new manuscript entitled 'When to prespecify a model and in which cases to consider variable selection?' was proposed by Frank Harrell.

TG3: Initial data analysis

Discussions and interactions

Four members, including the co-chairs, of the topic group were present, and one member joined via conference call for a group meeting. All were engaged in discussions and plans with other TG's (TG2, TG4, TG5, and TG9) as initial data analysis (IDA) is relevant for most other TGs, as outlined below, in the section on Between Groups Collaborations.

Research: current

- The manuscript on a systematic literature review on IDA reporting was discussed and revised. It has been approved by the STRATOS Publication Panel and has been submitted to *BC Medical Res. Meth*.

- Initial Outcome Data Analysis (IODA). Werner Vach described a randomized trial with several outcome variables and analyses that could be termed "Initial Outcome Data Analysis" (IODA). We discussed what might be considered IODA and other examples were shared.

- Saskia le Cessie developed a module with videos on IDA to be included in a MOOC by the University of Leiden. This course will run on the *Coursera* platform.

Research: future

As discussed below, several projects have been identified with other TGs. In addition:

- Carsten Schmidt obtained permission to use data from the large cohort Study of Health in Pommerania (SHIP). This will lead to a manuscript illustrating the IDA concepts and will serve as an example of reporting. In addition, recommendations for automatization of IDA can be developed.
- A conceptual paper on IDA in the context of multivariable regression analyses will be led by Werner Vach.
- New project on IDA for longitudinal studies will be led by Lara Lusa.
- TG3 will work with Mark Baillie and the STRATOS Data Visualization Panel to develop examples and recommendations for enhancing visual displays of the IDA results.

TG4: Measurement errors and misclassification

Discussions and interactions

Seven members, including the co-chairs, of the topic group were present, as well as 2 trainees (1 post-doctoral fellow and 1 PhD student). Current Research and progress was presented jointly in a plenary session. Veronika Deffner will be setting up a website for TG4, in line with the other TGs. Explorations for future joint papers with TG3, TG5, and TG8 took place, as outlined below.

Research: current

- A paper on a literature survey of the use of methods to adjust for measurement error in four areas of epidemiology was published in *Annals of Epidemiology*.
- A paper in *Statistics in Medicine* is under revision, after a favorable first review, which will be a guidance paper (in two parts) on measurement error and misclassification of variables in epidemiology, aimed at biostatisticians (level 2-3 paper).
- A paper on the general problem of measurement errors in epidemiology will be submitted to the journal *Significance*. This paper is written for the researchers without formal statistical background (level 1 paper).
- TG4 is conducting research into methods of handling the Berkson measurement error that occurs, for example, when prediction equation variables, or aggregate variables, are used in regression analyses.

Research: future

As discussed below, several future interdisciplinary collaborative projects have been identified with different other TGs. In addition, the following topics will be addressed in future TG4 research:

- Handling error-prone variables that are truly continuous but have been categorized for data analyses;
- A case-study paper on how to account and correct for measurement errors in practice (with real-life examples);
- A guidance paper for nutritional epidemiologists on handling measurement errors in nutritional epidemiology.

TG5: Study design

Discussions and interactions

Both co-chairs were in attendance, and they concentrated on discussions about collaborations with other Topic Groups. This focus was in agreement with the Workshop Organizers who had invited Mitch to give a Plenary talk designed to promote collaborations between TG5 and other TGs. Mitch and Suzanne had discussions with members of several TGs about joint projects, resulting in plans for projects with TGs 3 and 4. For more details see section 5 below. Discussions about approaches to increase the TG5 membership, and the related criteria, played also an important role.

Research: current

The first TG5 paper has been recently accepted for publication:

1. Final corrections of the revised version of an overview paper on study design were discussed among the TG5 members. The revised paper was resubmitted and will be published in *BMJ Open*:
Gail MH, Altman DG, Cadarette SM, Collins G, Evans SJW, Sekula P, Williamson E, Woodward M, for the STRATOS initiative (STRengthening Analytical Thinking for Observational Studies). Design Choices for Observational Studies of the Effect of Exposure on Disease Incidence. *BMJ Open* (In Press).

2. In addition, the short paper introducing TG5 to the members of the International Biometric Society was completed and published in *Biometric Bulletin*:
Gail M, Cadarette SM on behalf of TG5. STRengthening Analytical Thinking for Observational Studies (STRATOS): Introducing the Study Design Topic Group (TG5). *Biometric Bulletin* 2019; 36(2): 12-13.

Research: future

Interactions, during the BIRS Workshop, and plans for future collaborative projects with STRATOS TG3 and TG4 are described below, in the section 5 on Between-Groups Collaborations. In addition to the joint projects with other TGs, members of TG5 started work on two new papers, with the following preliminary titles:

- *'How to choose a design to study associations between prescription medications and risk of osteoporotic fracture.'* (This paper will focus on controlling for 'confounding by indication', which represents a paramount challenge for design of observational studies of medication effects. It will target a clinical audience).

- *'Design issues in prognostic studies.'*

TG6: Evaluating diagnostic tests and prediction models

Discussions and interactions

Three members attended, including the two co-chairs. Several topics were discussed, including some that had active involvement of the TG6 members, while not published under the umbrella of STRATOS. Potential new TG6 members were approached at the BIRS meeting.

Research: current

Three TG6 papers, being prepared for publication, have been discussed:

- "Performance assessment of survival models: a review". D McLernon and various STRATOS members: B van Calster, M van Smeden, E Steyerberg, T Therneau (TG8).

- "Myths about risk thresholds in prediction models". Laure Wynants, Maarten van Smeden, David J. McLernon, Dirk Timmerman, Ewout W. Steyerberg, Ben Van Calster. (This paper is now available at https://bmcmedicine.biomedcentral. 019-1425-3).

- "Calibration: the Achilles heel of predictive analytics". Ben Van Calster; David J McLernon; Maarten van Smeden; Laure Wynants; Ewout W Steyerberg. *BMC Medicine*.

Research: future

In collaboration with TG8, two future review papers on: 1/ performance assessment of competing risk and 2/ dynamic risk prediction models are planned.

TG7: Causal inference

Discussions and interactions

Four members were in attendance, including one of the two co-chairs. One of the main focus of the discussions were the Knowledge Translation (KT) activities of the TG7, in addition to initiation of collaborations with other STRATOS TG's (outlined below). TG7 created several short courses taught in an international setting. The output generated so far, consists of a TG7 website, www.ofcaus.org, that contains educational material on the concepts and methods of causal inference (using the potential outcomes framework). The website gives free access to presentation slides, practical assignments with questions and answers, data analysis problems with solutions and software code in R, SAS and stata, and source code for a 'simulation learner.'

Research: current

Saskia le Cessie gave a plenary talk on implementation, code, guidance, as well as potential and new statistical insights derived from the simulation learner. This is a large-scale, real-world based, simulated experiment in R that not only generates the 'observed data' but, for every subject, simulates also a set of possible alternative exposures with their potential outcomes. It allows to illustrate concepts, target estimands and statistical techniques with their practical properties for causal effect estimation in a unique way that has proven to be a great learning tool.

Research: future

Future joint collaborative projects were identified with TG8 and TG4, respectively, as described below.

TG8: Survival Analysis

Discussions and interactions

Six of the nine current TG8 members participated in the BIRS Workshop, including all three co-chairs, in addition to two trainees (1 PhD student and one Research Associate). Per Kragh Andersen gave a Plenary talk for all meeting participants. His talk focused on the methodological issues, as well as on their practical advantages in real-life applications, related to use of pseudo-values in survival analysis. Terry Therneau gave a plenary talk in which he summarized the recent TG8 progress and plans for future. Excellent representation of TG8 members (from 6 different countries on two continents) at the BIRS Workshop largely facilitated in-person exchanges and led to productive discussions. An after-hours TG8 meeting was held during the BIRS Workshop, in addition to regular program, to discuss both the ongoing research and plans for future TG8 activities. In addition, as outlined below, two small-group meetings with other STRATOS TG's were held to initiate and outline future collaborative projects involving TG8 members.

Research: current

The main focus of the within-group discussions was on the final steps of the revisions of the TG8 review/tutorial paper that provides guidance on the fundamental issues and analytical challenges typically encountered in survival analysis (or 'time-to-event' analyses), in the classic setting of single-event studies (e.g. of all-cause mortality). This paper, co-authored by all nine TG8 members, is oriented toward researchers with solid general statistical training who, however, do not have in-depth expertise in survival analysis (considered 'level 2' paper according to the STRATOS criteria). The BIRS meeting gave an excellent opportunity to exchange ideas regarding some specific details of the content of this first TG8 paper, mathematical notation and – above all – the final choice, and presentation, of the real-life examples that will clearly illustrate different methodological challenges, and the methods recommended to avoid the potential pitfalls. During the BIRS meeting, a consensus was reached regarding these outstanding issues, and the manuscript is currently undergoing the final revision and will be submitted for publication in Statistics in Medicine in December 2019.

Research: future

As a logical extension of the discussions about the first TG8 paper, the group members present in Banff had also an opportunity to consider different options for how to address several further, more 'advanced' analytical challenges. These discussions, together with earlier discussions among six TG8 members present at the IBC 2018 meeting in Barcelona, identified several issues that are also highly relevant for time-to-event analyses of observational data, but – largely because of the space limitations – could not be adequately covered in the initial TG8 'tutorial', outlined above. These future activities will aim at providing further guidance regarding such, more complex topics as, for example (in random order): (i) competing risks and modeling of multi-state transitions, (ii) alternatives to the ubiquitous Cox's proportional hazards model (Accelerated Failure Time and Additive Hazards models), (iii) interval-censored data, (iv) modeling of time-varying covariates (lagged or cumulative effects, impact of sparse, irregular measurements), and (v) net survival methods to correct for unknown causes of death. It was generally agreed upon that different (though partly overlapping) subgroups of the TG8 members may collaborate more closely on each specific topic, and preliminary ideas regarding who may take a lead on particular future manuscripts were also considered. It was decided to start developing concrete plans for the future papers, to deal with some of the above issues, in the Winter/Spring of 2020. These plans will be then ironed out during an in-person meeting of the most TG8 members during or after the 41st International Society for Clinical Biostatistics (ISCB) meeting in August 2020 (several TG8 members are either Invited Speakers or members of the Scientific Program Committee for the ISCB 2020 conference).

In parallel, TG8 started discussions about new inter-group collaborative projects with the STRATOS TG7 (Causal Inference), TG5 (Predictive Models) and TG4 (Measurement Errors), as outlined below.

TG9: High dimensional data

Discussions and interactions

Six members, including the two co-chairs, were in attendance. and an overview paper for high dimensional data was discussed. Key issues were presented by Lisa McShane in a Plenary presentation to the full STRATOS group at BIRS. Details of the development, and of the future content, of the dedicated TG9 website, to be linked to the STRATOS main website, was agreed upon.

Research: current

- The overview paper for the high dimensional data group was further refined. Data analysis pipelines for a wide variety of omics data with detailed worked examples would serve as guidance to practitioners. While this is geared toward "omics" data, other types of high-dimensional data (e.g., medical records databases with large numbers of variables per individual) are potential examples. Real-life examples of how and why standard statistical approaches can "break down" in high dimensional data settings will be important to include.

- A paper on the topic of simulation of high dimensional data, in collaboration with the STRATOS Simulation Panel, is planned to address those aspects and challenges of designing and carrying out complex simulations that are particular for high dimensional data.

Research: future

- Needs already identified include better guidance and methods for design of studies involving high-dimensional data and methods for simulation of high-dimensional data. Better methods to simulate realistic high-dimensional data will be critical for assessing performance of new analysis methods and for comparison of existing methods and are therefore essential to many aspects of TG9's work.
- Design of studies is particularly challenging given the often broad aims of these studies, e.g., identification of clusters, and likely complex distributions of these data.
- Several members of TG9 will be actively involved in a STRATOS-wide project to evaluate machine learning methods and better understand their strengths and weaknesses compared to more conventional statistical methods.

New Collaborative research projects involving Joint Efforts of different Topic Groups

In addition to enhancing the aforementioned research activities of individual Topic Groups (TG), the BIRS Workshop created a unique opportunity to identify, stimulate and foster new 'inter-disciplinary' collaborations between members of different TG's. Indeed, as reflected in the Workshop's title, one of our major focuses was on *integrating* recent developments made in different areas of statistical research of major relevance for the analyses of complex observational studies. This aspect of the Workshop drew directly on the rich range of the expertise of the members of separate TG's, who – in most cases – had no earlier opportunities to work together on common collaborative projects. Figure 1 below summarizes different new between-TG's collaborative links created during the BIRS Workshop. Later, in this section, we outline the scope of 10 new between-groups collaborations, and provide a brief summary of respective discussions.

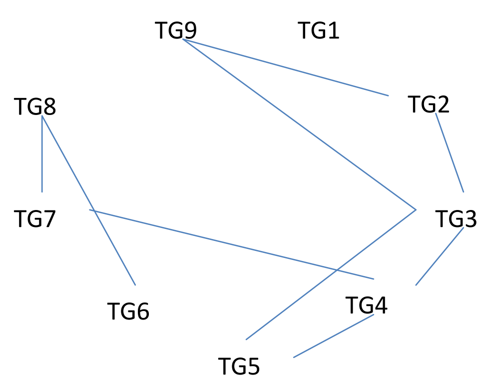

Figure 11.1: New between-TG's collaborative links

TG2 and TG3. Our meeting included 4 TG3 members (Mark Baillie, Marianne Huebner, Werner Vach, and Carsten Oliver Schmidt) and 5 TG2 members (Frank Harrell, Georg Heinze, Aris Perperoglou, Matthias Schmid, and Willi Sauerbrei). Two joint TG2-TG3 papers have been proposed: one more theoretical under the lead of Werner Vach (TG3) and one applications-oriented to be co-led by Marianne Huebner (TG3) and Georg Heinze (TG2). For the latter, five initial data analysis (IDA) topics are to be included (distribution of a single variable, associations between variables, missing data, measurement error, levels of measurements) and the paper will illustrate how these activities addressing these might impact the set-up of the multivariable regression analysis. Three data sets were proposed by MH, FH, and COS. Work on illustrating the IDA topics with these data sets will be divided between the participants. Georg Heinze and Marianne Huebner will co-present the results at the Invited STRATOS Session at the 41st ISCB meeting in Poland, in August 2020.

TG2 and TG9 and Simulation panel. Issues of model-based simulation and data-based (plasmode) simulation were discussed. Michael Kammer (PhD student of Georg Heinze, TG2) presented his R package 'SimulatoR' which implements the ideas of e.g. [Binder et al 2013, Stat Med], and [Royston and Sauerbrei, 2008 monograph, Wiley], for model-based simulation of realistic data. The package will soon be made available on CRAN. Further discussions focused on issues specific to simulating high-dimensional data. Michal Abrahamowicz (TG2/TG8), a co-chair of the Simulation Panel, made some suggestions based on his experience, and it was decided to pursue this challenging theme in a future in-person meeting during the ISCB 2020.

TG3 and TG9. Marianne Huebner (TG3) and Joerg Rahnenfuehrer (TG9) worked on the TG9 overview paper to align initial data analysis (IDA) steps for high dimensional data with those already developed by TG3 for 'standard' settings, where the number of subjects largely exceeds the number of variables.

TG3 and TG4. Marianne Huebner, Werner Vach, and Carsten Schmidt from TG3 met with Laurence Freedman, Victor Kipnis, Pamela Shaw, Michael Wallace, Paul Gustafson, and Veronika Deffner from TG4 to discuss possible future collaborations and the need to develop a common approach to measurement errors. TG4 approaches to measurement error rely mostly on modeling such errors in the context of specific application areas, e.g. nutrition and physical activities, or validation studies. On the other hand, TG3, so far, has discussed examples of detecting possible measurement errors through investigating data properties. CS shared examples of examiner effects over time in the SHIP data (see TG3 report above). LF suggested that CS shall come up with a concrete proposal on which the two TGs can work together.

TG3 and TG5. An informal discussion of Carsten Schmidt (TG3) and Mitchell Gail (TG5) aimed at identifying and initiating potential collaborations concerning study design set up that will facilitate the IDA activities. CS has sent a draft with ideas on study design relevant issues for IDA approaches being promoted by TG3.

TG4 and TG5. Mitchell Gail and Suzanne Cadarette (TG5 co-chairs) met with Laurence Freedman, Victor Kipnis, Pamela Shaw, Michael Wallace, Paul Gustafson, and Veronika Deffner from TG4 to discuss the objectives and the content of a future joint paper on design issues related to measurement error. The focus will be on the introduction of previously proposed two-phase designs in case-cohort or nested case-control studies (e.g. by N. Breslow) to researchers who may be unfamiliar with these techniques, in the context of investigating the safety or comparative effectiveness of treatments in observational data. We decided to focus on validation studies where there is gold standard (or at least accepted) measurement against which to assess error. A motivating example might be the use of electronic health records (EHRs), which are subject to measurement errors in both covariates and outcomes. Validation studies within and EHR study might improve inference. Ideally, one would have a test example with validated measurements on all subjects. Using these data we could estimate the "true" model. Then we could see how well limited-size subsamples used for validation led to estimates approximating the true model, and we could see how far off were the original estimates, based on the model fit to error-prone EHR data. Pamela Shaw will liaise with Mitchell Gail on taking this plan further.

TG7 and TG4. Members of TG7 (Causal inference) met with Ruth Keogh (TG4) to discuss potential issues of common interest to both groups. Two topics emerged for future collaborations:

- Guidance on design and analysis of observational population-based studies on the real-life effectiveness and safety of cancer treatments, and their impact on the patients' quality of life.

- Developing further insights and guidance on landmark analysis and its ability to allow for additional causal effect insights under well understood assumptions.

TG6 and TG8. Discussion between TG6 members (Ewout Steyerberg, Ben van Calster, Marteen van Smeden) and Terry Therneau (TG8 co-chair) revolved around a planned review paper on the new approaches and criteria for performance assessment of the predictive models in time to event analyses of right-censored data. The content and methods of the paper were outlined and the design of future simulations, to validate and compare alternative approaches, was considered. Additional TG8 members may join this collaborative project in future.

TG4 and TG8. Michal Abrahamowicz (one of the TG8 co-chairs), and his two trainees, met with TG4 members: Laurence Freedman, Victor Kipnis, and Pamela Shaw, as well as a PhD student of Ruth Keogh, to discuss possible new collaboration on correcting for measurement errors in the context of flexible modeling of the effects of time-varying covariates (TVC) in survival analysis. These discussions identified 2 different sources of potential measurement errors: (i) ‘classic’ errors in the observed TVC values, and (ii) errors specific to TVC‘s, related to sparse and/or irregular measurements during the follow-up time (e.g. at the time of clinic visits), each of which requires different analytical tools. Additional challenges may need to be addressed if the hazard does depend not only on the current TVC value but possibly also on its past values (due e.g. to the lagged or cumulative effects). As a preliminary step, the participants exchanged some ideas regarding whether and how the existing approaches to handling measurement errors, such as SIMEX or regression calibration, could be adapted to this complex setting. It was decided that Michal Abrahamowicz will update the interested TG4 members on the progress in implementing these ideas and evaluating them in preliminary simulations.

TG7 and TG8. Most members of both TG7 (Causal Inference) and TG8 (Survival analysis) met to discuss topics of joint interest. Several topics were identified as promising, relevant and targets for future collaboration:

- A sequel of the original TG8 tutorial paper, where right censored survival times are considered as the key outcome, and all specifics and key complications for that setting are explained and similarly worked out, taking into account considerations relevant for causal inference . This joint project may represent an important step toward reconciliation of the survival analytical vs. causal inference research paradigms.

- An extension of the currently available methods that allow for more accurate modelling of the effects of measured time-varying confounders and time-varying exposures. The possibility of a future contribution, regarding this complex challenge, to the new book on survival analysis being written by Terry Therneau (TG8 co-chair) and co-authors was suggested.

- A further similar extension that will allow for mediation analysis.

- Development of a graph-based tool (DAG-oriented) and method to help researchers decide on the covariates they need to measure and adjust for in a given setting where the causal effect of an observational exposure is targeted, in time-to-event analyses, and the ‘no unmeasured confounders assumption’ will be relied upon.

Outline of the progress and future plans by selected STRATOS Panels

Eleven cross-cutting STRATOS panels have been created to coordinate the activities of different TGs, share best research practices, and disseminate the research tools and the results across the TGs. These panels address common issues such as creating a glossary of statistical terms, giving advice on how to conduct literature reviews or simulation studies, and setting publication policies for the initiative. The recommendations of the cross-cutting panels are intended to support, integrate and harmonize work within and across the TGs, and to increase transparency in producing guidance. The STRATOS website www.stratos-initiative.org provides an overview of all 11 panels.

Discussions about the structure, objectives and modus operandi of several panels played a key role in the first BIRS meeting, in 2016. Since then, several panel-specific issues have been resolved, so that during the 2019 Workshop, it was decided to focus more detailed panel presentations and discussions on the issues relevant mostly to three panels: the Simulation Panel, the (newly created) Visualization Panel, and the Glossary Panel. Below, we briefly summarize the goals of these three panels, and the relevant discussions during the 2019 BIRS Workshop.

Simulation Panel (SP)

Simulation studies are key to the work of all STRATOS TGs. They are essential to (i) validate some of the recently developed methods, (ii) compare how the relative advantages and disadvantages of alternative methods depend on the true underlying data structure, and (iii) at time, illustrate the pitfalls and potentially serious errors induced by conventional methods (frequently used in the applied research), especially when the underlying assumptions are violated. This panel develops and promotes principles for, and provides examples of, best practice for simulation studies.

Discussions during the BIRS workshop focused on drawing on the literature to identify the key principles, and find useful published examples, which will help TG members with the design, conduct, analysis and reporting of targeted simulation studies, addressing issues most relevant for their areas of expertise. This will help ensure that the conduct of simulation studies is as consistent as possible across TGs (especially when they touch on similar issues), and support the accessibility, transparency, and reproducibility principles, that are fundamental to all STRATOS research activities. Moreover, there were specific discussions on a project for a level 1 paper on simulation studies, and a potential collaboration with TG9 about the design of simulations for high-dimensional data.

Visualization Panel (VP)

The goal of quantitative science is to enable informed decisions and actions through a data-driven understanding of complex scientific questions. It is the role of any quantitative scientist (e.g. psychometrician, statistician, epidemiologist, etc.) to support this goal through (1) identification of the scientific question of interest (2) choice of the appropriate quantitative methods to address this question (experimental design, statistical or mathematical models, etc.), and (3) effective communication of the results. All of these aspects have to work in concert, including the 3rd challenge, which often receives less attention in the conduct of scientific studies. Yet, the ability of a scientific study to make an impact depends strongly on effective communication, and neglecting this essential component may be often the reason why many sophisticated investigations remain without a material impact. Effective visual communication is a core competency for the quantitative scientist. It is essential in every step of the quantitative workflow, from scoping to execution and communicating results and conclusions. With this competency, we can better understand data and influence decisions towards appropriate actions. Without it, we risk missing an opportunity to turn the research results into clear conclusions and evidence-based actions. These considerations motivated the STRATOS Steering Group to create, in 2018, a new Visualization Panel (VP), whose overall goal is to promote the use of good graphical principles for effective visual communication. The aim of the panel is to provide guidance and recommendations covering all aspects relevant for the statistical analyses, from the study design, to implementation of specific analytical methods, to the choice of most effective graphical displays and tools. Discussions during the BIRS workshop focused on membership and direction of this newly formed Panel, with the aim to have a formal kick-off meeting around the end of 2019.

Glossary Panel (GP)

The status of the STRATOS glossary and a web-based user interface for its editing were reported.

The STRATOS glossary is based on the second edition of the ”Dictionary for Clinical Trials” by Simon Day. All terms and definitions relevant to STRATOS have been imported from the original text source into a database. Links between dictionary entries have been conserved. Agreement has been given by NICE to use terms from their glossary (https://www.nice.org.uk/glossary). Relevant terms from there are currently being extracted and will be included into the database together with a source indicator (provenance) of each entry.

The current graphical user interface of the STRATOS glossary allows a limited number of editors to read and write proposals for changes and new entries. All users can see what the other editors proposed. They can individually add/comment/propose. The current editor user interface is technically based on Jupyter which allows for a rapid integration of new requirements. The current interface will not be the definitive end user interface.

The development of a STRATOS glossary is an important step for the overall STRATOS project. As a mid-term objective a machine-readable STRATOS terminology/ontology derived from the glossary should be developed integrating with already existing terminologies (e.g. from https://bioportal.bioontology.org/).

The next step will be to roll the database out to all STRATOS members, along with a little training/tutorial on how it can be used.

Further issues discussed at BIRS and plans for the future

STRATOS representation at future international conferences

Presentations at scientific conferences are one of the most important activities to disseminate knowledge developed within the STRATOS Initiative to a broader audience of analysts with varying levels of statistical education, experience and interests. Invited sessions, mini-symposia and courses are highly relevant to increase both the efficiency and the timeliness of dissemination of the STRATOS results. We discussed details of presentations in the near future (e.g. Mini symposium at the 40th ISCB meeting in July 2019) but also more detailed plans for future presentations (eg. Invited STRATOS Sessions at the two most important international biostatistical conferences in 2020: (i) the 41st ISCB conference in Poland (August) 2020, and (ii) the 30th IBC meeting in South Korea (July 2020), as well as mini-symposia at the CEN & GMDS 2020 meetings in Germany) and discussed to approach organizers of other meetings relevant for topics of STRATOS. After the BIRS Workshop we were invited to give a short presentation and present a poster (attached at the end) at the European Public Health Conference in November 2019.

STRATOS series in the *Biometric Bulletin*

After the invited session at the International Biometric Conference (IBC) in 2016 we were invited to write a series of short papers in the Biometric Bulletin, summarizing quarterly the news for members from the International Biometric Society (IBS). In 2019, IBS has approximately 6,000 members from 80 countries. We had started with an overview paper in Issue 3 of 2017, followed by a series of TG-specific short papers, in the consecutive issues in 2018 and 2019. During the BIRS Workshop, we discussed our interest to proceed with further STRATOS papers in the Biometric Bulletin and agreed that papers from several panels could also be very helpful to transfer STRATOS-generated knowledge to a wider community of for IBS members. Following on these discussions, more recently we have agreed with the IBS President and the Bulletin Editor to start with papers from STRATOS panels in issue 1/2020. The first two papers will be written by the Simulation and the Visualization Panels.

STRATOS involvement in the SISAQOL Consortium

Two weeks before the BIRS Workshop, the Consortium on Setting International Standards in Analyzing Patient-Reported Outcomes and Quality of Life Endpoints Data (SISAQOL, https://qol.eortc.org/projectqol/sisaqol/) has invited us to join a large grant application in the Innovative Medicines Initiative of the European Union. Viktor Kipnis (TG4) has agreed to review some of the related papers and gave a short presentation about the intended project. We discussed the potential interest for STRATOS and agreed having a first meeting with leading members of the SISAQOL Consortium in July 2019. Led and coordinated by members of the European Organisation for Research and Treatment of Cancer (EORTC) a grant application was submitted recently. Several STRATOS members lead a work package about recommendations from observational studies.

STRATOS paper on 'Methodological issues in medical research and patient care-critical appraisal of statistical and machine learning techniques'

Many stakeholders (researchers, companies, funders, the public, doctors, patients and more) consider 'Data Science' as a key part to improve issues related to patient care and health research. However, most people do not understand what's behind such complex concepts as 'Artificial Intelligence (AI)', personalized treatment, individual predictions, or causal effects. Even many researchers do not (fully) understand that AI related methods not only have an exciting potential but they also need to confront several important challenges. Aiming to provide more evidence supported knowledge about advantages and disadvantages of various techniques, during the Workshop we have proposed to write a STRATOS paper with the working title "Methodological issues in patient care and medical research - critical appraisal of statistical modeling and machine learning techniques". It was decided that Jörg Rahnenführer (TG9) and Matthias Schmid (TG2) will co-lead the development of this paper. In the four months after the BIRS Workshop, joint work on this complex paper has started and more than ten members from several STRATOS Topic Groups and Panels have joined the project and participated in discussions about its content and methods.

Summary of the BIRS Workshop activities and achievements

Activities:

Over the course of several plenary meetings, Topic Groups and selected Panels presented progress in identifying those issues within their areas of statistical expertise that need guidance, and in the steps undertaken to prepare and develop the guidance. This helped to inform and learn not only about the successes obtained so far, but also about the challenges having been encountered, and that solutions that either were already implemented and found to have worked or were planned to address these challenges. All members benefitted immensely from face-to-face meetings. This was vital for establishing new long-term research collaborations, the continuation of which will be almost exclusively by email, teleconferences and meetings of smaller groups.

Interactions between topic groups and establishing new cross-TG collaborative projects was one of the main themes of the BIRS Workshop. Topic groups came prepared with proposals of such projects and were able to connect in break-out sessions, which resulted in 10 concrete new collaborative projects (summarized in section 5 of this Report). In addition, to the inter-group collaborative plans, each TG discussed current and future STRATOS manuscripts and project management. In general, for each such collaboration, one or two leading researchers within the relevant TG have been identified, and all TG members who express an interest are invited to actively contribute to a given project. Input from the other TG members will be sought at various stages, e.g. before presentations and for revisions of manuscript drafts. Moreover, TG-specific websites with a common format were proposed in the interest of up-to-date information, activities, and resources. All participants expressed the strong wish having more regular meetings in smaller groups, and plans for several future TG meetings, joint meetings of the members from two or more TGs and/or one or two panels with somewhat overlapping mandates (e.g. Knowledge Translation vs Publication panels) were outlined during the Workshop small-group meetings and discussions.

Achievements:

The participants were unanimous in that the 2019 BIRS workshop was very successful in stimulating both: (i) further progress in research activities of individual Topic Groups (summarized in section 4 of this Report); and (ii) initiation of new, creative, multi-disciplinary inter-TG collaborative projects, tackling complex analytical challenges and issues that require joint expertise of the members of two or more different TG's (section 5 of the Report). Indeed, there was a general consensus that the BIRS Workshop created a unique opportunity for in-person exchanges and productive discussions between experts in different areas of statistics, and from 14 different countries on 3continents, without which such fruitful, dynamic interactions would not be possible. Each of the eight Topic Groups (TGs) represented at the Workshop made an impressive progress in developing and finalizing their respective research papers, as summarized in individual TG reports in section 4 above. Furthermore, the longer-term scientific yield of the BIRS Workshop activities will be reflected in many research papers designed or enhanced through the Workshop discussions (please see sections 4, 5 and 7.4 for more details on the manuscripts being prepared or planned through, respectively, (i) joint efforts of several members of specific TG's and (ii) new inter-TG collaborations initiated during the Workshop). Thus, the Workshop met its overarching objectives, outlined in section 2 above, of both enhancing and integrating the research activities of individual STRATOS Topic Groups. Given the achievements of the 2019 BIRS Workshop, there was also an overwhelming consensus that it will be essential to organize the next general meeting of the STRATOS team in about two years.

Participants

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Chapter 12

Women in Analysis (WoAN) - A Research Collaboration Conference for Women (19w5082)

June 9 - 14, 2023

Organizer(s): Donatella Danielli (Purdue University), Irina Mitrea (Temple University)

Short Overview

Following the successful models of the mathematical communities WIN, WINASc, WiSh, WhAM!, WIT, the one-week collaboration workshop 19w5082 co-organized by Donatella Danielli (Purdue University) and Irina Mitrea (Temple University), was the first international activity of the newly founded Women in Analysis (WoAN) research group. The workshop hosted the following collaborative research teams:

1. **Complex Analysis**
2. **Free Boundary Problems**
3. **Geometric Analysis**
4. **Harmonic Analysis**
5. **Inverse Scattering Theory**
6. **Nonlinear Dispersive Equations**

Each team was led by internationally recognized women experts in these fields. Scientific activities at the workshop included introductory lectures and discussions, collaborative research time, a poster session for junior participants, and wrap-up sessions in which teams reported on their progress. The workshop schedule also included a professional development session. Below we will elaborate on the scientific content of the workshop and the progress registered by the various collaboration teams.

Introductory Lectures/Discussions

The goal of these colloquium style lectures and discussions were to introduce *all* workshop participants to the history and general developments in each of the emphasis areas.

- **Complex Analysis**. One of the main themes discussed in the Complex Analysis group was the Hartog's triangle in complex Euclidean space and its corresponding formulation in complex projective space. The Hartog's triangle in $\mathbb{C}^2$ is defined by:

  $$H =: \{(z, w) \in \mathbb{C}^2 : \ |z| < |w| < 1\}.$$

  and is an important example in Several Complex Variables (SCV) as it provides many interesting phenomena in SCV which do not exist in one complex variable. It is the first example of a pseudoconvex domain which does not admit a Stein neighborhood basis. At the same time, H is rectifiable but not Lipschitz. It is also a non-tangentially accessible domain, a recent subject of intense research by many leading harmonic analysts. The specific problems on the Hartog's triangle in Complex Euclidean space discussed during the program were:

  1. the density and extension problems in the Sobolev spaces for the Hartog's triangle in complex Euclidean space;
  2. boundary integral representation formulas for functions holomorphic in the interior of the Hartog's triangle that satisfy suitable regularity up to the boundary, and related questions concerning the notion of Shilov boundary; theory of holomorphic Hardy spaces, Szegö projection, etc.

  The presence of even just a single non-Lipschitz boundary point makes the study of any aspect of boundary behavior of holomorphic functions much more involved than the analysis of their interior behavior, and it accounts for the minimal progress to date in the existing literature for item 2 above.

- **Free Boundary Problems.** Reaction-diffusion systems with strong interaction terms appear in many multi-species physical problems as well as in population dynamics. The qualitative properties of the solutions and their limiting profiles in different regimes have been at the center of the community's attention in recent years. A prototypical example is the system of equations

  $$\begin{cases} -\Delta u + a_1 u = b_1 |u|^{p+q-2} u + cp|u|^{p-2}|v|^q u, \\ -\Delta v + a_2 v = b_2 |v|^{p+q-2} v + cq|u|^p |v|^{q-2} v \end{cases}$$

  in a domain $\Omega \subset \mathbb{R}^N$ which appears, for example, when looking for solitary wave solutions for Bose-Einstein condensates of two different hyperfine states which overlap in space. The sign of b_i reflects the interaction of the particles within each single state. If b_i is positive, the self interaction is attractive (focusing problems). The sign of c, on the other hand, reflects the interaction of particles in different states. This interaction is attractive if $c > 0$ and repulsive if $c < 0$. If the condensates repel, they eventually separate spatially giving rise to a free boundary. Similar phenomena occurs for many species systems. As a model problem, we consider the system of stationary equations:

  $$\begin{cases} -\Delta u_i = f_i(u_i) - \beta u_i \sum_{j \neq i} g_{ij}(u_j) \\ u_i > 0 \ . \end{cases}$$

  The cases $g_{ij}(s) = \beta_{ij} s$ (Lotka-Volterra competitive interactions) and $g_{ij}(s) = \beta_{ij} s^2$ (gradient system for Gross-Pitaevskii energies) are of particular interest in the applications to population dynamics and theoretical physics respectively.

The introductory lecture discussed recent advances in the analysis of phase separation phenomena arising in competition-diffusion system. Indeed, phase separation has been described in the recent literature, both physical and mathematical. Relevant connections have been established with optimal partition problems involving spectral functionals. The classification of entire solutions and the geometric aspects of phase separation are of fundamental importance as well. The lecture focused on the most recent developments of the theory in connection with problems featuring:

1. Competition-diffusion problems with fractional laplacians.
2. Competition-diffusion problems with non local interactions.
3. Spiralling solutions in the non symmetrical case.

- **Geometric Analysis**. The field of geometric flows has been thriving in the past few decades because of its powerful applications to topology, geometry, analysis, and general relativity. In many applications, it is important to understand how the flow could continue after a singular time, by a better understanding of singular formation, which is the focus of our discussion during the workshop.

  Let (M, g_0) by a compact Riemannian manifold without boundary. A solution to the Ricci flow is a family of metrics $\{g(\cdot,t)\}$ on M satisfying the deformation $\frac{\partial g}{\partial t} = -2\mathrm{Ric}$ where Ric is the Ricci curvature of $g(\cdot,t)$ with $g(\cdot,0) = g_0$. We say that T is a singular time if there is a sequence of points $p_k \in M$ and a sequence $t_k \to T$ such that
  $$Q_k = |\mathrm{Rm}|(p_k,t_k) = \max_{M\times[0,t_k]} |\mathrm{Rm}| \to +\infty \quad \text{as } k \to \infty.$$
  A singular model is the limiting metric $g_\infty = \lim_{k\to+\infty} g_k$ where $g_k(\cdot,t) = Q_k g(\cdot, t_k + tQ_k^{-1})$ are the appropriate rescaling metrics corresponding to $\{p_k\}$. If the blow-up rate of Q_k is sublinear in $T - t_k$, which in particular implies it must be linear in $T - t_k$, the singularity is called Type I. All other singularities are called Type II.

  We now turn to the mean curvature flow, which is an extrinsic geometric flow that deforms hypersurfaces in $\mathbb{R}^{n+1}$. Let M be a complete hypersurface in $\mathbb{R}^{n+1}$ and let $F(x,t) : M \times [0,\varepsilon) \to \mathbb{R}^{n+1}$ be a family of immersions parametrized by t with $F(\cdot,0) = M$. The mean curvature flow is a solution F whose speed of deformations is given by the mean curvature vector at each instant time, that is, $\frac{\partial F}{\partial t} = -H\nu$, where ν is the outward unit normal to $M_t = F(\cdot,t)$ and the mean curvature is $H = -\mathrm{div}_{M_t}\nu$. If M is compact, the mean curvature flow must stop at a finite time by avoidance principle. One can similarly define the singular models and types as for the Ricci flow.

  There are many similarities between the two flows, they are both gradient flows and in both flows the monotonicity formula has been discovered, in the mean curvature flow by Huisken and in the Ricci flow by Perelman. Those monotonicity formulas play important role in singularity analysis in both flows. Three main topics that the Geometric Analysis groups is interested in pursuing are (1) Ricci flow solutions with degenerate neck-pinches, (2) Stability of cylindrical solutions to the Ricci flow, and (3) Stability of translating solutions to the mean curvature flow.

- **Harmonic Analysis.** Pattern identification in sets has long been a focal point of interest in geometry, combinatorics and number theory. No doubt the source of inspiration lies in the deceptively simple statements and the visual appeal of these problems. A few prototypical examples discussed in the introductory part of the workshop where:

  [1.]

  1. A set occupying a positive proportion of the natural numbers contains arbitrarily long arithmetic progressions (AP-s). This affirmative answer by Szemerédi to the famous Erdös-Turán conjecture is one of the masterpieces

of modern mathematics [24, 14], and a trendsetter in this field. More generally, given a set $A \subseteq \mathbb{Z}^d$ with positive density, i.e.,

$$\limsup_{N\to\infty} \frac{\#\left(A \cap [-N,N]^d\right)}{\#\left([-N,N]^d\right)} = d(A) > 0, \quad \text{where } \#(A) = \text{cardinality of } A,$$

and any finite configuration $S \subseteq \mathbb{Z}^d$ (say a polytope), A has infinitely many $\mathbb{Z}$-affine copies of S.

2. Contrast this with a problem in the Euclidean setting. A set $S \subset \mathbb{R}$ is said to be universal if every set of positive Lebesgue measure contains an affine copy of S. A classical theorem of Steinhaus shows that all finite sets are universal. A famous question of Erdös [12] asks: does there exist an infinite universal set? Despite its superficial analogy with Szemerédi-type questions in $\mathbb{Z}^d$, this problem remains unsolved. All results to date merely establish that certain infinite structures are non-universal [13, 6, 16]. In particular, we do not even know if $\{2^{-n} : n \geq 1\}$ is universal.

3. Alternatively, one could ask for a set containing all sufficiently large copies instead of infinitely many affine copies. A result of Bourgain [5] says that if $A \subseteq \mathbb{R}^d$ has positive upper density, i.e.,

$$\limsup_{R\to\infty} \frac{|A \cap B_R|}{|B_R|} = \delta(A) > 0, \text{ where } |\cdot| = \text{Lebesgue measure}, \; B_R = \{x \in \mathbb{R}^d : |x| < R\},$$

and $S \subseteq \mathbb{R}^d$ is any set of d points spanning a $(d-1)$-dimensional hyperplane (e.g. a line in $\mathbb{R}^2$ or a triangle in $\mathbb{R}^3$), then there exists ℓ_0 such that A contains an isometric copy of ℓS for every $\ell > \ell_0$. The corresponding statement when $\#(S) > d$ is not known, though there are some partial results [25]. For instance, we do not know if a set in $\mathbb{R}^3$ of positive upper density contains all sufficiently large regular tetrahedra.

These problems share the common feature that they aim to identify patterns in thick sets. There is now an immense variety of results in this genre, asserting existence or avoidance of configurations under assumptions on size, often stated in terms of measure, dimension or density. While this body of work has contributed significantly to our understanding, a complete picture is yet to emerge. Not surprisingly, such questions are nontrivial when posed for a thin set whose content is insignificant when measured on some of these scales.

- **Inverse Scattering Theory**. The introductory lecture/discussion was concerned with inverse scattering, i.e., inverse problems for linear hyperbolic partial differential equations which model sound, electromagnetic or elastic waves. We discussed in particular setups where a collection (array) of sensors probes a heterogeneous medium with signals and measures the resulting wave. The goal of the inverse scattering problem is to process these measurements in order to determine the heterogeneous medium, the so-called reflectivity function.

  The introductory lecture considered such a problem, for the case of broadband probing signals and time resolved array measurements, at regular time sample intervals T. It discussed a novel reduced order modeling (ROM) strategy, where the reduced order model is a proxy of the wave propagator, which is the operator that takes the wave at a given time t and maps it to the wave at the next time step $t + T$. The ROM has the following important properties:

  1. It is data driven, meaning that it can be obtained just from the array measurements, without any knowledge of the medium.
  2. It is a matrix of size determined by the number of sensors in the array and the duration of the measurements and yet, it fits the array measurements exactly.
  3. The ROM corresponds to a Galerkin projection of the wave propagator operator on an approximation space that is spanned by the wave field at the sample time instants (so called solution snapshots).

4. The ROM is a matrix with special algebraic structure that allows an efficient (well conditioned, almost linear) inversion procedure for determining the unknown reflectivity of the medium.

The lecture described the construction of the ROM, proved its main properties and showed how it can be used for solving inverse scattering. The theoretical analysis of the ROM based inversion requires further analysis, which is why it was presented at the beginning of the conference.

- **Nonlinear Dispersive Equations**. The introductory efforts of this group were focused on presenting recent results on the short and long time dynamics of solutions to nonlinear Schrödinger equations (NLS). The Schrödinger equation is arguably the most famous one in the class of dispersive nonlinear equations, and it plays a fundamental role in quantum mechanics.

  The team leaders emphasized the striking difference between the behavior of solutions to the NLS when no boundary data are imposed, hence wave solutions can *disperse*[1] without encountering any obstacle, versus when boundary data, such as the periodic ones, are given as a constraint. In this case dispersion does not happen, and to the contrary, the wave solutions may be periodic in time, a situation that happens for example in 2d, when the ratio between the two periods is a rational number. The leaders reported on the most recent advances in the study of periodic solution to the NLS equation, while emphasizing the many different mathematical tools, taken for example from analytic number theory, probability, dynamical systems, symplectic geometry and more, that have been used to make this progress. An idea of how these tools have been used and a list of open questions were also presented during the lecture.

Team Progress Reports

A summary description of the specific problems attacked by the research groups participating in the workshop is as follows.

- **Complex Analysis**. With the participation and involvement of the Harmonic Analysis group, led by Almut Burchard and Malabika Pramanik, during the workshop significant progress was made towards the solution of the aforementioned density and extension problems in the Hartog's triangle. Though details are yet to be verified, it seems that recently obtained results in harmonic analysis can be employed to resolve the questions raised in the density and extension problems in the Sobolev spaces for the Hartog's triangle in complex Euclidean space. Group discussions lead by Loredana Lanzani ignited a new and ongoing collaboration involving Anne-Katrine Gallagher; Purvi Gupta; Loredana Lanzani and Liz Vivas. Progress has already been made on several among the questions raised on the boundary integral representation formulas for functions holomorphic in the interior of the Hartog's triangle that satisfy suitable regularity up to the boundary.

  Further activities at the workshop included a follow-up discussion led by Mei-Chi Shaw on the Hartog's triangle in complex projective space, which exhibits distinct features from its Euclidean counterpart due to the presence of positive curvature. In this context several questions were raised pertaining complex foliations, which are equivalent to limit cycles in the real setting; also the question of existence of Levi-flat hyper surfaces without singularities, which arises from complex foliation theory and is of interest to the complex dynamics, topology and geometry communities.

- **Free Boundary Problems**. The following problem has been introduced to the junior team members by Susanna Terracini. A classic free boundary problem arises by considering a model of segregated populations. Suppose that there are N segregated populations occupying a bounded domain Ω. The optimal space occupied by each population is represented by the positivity set of the respective function u_i, for

[1] In this case *dispersion* means that the amplitude of the wave tends to zero as the time tends to infinity, while the energy of the system remains constant.

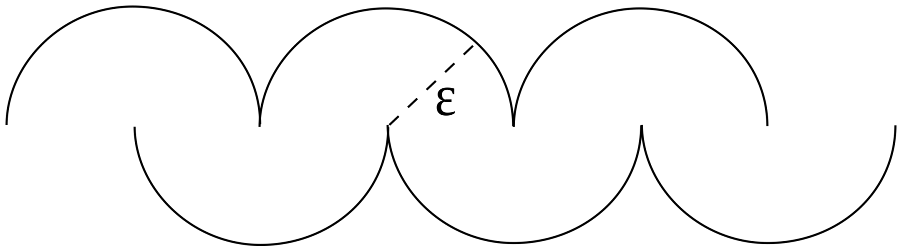

Figure 12.1: A potential buffer region between two populations that are ε apart.

$i \in \{1, 2, \ldots, N\}$, and where the u_i minimize the following energy:

$$\mathcal{E} = \min \Big\{ \int_\Omega \sum_{i=1}^{N} |\nabla u_i|^2 : u_i|_{\partial\Omega} = \varphi_{u_i} \text{ and } u_i u_j = 0 \text{ for } i \neq j \Big\},$$

under a boundary condition induced by given functions φ_{u_i} on $\partial\Omega$. A major problem is to understand the free boundary, which in this case is the boundary between the different populations within Ω. To understand the free boundary, it is useful to look at the domain variation formula. For $Y \in C_0^\infty(\Omega)$ let

$$\begin{cases} \dot{\Phi}_t = Y(\Phi_t) \\ \Phi_0(x) = x. \end{cases}$$

be a local variation. Then the domain variation formula is found by computing

$$\frac{d}{dt}\Big|_{t=0} \mathcal{E}(\Phi_t(\Omega))\,.$$

From the expansion of the first variation one may recover a reflection law which describes the symmetry with which two functions u_i and u_j approach their common boundary, and using Almgren's monotonicity formula, further regularity results, including that the boundary is mostly regular outside of a small singular set which is small in the sense of dimension.

A related problem is to understand segregated populations in the case where there is a buffer zone between the populations. In this case one minimizes:

$$\mathcal{E}_\varepsilon(u) = \min \Big\{ \int_\Omega \sum_{i=1}^{N} |\nabla u_i|^2 : u_i|_{\partial\Omega} = \varphi_{u_i} \text{ and } \operatorname{dist}(\operatorname{spt}\{u_i\}, \operatorname{spt}\{u_j\}) \geq \varepsilon \text{ for } i \neq j \Big\}$$

where spt is the support of the given function.

Progress on this problem has been made in the works of Soave, Tavares, Terracini, and Zilio (2018) and of Caffarelli, Patrizi, and Quitalo (2017). More work is required to get regularity of the free boundary because they need to address shapes like the following: suppose that you have two populations in a cylinder, where the boundary takes a scalloped shape for each population formed by semi-circles of radius ε connected in a line, and offset so that the boundaries are constantly ε apart. While this set does have singular set of small dimension, it is expected that one should be able to show that this arrangement is not a candidate even to be a local minimizer, perhaps by using the domain variation formula. This problem is interesting for fixed $\varepsilon = 1$, or as a variational problem where ε is sent to 0, so that the potentially invalid arrangement approaches a minimizer for the classic segregation problem in the limit.

- **Geometric Analysis**. The team reported work in the following directions.

1. **Ricci flow solutions with degenerate neck-pinches**. For Ricci flow, a family of "dumbbell" initial metrics leads to two drastically different singular models: either spherical or non-degenerate cylindrical singular model, depending on the ratio between the radius of the neck and the radii of two balls of the initial dumbbell manifold. A dumbbell metric at the threshold ratio gives rise to the so-called peanut solution, which was shown to exist rigorously by Angenent, Isenberg, Knopf in 2015. The peanut solution gives two different singular models, depending on the choice of the sequence of points p_k. If $\{p_k\}$ goes to the neck region, the resulting singular model is degenerate cylindrical and if $\{p_k\}$ goes to the ball region, the resulting singular model is the Bryant soliton. Such peanut solution is expected to be an unstable solution to the Ricci flow, so it is in general difficult to construct. Our ultimate goal is to show that the peanut solution is unstable. A closely related counterpart is the following question.

   Problem 12.0.1. *Show that a doubly warped Berger metric on $S^1 \times S^3$ gives rise to a Ricci flow solution similar to the peanut solution, in the sense that its normalized Ricci flow converges to a normalized peanut solution.*

   The group discussed how the peanut solution (with rotational symmetry) is constructed in the original two papers of Angenent, Isenberg, and Knopf. Their approach suggests to first derive a formal expansion of the warping factors of the metrics and then show the formal solution exists.

2. **Stability of cylindrical solutions to the Ricci flow**. As discussed above, the cylindrical solution to the Ricci flow appears naturally as a singular model. It gives rise to the natural question of how "stable" a cylindrical solution is.

   Problem 12.0.2. *Let g_0 be the standard cylindrical metric defined on $\mathbb{R} \times S^3$. Show that there is $\varepsilon > 0$ so that if g is in an ε-neighborhood of g_0 (in a suitable topology), then the Ricci flow solution of g converges to the solution of g_0, in the sense that the normalized solution converges to g_0, after a diffeomorphism change.*

   The group discussed the first step to understand the long time existence of the normalized solution $\tilde{g}_t$. It relies on analyzing the linearized normalized Ricci flow equation and employing the de Turck trick to eliminate the diffeomorphism group. The second step is to provide estimates on $\tilde{g}_t$ and show that up to a diffeomorphisms the flow converges to a normalized cylindrical solution as $t \to \infty$. We plan to understand the work of Schnürer, Schulze, and Simon where they prove stability of Euclidean space, as well as hyperbolic space, under the Ricci flow.

3. **Stability of translating solutions to the mean curvature flow**. Let M be a hypersurface in $\mathbb{R}^{n+1}$. We say that M is a translating solution if $F : M \times [0, \varepsilon)$ satisfies $\frac{\partial F}{\partial t} = -w$ for a w is a constant vector in $\mathbb{R}^{n+1}$, where F a family of immersions parametrized by t. Comparing with the mean curvature equation discussed above, a translating solution to the mean curvature flow, sometimes called the translator, must satisfy $H = \langle \nu, w \rangle$. Much progress has been made to classify translators. For surfaces in $\mathbb{R}^3$ that are contained in a slab $(-\pi/2, \pi/2) \times \mathbb{R}^2 \subset \mathbb{R}^3$, there are only three types of translators: Bowl solitons, Grim reaper planes, and the delta-wing solutions.

   Problem 12.0.3. *Let M_0 be a graphical surface in $\mathbb{R}^3$ defined on a slab $(-\pi/2, \pi/2) \times \mathbb{R} \subset \mathbb{R}^3$. Suppose that M_0 is asymptotic to the two vertical planes that bound the slab. Then the mean curvature flow M_t converges to either grim reaper plane or the delta-wing solution.*

   The team first discussed the long time existence of M_t. It relies on a general interior gradient estimate of Ecker and Huisken and the gradient estimate toward the boundary in the recent work of Spruck and Xiao. We believe that the pancake solutions of Bourni, Langford, and Tinaglia would give barriers to guarantee that the solution M_t stays in the same slab and converges to a nontrivial solution. Last, to show that the solution converges to a translating solution, the group may employ the techniques in the recent work to Choi, Choi, and Daskalopoulos for the Gauss curvature flow.

- **Harmonic Analysis.** The introductory harmonic analysis discussions provided an overview of results concerning geometric and analytic configurations that exist in sparse sets in Euclidean spaces. Here sparsity implies zero Lebesgue measure and size is phrased in terms of finer notions such as Hausdorff or Fourier dimensions, occasionally with additional structures. The background literature on a few questions of the following flavor were discussed in the group meetings:

  1. Does a set in $\mathbb{R}$ with dimension $\alpha < 1$ contain algebraic patterns, such as arithmetic progressions, or solutions of a translation-invariant linear equation? If so, are such patterns abundant in some quantifiable sense?
  2. Does a sparse set in $\mathbb{R}^2$ contain geometric configurations such as vertices of a right triangle?

  Looking ahead, one can formulate more refined questions. Lower-dimensional surfaces such as curves and hypersurfaces yield a class of thin sets in $\mathbb{R}^d$ for $d \geq 2$ that arise naturally from the differential geometry of Euclidean spaces. The induced surface measure on such sets is rich in geometric and analytic structure. It is the source of a vast literature and the inspiration of the following genre of questions, the study of which is one of the long-term research goals of the harmonic analysis group:

  1. For $d \geq 1$ and $0 < \alpha < d$, $\alpha \notin \mathbb{Z}$, do there exist sparse subsets of $\mathbb{R}^d$ with Hausdorff dimension α supporting measures that behave in some quantifiable sense like the induced Lebesgue measure on surfaces in $\mathbb{R}^d$?
  2. What properties of fractal sets ensure/prevent analytic and geometric phenomena seen on manifolds?
  3. What are the scope and the limitations of Fourier-analytic methods in such problems?

  The group also discussed four problems on sumsets and convolutions. The Minkowski sum $A + B = \{a + b \mid a \in A, b \in B\}$ arises frequently in the study of convolution operators. It is typically large compared to the individual sets; the general principle is that small sumsets imposes strong geometric and arithmetic constraints on the sets. We propose four problems that seek to quantify these constraints.

  For non-empty sets $A, B \subset \mathbb{R}^d$, the Brunn-Minkowski inequality $|A + B|^{\frac{1}{d}} \geq |A|^{\frac{1}{d}} + |B|^{\frac{1}{d}}$ provides a fundamental lower bound on the volume of the sumset. Equality holds only if the sets A and B are scaled and translated copies of the same convex set K [Henstock-Macbeath 1953, Hadwiger-Ohmann 1956].

  1. If the Brunn-Minkowski inequality holds with near-equality for two sets A, B, must they be close to homothetic and convex? (How close?)

  Affirmative answers are known in certain cases, for example when A and B are convex, when the two sets are comparable in volume, and in one dimension [Christ, Figalli, Jerison, Maggi, Pratelli and others since 2010]. The general problem, for sets of disparate size, is open.

  Much of the recent progress on this problem is motivated by additive combinatorics, where the study of sets with small sumsets has been a core problem for almost 100 years. For finite sets of integers, the cardinality of $A + B$ can be as large as the product $|A| \cdot |B|$; a lower bound is $|A + B| \geq |A| + |B| - 1$. Equality occurs only if A and B are arithmetic progressions with the same increment. Large sets with small sumsets were characterized in terms of generalized arithmetic progressions by Freiman [1973] and Ruzsa [1994].

  2. Among subsets $C \subset \mathbb{N}$ of given cardinality, which have the largest number of decompositions as sumsets (modulo translations)?

  One may suspect that arithmetic progressions may be the answer also here. there is a surprising connection with lunar arithmetic, an exotic algebra on the nonnegative integers [Applegate-LeBrun-Sloane 2011, G. Gross 2019].

One of the functional versions of the Brunn-Minkowski inequality is the Riesz-Sobolev inequality, that convolution integrals of the form $\int_{\mathbb{R}^d} f*gh$ can only increase under symmetric decreasing rearrangement of the three functions. The characterization of equality cases is quite complicated and depends on the relative size of the level sets of the three functions [Burchard 1994]. The Brunn-Minkowski inequality is equivalent to the special case of indicator functions of sets that are in a critical size relation. Analogous inequalities hold on the integers [Hardy-Littlewood-Polya 1934] and on the unit circle S^1 [Baernstein 1989]. Equality and near-equality cases on $\mathbb{R}$ and S^1 were classified by Christ [2013] and Christ-Iliopoulou [2018].

3. Are there any other groups that admit rearrangement inequalities of Riesz-Sobolev type? What are the obstructions?

It is a folklore result that Riesz-Sobolev inequalities cannot hold on the special orthogonal groups $SO(d)$ for $d > 2$, and perhaps on no other groups. It would be interesting to work out a rigorous proof and identify the precise nature of the geometric obstruction. Part of the question is how to define a suitable rearrangement. One possible approach is to construct the rearrangement in a different space. For example, S^1 has proved useful as a comparison space for compact connected Abelian groups [Kneser 1956, Candela-De Roton 2016, Tau 2018, Christ-Iliopoulou 2018].

We close with an intriguing problem that connects additive combinatorics with the geometry of Banach spaces, due to Oleskiewicz [2016]. To state the question, let us call a subset of a metric space well-separated, if any two distinct points in the set have distance at least 1.

4. Let A, B be non-empty finite subsets of a normed vector space. If A and B are well-separated, does $A + B$ contain a well-separated subset C of cardinality $|C| = |A| + |B| - 1$?

The answer is known to be positive when the norm is Euclidean [Oleskiewicz 2016], and when one of the sets has only one or two elements. It is open in all other cases, even for the spaces ℓ^p with $p \neq 2$ in dimension two.

- **Inverse Scattering Theory**. The team reported on two research problems:

  1. **Reduced order model**: The ROM based inversion methodology was discussed by our group throughout the week, for both the setup in the lecture as well as for inversion with time harmonic waves and in anisotropic media. The group identified a few analysis problems to work on. In particular, the study of the dependence of the Galerkin projection on the unknown reflectivity was determined to be important and of interest to the group.
  2. **Transmission eigenvalues**: This problem arises in the analysis of scattering operator for inhomogeneous media of compact support. It is a non-selfadjoint and non-linear eigenvalue problem for a set of two elliptic PDEs defined in the support of inhomogeneity and sharing the same Cauchy data on the boundary. Transmission eigenvalues relate to interrogating frequencies for which there is an incident field that does not scatter. They can be determined from scattering data, hence can be used to obtain information about scattering media. Our group was interested in two main open theoretical questions: a) spectral properties of this eigenvalue problem in the case when contrast in the media changes sign up to its boundary, and b) regularity assumptions on the given media for which a transmission eigenvalue is indeed a non-scattering frequency, i.e. understanding when it is possible to extend eigenfunctions corresponding to incident waves outside the support of inhomogeneity as a solution of PDEs governing the background.

- **Nonlinear Dispersive Equations**. During the week spent at Banff the Nonlinear Dispersive PDE group centered their discussion mainly on two projects.

1. The first project, that involves D. Mendelson, A. Nahmod, N. Pavlovic and G. Staffilani, is related to the active area of research of deriving effective evolution equations from many-body quantum systems. One important and ubiquitous example of a limiting effective equation is the NLS equation mentioned above, which more in details is a scalar dispersive equation which describes in a certain regime the evolution of a system of infinitely many bosons with a two particle interaction. The NLS equation is an important model in its own right, as both a representative example of an infinite dimensional Hamiltonian system, and, in the one dimensional cubic case, an example of an integrable PDE. Recently, our group together with M. Rosenzweig, a PhD student at UT Austin under the supervision of N. Pavlovic, has been able to derive geometric aspects of the Hamiltonian structure of the NLS equation from the many-body quantum model. Moreover, we have been able to connect the integrability of the scalar NLS equation with integrability for a certain system of equations, called the GP hierarchy, which models the interaction between infinitely many quantum particles and arises in the derivation of the NLS equation from the finite particle models.

   While at the workshop at BIRS, the group discussed several possible extensions to this recent work. The first direction, which seems very promising, is related to the connection between the NLS equation and the Vlasov equation. Specifically, in the so-called semi-classical limit, solutions of the NLS equation tend to solutions of the Vlasov equation. A natural question is thus "what happens to the geometric Hamiltonian structure associated to the NLS?". We believe, after some preliminary investigation, that our techniques should enable us to derive a Hamiltonian structure for the Vlasov equation from a classical finite particle system.

2. The second project, which involves M. Czubak, A. Nahmod, G. Staffilani and X. Yu, is based on a question proposed by Luis Vega. Consider the following NLS equation in one spatial dimension:

$$iu_t + u_{xx} = |u|^8 u. \tag{0.1}$$

   Here $u : \mathbb{R} \times \mathbb{R} \to \mathbb{C}$ is a complex-valued function of time and space and the scaling invariant Sobolev norm is $H^{\frac{1}{4}}$. The goal is to study the long time dynamics for this initial value problem, namely global well-posedness (GWP) and scattering when the initial data are taken in $H^{\frac{1}{4}}$.

   It is known that given an initial data u_0 with finite energy, that is $u_0 \in H^1$, due to energy conservation, and the fact that H^1 is a subcritical norm in this case, GWP and scattering is well understood, while at the critical regularity, $u_0 \in \dot{H}^{\frac{1}{4}}$, a similar argument only gives *small* data GWP and scattering results. If one considers intermediate (but still subcritical) regularity, that is $u_0 \in H^s$, $\frac{1}{4} < s < 1$, then one can combine the I-method and the following Morawetz estimate for the solution u of (0.15):

$$\|u\|_{L^8_{t,x}}^8 \lesssim \|u_0\|_{L^2_x}^6 \|u\|^2_{L^\infty_t \dot{H}^{\frac{1}{2}}_x} \tag{0.2}$$

   to prove the GWP and scattering for data $u_0 \in H^s$, $s > \frac{8}{11}$. During the discussion at Banff X. Yu noticed that if we replace the Morawetz estimate (0.2) by the one derived in Planchon-Vega [21]:

$$\|u\|_{L^{12}_{t,x}}^{12} \lesssim \|u_0\|_{L^2_x}^2 \|u\|^2_{L^\infty_t \dot{H}^{\frac{1}{2}}_x}, \tag{0.3}$$

   we are able to improve the index for GWP and scattering to $s > \frac{4}{7}$. Note that this index still leaves a gap if one want to reach the critical regularity. Following a suggestion by L. Vega we would like to consider this GWP and scattering problem from another point of view, which would be new also for other dispersive equations. Instead of concentrating the study of the global dynamics for the NLS equation (0.15) on the analysis of the behavior in time of the solution in terms of Sobolev and L^p norms, we want to analyze the asymptotic behavior in time of the more natural $h(t)$ quantity defined in the proof of Planchon-Vega [21]:

$$h(t) := \int_{\mathbb{R}} \int_{\mathbb{R}} |u(t,x)|^2 |u(t,y)|^2 |x-y| \, dxdy. \tag{0.4}$$

The second derivative of $h(t)$ in essence gives the Morawetz estimates, which encodes the fact that some L^p norm is decaying in time, which in turn implies scattering. Therefore this $h(t)$ function is closely linked to the scattering of the NLS equation (0.15), and it should be the right quantity to look at to prove scattering.

Poster Session Research Themes

The following scientific themes have been discussed at the poster session.

- **A generalized radial Brèzis-Nirenberg problem**. In a poster presentation by Soledad Benguria, Mathematics Department, University of Wisconsin the following problem was discussed. In an 1983 paper Brèzis and Nirenberg consider

  $$-\Delta u = \lambda u + u^p \qquad \text{in} \qquad \Omega, \tag{0.5}$$

  where Ω is a bounded, smooth, open subset of $\mathbb{R}^n$, $n \geq 3$, with $u > 0$ in Ω and $u = 0$ in $\partial\Omega$. Here $p = (n+2)/(n-2)$ is the critical Sobolev exponent. They show there are no positive solutions to (0.5) if $\lambda \geq \lambda_1$, where λ_1 is the first eigenvalue of $-\Delta$ in Ω. And if Ω is star-shaped, there are no solutions if $\lambda \leq 0$. However, the existence of solutions for $0 < \lambda < \lambda_1$ depends on the dimension of the space.

  In fact, if $n \geq 4$, then there is a solution $u \in H_0^1(\Omega)$ for all $\lambda \in (0, \lambda_1)$. But if $n = 3$, there is a positive $\lambda_*(\Omega)$ such that (0.5) has no solution if $\lambda \leq \lambda_*$, and (0.5) has a solution if $\lambda \in (\lambda_*, \lambda_1)$. If Ω is a ball, then $\lambda_* = \lambda_1/4$. Many variants of (0.5) have been studied. Among others, the Brèzis-Nirenberg problem in other spaces of constant curvature, such as $\mathbb{S}^n$ and $\mathbb{H}^n$ (see, e.g., [3], [22], [8], [4]).

  The problem that Benguria and her collaborators attacked is as follows. Let $R \in (0, \infty)$ and let a be a smooth function such that $a \in C^3[0, R]$; $a(0) = a''(0) = 0$; $a(x) > 0$ for all $x \in (0, R)$; and $\lim_{x\to 0} a(x)/x = 1$. Given $n \in (2, 4)$, the goal is to study the existence of positive solutions $u \in H_0^1(\Omega)$ of

  $$-u''(x) - (n-1)\frac{a'(x)}{a(x)}u'(x) = \lambda u(x) + u(x)^p \tag{0.6}$$

  with boundary condition $u'(0) = u(R) = 0$. Notice that the radial Brèzis-Nirenberg problem on the Euclidean space corresponds to taking $a(x) = x$; on the hyperbolic space, to taking $a(x) = \sinh(x)$; and on the spherical space, to taking $a(x) = \sin(x)$. Benguria shows that this boundary value problem has a positive solution if $\lambda \in (\mu_1, \lambda_1)$. Here, λ_1 is the first positive eigenvalue of $y'' + \frac{a'}{a}y' + \left(\lambda - \alpha^2\left(\frac{a'}{a}\right)^2 + \alpha\frac{a''}{a}\right)y = 0$ with boundary conditions $\lim_{x\to 0} y(x)x^{\alpha} = 1$; and μ_1 is the first positive eigenvalue with boundary conditions $\lim_{x\to 0} y(x)x^{-\alpha} = 1$, with $\alpha = (2-n)/2$. She also obtains non-existence and uniqueness results.

- **Aharonov–Bohm operators in planar domains.** The poster by Laura Abatangelo (University of Milan - Bicocca) concerned possible multiple eigenvalues for the so-called Aharonov–Bohm operators. These operators are special as they present a strong singularity at a point (pole), for they cannot be considered small perturbations of the standard Laplacian. More precisely, for $a = (a_1, a_2) \in \mathbb{R}^2$ and $\alpha \in \mathbb{R} \setminus \mathbb{Z}$, we consider the vector potential

  $$A_a^{\alpha}(x) = \alpha\left(\frac{-(x_2 - a_2)}{(x_1 - a_1)^2 + (x_2 - a_2)^2}, \frac{x_1 - a_1}{(x_1 - a_1)^2 + (x_2 - a_2)^2}\right), \quad x = (x_1, x_2) \in \mathbb{R}^2 \setminus \{a\},$$

  which generates the Aharonov-Bohm delta-type magnetic field in $\mathbb{R}^2$ with pole a and circulation α; such a field is produced by an infinitely long thin solenoid intersecting perpendicularly the plane (x_1, x_2) at the point a, as the radius of the solenoid goes to zero and the magnetic flux remains constantly equal to α. So, they are responsible of the so-called Aharonov–Bohm effect: in a quantum mechanics context, a charged particle living in this region is affected by the presence of a magnetic field even if this is zero almost everywhere.

From an analytic point of view, the particle's dynamics is described by solutions to Schrödinger equations, where the (stationary) operators are defined as

$$(i\nabla + A_a)^2 u = -\Delta u + 2iA_a \cdot \nabla u + |A_a|^2 u$$

acting on functions $u : \Omega \subset \mathbb{R}^2 \to \mathbb{C}$. As one can easily understand, in the last years, a particular interest has been devoted to the spectrum of the stationary operator defined above. In particular, the spectrum is stable under small movement of the pole. Moreover, small movements of the pole can make a double eigenvalue to be simple in many situations. When the domain posseses strong symmetries, it seems that it can remain simple not only for small movements, but also globally in the domain.

The two main results achieved in this direction are the following

Theorem 12.0.4 ([2]). *Let $0 \in \Omega$ and $\alpha_0 \in \{\frac{1}{2}\} + \mathbb{Z}$. Let $n_0 \geq 1$ be such that the n_0-th eigenvalue $\lambda := \lambda_{n_0}^{(0,\alpha_0)}$ of $(i\nabla + A_0^{\alpha_0})^2$ with Dirichlet boundary conditions on $\partial\Omega$ has multiplicity two. Let φ_1 and φ_2 be two orthonormal in $L^2(\Omega, \mathbb{C})$ and linearly independent eigenfunctions corresponding to λ. Let c_k, $d_k \in \mathbb{R}$ be the coefficients in the expansions $\varphi_k^{(a,\alpha)}(a + r(\cos t, \sin t)) = e^{i\frac{t}{2}}\, r^{1/2} \left(c_k \cos\frac{t}{2} + d_k \sin\frac{t}{2}\right) + o(r^{1/2})$. If φ_1 and φ_2 satisfy both the following*

$$(i)\ c_k^2 + d_k^2 \neq 0 \text{ for } k = 1, 2; \qquad (ii)\ \int_\Omega (i\nabla + A_0^{\alpha_0})\varphi_1 \cdot A_0^{\alpha_0}\overline{\varphi_2} \neq 0;$$

$$(iii) \text{ there does not exist } \gamma \in \mathbb{R} \text{ such that } (c_1, d_1) = \gamma(c_2, d_2);$$

then there exists a neighborhood $U \subset \Omega \times \mathbb{R}$ of $(0, \alpha_0)$ such that the set

$$\{(a, \alpha) \in U \,:\, (i\nabla + A_a^\alpha)^2 \text{ admits a double eigenvalue close to } \lambda\} = \{(0, \alpha_0)\}\,.$$

Theorem 12.0.5 ([1]). *Let $\lambda_1^{(a,\frac{1}{2})}$ be the first eigenvalue on the disk. Then $\lambda_1^{(a,\frac{1}{2})}$ is simple if and only if $a \in (-1, 1) \setminus \{0\}$.*

- **Recovering Riemannian metrics from least-area data**. This poster was presented by Tracey Balehowsky (Postdocoral Researcher at the University of Helsinki) and contained her joint work with Spyros Alexakis and Adrian Nachman (Professors at the University of Toronto). The following question was considered: Given any simple closed curve γ on the boundary of a Riemannian 3-manifold (M, g), suppose the area of the least-area surfaces bounded by γ are known. From this data may we uniquely recover g?

  This question can be thought of as an $n - 2$ codimensional version of boundary rigidity, wherein one seeks to determine the metric g given knowledge of the geodesic distance $d(x, y)$ between any two points x, y on the boundary of M. In the cases where this is possible, we say the manifold is boundary rigid. The problem of boundary rigidity has been solved in 2 dimensions, but remains open in higher dimensions.

  The poster summarized some of the history of the problem of boundary rigidity, highlighting the works of Michel [18], Gromov [15], Croke [11], Pestov and Uhlmann [20] (which settled the 2D case), Lassas et. al. [17], Burago and Ivanov [9, 10], and Stefanov et. al. [23]. It also contained a brief description of the obstacles to boundary rigidity as motivation for the analogous obstacles one faces when instead considering least-area data instead of distances.

Next presented were three theorems which gave conditions when one can uniquely recover (up to boundary-fixing diffeomorphisms) the Riemannian metric g, given knowledge of the areas of least-area surfaces circumscribed by simple curves on the boundary of M. The results do not require this area data for all such simple curves on the boundary; rather just certain families of curves.

1. The first theorem addressed the question of what is the least amount of area data possible to achieve global uniqueness. It showed that if the metric was either C^3-close to Euclidean or "straight-thin", knowledge of the areas of least-area surfaces with boundary given by a leaf of a particular 1-parameter family of foliations of the boundary by simple curves was enough to uniquely determine the metric.
2. The second theorem was a global uniqueness result which demonstrated that the curvature conditions of the first theorem could be relaxed if more data was given and an additional foliation structure was assumed. This theorem showed that if the manifold was of the type which "admitted foliations from all directions", knowledge of the areas of the least-area surfaces arising as leaves in the admitted foliations uniquely recovered the metric.
3. The third theorem was a local result which showed that if the boundary ∂M was strictly mean convex at $p \in \partial M$ and one knows the areas of a certain 2-parameter family of least-area surfaces which are near p, then the metric is uniquely determined in a small neighbourhood $V \subset M$ containing p. It was emphasized that a key starting point for all the results presented was that the area data gave information about the Dirichlet-to-Neumann map for the Jacobi operator on the 2-dimensional least-area surfaces, from which curvature information was determined via the result of Nachman [19].

- **The Mixed Boundary Value Problem for the Laplacian in Non-Smooth Domains**. The poster, presented by Katharine Ott from Bates College, summarized results regarding well-posedness of the L^p-mixed boundary value problem in Lipschitz domains for the Laplacian. The theorems presented have appeared in a series of recent papers with coauthors H. Awala, R. Brown, S. Kim, I. Mitrea, and J. Taylor.

  To give a sense of the work presented, consider the case of the L^p-mixed problem for the Laplacian. In this setting, let Ω be a bounded open set in $\mathbb{R}^n$, $n \geq 2$, and let $\partial\Omega = D \cup N$, where D is an open subset of the boundary and $D \cap N = \emptyset$. Then the boundary problem is given by

$$\begin{cases} \Delta u = 0 \quad \text{in} \quad \Omega, \\ u\,|_D = f_D \in W^{1,p}(D), \\ \partial_\nu u\,|_N = f_N \in L^p(N), \\ (\nabla u)^* \in L^p(\partial\Omega). \end{cases} \tag{0.7}$$

  Above, ∂_ν denotes differentiation in the normal direction. For any function $v : \Omega \to \mathbb{R}$, v^* stands for the non-tangential maximal function.

  The first result is well-posedness (meaning existence and uniqueness of solutions) of the L^p-mixed problem for the Laplacian in Lipschitz domains for a range $p \in (1, 1 + \varepsilon)$ under a mild assumption on the boundary between D and N (the Dirichlet and Neumann portions of the boundary, respectively). It is important to note that well-posedness in L^2 may actually fail and thus the result for small $p > 1$ is, in a sense, optimal. An important step in the proof of well-posedness of (0.7) (and similarly in the case where the Laplacian is replaced with the Lamé system of elastostatics) is establishing decay of solutions when the boundary data is an atom. This decay is encoded in estimates for the Green function for the mixed problem, which constituted the second theorem of the poster.

  The final portion of the poster addressed an alternative approach to studying the L^p-mixed problem for the Laplacian in the special case where $\Omega \subset \mathbb{R}^2$ is the infinite upward sector with vertex at zero and aperture $\theta \in (0, 2\pi)$. Here, we define the left edge of the sector to be D and the right edge of the sector to be

N. Under these conditions, we can translate (0.7) into an integral boundary equation. The solvability of this aforementioned equation hinges on whether or not an associated integral operator is invertible on the prescribed function spaces. This approach results in a sharp well-posedness results for (0.7).

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Chapter 13

Reconstruction Methods for Inverse Problems (19w5092)

June 23rd - 29th, 2019

Organizer(s): Uri Ascher (UBC, Vancouver), Elena Beretta (New York University Abu Dhabi), Otmar Scherzer (University of Vienna), Luminita Vese (UCL, Los Angeles)

The report as written surveys parts of the original submission to review the state of the art in the field. Then come the presentations and their abstracts, and then outcomes of the meeting where we put the talks in perspective.

Overview of the Field

Inverse problems require to determine the cause from a set of observations. Such problems are of importance in medical imaging, non destructive testing of materials, computerized tomography, source reconstructions in acoustics, computer vision, and geophysics, to mention but a few, and their mathematical solutions represent breakthroughs in applications. In many situations the mathematical modeling of these problems leads to the study of inverse boundary value problems for partial differential equations and systems that are highly non-linear and ill-posed in the sense of Hadamard; small errors in the data may cause uncontrollable errors in the solution. It is precisely this feature that makes crucial the analysis of these instabilities and their regularization towards a successful computational reconstruction. The strategy of reconstruction is the following: Given a discrete set of (noisy) measurements, reconstruct an image of the unknown physical quantity inside the examined object. The natural approach is to reduce the problem to a minimization problem for a least-square constrained type functional. Due to the ill-posedness of the underlying inverse problems, all the functional reconstruction methods involve some form of regularization which enables stable reconstruction. These methods are called regularization techniques (see for instance [8]).

An illuminating example of ill-posed nonlinear inverse problem is the inverse conductivity problem modelling electrical impedance tomography (EIT), a nondestructive imaging technique with applications in medical imaging, geophysics and testing of materials, respectively. The problem was introduced the first time by Calderon in the early 80's motivated by an application in geophysical prospection. The goal is to detect the conductivity inside an object from boundary measurements encoded by the so-called Dirichlet to Neumann map. The conductivity problem is severely ill-posed as was proved in 1988 by Alessandrini [1]. In fact, despite of a-priori smoothness assumptions on the unknown conductivity, a conditional stability estimate of logarithmic type is the best possible. This has led to tackle the ill-posedness of the problem establishing regularization strategies for the effective determination of the solution to the problem. A recent trend is to restrict the set of admissible conductivities; for example assuming a smooth background conductivity containing a finite number of unknown small inclusions with a significantly different conductivity [9] or considering conductivities that are linear combinations of finitely many (known) profiles [2]. In fact, under these assumptions it is possible to prove Lipschitz stability estimates that imply local convergence of iterative methods, see for instance [7, 4].

We would like to mention several numerical approaches, that have been developed in the context of nonlinear tomographic problems, in particular EIT, inverse scattering, and inverse conductivity problems: these are for instance, level set methods (Santosa [17] based on Osher & Sethian [16]), shape derivatives (based on Sokolowski & Zolesio [18]), Statistical methods (Kaipio & Somersalo [11]), Dbar methods (Nachman [15]), Iterative regularization methods for nonlinear problems (Hanke [10]), Regularization by projection (Kaltenbacher [12]), Topological gradients (Masmoudi), variational regularization methods (Mueller & Siltanen [14]), PDE constraint optimization (Haber [3]).

The year 2016 marks the 110th birthday of the great Russian academician Andrey Nikoayevich Tikhonov (1906 - 1993). Tikhonov's work provides the mathematical foundations of regularization theory for solving inverse problems, which is a core topic of this workshop. Exciting experimental developments and the possibility of implementing regularization algorithms on computers made the mathematical results as prominent as they appear today. In 1979 Allan MacLeod Cormack (1924-1998) and Godfrey Hounsfield (1919-2004) won the Nobel Prize in "Physiology or Medicine" for the first development of a CT-scanner, which was based on inversion of the parallel beam transform, which is probably the most prominent inverse problem. Today new imaging concepts are the major driving force for discoveries in a variety of research areas, ranging from the nanoscale of single molecule imaging, via biomedical research, to macroscopic scales in Astrophysics.

This workshop tried to survey the zoo of regularization methods and to stimulate new research by productive interactions of the different computational and theoretical fields which were represented in the workshop.

Recent Developments and Open Problems

The primary goal of the workshop has been to provide a forum on theoretical and numerical aspects related to stability in inverse problems. In particular we emphasize stability estimates for inverse problems, such as parameter estimation problems in wave equations, regularization methods in the discrete and continuous formulations, and multi-level techniques that make use of theoretical stability estimates and numerical algorithms. The workshop brought together fields which usually do not interact. Numerically oriented researchers usually do not make use of theoretical stability estimates and regularization researchers working on discrete and continuous formulations have focus on different aspects of numerics and analysis. The situation with interactions actually changed with the fundamental work of Alessandrini and Vessella [2], who derived stability estimates based on a continuous formulation for piecewise constant Ansatz functions. Their work bridged the gap between the discrete and continuous regularization world and also found its way to numerics recently. The recently very active topic of uncertainty quantification in continuous and discrete formulations is another example, considered by different communities, but solves the same problems (like the inverse aquifer problem). These communities use completely different computational approaches like Markov Chain Monte Carlo (MCMC), Kalman Filter (KF). The stochastic analysis can be considered the analog to the deterministic stability estimates. As with all workshops on inverse problems at BIRS, which were predominantly on theoretical aspects and concrete developments, we observed a broad and lively discussion of the theoretical developments, analytical and computational methodologies and new and existing applications. Moreover, we observed a growth in understanding of analysis, algorithms, and mathematical modeling. We aimed to bring mathematicians working on more abstract stability estimates in concrete examples as well as researchers working on more concrete computational algorithms.

Presentation Highlights

We start by giving a list of the titles and abstracts in chronological order:

Monday:

Peter Kuchment: Detecting presence of emission sources with low SNR. "Analysis" vs deep learning: The talk will discuss the homeland security problem of detecting presence of emission sources at high noise conditions. (Semi-)analytic and deep learning techniques will be compared. This is a joint work with W. Baines and J. Ragusa.

Luca Rondi: A multiscale approach for inverse problems: We extend the hierarchical decomposition of an image as a sum of constituents of different scales, introduced by Tadmor, Nezzar and Vese in 2004 [19], to a general setting. We develop a theory for multiscale decompositions which, besides extending the one of Tadmor, Nezzar and Vese to arbitrary L^2 functions, is applicable to nonlinear inverse problems, as well as to other imaging problems. As a significant example, we present applications to the inverse conductivity problem. This is a joint work with Klas Modin and Adrian Nachman.

Adrian Nachman: Two nonlinear harmonic analysis results: a Plancherel theorem for a nonlinear Fourier transform arising in the Inverse Conductivity Problem and multiscale decomposition of diffeomorphisms in Image Registration: The first part of this talk will be devoted to a well-studied nonlinear Fourier transform in two dimensions for which a proof of the Plancherel theorem had been a challenging open problem. I will describe the solution of this problem, as well as its application to reconstruction in the inverse boundary value problem of Calderon for a class of unbounded conductivities. This will include new estimates on classical fractional integrals and a new result on L^2 boundedness of pseudodifferential operators with non-smooth symbols. (Joint work with Idan Regev and Daniel Tataru).

The second part will be a continuation of Luca Rondi's lecture. It will be devoted to a multiscale decomposition of diffeomorphisms in image registration, inspired by the Tadmor Nezzar Vese hierarchical decomposition of images, with the sum replaced by composition of maps. (Joint work with Klas Modin and Luca Rondi).

Elisa Francini: Stable determination of polygonal and polyhedral interfaces from boundary measurements: We present some Lipschitz stability estimates for the Hausdorff distance of polygonal or polyhedral inclusions in terms of the Dirichlet-to-Neumann map based on a series of papers in collaboration with Elena Beretta (New York University AbuDhabi) and Sergio Vessella (Universit?? di Firenze).

Matteo Santacesaria: Infinite-dimensional inverse problems with finite measurements: In this talk I will discuss how ideas from applied harmonic analysis, in particular sampling theory and compressed sensing, may be applied to inverse problems for partial differential equations. The focus will be on inverse boundary value problems for the conductivity and the Schrodinger equations, but the approach is very general and allows to handle many other classes of inverse problems. I will discuss uniqueness, stability and reconstruction, both in the linearized and in the nonlinear case. This is joint work with Giovanni S. Alberti.

Ekaterina Sherina: Quantitative PAT-OCT Elastography for Biomechanical Parameter Imaging: Diseases like cancer or arteriosclerosis often cause changes of tissue stiffness in the micrometer scale. Our work aims at developing a non-invasive method to quantitatively image these biomechanical changes and study the potential of the method for medical diagnostics. We focus on quantitative elastography combined with photoacoustic (PAT) and optical coherence tomography (OCT). The problem we deal with consists in estimating elastic material parameters from internal displacement data, which are evaluated from OCT-PAT recordered successive images of a sample.

Tuesday:

Gabriele Steidl: Regularization of Inverse Problems via Time Discrete Geodesics in Image Spaces: This talk addresses the solution of inverse problems in imaging given an additional reference image. We combine a modification of the discrete geodesic path model of Berkels, Effland and Rumpf [5] with a variational model, actually the L^2-TV model, for image restoration. We prove that the space continuous model has a minimizer and propose a minimization procedure which alternates over the involved sequences of deformations and images. The minimization with respect to the image sequence exploits recent algorithms from convex analysis to minimize the L 2 -T V functional. For the numerical computation we apply a finite difference approach on staggered grids together with a multilevel strategy. We present proof-of-the-concept numerical results for sparse and limited angle computerized tomography as well as for superresolution demonstrating the power of the method. Further we apply the morphing approach for image colorization. This is joint work with Sebastian Neumayer and Johannes Persch (TU Kaiserslautern).

Uri Ascher: Discrete processes and their continuous limits: The possibility that a discrete process can be closely approximated by a continuous one, with the latter involving a differential system, is fascinating. Important theoretical insights, as well as significant computational efficiency gains may lie in store. A great success story in this regard are the Navier-Stokes equations, which model many phenomena in fluid flow rather well. Recent years saw many attempts to formulate more such continuous limits, and thus harvest theoretical and practical advantages, in diverse areas including mathematical biology, image processing, game theory, computational optimization, and machine learning. Caution must be applied as well, however. In fact, it is often the case that the given discrete process is richer in possibilities than its continuous differential system limit, and that a further study of the discrete process is practically rewarding. I will show two simple examples of this. Furthermore, there are situations where the continuous limit process may provide important qualitative, but not quantitative, information about the actual discrete process. I will demonstrate this as well and discuss consequences.

Markus Grasmair: Total variation based Lavrentiev regularisation: In this talk we will discuss a non-linear variant of Lavrentiev regularisation, where the sub-differential of the total variation replaces the identity operator as regularisation term. The advantage of this approach over Tikhonov based total variation regularisation is that it avoids the evaluation of the adjoint operator on the data. As a consequence, it can be used, for instance, for the solution of Volterra integral equations of the first kind, where the adjoint would require an integration forward in time, without the need of accessing future data points. We will discuss first the theoretical properties of this method, and then propose a taut-string based numerical method for the solution of one-dimensional problems.

Andrea Aspri: Analysis of a model of elastic dislocation in geophysics: In this talk we will discuss a model for elastic dislocations describing faults in the Earth???s crust. We will show how to get the well-posedness of the direct problem which consists in solving a boundary-value/transmission value problem in a half-space for isotropic, inhomogeneous linear elasticity with Lipschitz Lam?? parameters. Mostly we will focus the attention on the uniqueness result for the non-linear inverse problem, which consists in determining the fault and the slip vector from displacement measurements made on the boundary of the half-space. Uniqueness for the inverse problem follows by means of the unique continuation result for systems and under some geometrical constrains on the fault. This is a joint work with Elena Beretta (Politecnico di Milano & NYU ??? Abu Dhabi), Anna Mazzucato (Penn State University) and Maarten de Hoop (Rice University).

Barbara Kaltenbacher: Regularization of backwards diffusion by fractional time derivatives: The backwards heat equation is one of the classical inverse problems, related to a wide range of applications and exponentially ill-posed. One of the first and maybe most intuitive approaches to its stable numerical solution was that of quasireversibility, whereby the parabolic operator is replaced by a differential operator for which the backwards problem in time is well posed. After a short overview of approaches in this vein, we will dwell on a new one that relies on replacement of the first time derivative in the PDE by a fractional differential operator, which, due to the asymptotic properties of the Mittag-Leffler function as compared to the exponential function, leads to an only moderately ill-posed problem. Thus the order alpha of (fractional) differentiation acts as a regularization parameter and convergence takes place in the limit as alpha tends to one. We study the regularizing properties of this approach and a regularization parameter choice by the discrepancy principle. Additionally, a substantial numerical improvement can be achieved by exploiting the linearity of the problem by breaking the inversion into distinct frequency bands and using a different fractional order for each. This is joint work with William Rundell.

Bernd Hofmann: The impact of conditional stability estimates on variational regularization and the distinguished case of oversmoothing penalties: Conditional stability estimates require additional regularization for obtaining stable approximate solutions if the validity area of such estimates is not completely known. The focus of this talk is on the Tikhonov regularization under conditional stability estimates for non-linear ill-posed problems in Hilbert scales, where the case that the penalty is oversmoothing plays a prominent role. This oversmoothing problem has been studied early for linear forward operators, most notably in the seminal paper by Natterer 1984. The a priori parameter choice used there, just providing order optimal convergence rates, has in the oversmoothing case the unexpected property that the quotient of the noise level square and the regularization parameter tends to infinity when the noise level tends to zero. We provide in this talk some new convergence rate results for nonlinear problems and moreover case studies that enlighten the interplay of conditional stability and regularization. In particular, there occur pitfalls for oversmoothing penalties, because convergence can completely fail and the stabilizing effect of conditional stability may be lost.

Antonio Leitao: A convex analysis approach to iterative regularization methods: We address two well known iterative regularization methods for ill-posed problems (Landweber and iterated-Tikhonov methods) and discuss how to improve the performance of these classical methods by using convex analysis tools. The talk is based on two recent articles:

Range-relaxed criteria for choosing the Lagrange multipliers in nonstationary iterated Tikhonov method (with R.Boiger, B.F.Svaiter [6]), and On a family of gradient type projection methods for nonlinear ill-posed problems [13]

Lars Ruthotto: Deep Neural Networks motivated by PDEs: One of the most promising areas in artificial intelligence is deep learning, a form of machine learning that uses neural networks containing many hidden layers. Recent success has led to breakthroughs in applications such as speech and image recognition. However, more theoretical insight is needed to create a rigorous scientific basis for designing and training deep neural networks, increasing their scalability, and providing insight into their reasoning.

This talk bridges the gap between partial differential equations (PDEs) and neural networks and presents a new mathematical paradigm that simplifies designing, training, and analyzing deep neural networks. It shows that training deep neural networks can be cast as a dynamic optimal control problem similar to path-planning and optimal mass transport. The talk outlines how this interpretation can improve the effectiveness of deep neural networks. First, the talk introduces new types of neural networks inspired by to parabolic, hyperbolic, and reaction-diffusion PDEs. Second, the talk outlines how to accelerate training by exploiting multi-scale structures or reversibility properties of the underlying PDEs. Finally, recent advances on efficient parametrizations and derivative-free training algorithms will be presented.

Wednesday:

Simon Arridge Combining learned and model based approaches for inverse problems: Deep Learning (DL) has become a pervasive approach in many machine learning tasks and in particular in image processing problems such as denoising, deblurring, inpainting and segmentation. The application of DL within inverse problems is less well explored because it is not trivial to include Physics based knowledge of the forward operator into what is usually a purely data-driven framework. In addition some inverse problems are at a scale much larger than image or video processing applications and may not have access to sufficiently large training sets. In this talk I will present some of our approaches for i) developing iterative algorithms combining data and knowledge driven methods with applications in medical image reconstruction ii) developing a learned PDE architecture for forward and inverse models of non-linear image flow. Joint work with : Marta Betcke, Andreas Hauptmann, Felix Lucka

Giovanni Alberti "Combining the Runge approximation and the Whitney embedding theorem in hybrid imaging":

Abstract The reconstruction in quantitative coupled physics imaging often requires that the solutions of certain PDEs satisfy some non-zero constraints, such as the absence of critical points or nodal points. After a brief review of several methods used to construct such solutions, I will focus on a recent approach that combines the Runge approximation and the Whitney embedding theorem.

Eldad Haber "Conservative architectures for deep neural networks": In this talk we discuss architectures for deep neural networks that preserve the energy of the propagated signal. We show that such networks can have significant computational advantages for some key problems in computer vision

Robert Plato "New results on a variational inequality formulation of Lavrentiev regularization for nonlinear monotone ill-posed problems": We consider nonlinear ill-posed equations $Fu = f$ in Hilbert spaces $\mathcal{H}$, where $F : \mathcal{H} \to \mathcal{H}$ is monotone on a closed convex subset $\mathcal{M} \subset \mathcal{H}$. For given data $f^\delta \in \mathcal{H}, \|f^\delta - f\| \le \delta$, a standard approach is Lavrentiev regularization $Fv_\alpha^\delta + \alpha v_\alpha^\delta = f^\delta$, with $v_\alpha^\delta \in \mathcal{M}$ and $\alpha > 0$ small. Since existence of a solution $v_\alpha^\delta \in \mathcal{M}$ may only be guaranteed for special cases, e.g., $\mathcal{M} = \mathcal{H}$ or $\mathcal{M} =$ ball, we replace this equation by a regularized variational inequality, i.e., we consider $u_\alpha^\delta \in \mathcal{M}$ satisfying

$$\langle Fu_\alpha^\delta + \alpha u_\alpha^\delta - f^\delta, w - u_\alpha^\delta \rangle \ge 0 \quad \text{for each } w \in \mathcal{M}.$$

We present new estimates of the error $u_\alpha^\delta - u_*$ for suitable choices of $\alpha = \alpha(\delta)$, if the solution $u_* \in \mathcal{M}$ of $Fu = f$ admits an adjoint source representation. Examples like parameter estimation problems or the autoconvolution equation are considered, and numerical illustrations are also given.

This is joint work with B. Hofmann (TU Chemnitz, Germany), to appear in JOTA.

Thursday:

Erkki Somersalo "A stable Bayesian layer stripping algorithm for electrical impedance tomography": In electrical impedance tomography (EIT) the goal is to estimate an unknown conductivity distribution inside a body based on current-voltage measurements on the boundary of the body. Mathematically, the problem is tantamount to recovering a coefficient function of an elliptic PDE from the knowledge of complete Cauchy data at the boundary. Layer stripping method is based on the idea that the Dirichlet-to-Neumann map of the elliptic PDE can in principle be propagated into the body using an operator-valued backwards Riccati equation, while simultaneously estimating the unknown coefficient around the inwards moving artificial boundary. The ill-posedness of the inverse problem manifests itself as instability of the approach: among other things, the backwards Riccati equation may blow up in finite time. In this talk, the layer stripping algorithm is revisited in a Bayesian framework, and using novel ideas from particle filtering and sequential Monte Carlo methods, a stable computational scheme is proposed and tested numerically.

Daniela Calvetti "Reconstruction via Bayesian hierarchical models: convexity, sparsity and model reduction": The reconstruction of sparse signals from indirect, noisy data is a challenging inverse problem. In the Bayesian framework, the sparsity belief can be encoded via hierarchical prior models. In this talk we discuss the convexity - or lack thereof - of the functional associated to different models, and we show that Krylov subspace methods for the computation of the MAP solution implicitly perform an effective and efficient model reduction.

Jari Kaipio "Born approximation for inverse scattering with high contrast media": Born approximation is widely used for inverse scattering problems with low contrast media. With high constrast media, the single scattering approximation is not a feasible one and the respective reconstructions are often rendered useless. In this talk, we consider the inverse scattering problem in the Bayesian framework for inverse problems. We show that with approximative marginalization, one may be able to use the Born approximation and, furthermore, compute statistically meaningful error estimates for the index of refraction.

Claudia Schillings "On the Analysis of the Ensemble Kalman Filter for Inverse Problems and the Incorporation of Constraints": The Ensemble Kalman filter (EnKF) has had enormous impact on the applied sciences since its introduction in the 1990s by Evensen and coworkers. It is used for both data assimilation problems, where the objective is to estimate a partially observed time-evolving system, and inverse problems, where the objective is to estimate a (typically distributed) parameter appearing in a differential equation. In this talk we will focus on the identification of parameters through observations of the response of the system - the inverse problem. The EnKF can be adapted to this setting by introducing artificial dynamics. Despite documented success as a solver for such inverse problems, there is very little analysis of the algorithm. In this talk, we will discuss well-posedness and convergence results of the EnKF based on the continuous time scaling limits, which allow to derive estimates on the long-time behavior of the EnKF and, hence, provide insights into the convergence properties of the algorithm. This is joint work with Dirk Bloemker (U Augsburg), Andrew M. Stuart (Caltech), Philipp Wacker (FAU Erlangen-Nuernberg) and Simon Weissmann (U Mannheim).

Noemie Debroux "A joint reconstruction, super-resolution and registration model for motion-compensated MRI": This work addresses a central topic in Magnetic Resonance Imaging (MRI) which is the motion-correction problem in a joint reconstruction, super-resolution and registration framework. From a set of multiple MR acquisitions corrupted by motion, we aim at -jointly- reconstructing a super-resolved single motion-free corrected image and retrieving the physiological dynamics through the deformation maps. To this purpose, we propose a novel variational model relying on hyperelasticity and compressed sensing principles. We demonstrate through numerical results that this combination creates synergies in our complex variational approach resulting in higher quality reconstructions. This is a joint work with A. Aviles-Rivero, V. Corona, M. Graves, C. Le Guyader, C. Sch??nlieb, G. Williams.

Shari Moskow "Reduced order models for spectral domain inversion: Embedding into the continuous problem and generation of internal data": We generate reduced order Galerkin models for inversion of the Schrödinger equation given boundary data in the spectral domain for one and two dimensional problems. We show that in one dimension, after Lanczos orthogonalization, the Galerkin system is precisely the same as the three point staggered finite difference system on the corresponding spectrally matched grid. The orthogonalized basis functions depend only very weakly on the medium, and thus by embedding into the continuous problem, the reduced order model yields highly accurate internal solutions. In higher dimensions, the orthogonalized basis functions play the role of the grid steps, and highly accurate internal solutions are still obtained. We present inversion experiments based on the internal solutions in one and two dimensions. This is joint with: L. Borcea, V. Druskin, A. Mamonov, M. Zaslavsky.

Weihong Guo "PCM-TV-TFV: A Novel Two-Stage Framework for Image Reconstruction from Fourier Data": We propose in this paper a novel two-stage projection correction modeling (PCM) framework for image reconstruction from (nonuniform) Fourier measurements. PCM consists of a projection stage (P-stage) motivated by the multiscale Galerkin method and a correction stage (C-stage) with an edge guided regularity fusing together the advantages of total variation and total fractional variation. The P-stage allows for continuous modeling of the underlying image of interest. The given measurements are projected onto a space in which the image is well represented. We then enhance the reconstruction result at the C-stage that minimizes an energy functional consisting of a delity in the transformed domain and a novel edge guided regularity. We further develop ecient proximal algorithms to solve the corresponding optimization problem. Various numerical results in both one-dimensional signals and two-dimensional images have also been presented to demonstrate the superior performance of the proposed two-stage method to other classical one-stage methods. This is a joint work with Yue Zhang (now at Siemens Corporate Research) and Guohui Song (Clarkson University).

Friday:

Fioralba Cakoni "Inverse Scattering Problems for the Time Dependent Wave Equation": In this presentation we will discuss recent progress in non-iterative methods in the time domain. The use of time dependent data is a remedy for the large spacial aperture that these method need to obtain a reasonable reconstructions. Fist we consider the linear sampling method for solving inverse scattering problem for inhomogeneous media. A fundamental tool for the justification of this method is the solvability of the time domain interior transmission problem that relies on understanding the location on the complex plane of transmission eigenvalues. We present our latest result on the solvability of this problem. As opposed to the frequency domain case, in the time domain there are no known qualitative methods with a complete mathematical justification, such as e.g. the factorization method.This is still a challenging open problem and the second part of the talk addresses this issue. In particular, we discuss the factorization method to obtain explicit characterization of a (possibly non-convex) Dirichlet scattering object from measurements of time-dependent causal scattered waves in the far field regime. In particular, we prove that far fields of solutions to the wave equation due to particularly modified incident waves, characterize the obstacle by a range criterion involving the square root of the time derivative of the corresponding far field operator. Our analysis makes essential use of a coercivity property of the solution of the Dirichlet initial boundary value problem for the wave equation in the Laplace domain that forces us to consider this particular modification of the far field operator. The latter in fact, can be chosen arbitrarily close to the true far field operator given in terms of physical measurements. Finally we discuss some related open questions.

Marco Verani "Detection of conductivity inclusions in a semilinear elliptic problem via a phase field approach": We tackle the reconstruction of discontinuous coefficients in a semilinear elliptic equation from the knowledge of the solution on the boundary of the planar bounded domain. The problem is motivated by an application in cardiac electrophysiology. We formulate a constraint minimization problem involving a quadratic mismatch functional enhanced with a phase field term which penalizes the perimeter. After computing the optimality conditions of the phase-field optimization problem and introducing a discrete finite element formulation, we propose an iterative algorithm and prove convergence properties. Several numerical results are reported, assessing the effectiveness and the robustness of the algorithm in identifying arbitrarily-shaped inclusions. (Joint work with E. Beretta and L. Ratti)

Peter Elbau "About using dynamical systems as regularisation methods and their optimal convergence rates": A regularisation method for a linear, ill-posed problem may be seen as a family of bounded approximate inverse operators; for example, this family could be given as the solution of a dynamical system whose stationary limit corresponds to the exact inverse. Showalter's method, where the dynamical system is the gradient flow for the squared norm of the residuum, is a classical example of this sort of regularisation. Recently, second order dynamical systems have been used for this construction (despite their oscillating behaviour), and this setting allowed for a continuous formulation of Nesterov's algorithm which gave an explanation of its fast rate of convergence. In this talk, we want to restrict ourselves to the case where the inverse problem enters the dynamical system only via the gradient of the squared norm of the residuum so that we can apply spectral theory to solve the dynamical system explicitly, which allows us to characterise the convergence rate of the regularisation method uniquely by, for example, variational source conditions.

Outcome of the Meeting and Scientific Progress Made

The meeting took place in a friendly environment with a lot of interactions and many stimulating discussions. In addition to the scientific talks also a poster presentation was held, which yielded to lively interactions of the participants.

The workshop combined different aspects and techniques for the solution of inverse problems and image reconstruction, like machine learning, neural networks, stability, regularization methods in deterministic and stochastic settings and uncertainty quantification. The participants could identify some common view points. For instance, dynamical methods for solving inverse problems in a deterministic and a stochastic setting differ by the consideration of noise. Indeed, while in uncertainty quantification a time dependent noise process is considered, in the deterministic setting noise is static. However, both approaches have the same goal: to establish and analyze new methods for solving applied inverse problems. The similarities became evident in the talks of Daniela Calvetti, Claudia Schilling and Peter Elbau, respectively, and allow for a synergetic point of view. Dynamical approaches for registration and general imaging problems where discussed in the talks of Gabriele Steidl, Adrian Nachman and Luca Rondi. Here the considered analytical methods are the calculus of variations.

When discretizing inverse problems, stability becomes the dominant question, and the analysis of such was a common topic along many presenters, like Elisa Francini, Matteo Santacesaria and Bernd Hoffman. Stability could be investigated in a deterministic and a stochastic setting as well. Interestingly merging of the discrete setting with the continuous world is still not fully understood and a series of open questions needs to be solved. In particular, appropriate discretization spaces are still limited to piecewise constant and simple finite element spaces, while adaptive and advanced spaces like reduced basis spaces have not been investigated. The need of appropriate discretization in electrical impedance tomography has been documented in the talk by Matteo Santacesaria as an open question. Erkki Somersalo presented a stable layer stripping method for solving the problem of EIT in a stochastic setting. Similar as EIT also inverse scattering problems have been a driving source for inverse problems in general and regularization theory in particular. Fioralba Cakoni has reported on scattering problems for the wave equation. Jari Kaipio presented Born approximation methods for solving inverse scattering problems, which then were solved by a Bayesian regularization method.

Uniqueness of inverse problems was the main issue in the talk of Giovanni Alberti, who showed uniqueness results for hybrid inverse problems. While on the other hand Shari Moskow showed how to generate highly accurate internal data using reduced order models that are used in hybrid inverse problems.

Machine learning has become a major research topic in inverse problems: the expanding area is yet not well structured scientifically and it is indeed necessary to provide mathematically well defined problem formulations. The talks of Lars Ruhotto and Eldad Haber were highlights in this perspective: by presenting a class of neural networks with connections between layers at distance greater than one, which is the standard setting, they introduced a links to dynamical systems and differential equations; this approach relates the usual problem of weight determination in machine learning to parameter identification in partial differential equations. In the reverse direction, deep Learning and methods from artificial intelligence have been identified as new tools for solving inverse problems. Although the mathematical theory of machine learning is still at a premature stage there are already a series of well-established connections, such as to constrained optimization and to parameter identification in partial differential equations. Therefore this workshop can be considered as one of the first in which continuous limits of machine learning algorithms (layer to infinity) were shown. A careful investigation of continuous limits of discrete dynamical systems was presented in Uri Ascher's talk - he also showed how this algorithms can be used to solve inverse problems. Very intriguing was the talk of Peter Kuchment who explained his point of view of machine learning in the context of highly ill–posed problems in security applications with very little information on the object. In this case data driven models might outperform model driven approaches.

The field of regularization was covered in a wide generality: Novel aspects of infinite dimensional regularization theory in a deterministic setting were discussed in the talks of Markus Grasmair, Robert Plato, Barbara Kaltenbacher and Bernd Hofmann. Numerical methods for solving convex optimizations problems of regularized inverse problems were discussed in several talks, such as in particular in Antonio Leitao's talk.

Imaging problems, in particular with magnetic resonance data has been considered by Noemie Debroux, Weihong Guo and Simon Arridge. Here one could learn about (dynamical) total variation denoising and filtering. Simon Arridge combined and replaced filtering techniques by learning methods.

The speakers were chosen from all levels of the academic career: recent Ph.D.s (e.g., Noemie Debroux) were given the possibility to present their work alongside the more senior researchers in the field of inverse problems.

Peter Kuchment: Detecting presence of emission sources with low SNR. "Analysis" vs deep learning. Emission problems with detective sensitive sensors. $<< 0.1\%$ SNR. Anger Camera (collimination) not useful. Alternatives Compton cameras (better suited), Measures integrals over cones (a lie when the counts are low). Survey in IP in 2018 on Compton imaging. Deep learning techniques as alternative for source location by backprojection. Elisa Francini: Stable determination of polygonal domains. Stability in the Calderon problem with pw constant functions and polygonal domains.

Matteo Santacesaria: Infinite-dimensional inverse problems with finite measurements. Stability estimates with only a finite number of measurements.

Ekaterina Sherina: Quantitative PAT-OCT Elastography for Biomechanical Parameter Imaging. Parameter estimation. Lars Ruhotto: Convolution neural networks motivated from PDEs. Deep learning and optimal controls. Claudia Schillings Giovanni Alberti

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Chapter 14

Algebraic and Statistical ways into Quantum Resource Theories (19w5120)

July 21 - 26, 2019

Organizer(s): Francesco Buscemi (Nagoya University), Eric Chitambar (University of Illinois Urbana-Champaign), Gilad Gour (University of Calgary)

Overview of the Field

Quantum information science is one of the most active, intellectually stimulating, and technologically promising areas in science. It offers a unique opportunity to engage in a wide variety of topics, such as the mathematical and logical foundations of quantum theory, the theory of quantum computation and quantum Shannon theory, and practical applications like quantum cryptography and quantum sensing. Within quantum information science, an increasingly important role is played by quantum resource theories (QRTs), a collective name accounting for the fact that some distinctive features of quantum mechanics, like entanglement and coherence, are not just qualitative traits of quantum systems, but are "tangible resources" that can be extracted, transformed, traded for one another, and transferred from one system to another [1]. It is quite natural to apply a resource-theoretic outlook to the study of quantum systems since processes like decoherence rapidly eliminate most quantum behavior of a system. Like an oil digger, one must exert considerable experimental effort to witness and control the subtle effects of quantum mechanics.

The basic idea of a quantum resource theory is to study quantum information processing under a restricted set of physical operations. The permissible operations are called "free," and because they do not encompass all physical processes that quantum mechanics allows, only certain physically realizable states of a quantum system can be prepared. These accessible states are likewise called "free," and any state that is not free is called a resource state. Thus a quantum resource theory identifies every physical process as being either free or prohibited, and similarly it classifies every quantum state as being either free or a resource.

The most celebrated example of a quantum resource theory is the theory of entanglement. For two or more quantum systems, entanglement can be characterized as a resource when the allowed dynamics are local quantum operations and classical communication (LOCC). For example, as depicted in Fig. 14.2, Alice and Bob may be working in their own quantum laboratory while being separated from each other by some large distance. Due to current technological limitations, the only communication channel connecting their laboratories is classical, such as a telephone. Hence Alice cannot directly send quantum states to Bob and vice versa, and the free operations in this resource theory consists of LOCC. While the classical communication channel allows for the preparation of classically correlated states between the two laboratories, not every type of joint quantum state can be realized for Alice and Bob's systems using LOCC. A state is said to be entangled, and therefore a resource, precisely when it *cannot* be generated using the free operations of LOCC. For instance, if Alice and Bob each control a single spin-1/2 quantum system, the singlet state $\sqrt{1/2}(|01\rangle - |10\rangle)$ cannot be created by LOCC and it is therefore called an entangled state.

Inspired by the success of entanglement theory, researchers have adopted the resource theory framework within many other areas of quantum information and physics. For example, asymmetry and quantum reference frames, quantum thermodynamics, quantum coherence and superposition, secret correlations in quantum and classical systems, non-Gaussianity in bosonic systems, "magic states" in stabilizer quantum computation, non-Markovianity in multi-part quantum processes, nonlocality, and quantum correlations have all been studied as resource theories. Even more foundational objects such as contextuality and Bell non-locality have been envisioned as resources within quantum information theory.

At the same time, operator theory and mathematical statistics represent two very deep, extremely active, and intimately interconnected areas of mathematics that have provided the formal basis for the development of statistical mechanics, quantum theory, and quantum field theory. Notions like "algebra of observables," "complete positivity," or "quantum hypothesis testing" have appeared very soon after the inception of quantum theory and have been used ubiquitously ever since. Developments in quantum physics have often served as inspiration for new results in operator theory and statistics. These fields have largely benefited from mutual influences, cross-breeding, and feedbacks.

It has recently been discovered how generalized resource theories carry many similarities with the theory of "statistical comparisons" in mathematical statistics. In the latter, the statistician is interested in answering questions like, "Is one statistical test more informative than another one in deciding between alternative hypotheses?" or "Which statistical test, chosen among a set of alternatives, is the most informative one?" The theory of statistical comparison was established in the 1950s by work of Blackwell, Sherman, and Stein (BSS), as a generalization of the theory of majorization.

The theory of quantum statistical comparison has advanced as an emerging area in quantum statistics, with important contributions that extends initial quantum generalizations of the classical BSS theory [6] to the approximate case [29] and the case of infinite dimensional quantum systems [7]. Extremely important connections with the theory of operator Schur-convexity have also been explored [42]. The program of quantum statistical comparison has become intertwined with the program of characterizing generalized entropy for quantum systems via the notion of "reverse tests" [9].

Recent work has shown how the theory of statistical comparison can provide a new insight into quantum re-

Figure 14.1: In a quantum resource theory, the precious commodity is some physical property or phenomenon that emerges according to the principles of quantum mechanics. The paradigmatic example is quantum entanglement.

source theories, in particular, quantum nonlocality [10], and quantum thermodynamics and the resource theories of asymmetry and coherence [2, 3]. Indeed, the only (to date) known complete set of necessary and sufficient conditions for arbitrary quantum state transformation under thermodynamic processes [4] has been obtained using the framework of quantum relative majorization [5] and quantum statistical comparison [6]. This workshop aimed to create new links between operator theory, mathematical statistics, and the burgeoning field of quantum information science – in particular, quantum thermodynamics and generalized resource theories.

Presentation Highlights and Scientific Progress Made

This workshop united over forty international researchers to present their work on QRTs, discuss recent results, and stimulate new research directions. The results and scientific work covered in the workshop are summarized in the following.

- **General Structures of QRTs**

  One of the advantages to adopting a resource-theoretic approach to studying some quantum phenomenon is that it allows one to leverage techniques and analytic tools that apply to general QRTs. Recent work has focused on identifying key structural properties shared by all QRTs that satisfy certain mild conditions. In this workshop, some general features that emerge when casting QRTs in terms of von Neumann subalgebras were covered [11]. Complementary findings for the task of one-shot resource cost and distillation in general QRTs were also discussed [12]. It was further shown how the resource objects in any QRT with convex structure have an operational interpretation of being advantageous in some channel discrimination task [13].

- **Quantum coherence and thermodynamics**. The QRT of quantum coherence analyzes the operational utility of superposition and off-diagonal elements in the density matrix. In this workshop, techniques for computing the robustness measure of coherence were demonstrated [14]. Recent work on extending coherence theory to the level of quantum operations and superchannels was also presented [15]. Applications to clock synchronization via coherence distillation were discussed [16]. In the QRT of thermodynamics, an application to molecular transitions and their thermodynamics costs was described [17].

- **Entanglement and nonlocality** Quantum entanglement and nonlocality are two quintessential quantum resources that emerge in multipartite systems. In the workshop, recent efforts to understand the structure of multipartite entanglement from a QRT perspective were described [18]. Quantum entanglement is the key resource in performing quantum teleportation, and new bounds in the asymptotic cost of port-based teleportation were presented [19]. Entanglement is also used for "embezzling" state transformations, and a rigorous analysis of quantum embezzlement was conducted within the context of a QRT [20]. A resource related to entanglement is quantum nonlocality, and its presence is detected through the violation of a Bell Inequality. Recently, such violations have been shown to certify the type of quantum state shared between the different parties, and some results in this direction were presented [21].

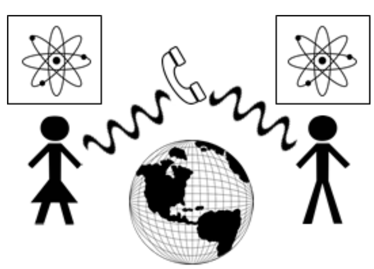

Figure 14.2: Quantum entanglement is a quantum resource in the "distant-lab" scenario where the free operations are LOCC.

- **Quantum computation**. QRTs for quantum computation attempt to identify the properties of quantum systems that enable them to perform certain computations seemingly faster than the best classical algorithms. New measures of quantum computational "magic" were discussed as well as new bounds on magic state convertibility [22, 23]. In addition, an updated analysis of the matchgate quantum computational model and its classical simulation were presented [24].

- **Pairwise conversion of resources**. A particular problem arising in all QRTs is to determine when one pair of resource states (ρ_1, σ_1) can be transformed into another (ρ_2, σ_2) using a free operation in the QRT. An analysis of this problem in general majorization-based QRTs was presented [25, 26]. These results included the case of converting pairs of states from one to the other, and variations to this central problem were analyzed both in the one-shot and asymptotic settings [27, 28]. The problem was also extended to the pairwise convertibility of quantum channels [29].

- **Quantum Shannon Theory** Quantum Shannon Theory exemplifies a QRT in that it studies the convertibility between different information-theoretic resources in the presence of restrictions. New tools in the study of quantum information systems were presented including entropic continuity bounds [30], improved decoupling techniques [31], and De Finetti Theorems for Quantum Channels [41].

- **Quantum channels and superchannels**. A dynamical QRT studies properties of quantum channels and quantum measurements. Work was presented showing how the structure of devices can be inferred from the study of classical output data [33, 34, 35]. The general theory of quantum superchannels and quantum combs was surveyed [36]. In addition, a framework for quantifying the resourcefulness of quantum channels was described in considerable detail [37, 38]. Specific applications discussed include the Quantum Zeno Effect [39].

Open Problems

A highlight of the workshop was the two open problem sessions. All participants were encouraged to pose an interesting problem to the community related to quantum resource theories. Here we record the open problems that were presented.

- **Parallel versus sequential strategies for quantum channel discrimination** - Presenter: Mark Wilde. **Comment: A solution to this problem has recently been given in arXiv:quant-ph/1909.05826 with an acknowledgement of the workshop.**. An experimenter has access to one of two unknown quantum channels, $\mathcal{N}_1$ or $\mathcal{N}_2$, that both act on system S. The goal is to identify which of the two channels is given in the many-copy setting. A *parallel discrimination strategy* involves applying n copies of the channel to an entangled state ρ^{RS^n} and them performing a joint measurement on the outcome state $\mathrm{id}^{\otimes n} \otimes \mathcal{N}_i^{\otimes n}(\rho^{RS^n})$. Based on the measurement outcome, a guess is made to the channel's identity i. In the language of hypothesis testing, it is known that the optimal rate for the type-two error exponent is given by a regularized channel relative entropy [40]: $D^\infty(\mathcal{N}_1\|\mathcal{N}_2) = \lim_{n\to\infty} \frac{1}{n} D(\mathcal{N}_1^{\otimes n}\|\mathcal{N}_2^{\otimes n})$, where
$$D(\mathcal{N}_1\|\mathcal{N}_2) = \sup_{\psi^{RS}} D(\mathrm{id}^R \otimes \mathcal{N}_1(\psi^{RS})\|\mathrm{id}^R \otimes \mathcal{N}_2(\psi^{RS})).$$

  In contrast, a *sequential discrimination strategy* does not involve using all n channels at once; rather, the output of the j^{th} channel can be used in the $j^{th}+1$ input. In the sequential setting, the optimal discrimination rate is given by the amortized relative entropy [41]:
$$D^A(\mathcal{N}_1\|\mathcal{N}_2) = \sup_{\rho^{RS},\sigma^{RS}} D(\mathrm{id}^R \otimes \mathcal{N}_1(\rho^{RS})\|\mathrm{id}^R \otimes \mathcal{N}_2(\sigma^{RS})) - D(\rho^{RS}\|\sigma^{RS}).$$

  In general the adaptive strategy is no worse that the parallel strategy, in the sense that
$$D^\infty(\mathcal{N}_1\|\mathcal{N}_2) \leq D^A(\mathcal{N}_2\|\mathcal{N}_2). \tag{0.1}$$

For classical channels and quantum-classical channels it is known that this inequality is tight. The open problem is to determine whether there exists quantum channels in which this is a strict inequality, that is, whether adaptive discrimination can be strictly more powerful than parallel discrimination.

- **Second-order asymptotics in pairwise state convertibility** - Presenter: Marco Tomamichel. Given two pairs of quantum states (ρ_1, σ_1) and (ρ_2, σ_2), a general problem is to decide whether there exists a quantum channel $\mathcal{E}$ such that $\mathcal{E}(\sigma_1) = \sigma_2$ and $\mathcal{E}(\rho_1) \approx_\varepsilon \rho_2$. Such a transformation can be denoted as

$$(\rho_1, \sigma_1) \to_\varepsilon (\rho_2, \sigma_2),$$

this question arises in QRTs defined by some fixed point constraint on the allowed maps $\mathcal{E}(\sigma_1) = \sigma_1$, such as Gibbs-preserving maps in thermodynamics. In the special case of $\varepsilon = 0$, the solution is known [42, 5]. The asymptotic version of this problem considers the largest rate R such that for all $\varepsilon > 0$ there exists a sufficiently large n such that

$$(\rho_1^{\otimes n}, \sigma_1^{\otimes n}) \to_\varepsilon (\rho_2^{\otimes Rn}, \sigma_2^{\otimes Rn}).$$

It is known that the optimal R_∞ is given by [28, 43]

$$R_\infty = \frac{D(\rho_1 \| \sigma_1)}{D(\rho_2 \| \sigma_2)}. \tag{0.2}$$

However, the second-order terms in the rate are not known, and the open problem is to characterize, for a given n and ε, the exact achievable values $R_{n,\varepsilon}$ such that $(\rho_1^{\otimes n}, \sigma_1^{\otimes n}) \to_\varepsilon (\rho_2^{\otimes R_{n,\varepsilon} n}, \sigma_2^{\otimes R_{n,\varepsilon} n})$.

- **Sequential channel simulation** - Presenter: Andreas Winter. The Reverse Shannon Theorem addresses the problem of simulating a given quantum channel $\mathcal{N}$ using one-way classical communication channels plus local operations with unlimited shared entanglement (LOSE) [44, 45]. In terms of resource transformation, this can be expressed as

$$lR \cdot [c \to c] + (LOSE) \to \mathcal{N}^{\otimes l},$$

which says that lR bits of classical communication with LOSE can simulate l copies of $\mathcal{N}$. In this setting, LOSE represents the free operations in the QRT, and the goal is to find the minimal rate R for which this transformation is possible. Notice that this describes a parallel simulation of $\mathcal{N}$ in the sense that $\mathcal{N}^{\otimes l}$ is an object that acts on l input spaces all at once. A more general simulation involves reproducing l uses of $\mathcal{N}$ that may be applied in a sequential manner. Figure 14.3 provides an example of three sequential uses of $\mathcal{N}$. The goal is to simulate such a dynamical resource using classical communication and LOSE, and the

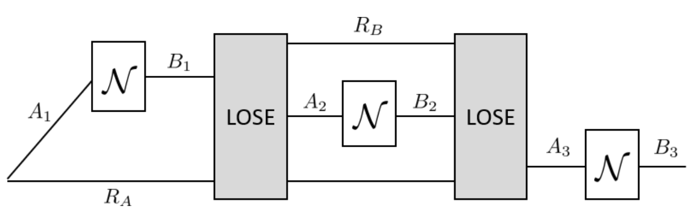

Figure 14.3: Three sequential uses of $\mathcal{N}$.

sequential simulation cost is the smallest rate of classical communication needed to faithfully simulate n sequential uses of $\mathcal{N}$, as $n \to \infty$. The open question is whether there exists channels in which the sequential simulation cost is strictly larger than the parallel simulation cost.

- **Catalytic entropy conjecture** - Presenter: Paul Boes. The catalytic entropy conjecture proposes necessary and sufficient conditions for the catalytic convertibility of one state ρ_1^S into another ρ_2^S by unitary evolution.

Namely, it says that when the spectrum of ρ_1 and ρ_2 are inequivalent, there exists a catalytic state σ^C and joint unitary U^{SC} such that

$$\mathrm{Tr}_C\left[U(\rho_1^S \otimes \sigma^C)U^\dagger\right] = \rho_2 \quad \text{and} \quad \mathrm{Tr}_S\left[U(\rho_1^S \otimes \sigma^C)U^\dagger\right] = \sigma \tag{0.3}$$

if and only if $S(\rho_1) > S(\rho_2)$ and $rk(\rho_1) \geq rk(\rho_2)$. Eq. (0.3) characterizes the catalytic convertibility of ρ into ρ', and such a problem appears naturally in the QRTs of thermodynamics and entanglement [46]. The conjecture here is that the von Neumann entropy is unique measure for deciding catalytic convertibility. If true, it would provide an operational interpretation of the von Neumann entropy in the single-shot setting, in contrast to standard i.i.d. interpretations of the von Neumann entropy. The open problem is to prove or disprove the catalytic convertibility conjecture, and recent work in this direction can be found in Refs. [46, 47], as well as a formal statement of the problem at [48].

- **Realization of Completely PPT-Preserving Superchannels** - Presenter: Gilad Gour. A bipartite quantum channel $\mathcal{N}^{A_0B_0\to A_1B_1}$ is called PPT if it remains completely positive when composed with partial transpose maps. That is, $\mathcal{N}^{A_0B_0\to A_1B_1}$ is PPT if $T^{A_1} \circ \mathcal{N}^{A_0B_0\to A_1B_1} \circ T^{A_0} \geq 0$, where T is the transpose operation on the given system. Such maps play an important role in the study of entanglement since they provide a mathematically-friendly relaxation on the class of LOCC [49]. A superchannel $\Theta^{AB\to A'B'}$ is called completely PPT-preserving if $1^{\overline{AB}} \otimes \Theta[\mathcal{N}^{A\overline{A}B\overline{B}}]$ is PPT for any PPT channel $\mathcal{N}^{A\overline{A}B\overline{B}}$, where $\overline{A}$ and $\overline{B}$ are arbitrary auxiliary systems and $1^{\overline{AB}}$ is the identity supermap [50]. A general superchannel can be realized by pre-processing quantum channel that is connected to some post-processing channel via an auxiliary memory system. If these pre- and post-processing channels are themselves PPT, then the resulting superchannel is completely-PPT preserving (see Fig. 14.4). The open problem is whether every completely PPT-preserving superchannel can be realized in this way.

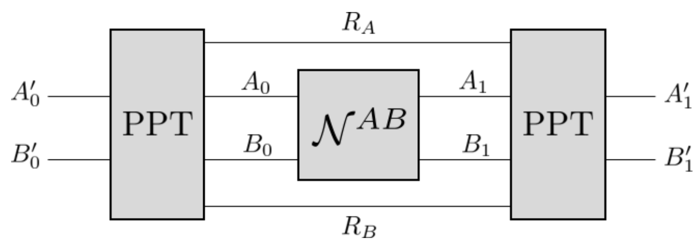

Figure 14.4: One type of completely PPT-preserving superchannels is composed of pre- and post-processing PPT channels. Can all completely PPT-preserving superchannels be built in this way?

- **Entanglement Distillation using Local Incoherent Operations** - Presenter: Eric Chitambar. In the quantum resource theory of coherence, one is restricted to performing some family of quantum operations that cannot generate coherence. The most commonly studied are the so-called incoherent operations [51]. These operations can be extended to bipartite systems, and when additional locality constraints are placed on the operations, one arrives at a resource theory in which only local incoherent operations and classical communication (LIOCC) are free. The canonical resource states are local maximally coherent bits (cobits), $|\phi_+\rangle^A$ and $|\phi_+\rangle^B$ where $|\phi_+\rangle = \sqrt{1/2}(|0\rangle + |1\rangle)$, as well as a maximally entangled coherent bit (ecobit) $|\Phi^+\rangle = \sqrt{1/2}(|00\rangle + |11\rangle)$. A general distillation protocol then involves converting a given bipartite state ρ^{AB} into a triple of cobits and ecobits (see Fig. 14.5). The problem of asymptotic distillation for a pure state $|\Psi\rangle^{AB}$ has been studied in Ref. [52], and an optimal point in the rate region has been identified as

$$(R^A_{co}, R^B_{co}, R^{AB}_{eco}) = (0, S(Y|X)_{\Delta(\Psi)}, I(X:Y)_{\Delta(\Psi)}),$$

where $\Delta(\Psi)^{XY}$ is the fully classical state obtained from locally dephasing $|\Psi\rangle^{AB}$. However, it is known that higher entanglement rates R_{eco}^{AB} are achievable at the cost of reducing the coherence rate R_{co}^{B}, but optimal rate has not been solved. The open problem is to determine the largest achievable rate of ecobit distillation from an arbitrary pure state $|\Psi\rangle^{AB}$ using LIOCC.

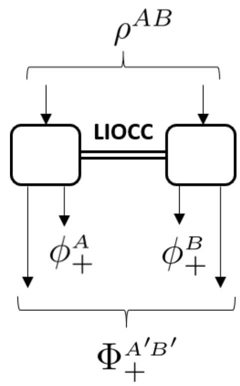

Figure 14.5: In the resource theory of distributed coherence, an operational task is to distill local coherent bits $\phi+^A$ and ϕ_+^B as well as entangled coherent bits Φ_+^{AB}. In general there will be a trade-off in distillation rates.

- **Tightening of the Alicki-Fannes Inequality** - Presenter: Mark Wilde. The Alicki-Fannes Inequality puts a bound on the difference of conditional von Neumann entropies [53], and it reads

$$|S(A|B)_\rho - S(A|B)_\sigma| \leq 4\varepsilon \log_2 |A| + 2h(\varepsilon), \quad (0.4)$$

where $\varepsilon \geq \|\rho - \sigma\|_1$ and $h(\varepsilon) = -\varepsilon \log_2 \varepsilon - (1-\varepsilon)\log_2(1-\varepsilon)$. This is a useful inequality in quantum information theory as it establishes a uniform continuity bound on the conditional von Neumann entropy. Recently, the RHS has been tightened to $2\varepsilon \log_2 |A| + (1+\varepsilon)h(\frac{\varepsilon}{1-\varepsilon})$ [54], however it is not known whether this is optimal in the sense that it can be satisfied by certain pairs of states. For classical-quantum (CQ) states, an improvement can be made by replacing the RHS with $\varepsilon \log_2(|A|-1) + h_2(\varepsilon)$, and this is known to be optimal [55]. The open problem is whether the Alicki-Fannes Inequality can be improved in the fully quantum case to the following form, which would be tight using the pair of states used in Remark 3 of [54]:

$$|S(A|B)_\rho - S(A|B)_\sigma| \leq \varepsilon \log_2(|A|^2 - 1) + h(\varepsilon). \quad (0.5)$$

Outlook

A common theme in physics is the unification of theories and models that at first glance may seem completely unrelated. Most notable in this regard is the successful unification of the three non-gravitational forces in nature. Such an amalgamation not only leads to new discoveries, but it also has the potential to profoundly change the way we perceive the world around us. With the advent of quantum information science, many seemingly unrelated properties of physical systems, such as entanglement, asymmetry, and athermality, have now become recognized as resources. This recognition is profound as it allows them to be unified under the same roof of quantum resource theories. Entanglement, athermality, and asymmetry, are no longer regarded as just interesting physical properties of a quantum system, but they now emerge as resources that can be utilized and manipulated to execute a variety of remarkable tasks, such as quantum teleportation.

This BIRS workshop has focused on the interface between quantum resource theories, operator theory, and (quantum) mathematical statistics. We believe the results presented at the workshop and the discussions shared by its participants will have a lasting impact on all the fields involved. It is an exciting time for quantum resource theories, and we thank BIRS for providing the opportunity to further advance this important subject.

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Chapter 15

From Many Body Problems to Random Matrices (19w5176)

August 4 - 9, 2019

Organizer(s): Paul Bourgade (New York University), Laszlo Erdős (Institute of Science and Technology Austria), Jeremy Quastel (University of Toronto), Tai-Peng Tsai (University of British Columbia)

Overview of the Field

Overview of the subject area of the workshop

Universality and integrability. Complex physical systems with many degrees of freedom cannot typically be described deterministically; solving an equation with $N = 10^{23}$ variables is not feasible unless it has a special structure allowing for explicit solutions. Moreover, precise details of the system and the initial conditions are often known only statistically and not exactly. On the crudest level of description, random effects cancel out and effective equations for a few macroscopic physical variables become accurate - a fundamental mechanism that justifies thermodynamics, statistical physics and fluid dynamics. On a finer scale, quite surprisingly, fluctuations around these macroscopic variables tend to exhibit universal behavior.

Universality within and between complex random systems is a striking concept which has played a central role in the direction of research within probability, mathematical physics and statistical mechanics. Complementary to universality, is the exact description of the behaviors that are supposed to be universal as well as the determination which systems are supposed to display them.

The historical example is the Gaussian distribution emerging from the central limit theorem. Since its discovery more than two hundred years ago, it has proved to be an incredibly versatile and robust tool explaining randomness in the physical world, under the assumption of some underlying independence. Systems accurately described in terms of this distribution are said to be in the Gaussian universality class.

Ongoing efforts to understand this universality class are essentially of two types. First, integrability consists in finding possibly new statistics for a few, rigid models, with methods including combinatorics and representation theory. Second, universality means enlarging the range of models with random matrix statistics, through probabilistic methods.

In recent years there has been an immense amount of progress in the rigorous mathematical understanding of certain universal scaling limits, not only on the universality and integrability fronts, but also both in equilibrium and non-equilibrium statistical physical systems. On the random matrix side, microscopic scaling limits are often described in terms of determinantal or pfaffian point processes. On the non-equilibrium side, systems like growth processes are described through the Kardar-Parisi-Zhang universality class. There is reason to believe that these two directions share many (as of yet) unexploited relationships. For instance, the field of quantum integrable systems was developed to study equilibrium systems, but has now found itself center stage in the KPZ universality class. Conversely, methods developed in stochastic PDEs for non-equilibrium systems have begun to make their way into constructive field theory, and the dynamics of Dyson Brownian motion proved to be essential to understand static spectral universality.

We give below a succinct overview of recent progress for random matrices, with the key technique of dynamics, and the recent progress on the KPZ universality class.

The Wigner-Dyson-Mehta conjecture. As a first test for his paradigm, Wigner conjectured - together with Dyson and Mehta - that the microscopic eigenvalue statistics of large symmetric matrices with independent entries - so-called Wigner matrices - do not depend on the distribution of the matrix elements [57, 46]. This is an analogue of the central limit theorem for eigenvalue statistics at the microscopic scale, but with a non-Gaussian limit. Along an important series of breakthroughs in the past ten years, the Wigner-Dyson-Mehta conjecture has been proved, enlarging the universality class from the integrable Gaussian ensembles to the Wigner matrices: the Gaudin-Mehta and Tracy-Widom distributions appear naturally as a simple transform with input independent, arbitrarily distributed, random variables (see e.g. [28, 56, 30, 29]).

The universality class has subsequently been enlarged to many other models, as was done recently for covariance matrices, β-ensembles, matrices with correlated entries, matrices of free-convolution type, Erdős-Rényi and d-regular random graphs.

Universality for these models may use a variety of tools including the Itzykson Zuber integral, the Lindeberg principle, transport maps and multiscale analysis. However, for all of these models, possibly the most fundamental idea - introduced by Erdős, Schlein and Yau [28] - consists in using dynamics to prove the - static - universality result by interpolation.

Dynamics. The Dyson Brownian motion [10] describes the dynamics of eigenvalues of random matrices, when matrix entries follow standard independent Brownian paths. At the technical level, the analysis of Dyson Brownian motion can be performed either through hydrodynamics or probabilistic coupling. Erdős, Schlein, Yau and Yin proved that this dynamics reaches local equilibrium very rapidly, so that the noise regularization could be effectively removed by density arguments.

From a more general perspective, non-equilibrium dynamics describes systems which are in motion. Examples include fluid dynamics, weather, and models in the biological sciences. Although nonequilibrium dynamics are ubiquitous in the real world, it is one of the most challenging domains of mathematics and physics. Unfortunately we still have only limited mathematical tools to analyze general dynamics, but at least the Dyson Brownian motion is now well understood even for arbitrary initial conditions.

The following two particular models of stochastic dynamics became better understood in recent years and are of particular interest: the Kardar- Parisi-Zhang (KPZ) equation for its own sake, and Dyson Brownian motion for its applications, as previously mentioned. It is a remarkable fact that the fluctuations of the KPZ solutions are very closely connected to random matrix theory, through the Tracy Widom distribution(s).

Kardar-Parisi-Zhang. The KPZ equation is a stochastic equation in one dimension which has elements of “stochastic integrability”. It is also related to asymptotic representation theory. A substantial part of the program was centered around the KPZ equation. Originally, the equation was proposed by Kardar, Parisi, and Zhang (1986) [42] to describe the motion of growing fronts. Large scale mathematical activities started in the seminal work of Baik, Deift and Johansson (2000) [4]. The wide interest in the KPZ equation stems from its role in connecting seemingly different mathematical worlds, in particular, Dyson's Brownian motion, quantum Toda chain and related integrable models, statistical mechanics of line ensembles, directed polymers in a random medium, tilings, stochastic lattice gases, and stochastic conservation laws in one dimension. During recent years, a wide spectrum of advances have been achieved. We list only a few examples:

(i) Hairer's rigorous and robust regularity theory structures gave firm grounds to the KPZ equation [36, 37].

(ii) Universality of the KPZ equation. Based on heuristic arguments, one expects the KPZ equation to be "universal" in the sense that microscopic models of surface growth presenting either weak noise or a weak asymmetry is expected to converge to the KPZ equation when viewed at a suitable large scale. Some results were recently established rigorously for a class of continuous models. (Hairer, Quastel [39]).

(iii) More recently, a clear understanding of the KPZ fixed point for any initial data was provided in a key result of Quastel, Matetski and Remenik [45].

These recent progresses raise questions about universality of discrete models supposed to converge to the KPZ fixed point. For example, one natural question is whether ASEP models exhibit the whole range of possible limiting behaviors discovered in (iii).

Delocalization and universality beyond mean field. In Wigner's original theory, the eigenvectors play no role. However, their statistics are essential in view of a famous dichotomy of spectral behaviors, widely studied since Anderson's tight binding model [3] for conductor-insulator transition: random matrix eigenvalue distributions should coincide with delocalization of eigenstates, while Poisson and Gaussian universality classes for the spectrum occur together with localization. The localized phase is well understood since the early work of Fröhlich and Spencer [33], but delocalization and random matrix universality have still not been proved for any operator relevant in physics. Indeed Wigner matrices are mean field models - all matrix entries are random - which strongly limits their physical relevance. An outstanding problem consists in proving the Anderson transition phenomenon for at least one model.

One well-known such model is given by band matrices (see e.g. [55]): each point in space randomly interacts only with a finite-range of neighbours. These matrices are believed to exhibit the insulator-conducting transition, as famously conjectured twenty five years ago by Fyodorov and Mirlin [34]: for example, in dimension 1, if the random band has width greater than $N^{1/2}$, with N the matrix dimension, the system is supposedly delocalized, otherwise it is localized. Very little is known about the delocalized phase. Recently, a mean field reduction technique was introduced to identify the eigenvalue statistics for some non mean field band matrices [9, 10]. Interestingly, this reduction technique means that universal spectral statistics follow from quantum unique ergodicity of the eigenvectors, a notion of delocalization introduced by Rudnick and Sarnak in the context of the Laplacian on manifolds [50].

Another very intriguing idea is the supersymmetric (SUSY) approach that explicitly computes local statistics of quite general disordered models, including the Anderson model, but it uses mathematically ill-defined saddle point analysis on Grassmann integrals [27]. Currently there is no idea how to remedy this unfortunate situation where physicists have found an obviously powerful tool but mathematicians failed to create its rigorous foundations. Nevertheless, some aspects of SUSY analysis can be made rigorous and have been used to analyse band matrices [24, 51, 52, 53, 54].

Statement of the objectives of the workshop

The focus of this workshop was to enlarge the basin of attraction of integrable models, by developing new analytic tools to advance our understanding of universality, both for random matrices and stochastic growth models. It brought together leading figures that are working on questions related to this field and place them in contact with young researchers. The chief interests did not only include the exposition of recent work, but also a collaborative effort to understand the relationships between the seemingly disparate results and techniques and foster new collaborations.

Organisational aspects. The workshop had 19 speakers and 35 participants in a very active and fundamental area at the intersection of probability, analysis and mathematical physics. The organizers have invited leading researchers in this field, including women mathematicians, and made sure promising postdocs attend the meeting for their scientific development. The organizing committee also made sure that the meeting contribute to the enhancement and improvement of scientific and educational activities through the dissemination of the results. Most speakers provided slides which have become immediately available through the workshop webpage. The video facilities at BIRS have allowed wide range dissemination of this very active research field.

Why now? A special year was organized on random matrix theory and the KPZ equation at the Institute for Advanced Study in 2013-2014. The organizing committee felt that now is a good time to join again these research groups, after five years of intensive progress.

Probability as a field has seen tremendous advances in recent years with breakthroughs in random matrix theory, stochastic PDEs and the Kardar-Parisi-Zhang universality class. For instance, random matrix theory has found some new uses in the study of random 2d geometries, as have stochastic PDEs; stochastic PDEs and random matrix theory have found new uses in the study of random growth. In light of all of these new techniques and advances, it also seems quite appropriate to try to reintroduce many of the fundamental challenges related to localization, delocalization, dynamics and perhaps refocus people's attention (and new methods) on some of these questions.

Some major open problems

This conference brought together international experts working on the broad theme of dynamics and universality of complex disordered systems, who are at the forefront of current progress in these fields. These areas provided a vast source of open questions and interesting phenomena for the past 50 years. Despite the long investigation and remarkable progress, several fundamental problems remain unsolved:

(i) Random Matrix Universality beyond mean field models, in particular delocalization

(ii) A robust characterization for convergence of discrete models to the KPZ fixed point

(iii) Universality of the Tracy Widom distribution in first passage percolation

(iv) Random matrix statistics in semiclassical analysis, i.e. the Bohigas Giannoni Schmidt conjecture [7]

Problems number (iii) and (iv) seem out of reach with current techniques, but there is some starting point for problems (i) and (ii) and some progress was mentioned during the workshop. This progress, and some more specific open problems, are detailed in the next section.

Presentation Highlights

The meeting "From Many Body Problems to Random Matrices" was held Aug 4-9, 2019. There were many very high level talks surveying the latest developments in the general field spanning mathematical physics and probability, mostly by junior researchers, with many interesting comments and discussions with the more senior attendants. Some key progress and ideas of the talks are mentioned in te next paragraph. Some more details (and possibly some open problems) for each talk are given just after.

Monday morning was devoted to several talks on the recent proofs of the Lee-Huang-Yang asymptotics for the ground state energy of the Bose-Einstein condensate, a problem that has been worked on intensively in the math-physics community for the last several decades. In the afternoon there were a variety of results on hydrodynamic limits without local equilibrium, quantum lattice models, and the dynamical approach to eigenvalue empirical distributions of complex matrix ensembles. As well, there was the talk of Novak on the successful culmination of a decade work on deriving Hurwitz numbers from matrix integrals. Tuesday had a breakthrough result of Ding on the mathematical approach to Anderson localization problems, as well as Tatyana Shcherbyna on the supersymmetric approach to random band matrices. Wednesday morning concentrated on large random graphs, then some hints at new universality classes for statistics in numerical algorithms. The final talks of the meeting contained remarkable new results by a number of young researchers: Bauerschmidt has found a way to extend the Bakry-Emery arguments to non-convex potentials, with an application to obtain the log-Sobolev inequality for dynamical sine-Gordon; Aggarwal has managed to extend the three step program for universality of random matrices to obtain the local statistics in the bulk of lozenge tiling models for general domains; Sosoe and coauthors have extended the Fields medal work of Martin Hairer to certain stochastically forced wave equations; Cipolloni extended the random matrix universality to places where there is a cusp in the eigenvalue density, and to the edge of non Hermitian random matrix models; finally, Landon calculated the fluctuations of the overlap in the spherical spin glass model.

Benjamin Schlein: Excitation spectrum of Bose Einstein condensates [7]. This talk considered systems of N trapped bosons interacting through a repulsive potential with scattering length of the order 1/N, i.e. in the Gross-Pitaevskii regime. Schlein and collaborators determined the low-energy spectrum of the Hamilton operator in the limit of large N, confirming the predictions of Bogoliubov theory.

Jan Phillip Solovej: On the Lee-Huang-Yang universal asymptotics for the ground state energy of a Bose gas in the dilute limit. [5, 13, 31, 32] In 1957 Lee, Huang, and Yang (LHY) predicted a universal expression for a two-term asymptotic formula for the ground state energy of a dilute Bose gas. The formula is universal in the sense that the two terms depend on the interaction potential only through its scattering length. In 2009 Yau and Yin proved an upper bound of the LHY form for a fairly large class of potentials [58]. The speaker discussed recent joint work with Fournais complementing this by a corresponding lower bound, establishing the LHY universality formula.

Stefano Olla: Some problems in hyperbolic hydrodynamic limits: random masses and non-linear wave equation with boundary tension. The speaker illustrated some recent results about hydrodynamic limit in Euler scaling for one dimensional chain of oscillators:

(1) in the harmonic case with random masses, Anderson localization allows to obtain Euler equation in the hyperbolic scaling limit, while temperature profile does not evolve in any time scale.

(2) If the chain is in contact with a Langevin heat bath conserving momentum and volume (isothermal evolution), we prove convergence to L^2-valued weak entropic thermodynamic solutions of the non-linear wave equation, even in presence of boundary tension.

Open problem related to this talk. Uniqueness of the solution to the limiting hydrodynamic equation.

Bruno Nachtergaele: Stability of the superselection sectors of two-dimensional quantum lattice models [15]. Kitaev's quantum double models provide a rich class of examples of two-dimensional lattice systems with topological order in the ground states and a spectrum described by anyonic elementary excitations. The infinite volume ground states of the abelian quantum double models come in a number of equivalence classes called superselection sectors. Nachtergaele and collaborators showed that the superselection structure remains unchanged under uniformly small perturbations of the Hamiltonians.

Open problems related to this talk. Among important remaining questions are the thermodynamics and effective equations for many-anyon systems, and interesting examples of stable non-abelian anyons.

Todd Kemp: Geometric Matrix Brownian Motion and the Lima Bean Law. [25] The non-normality (and lack of explicit symmetry) of the Geometric matrix Brownian motion has made understanding its large-N limit empirical eigenvalue distribution quite challenging. There are two sides to this problem: proving that the empirical law of eigenvalues converges (which amounts to certain tightness conditions on singular values), and computing what it converges to. In the case of the geometric matrix Brownian motion, the speaker exposed the explicit calculation of the conjectured limit empirical eigenvalue distribution. It has an analytic density with a nice polar decomposition, supported on a region that resembles a lima bean for small time, then folds over and becomes a topological annulus for large time.

Open problems related to this talk. The question of convergence is still a work in progress.

Jonathan Novak: A tale of two integrals. The Harish-Chandra/Itzykson-Zuber integral [40] and its additive counterpart, the Brezin-Gross-Witten integral, play an important role in random matrix theory. The author presented his recent work which proves a longstanding conjecture on the large dimension asymptotic behavior of these special functions. Hurwitz and monotone Hurwitz numbers play an important role.

Jian Ding: Localization near the edge for the Anderson Bernoulli model on the two dimensional lattice. [16] The speaker considers a Hamiltonian given by the Laplacian plus a Bernoulli potential on the two dimensional lattice. He explained how, for energies sufficiently close to the edge of the spectrum, the resolvent on a large square is likely to decay exponentially. This implies almost sure Anderson localization for energies sufficiently close to the edge of the spectrum, answering a longstanding open question. The proof follows the program of Bourgain-Kenig [8], using a new unique continuation result inspired by a Liouville theorem of Buhovsky-Logunov-Malinnikova-Sodin [14]. Tha speaker also explained how Li and Zhang [44] proved a similar result in 3d.

Open problems related to this talk. Key questions are localization through the spectrum for $d = 2$ with weak potentials, and localization/delocalization phase transition for $d \geq 3$ with weak potentials.

Alexander Elgart: Localization at the bottom of the spectrum of a disordered XXZ spin chain . Quantum spin chains provide some of the mathematically most accessible examples of quantum many-body systems. However, even these toy models pose considerable analytical and numerical challenges, due to the fact that the number of degrees of freedom involved grows exponentially fast with the system's size. The speaker discussed the recent progress in establishing many body localization at the bottom of the spectrum of a disordered XXZ chain. In particular, he mentioned in progress introducing a new approach to many body localization that works beyond the droplet phase.

Mariya Shcherbyna: Central Limit Theorem for the entanglement entropy of free disordered fermions. [48] The speaker considered the macroscopic disordered system of free lattice fermions with the one-body Hamiltonian, which is the Schrödinger operator with i.i.d. potential in $d > 1$. Assuming that the fractional moment criteria for the Anderson localization is satisfied, she proved a Central Limit Theorem for the large block entanglement entropy.

Tatyana Shcherbyna: Universality for random band matrices. [51, 52, 53, 54] As explained in Section 15, random band matrices (RBM) are natural intermediate models to study eigenvalue statistics and quantum propagation in disordered systems, since they interpolate between mean-field type Wigner matrices and random Schrodinger operators. In particular, RBM can be used to model the Anderson metal-insulator phase transition (crossover) even in 1d. The speaker discussed some recent progress in application of the supersymmetric method (SUSY) and transfer matrix approach to the analysis of local spectral characteristics of some specific types of 1d RBM. In particular she explained work in progress to obtain the localization-delocalization transition at the level of 2 point correlation function, for some Hermitian Gaussian random band matrices.

Open problems related to this talk. Important natural questions are higher order correlation functions, other symmetry classes, eigenvector statistics and universality of the transition for the RBM model.

Morris Yau: Convex relaxations for robust statistics. Much of the theory of machine learning is concerned with the optimization of non-convex functions. Convex relaxations and their associated hierarchies (sum-of-squares, Lassere) provide a systematic approach for approximately optimizing non-convex functions. Recent breakthroughs in robust statistics have produced the first polynomial time (efficient) algorithms for computing the robust mean of a high dimensional Gaussian. Building on these developments, the speaker constructed a framework for robust learning via convex relaxations yielding the first polynomial time algorithm for robust regression when the overwhelming majority of the dataset is comprised of outliers.

Amir Dembo: Large deviations of subgraph counts for sparse random graphs. [21] The speaker discussed recent developments in the emerging theory of nonlinear large deviations, focusing on sharp upper tails for counts of a fixed subgraph in large sparse random graphs, such as Erdős-Rényi or uniformly d-regular. He explained his approach via quantitative versions of the regularity and counting lemmas suitable for the study of sparse random graphs in the large deviations regime.

Open problems related to this talk. For example, Sidorenko's conjecture (see (1.31) in [21])

Antti Knowles: Extremal eigenvalues of sparse Erdos-Renyi graphs. [2] The speaker reviewed recent results on the extremal eigenvalues of the adjacency matrix A of the Erdos-Renyi graph G(N,p). If p is large then, after a suitable rescaling, A behaves like a Wigner matrix and its extremal eigenvalues converge to the edges -2, +2 of the asymptotic support of the eigenvalue distribution. If p is small, this is no longer true. The behaviour of the extremal eigenvalues for small p was explained, and in particular the transition around a critical p. The proof is based on a tridiagonal representation of A and on a detailed analysis of the geometry of the neighbourhood of the large degree vertices. An important ingredient is a matrix inequality obtained via the associated nonbacktracking matrix and an Ihara-Bass formula.

Open problems related to this talk. Delocalized or localized behavior of eigenvectors near energy levels $-2, 0, 2$, for small connectivity.

Percy Deift: Universality in numerical computation with random data [22, 49]. The speaker described various universality results in numerical computation with random data. The talk provided an overview of prior results, and also some recent developments.

Roland Bauerschmidt: Log-Sobolev inequality for the continuum Sine-Gordon model [6]. The speaker presented a multiscale generalisation of the Bakry-Emery criterion [10] for a measure to satisfy a Log-Sobolev inequality. It relies on the control of an associated PDE well known in renormalisation theory: the Polchinski equation. His criterion remains effective for measures which are far from log-concave. Indeed, he explained that the massive continuum Sine-Gordon model on R^2 with $\beta < 6\pi$ satisfies asymptotically optimal Log-Sobolev inequalities for Glauber and Kawasaki dynamics.

Open problems related to this talk. Applications of this new LSI criterion to other dynamics with equilibrium φ^4, Ising models, for example.

Amol Aggarwal: Universality for Lozenge Tiling Local Statistics [1]. The speaker considered uniformly chosen random lozenge tilings of essentially arbitrary domains and showed that the local statistics of this model around any point in the liquid region of its limit shape are given by the infinite-volume, translation-invariant, extremal Gibbs measure of the appropriate slope. It confirms a famous prediction of Cohn-Kenyon-Propp from 2001 [20] in the case of lozenge tilings.

Open problems related to this talk. Edge statistics of Tracy-Widom type in such tiling models.

Philippe Sosoe: On the two-dimensional hyperbolic sine-Gordon equation [47]. The speaker considered the two-dimensional stochastic sine-Gordon equation (SSG) in the hyperbolic setting. In particular, by introducing a suitable time-dependent renormalization, Sosoe and collaborators proved local well- posedness of SSG for any value of a parameter $\beta > 0$ in the nonlinearity. This is in contrast to the parabolic case studied by Hairer and Shen [38] and Chandra-Hairer-Shen [16], where the parameter is restricted to the subcritical range $\beta^2 < 8\pi$.

Giorgio Cipolloni: Universality at criticality: Cusp and Circular Edge [17, 18, 19]. As explained in Section 15, in the last decade, Wigner-Dyson-Mehta (WDM) conjecture has been proven for very general random matrix ensembles in the bulk and at the edge of the self consistent density of states (scDos). The speaker explained this recent work on universality at the cusp of the scDos. About universality for non-Hermitian matrices much less is known (see [35] for the integrable model). The author explained his proof of universality at the circular edge of any non-Hermitian matrix X with entries i.i.d. real or complex centered random variables.

Open problems related to this talk. Bulk universality in non perturbative setting for non-Hermitian random matrices. For the same model, edge universality beyond two moment matching.

Benjamin Landon: Fluctuations of the overlap of the spherical SK model at low temperature [43]. The speaker considered the fluctuations of the overlap between two replicas in the 2-spin spherical SK model in the low temperature phase. He showed that the fluctuations are of order $N^{-1/3}$ and are given by a simple, explicit function of the eigenvalues of a GOE matrix.

Open problems related to this talk. Fluctuations of overlaps in presence of a magnetic field, and a quenched result.

Outcome of the Meeting

The meeting was very well appreciated by all the attendees, who shared and learned some of the most important developments in probability and mathematical physics in the last several years. The younger researchers also had an opportunity to meet, interact with and discuss mathematics with several of the most senior people in the field. Several very recent breakthroughs were presented for the first time. It was an unambiguous success.

Participants

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Benigni, Lucas (Paris 7)
Bourgade, Paul (New York University)

Brennecke, Christian (Harvard)
Cipolloni, Giorgio (Institute of Science and Technology Austria)
Deift, Percy (New York University)
Dembo, Amir (Stanford)
Ding, Jian (University of Pennsylvania)
Elgart, Alex (Virginia Tech)
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Sarkar, Sourav (University of Toronto)
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Shcherbyna, Tatyana (Princeton University)
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Sosoe, Philippe (Cornell University)
Spencer, Thomas (Institute for Advanced Study)
Strain, Robert (University of Pennsylvania at Philadelphia)
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Yau, Horng-Tzer (Harvard University)
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Chapter 16

Convex Integration in PDEs, Geometry, and Variational Calculus (19w5130)

August 11-16, 2019

Organizer(s): Eduard Feireisl (Czech Academy of Sciences), Marta Lewicka (University of Pittsburgh), Emil Wiedemann (Ulm University)

There is vast ongoing interest in the so-called technique of convex integration in several areas of mathematics, as demonstrated by diverse recent contributions. Notably, the seemingly unrelated fields of materials science, fluid dynamics and symplectic geometry enjoyed significant advances through this method, to mention a few: flexibility of the energy-minimizing solutions in the description of shape memory alloys, the resolution of Onsager's conjecture formulated in the realm of statistical mechanics, or the classification of overtwisted contact structures in all dimensions; all based on Gromov's h-principle and further appropriate extensions of Nash and Kuiper's iterative convex integration scheme developed for the classical isometric embedding problem in Riemannian geometry.

This 5-day workshop brought together experts from geometry, variational calculus and mathematical fluid dynamics to share existing knowledge as well as to open up new perspectives and collaborations across different mathematical subfields.

Overview of the Field

The first example of convex integration, albeit avant la lettre, was given by John Nash in 1954 [34]. Nash considered a classical problem in differential geometry, namely the isometric embedding problem. He showed that the $(n-1)$-dimensional unit sphere admits a C^1-isometric embedding into a ball $B_\varepsilon \subset \mathbb{R}^n$ with arbitrarily small radius $\varepsilon > 0$. The ingenious idea leading to this counterintuitive result was to shrink the sphere so that it fits inside B_ε and, consequently, all distances decrease by the factor of ε, and then to successively add "wrinkles" in order to increase the intrinsic distances back to the Euclidean ones.

Considerably later, Gromov [24] vastly extended Nash's idea and suggested the term convex integration for the iterative procedure in the isometric embedding problem. He developed very general ideas how to apply such approach to solve differential inclusions; roughly speaking, the method works well with systems of very non-linear partial differential equations, such that the convex envelope of each small domain of the submanifold representing the equation in the jet space has a non-empty interior. Consequently, Gromov used convex integration in his studies of the symplectic rigidity and Eliashberg started using systematically this kind of ideas to classify the overtwisted contact forms in [19].

The 1990s and early 2000s saw a further application of ideas of a similar flavour in the calculus of variations, the theory of partial differential equations, and in materials science. Two landmark papers from this period are the one by Dacorogna-Marcellini [12] and the work of Müller-Šverák [33], together with other parallel developments concerning counterexamples to elliptic regularity, existence of mappings with incompatible gradients and fluid-like behaviour of shape memory alloys.

A renewed interest in convex integration techniques was sparked around ten years ago, when De Lellis–Székelyhidi showed that the method could be adapted for constructing weak solutions to the incompressible Euler equations of fluid dynamics [16]. Such applicability of convex integration to time-dependent partial differential equations of mathematical physics came highly unexpected (Gromov himself had previously expressed his disbelief in such a possibility), as it violates the supposedly deterministic nature of classical mechanics. There is an ongoing debate in the fluid dynamics community how to make sense of the solutions of De Lellis-Székelyhidi in terms of turbulence theory.

The resulting ideas and techniques have had important implications on the solvability of the Cauchy problem for the incompressible Euler equations [37], the non-uniqueness of entropy solutions in compressible fluid dynamics [6, 7], and the proof of Onsager's Conjecture of turbulence theory [28, 4].

There is a vast ongoing interest in the technique of convex integration in several fields of mathematics, as demonstrated by a number of diverse recent contributions. To mention a few: Conti et al. [11] improved the original Nash embedding result, Kim-Yan [29] treated an equation related to image processing, Lewicka-Pakzad [30] showed flexibility of the Monge-Ampère equations in appropriate Hölder continuity regimes, and Rüland et al. [35] examined higher regularity in the theory of elasticity.

Recent Developments and Open Problems

As explained above, convex integration is used in various fields of mathematics, including (symplectic and contact) geometry, elliptic partial differential equations, calculus of variations, materials science, and mathematical fluid dynamics. Researchers employing convex integration, however, are usually experts only in one of these fields. Accordingly, convex integration is mostly discussed at meetings that focus solely on one of these mathematical subfields and there seems to be little interaction in particular between geometers and analysts working with convex integration techniques.

It has therefore been our main goal to bring together a diverse poll of experts in order to acquire a broader horizon on these techniques and to make new connections between different fields. To this end, we had survey talks and specialised talks alike, presenting cutting-edge research of very recent years, or even work in progress. Ample time was left for discussion and collaboration.

To our knowledge, the proposed workshop has been unique in focusing on convex integration across different mathematical disciplines. We managed to bring together a group of mathematicians several of whom had never met before. Let us mention a few open problems related to convex integration that enjoyed lively discussion at the workshop:

1. Rigidity vs. flexibility of isometric embeddings and solutions to Monge-Ampere equation – what is the threshold Hölder exponent?

2. Higher regularity of convex integration solutions for realistic models of nonlinear elasticity.

3. Dissipative Hölder-continuous Euler flows satisfying the local energy inequality.

4. Fluid equations of Navier-Stokes type, cf. [9].

5. Admissibility criteria for systems of fluid dynamics of inviscid fluids, designed to eliminate the "wild" solutions. One of them could be the maximal dissipation principle proposed by Dafermos or the viscosity criterion.

6. The structure of the set of initial data that give rise to “wild” solutions for the compressible (barotropic) and full Euler system; are such initial data dense in the phase space?

Presentation Highlights

Incompressible Fluids
OVERVIEW TALK
Roman Shvydkoy: Mechanisms for energy balance restoration in the Onsager (super-)critical flows

In this talk, Roman gave an overview of the current state of the Onsager conjecture, its relevance in laws of turbulence, and a series of new results on flows that have Onsager-critical or even supercritical regularity. In a number of recent works it was observed that some solutions to the Euler equation still conserve energy despite being critical or supercritical. Such energy law restoration comes as a result of several additional mechanisms that are not taken into account in the classical commutator estimate approach of proving the law. In this talk Roman highlighted those mechanisms, which include the use of incompressibility in a geometric way, such as in the vortex-sheet case, transport structure of the equation that comes into light in the pressureless case, singularity set organized on a smooth structure, e.g. the case of a point singularity and Hamiltonian structure that comes into place in this situation or as in the case of Caffarelli-Kohn-Nirenberg theorem for suitable solutions, and finally the vanishing viscosity limit in 2D with supercritical condition on vorticity was discussed. Many of these cases set certain restrictions on the application of the convex integration method in constructing critical dissipative solutions to the incompressible systems.

This overview calls for a more systematic study of these mechanisms and their possible generalization to less structured flows.

RESEARCH TALKS

Alexey Cheskidov: Wild solutions to the 3D Navier-Stokes equations

Alexey showed that there exists a nontrivial finite energy periodic stationary weak solution to the 3D Navier-Stokes equations (NSE) with zero force. This provides the first proof of a non-uniqueness for the stationary Naiver-Stokes equations. Moreover, the result gives an alternative proof of a non-uniqueness for the evolutionary Naiver-Stokes equations, recently obtained by Buckmaster and Vicol. Indeed, a nontrivial stationary solution can be used as an initial value for the evolutionary problem. Leray's theorem implies the existence of a Leray-Hopf solution starting from this initial data, which cannot coincide with the constructed stationary solution. This solution exhibit what is called the anomalous energy influx, the backward energy cascade that precisely balances the energy dissipation at each scale. The stationary solution does not lose any energy even though its enstrophy is positive (in fact, infinite).

The construction relies on a convex integration scheme utilizing new stationary building blocks designed specifically for the NSE. In order to increase concentration and decreases the intermittency dimension, Alexey and his collaborator Xiaoyutao Luo design *viscous eddies*, compactly supported approximate stationary solutions of the NSE that are divergence-free up to the leading term. The constructed viscous eddies are also used to prove the existence of weak solutions of the NSE with energy profiles discontinuous on a dense set of positive Lebesgue measure.

Mimi Dai: Flexibility and rigidity for some incompressible flows

Mimi discussed some recent trends in the study of incompressible flows. The emphasis is on the topic of flexibility and rigidity of solutions to the governing PDE model which do not have high enough regularity. For the three dimensional magnetohydrodynamics with Hall effect, Mimi showed that weak solutions in Leray-Hopf class are not unique, by tailoring a convex integration scheme to combine with classical theory. It is worth to mention that the uniqueness of weak solutions in Leray-Hopf class for the three dimensional Navier-Stokes equation (NSE) remains an open problem. On the rigidity side of the 3D NSE with external force, she showed that two weak solutions coincide in the energy space for large time provided that they coincide on the low frequency part below a certain time-dependent wavenumber. This wavenumber is called determining wavenumber. She further proved that the time average of the determining wavenumber is bounded by Kolmogorov's dissipation wavenumber which separates the inertial range from the dissipation range. A stronger version of the result shows the uniqueness of trajectory on the global attractor under the constraint on the low modes part. Moreover, the work built a bridge to connect mathematical theory with phenomenological law of physics.

Sara Daneri: On non-uniqueness below Onsager's critical exponent

In this talk, Sara considered the following initial value problem for the Euler equations on the three-dimensional torus $\mathbb{T}^3$

$$\begin{cases} \partial_t v + \operatorname{div}(v \otimes v) + \nabla p = 0 & \text{in } (0,T) \times \mathbb{T}^3 \\ \operatorname{div} v = 0 & \text{in } (0,T) \times \mathbb{T}^3 \\ v(\cdot, 0) = v_0 & \text{on } \mathbb{T}^3 \end{cases} \tag{0.1}$$

In (0.1), $v : [0,T) \times \mathbb{T}^3 \to \mathbb{R}^3$ is the velocity field of the fluid, $p : [0,T) \times \mathbb{T}^3 \to \mathbb{R}^3$ the pressure field and $v_0 : \mathbb{T}^3 \to \mathbb{R}^3$ is a given divergence free velocity field, the prescribed initial datum for the Cauchy problem.

While for initial data in $C^{1,\alpha}$ one has short time existence and uniqueness of classical solutions, a completely different picture appears for weak solutions with lower regularity. In the seminal paper [16], De Lellis and Székelyhidi showed the existence of infinitely many bounded solutions of the Euler equations with compact support in space and time, in any dimension greater than or equal to two. A feature of these non-physical solutions is that the total kinetic energy of the fluid, namely the map

$$[0,T) \ni t \mapsto \int_{\mathbb{T}^3} |v(t,x)|^2 \, dx. \tag{0.2}$$

increases at time $t = 0$. Therefore, in [17] they considered solutions satisfying an additional admissibility condition, which among the possible formulations takes the form

$$\int_{\mathbb{R}^3} |v(t,x)|^2 \, dx \leq \int_{\mathbb{R}^3} |v_0|^2 \, dx, \qquad \forall \, t \geq 0, \tag{0.3}$$

and asked themselves if in this class one can prevent non-uniqueness. The answer turns out to be negative: there are initial data v_0 in L^∞, called by the authors wild initial data, which give rise to infinitely many bounded and admissible weak solutions of (0.1). Moreover, in [36] they were shown to be dense in the solenoidal fields in L^2. Notice that, due to the weak-strong uniqueness result by Brenier, De Lellis and Székelyhdidi [3], not any initial datum can be a wild initial datum, since whenever a classical solution exists, this is the unique solution in the class of weak admissible solutions with the same initial datum.

Therefore a natural question arises, namely whether there exists a regularity threshold above which solutions are unique, for all initial data, and below which non-uniqueness may happen.

The aim of this talk was to show, by reviewing some already published results [13, 15] and announcing a result obtained in collaboration with E. Runa and L. Székelyhidi [14], that such a threshold must be bigger than Hölder continuity in space of any order $\beta < 1/3$ (with Hölder constant uniformly bounded in time).

Compressible Fluids

OVERVIEW TALK

Eduard Feireisl: Convex integration and compressible Euler system

This was a survey of recent results obtained via the method of convex integration for the Euler system describing the motion of a compressible inviscid fluid. The system written in terms of the variables $\varrho = \varrho(t,x)$ - the mass density, $\mathbf{m} = \varrho\mathbf{u}$ - the momentum, $S = \varrho s$ - the total entropy, reads:

$$\partial_t \varrho + \operatorname{div} \mathbf{m} = 0,$$

$$\partial_t \mathbf{m} + \operatorname{div}\left(\frac{\mathbf{m} \otimes \mathbf{m}}{\varrho}\right) + \nabla p(\varrho, S) = 0,$$

$$\partial_t \left(\frac{1}{2}\frac{|\mathbf{m}|^2}{\varrho} + \varrho e(\varrho, S)\right) + \operatorname{div}\left[\left(\frac{1}{2}\frac{|\mathbf{m}|^2}{\varrho} + \varrho e(\varrho, S)\right)\frac{\mathbf{m}}{\varrho}\right] = 0,$$

supplemented in the context of weak solutions by the entropy inequality

$$\partial_t S + \operatorname{div}\left(S\frac{\mathbf{m}}{\varrho}\right) \geq 0.$$

The method of convex integration can be used to show the existence of infinitely many weak solutions for a rather vast class of initial data satisfying also the entropy inequality, see [8], [23]. There are more results available for the isentropic system, where $S = \varrho\overline{s}$, $\overline{s}$ suitable constant. The approach via convex integration is based on the original results of DeLellis and Székelyhidi proved in the context of incompressible Euler system [17] and a generalization of the so–called Oscillatory Lemma in [20].

RESEARCH TALKS

Martina Hofmanová: Ill-posedness in fluid dynamics — what can we do about it?

Martina discussed several puzzling results related to solvability and ill-posedness of the isentropic Euler system. It is nowadays well understood that the multidimensional isentropic Euler system is desperately ill–posed. Indeed, the method of convex integration can be used to construct infinitely many wild solutions as well as rather surprising approximation results. On the other hand, Martina and collaborators propose a new concept of dissipative solution to the compressible Euler system based on a careful analysis of possible oscillations and/or concentrations in the associated generating sequence. Unlike the conventional measure–valued solutions or rather their expected values, the dissipative solutions comply with a natural compatibility condition – they are classical solutions as long as they enjoy certain degree of smoothness. Moreover, ideas from Markov selections allow to select a semiflow of physically reasonable solutions and to exclude oscillation defects in certain cases. The solution semiflow enjoys the standard semigroup property and the solutions coincide with the strong solutions as long as the latter exist. Moreover, they minimize the energy (maximize the energy dissipation) among all dissipative solutions. Finally, Martina shows that any weakly converging sequence of solutions to the isentropic Navier–Stokes system on the full physical space R^d, $d = 2, 3$, in the vanishing viscosity limit either (i) converges strongly in the energy norm, or (ii) the limit is not a weak solution of the associated Euler system. The same result holds for any sequence of approximate solutions in the spirit of DiPerna and Majda. This is in sharp contrast to the incompressible case, where (oscillatory) approximate solutions may converge weakly to solutions of the Euler system.

Simon Markfelder: On some non-uniqueness results for the compressible Euler equations based on convex integration

Simon considered the compressible Euler equations in multiple space dimensions. These equations describe the time evolution of a compressible inviscid fluid. He gave an overview over some results showing existence of infinitely many solutions. All these results are based on the convex integration method, which was used by De Lellis and Székelyhidi in the context of the incompressible Euler equations. After considering general initial data, Simon and collaborators focussed on a special type of two-dimensional initial data, namely those which are constant in each of the two half spaces (Riemann data).

Conservation Laws

RESEARCH TALKS

Sam Krupa: Uniqueness of solutions versus convex integration for conservation laws in one space dimension

For hyperbolic systems of conservation laws in one space dimension, the best theory of well-posedness is restricted to solutions with small total variation (Bressan et al. 2000). Looking to expand on this theory, Sam pushes in new directions. One key difficulty is that for many systems of conservation laws, only one nontrivial entropy exists. In 2017, in joint work with A. Vasseur, Sam proved uniqueness for the solutions to the scalar conservation laws which verify only a single entropy condition. Their result was the first result in this direction which worked directly on the conservation law. Further, their method was based on the theory of shifts and a-contraction developed by Vasseur and his team. These theories are general theories and apply also to the systems case, leading one to hope the framework they built for the scalar conservation laws will apply to systems. In this talk, Sam reviewed the current progress on using the theory of shifts and a-contraction to push forward the theory of well-posedness for systems of conservation laws in one space dimension. On the other hand, he also briefly discussed the potential for non-uniqueness of solutions via convex integration. This is joint work with A. Vasseur and L. Székelyhidi.

Emil Wiedemann: Convex integration vs. the chain rule

Emil provided counterexamples to the chain rule for divergence-free vectorfields, based on a Gromov-type convex integration scheme. This was based on joint work with G. Crippa, N. Gusev, and S. Spirito.

Agnieszka Świerczewska-Gwiazda: Measure-valued–strong uniqueness for general conservation laws and some convex integration for nonlocal Euler system

In the last years measure-valued solutions started to be considered as a relevant notion of solutions if they satisfy the so-called measure-valued–strong uniqueness principle. This means that they coincide with a strong solution emanating from the same initial data if this strong solution exists. Following a result of Yann Brenier, Camillo De Lellis and Laszlo Székelyhidi Jr. [3] for the incompressible Euler equation, this property has been examined for many systems of mathematical physics, including incompressible and compressible Euler system, compressible Navier-Stokes system, polyconvex elastodynamics et al., [18, 21]. One observes also some results concerning general hyperbolic systems, [25]. Agnieszka's goal has been to provide a unified framework for general systems, that would cover the most interesting cases of systems. Additionally she introduced a new concept of dissipative measure valued solution to general hyperbolic system.

In the second part of the talk she considered several modifications of the Euler system of fluid dynamics including its pressureless variant driven by non-local interaction repulsive-attractive and alignment forces. These models arise in the study of self-organisation in collective behavior modeling of animals and crowds. Agnieszka discussed how to adapt the method of convex integration to show the existence of infinitely many global-in-time weak solutions for any bounded initial data. Then she considered the class of dissipative solutions satisfying, in addition, the associated global energy balance (inequality). She identified a large set of initial data for which the problem admits infinitely many dissipative weak solutions. Finally, she established a weak-strong uniqueness principle for the pressure driven Euler system with non-local interaction terms as well as for the pressureless system with Newtonian interaction, see [5]. Agnieszka directed her attention also to dissipative measure-valued solutions to the pressureless Euler system with non-local terms, and showed that the property of measure-valued - strong uniqueness holds.

Piotr Gwiazda: Onsager's conjecture for general conservation laws

A common feature of systems of conservation laws of continuum physics is that they are endowed with natural companion laws which are in such case most often related to the second law of thermodynamics. This observation easily generalizes to any symmetrizable system of conservation laws. They are endowed with nontrivial companion conservation laws, which are immediately satisfied by classical solutions. Not surprisingly, weak solutions may fail to satisfy companion laws, which are then often relaxed from equality to inequality and overtake a role of a physical admissibility condition for weak solutions. Piotr discussed what is the critical regularity of weak solutions to a general system of conservation laws to satisfy an associated companion law as an equality. An archetypal example of such result was derived for the incompressible Euler system by Constantin et al. [1] in the context of the seminal Onsager conjecture. This general result can serve as a simple criterion to numerous systems of mathematical physics to prescribe the regularity of solutions needed for an appropriate companion law to be satisfied. The talk was based on common results with C. Bardos, E. Feireisl, P. Gwiazda, E. S. Titi, and E. Wiedemann [10, 22, 26, 2].

Differential Geometry and Equations of Elliptic and Parabolic Type

RESEARCH TALKS

Dominik Inauen: Rigidity and Flexibilty of Isometric Embeddings

The problem of embedding abstract Riemannian manifolds isometrically (i.e. preserving the lengths) into Euclidean space stems from the conceptually fundamental question of whether abstract Riemannian manifolds and submanifolds of Euclidean space are the same. As it turns out, such embeddings have a drastically different behaviour at low regularity (i.e. C^1) than at high regularity (i.e. C^2). For example, by the famous Nash–Kuiper theorem it is possible to find C^1 isometric embeddings of the standard 2-sphere into arbitrarily small balls in $\mathbb{R}^3$, and yet, in the C^2 category there is (up to translation and rotation) just one isometric embedding, namely the standard inclusion. Analoguous to the Onsager conjecture, one might ask if there is a sharp regularity threshold in the Hölder scale which distinguishes these flexible and rigid behaviours. In his talk, Dominik reviewed some known results and argued why the Hölder Exponent 1/2 can be seen as a critical exponent in the problem.

Seonghak Kim: Fine phase mixtures in 1-D hyperbolic-elliptic problem

In this talk, Seonghak presented fine phase mixtures of weak solutions to the initial-boundary value problem for a class of hyperbolic-elliptic equations in one space dimension. Such solutions are constructed through a carefully modified method of convex integration to capture fine scale oscillations of spatial derivatives of solutions. Seonghak also included a numerical simulation via FEM to assert that his solutions are indeed reasonable candidates from infinitely many solutions to the problem.

Young-Heon Kim: The Monge problem in Brownian stopping optimal transport

Young-Heon discussed recent progress in an optimal Brownian stopping problem, called the optimal Skorokhod embedding problem, which is an active research area especially in relation to mathematical finance. Given two probability measures with appropriate order, the problem considers the stopping time under which the Brownian motion carries one probability measure to the other, while minimizing the transportation cost. Young-Heon focussed on the cost given by the distance between the initial and the final point. A strong duality result of this optimization problem is obtained, which enables one to prove that the optimal stopping time is given by the first hitting time to a barrier determined by the optimal dual solutions.

The main part of this talk was based on joint work of Young-Heon Kim with Nassif Ghoussoub (UBC) and Aaron Palmer (UBC).

Marta Lewicka: Convex integration for the Monge-Ampère equation

In this talk, Marta discussed the dichotomy of rigidity vs. flexibility for the $\mathcal{C}^{1,\alpha}$ solutions to the Monge-Ampère equation in two dimensions:

$$\mathcal{D}et\nabla^2 v := -\frac{1}{2}\text{curl curl}\,(\nabla v\otimes\nabla v) = f \qquad \text{in } \Omega\subset\mathbb{R}^2. \tag{0.4}$$

The reported results appeared in [30]. Fistly, they showed that below the regularity threshold $\alpha < 1/7$, the very weak $\mathcal{C}^{1,\alpha}(\bar\Omega)$ solutions to (0.4) are dense in the set of all continuous functions. This flexibility statement is a consequence of the convex integration h-principle, that is a method proposed by Gromov for solving certain partial differential relations and that, as Marta showed, turns out to be applicable to the Monge-Ampère equation. Here, she directly adapted the iteration method of Nash and Kuiper, in order to construct the oscillatory solutions to (0.4).

Secondly, Marta proved that the same class of very weak solutions fails the above flexibility in the regularity regime $\alpha > 2/3$: any $\mathcal{C}^{1,\alpha}(\Omega)$ solution to (0.4) with positive Hessian determinant f is necessarily convex, while when $f = 0$ the graph of u is necessarily developable. In these examples, convexity and developability are the two global characteristics displaying the solutions' rigidity. Their results and techniques are parallel with those concerning the low co-dimension isometric immersions, the Onsager conjecture for the Euler equation, the Perona-Malik equation, the active scalar equation, and also should be compared with results on the regularity of Sobolev solutions to the Monge-Ampère equation whose study is important in the variational description of shape formation [31, 32].

Baisheng Yan: Convex integration for the gradient flow of polyconvex functionals

In this talk, Baisheng discussed non-uniqueness and instability for a class of nonlinear diffusion equations, including the gradient flows of some nonconvex energy functionals, under the framework of partial differential inclusions by convex integration and Baire's category methods. The existence of infinitely many Lipschitz weak solutions to the initial-boundary value problem is proved if the diffusion flux function satisfies a structural condition called Condition (OC). For parabolic systems, this condition proves to be compatible with strong polyconvexity. As a result of such compatibility by brutal constructions, instability for the gradient flows of certain strongly polyconvex functionals is established in the sense that the initial-boundary value problem for the gradient flow possesses a weakly* convergent sequence of Lipschitz weak solutions whose limit is not a weak solution even for smooth initial-boundary data.

Materials Science

OVERVIEW TALK

Angkana Rüland: Convex integration in materials science

In this talk Angkana reviewed a number of applications of the method of convex integration in the calculus of variations and the theory of elasticity. She explained both the results and their applications. She covered:

- examples of irregular solutions to elliptic systems found by Müller-√Sverák as an application of convex integration within the quasiconvex theory of elasticity,
- the dichotomy between rigidity and flexibility in the modelling of shape-memory alloys as a non-quasiconvex model problem,
- the m-matrix problem and its resolution by Chlebík-Kirchheim-Preiss,
- the role of constraints, focusing particularly on the characterisation of gradient Young measures coming from sequences of gradients with a pointwise determinant bound at low integrability,
- elastic plates, folding and crumpling.

The method of convex integration appears here in a variety of different guises and roles.

RESEARCH TALK

Christian Zillinger: Convex integration arising in the modelling of shape-memory alloys: some remarks on scaling and numerical implementations

Christian studied convex integration solutions in the context of the modelling of shape-memory alloys. In a first part, he related the maximal regularity of convex integration solutions to the presence of lower bounds in variational models with surface energy. Hence, variational models with surface energy could be viewed as a selection mechanism allowing for or excluding convex integration solutions. Secondly, he presented the first numerical implementations of convex integration schemes for the model problem of the geometrically linearised two-dimensional hexagonal-to-rhombic phase transformation. This was based on joint work with Angkana Rüland

and Jamie Taylor.

Scientific Progress Made and Outcome of the Meeting

As indicated in the introduction, the main goal of this workshop has been the sharing of information and the exposition of various convex integration techniques used across different fields. Groups of mathematicians working in geometry and materials science often use closely related ideas but have little idea of progress made by the other group. The speakers from each group made an effort to address such a diverse audience, and all other speakers welcomed the opportunity to present their findings to colleagues they have not discussed with before. The schedule provided ample time for the unstructured mathematical discussions. Several new collaborations have been established: Hofmanova and Feireisl begun a project concerning the stochastic perturbations of the Euler system; Lewicka and Wiedemann started discussions on the possibility of extending the rigidity-flexibility results to the case with boundary conditions.

This mini-workshop had 20 participants, ranging from professors to graduate students. Among them were 6 female mathematicians. All participants gave talk. The participants list was international (USA, Czech Republic, Germany, Korea, Poland, Switzerland), with one participant from Canada.

Participants

Cheskidov, Alexey (University of Illinois at Chicago)
Dai, Mimi (University of Illinois at Chicago)
Daneri, Sara (Universität Erlangen)
Feireisl, Eduard (Institute of Mathematics, Czech Academy of Sciences)
Gwiazda, Piotr (Polish Academy of Sciences)
Hofmanova, Martina ()
Inauen, Dominik (Universität Zürich)
Kim, Seonghak (Kyungpook National University)
Kim, Young-Heon (University of British Columbia)
Kreml, Ondřej (Czech Academy of Sciences)
Krupa, Sam (The University of Texas at Austin)
Lewicka, Marta (University of Pittsburgh)
Markfelder, Simon (University of Würzburg)
Rüland, Angkana (Max Planck Institute for Mathematics in the Sciences)
Shvydkoy, Roman (University of Illinois at Chicago)
Świerczewska-Gwiazda, Agnieszka (University of Warsaw)
Weser, Daniel (University of Texas at Austin)
Wiedemann, Emil (Universität Ulm)
Yan, Baisheng (Michigan State University)
Zillinger, Christian (University of Southern California)

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Chapter 17

Charge and Energy Transfer Processes: Open Problems in Open Quantum Systems (19w5016)

Aug 18 - 23, 2019

Organizer(s): Aaron Kelly (Dalhousie), Marco Merkli (Memorial), Dvira Segal (Toronto)

Overview of the Field

Open quantum systems. A quantum system subjected to external influences is said to be open. The external degrees of freedom are often referred to as an environment, a bath, a reservoir or simply a noise. Typical examples of open quantum systems cover artificial and natural systems including a register of qubits (the system) in contact with a substrate they are mounted on (the environment), or a molecule undergoing a chemical reaction while immersed in a sea of surrounding substances (the solvent) influencing the process. Moreover, in large molecules the electrons and nuclear coordinates that do not directly take part in the reaction may act as a reservoir for the reaction coordinate(s). An open system may experience phase loss, energy and particle exchange with the surroundings, thus being open drastically impacts its dynamics. As even slight external influences can change the evolution of a quantum system considerably, it is important, both from a theoretical and practical standpoint, to be able to model and analyze such interactions. The study of open quantum systems is an important part of modern science. It carries a direct impact on different areas, such as the development of energy conversion and storage technologies based on organic or biological molecules and the realization of quantum-based technologies.

According to the postulates of quantum mechanics, the dynamical equation of a closed quantum system (not subjected to an external noise) is the Schrödinger equation, a differential equation governing the time evolution of the wave function (the state) of a system. A direct method to analyze the evolution of an open quantum system is to find the reduction of the evolution of the full system plus environment complex. In this approach, one first explicitly models the system and the environment including their interaction. These two components together form a closed system, and are thus described by the Schrödinger equation. (Most often, the latter is incredibly complicated since it encompasses all degrees of freedom of the system as well as the environment – and it cannot be used in practical applications.) One then takes the reduction of the full Schrödinger equation to find the effective evolution equation for the system alone. This procedure is often called tracing out the environment. It amounts to taking a partial expectation value with respect to the environment degrees of freedom. The resulting dynamical equation is still complicated, but it involves only the degrees of freedom of the system alone (dimensional reduction). The formally exact Nakajima-Zwanzig master equation [1] is an example of such a reduction process. Even in the simplest possible situation where the system is a single spin (qubit), the effective equation is one for a 2×2 hermitian matrix (spin density matrix), but it is not solvable analytically. Part of the problem is that the structure of the equation changes under the above explained reduction: While the original Schrödinger equation has a propagator generated by a hermitian Hamiltonian (generator of the dynamics) and is local in time, the effective, reduced equation is not local in time. It contains memory effects (is non Markovian) due to the flow of information back and forth between the system and its environment. The emergence of this complexity is not too surprising as the effective equation has to incorporate all noise effects and all properties of the reservoir. Finding theoretical and numerical approximation schemes to analyze and solve these effective equations has been a long standing challenge in various sub-disciplines of mathematics, physics and chemistry. It is of increasing interest in biology, engineering and even the social sciences [2, 20, 4, 26].

There is a classical, heuristic derivation of the effective open system dynamics in a parameter setting called the Markovian approximation. In this regime, the system–environment interaction is small and the environment has rapidly decaying correlations (fast memory loss). Using a perturbation theory based on heuristic (mathematically not justified) arguments, one can derive the so-called Markovian master equation. In this setting, the time-local property of the original Schrödinger equation is restored (memory effects are neglected) and one can define the analogous object to the Hamiltonian, called the Lindblad operator, which generates the reduced dynamics. One can then use the standard methodology to link the spectrum of the generator to dynamical properties. The real spectrum of the Hamiltonian turns into a complex spectrum of the non hermitian Lindblad operator. This means that effective energies are complex numbers. As such, they introduce irreversibility into the system dynamics, according to dynamical factors $\mathrm{e}^{-i\varepsilon t}$, where t is time and ε is an energy. The Markovian master equation is ubiquitous in applied and theoretical fields, sustaining an enormous body of research work. From a practical perspective, it is often in excellent agreement with numerical investigations of the true open system dynamics, and with experiments. From a theoretical perspective, the Markovian master equation is beautiful due to its inherent structure [18, 7], which in turn can be used to produce new models of open system dynamics, dispensing with the need to go through the reduction procedure described above.

Exciton and charge transfer processes. Many processes in chemistry involve reactions in which electrons are transferred between chemical compounds, moving from a reactant to a product. In realistic models, these transfer processes are influenced by the medium in which they are embedded. The Canadian chemist Rudolph Marcus established a formula describing the reaction rate of such processes, named after him as the Marcus formula. He was awarded the 1992 Nobel prize in Chemistry for his contributions to the theory of electron transfer reactions in chemical systems. The Marcus formula is widely used, designed to work for strong system-environment interactions and at high temperatures (room temperature), which are often encountered in chemistry and biology. In Marcus' original work, the environment was not treated as a quantum system. However, it was later shown in [8] that the Marcus formula can be derived from the fully quantum mechanical spin-Boson model where the environment is a quantum field in thermal equilibrium. The work [8] identifies the Marcus formula as the transition rate emerging from a (still heuristic) Markovian approximation to the open system dynamics. The latter is based on a derivation of the master equation given in [10].

A similar formalism can be used to describe exciton, or energy transfer processes. These are mechanisms encountered for example in light-sensitive molecules (chromophores) in plants and bacteria enabling photosynthesis [4]. In this context, excitation can be exchanged between molecular orbitals of electrons which lie spatially close together, but which are bound to nuclei belonging to different molecules. A donor chromophore, initially in its electronic excited state, can transfer energy to an acceptor chromophore through electrostatic dipole-dipole interaction, brought about by interaction with a common environment (a radiation field), which mediates the electrostatic coupling. No photons are emitted nor are any electrons transferred in these processes. According to the Förster resonance energy transfer theory (Theodor Förster), the reaction rate of such processes scales as $1/R^6$, where R is the distance between the donor and acceptor molecular units. The theory is based on heuristic arguments involving an application of the so-called Fermi Golden Rule within the realm of quantum electrodynamical calculations [11]. By measuring transfer rates one can estimate the distance between the donor and acceptor agents, which is important in chemistry and biology Nevertheless, to our knowledge, a mathematically satisfying derivation of the $1/R^6$ scaling does not exist up to now.

A mathematical approach: Davies theory. The first mathematically rigorous derivation of the Markovian master equation is due to E.B. Davies [9] in the mid 70ies. It is shown that up to times $t = O(\lambda^{-2})$ the Markovian master equation is correct, where λ is the system environment coupling constant, which is assumed to be small. More precisely, the difference between the true dynamics and the one given by the master equation converges to 0 as $\lambda \to 0$, uniformly on time scales $t \le c\lambda^2$ (where $c > 0$ is any fixed constant). While mathematically rigorous, Davies' results only prove the validity of the Markovian master equation for finite times – if interested in longer and longer time scales, one has to shrink at the same time the strength of the system-environment coupling. This regime is called the weak coupling, or Van Hove regime.

Numerically-exact methods. Complementing analytic treatments, the exact time evolution of an open quantum system can be approached numerically using various ideas. In such *numerically-exact techniques*, convergence (to hopefully the exact limit) is reached by pushing a numerical parameter as far as one can—limited by computing power and available memory of resources. Numerical parameters (unlike physical variables) include, for example, the time-step discretizing the dynamics, the size of the basis set that builds the model, or the 'depth' (history) of the memory function used to solve the non-Markovian Master equation. Due to the 'curse of dimensionality' – the cost of simulating a quantum system grows exponentially with the number of degrees of freedom – numerically exact methods are typically limited to simulate relatively small systems, specific type of baths (usually harmonic oscillators), and simple types of interactions between the two.

The dynamics of an open quantum system bilinearly coupled to a harmonic bath can be formally written as a path integral built around the Feynman-Vernon influence functional (IF), an object which incorporates the effect of the environment on the system. Several numerically exact methods are based on the IF description, including the celebrated quasi-adiabatic propagator path integral (QuAPI) method [12] and the Hierarchical Equations of Motion (HEOM) [13]. In particular, an efficient time evolution scheme can be developed based on the observation that in certain situations, the memory kernel of the IF decays within a finite time. This observation is utilized in QuAPI for the controlled truncation of the memory kernel within the path integral, and the development of an iterative time evolution scheme. The method converges to (hopefully) the exact limit by reducing the time step (Trotter error) and increasing the memory time in the path integral. The HEOM is similarly derived from the influence functional expression. It is organized as a sequence (layers) of Markovian Master equations, with convergence achieved by increasing the depth of the layer, thus covering memory (non-Markovian) effects increasingly well.

With the goal to describe more complex systems, beyond spin-boson type models, recent years have seen an explosion in efforts to develop numerically exact algorithms. Some examples include improvements of QuAPI [14, 15, 16] and the HEOM [17, 18], the development of a dynamical Quantum Monte Carlo algorithm [19], and advancements to wavefunction-based methods such as the Multi-configuration time-dependent Hartree (MCTDH) [20, 21, 22]. The latter approach solves the time-dependent Schrödinger equation for multidimensional systems by considering all degrees of freedom of a (finite-size) system-bath model. Altogether, while numerically exact methods are widely used for describing chemical processes, a rigorous understanding of their convergence behavior is generally missing. As yet, identifying convergence with these tools is based on the mere observation of a behavior that is seemingly focalizing and stabilizing to an acceptable physical solution.

Recent Developments and Open Problems

Markovian master equations. On the mathematical side, a derivation of the Markovian master equation for all time scales has been given recently using the so-called dynamical resonance theory. This result improves the above-mentioned Davies theory. In [23] it is shown that the difference between the true and the master equation approximated dynamics is of $O(\lambda^2)$, uniformly for all times $t \geq 0$. This work is based on the so-called resonance theory, which combines spectral techniques (complex scaling) with operator algebraic methods. So far, the rigorous theory assumes some technical conditions which translate, in particular, into exponential decay of the environment correlation function. It became apparent from discussion during the workshop that a substantial extension of the resonance theory is desirable. In particular, the following questions have emerged:

- Can one extend the resonance theory for polynomially decaying correlations?
- Can one describe the dynamics of a system coupled to several reservoirs at different temperatures?
- Is the formalism useful to describe the evolution of initially entangled system-environment states?
- What is the proper basis choice for the development of the Markovian master equation, the global (eigenenergy) or the local (spatial) one?

Strong system-bath coupling. A fundamental aspect of many real quantum dissipative systems is that they are not necessarily operating in the weak system-bath coupling regime, unlike macroscopic systems in which the boundary region between the system and its environment is small relative to the bulk volume. Treating open systems at strong coupling is challenging. It can be addressed by making use of perturbation theories [24] and through resummation techniques [25]. One may also apply a unitary transformation to the Hamiltonian, to reach a form that is more suitable for weak coupling techniques. Such approaches include the generalized quantum master equation based on the polaron transformation [26] (see e.g. [27] for a recent application), the reaction coordinate method [28], and mapping techniques [29]. Alternatively, one may retract from analytic methods and employ purely numerical techniques, which in principle can capture the exact dynamics at strong coupling. A partial list of numerically exact techniques includes QuAPI [12], HEOM [13], transfer matrix methods [30], and the wavefunction [20] and stochastic formalisms [31]. Open questions concern the accuracy and confluence of such different methods addressing the strong coupling limit:

- What should be the criteria for convergence in numerical algorithms?
- Is convergence necessarily monotonic if we take into account strong coupling effects (e.g. by a perturbative expansion)?
- How do we meaningfully compare results obtained from different tools?

Accuracy and predictive power. The Marcus formula beautifully describes the rate of electron transfer in donor-bridge systems at high temperatures. Motivated by this successful theory, a central goal in the research of open quantum systems has been to construct models, which are simple enough to perform calculations, yet sufficiently rich to be predictive. Of particular interest are light-sensitive molecules. In photosynthesis, the energy of solar photons generates an electronic excitation, which travels (as an exciton) through the biomolecular chromophores until it is captured at the reaction centre. Several aspects complicate simulations of this process, specifically: (i) The coupling of the system (localized exciton) to the environment (vibrations of the protein) cannot be treated as weak. (ii) The protein environment, described by the spectral density function, is highly structured. These two aspects render inapplicable the weak coupling Markovian maser equation. Understanding photochemical processes (photosynthesis, vision), and imitating them, has been a central theme in theoretical chemistry for decades. Open challenges include:

- Developing models and methods for light harvesting processes, specifically to take into account non-Markovian effects.

- Examining of the role of quantum coherences in condensed phases environments. Can quantum properties survive under thermal noise?

- Working closely with experimental data and developing models with predictive power.

Quantum thermodynamics and quantum control. Recent years have seen growing interest in "quantum thermodynamics", a discipline seeking to understand how the laws of thermodynamics emerge from quantum mechanics, without additional assumptions. The theory of open quantum systems offers a natural framework to examine this fundamental topic. In the context of heat engines, for example, the working fluid corresponds to the 'system', while the attached heat baths and the driving protocol constitute different environments. The field of quantum thermodynamics has a long history. The theory of the Laser is a prime example of its success. Recent experimental progress in building, controlling, and probing nanoscale systems, and even monitoring energy exchange at the single atom level, allows to meaningfully study basic questions regarding the role of quantum effects in the operation of thermal machines. Some goals in quantum thermodynamics are to:

- Develop a quantum theory that provides consistent definitions of thermodynamical concepts (heat, work, entropy) at strong system-bath coupling.

- Develop a master equation for driven systems, which is consistent with thermodynamic principles.

- Understand the impact of quantum resources, such as coherence and correlations (entanglement) on the performance of quantum heat engines.

- Learn how to treat the effect of multiple reservoirs on the system, since this interaction can become non-additive in the strong coupling limit.

New tools: Machine learning quantum and dynamics. Machine learning (ML) is revolutionizing many fields including manufacturing industries, healthcare, finance, transportation. In the sciences, so far its main impact has been in material science and pharmaceutics, accelerating e.g. drug discovery and providing predictions of molecular properties. Employing ML techniques to quantum molecular dynamics is a promising new avenue. Some of the exploratory questions we ask are: Can we probe open quantum systems using ML methods? What types of molecular dynamic methods would directly benefit from an integration with ML tools, providing for instance efficient interpolation, parameter optimization, guided search?

Statement on the objectives of the workshop. The goal of the workshop was to open the dialog between mathematicians, physicists and chemists, to identify important open theoretical problems surrounding charge and energy transfer processes, and to craft solution strategies. The workshop aimed at helping to break down "language barriers", which prevent mathematicians from applying their knowledge to relevant chemistry problems, and conversely, prohibit chemists from applying new mathematical tools. The idea of the workshop was to join research efforts of different communities working on similar problems, with the ultimate goal of creating collaborations, which could deliver mathematically rigorous results for realistic systems relevant to physics and chemistry.

Organizational aspects. The workshop had 32 participants, with 34 presentations. The organizers had invited leading researchers in the field, as well as young researchers and postdoctoral fellows who greatly benefited from the interaction with senior researchers. Participants came from mathematics, theoretical chemistry and physics departments. The meeting was international with scientists arriving from different parts of the world: Canada, the US, South America, Europe, Asia and Africa. The organizers actively worked to have participants from under-represented groups, particularly female scientists.

Presentation Highlights

The meeting Charge and Energy Transfer Processes: Open Problems in Open Quantum Systems was held Aug 18-23, 2019. There were 34 research talks. Here are the hightlights of the talks:

Marco Merkli presented an approach to mathematically prove the validity of the Markovian approximation for N-level quantum systems in contact with thermal reservoirs. Using quantum resonance theory, he showed that the true system dynamics is approximated by a completely positive, trace preserving dynamical group. The novelty is that the validity is proven to hold for all times.

Francesco Petruccione gave a systematic overview of the theory of open quantum walks. He discussed recent analytical and numerical results, along with some potential applications, and some open problems related to open quantum walks.

Christiane Koch discussed problems that arise when quantum information meets open quantum systems. For example, how fast can one export entropy in order to purify a qubit and erase its correlations with the environment? Christiane addressed this question via the paradigm of a qubit interacting with a structured environment, using a combination of geometric and numerical optimal control theory.

Martin B. Plenio discussed efficient numerical methods for simulating the dynamics of extended quantum system that are in contact with non-Markovian Environments. Specifically, he presented the time evolving density operator method with orthogonal polynomials (TEDOPA), and a selection of recent applications of this method to spatially extended systems at finite temperatures, and in fermionic environments.

Jonathan Keeling spoke about using time-evolving matrix product operators for efficient non-Markovian quantum dynamics simulations based on the numerically exact quasi-adiabatic path integral approach of Makri and Makarov. He showed that expressing the system state (and its propagator) as a matrix product state (and operator, respectively), provides an improvement of several orders of magnitude, in the size of the problem, as compared to using QuAPI.

David Limmer presented recent work on developing perturbative master equations to study the photoisomerization dynamics through conical intersections. These approaches leverage a separation of time an energy scales to treat different degrees of freedom at varying levels of accuracy, and they allow reactive pathways to be visualized.

Dominique Spehner presented a theory of adiabatic quantum transitions in a two-level system coupled to a free Boson reservoir. Assuming that the reservoir is initially decoupled from the system and in the vacuum state, Dominique showed how to compute the time-dependent transition probability in the limit of small system-reservoir coupling, and he analyzed the deviations from the adiabatic transition probability in absence of the reservoir.

Alain Joye presented work on the nonlinear quantum adiabatic approximation. Considering the adiabatic limit of a nonlinear Schrödinger equation, in which the Hamiltonian depends on time and on a finite number of components of the wave function, he proved the existence of instantaneous nonlinear eigenvectors and of solutions which remain close to them (up to a rapidly oscillating phases) in the adiabatic regime. Consequences on the energy content of these solutions were also discussed.

Janet Anders spoke about the possible energetic footprints of coherence and irreversibility in the quantum regime. She addressed the topic of work extraction in the quantum regime by constructing an optimal quantum thermodynamic process that removes quantum information in analogy to Landauer's erasure of classical information. Janet's thermodynamic analysis of this optimal process suggests that, in addition to the work that can be extracted from classical non-equilibrium states, work can be extracted from quantum coherences.

Luis A. Correa discussed how the performance enhancements that have been observed in various models of continuous quantum thermal machines have sometimes been linked to the buildup of coherences in a preferred basis. Then Luis showed that this connection is not always evidence of so-called 'quantum-thermodynamic supremacy'. He argued, through some nicely constructed examples, that even if coherence is present in a specific quantum thermal machine, it is often not essential to replicate the underlying energy conversion process.

Ronnie Kosloff presented work on the quantum Carnot engine and its quantum signature. Motivated by previous failed theoretical attempts to model the four-stroke quantum Carnot cycle, that were stymied by the difficulty in modeling the isothermal branches of the process, he derived a time-dependent nonadiabatic master equation (NAME) to overcome this challenge. Using this approach he also showed how a finite-time Carnot-like cycle could be studied, and explored its performance.

Jianshu Cao reviewed a number of aspects of quantum coherence in light-harvesting energy transfer. Using a minimal model of a three-level system, he showed how to systematically predict both its transient and steady-state coherences and demonstrated the interplay of exciton trapping at the reaction center and the non-canonical distribution due to the system-bath coupling. Further, he offered an analysis of the efficiency and energy flux of the three-level model, showing that the optimal performance lies in the intermediate range of temperature and coupling strength.

Javier Cerrillo introduced the transfer tensor method, which is an efficient tool for the simulation of open quantum systems. He showed that by extracting the information contained in short samples of the initial dynamics, this method has the ability to extend the simulation power of existing exact approaches. Currently, this technique is being applied in combination with the hierarchy of equations of motion approach, to facilitate quantum transport studies in the highly challenging strong-coupling and non-Markovian regimes.

Philipp Strasberg discussed quantifiers of non-Markovianity, and, based on linear response theory, presented a new definition for a measure of non-Markovianity. He went on to discuss how negativities in the entropy production rate may, or may not, imply non-Markovianity in the dynamics of an open system, and emphasized the subtleties involved in connecting the mathematical concept of non-Markovianity with a time-dependent physical observable.

Erik Gauger presented microscopically-derived master equation approaches for modelling quantum networks with multiple environments, with a particular focus on how the interplay between coherent and dissipative processes gives rise to a wide variety of non-equilibrium transport phenomena in nanoscopic systems.

Ahsan Nazir considered quantum systems coupled simultaneously to multiple environments, and showed that enforcing additivity of such combined influences can result in unphysical behaviour in both nonequilibrium and equilibrium scenarios. He also showed that by restoring environmental non-additivity, strong-coupling in non-equilibrium quantum systems can be studied through a reaction-coordinate type description.

Yuta Fujihashi presented HEOM simulations of the primary charge separation event at the photosystem II reaction center, to assess the impacts of the protein environment and intramolecular vibrations on the exciton and charge transfer dynamics. He suggested that intramolecular vibrations complement the robustness of the charge separation against the large static electronic disorder. He also presented some recent work on simulating electronic excitation dynamics initiated by entangled photons.

Gabriel Hanna presented mixed quantum-classical simulations of nonequilibrium heat transport in molecular junctions. He showed how calculations of the steady-state heat current in the nonequilibrium spin-boson model could be carried out in a variety of parameter regimes using a selection of quantum-classical approaches, and compared them with numerically exact, as well as weak-coupling-limit results.

Takaaki Aoki considered a single harmonic oscillator coupled to a bath of many harmonic oscillators. He defined a time-dependent temperature of the oscillator, and showed that this temperature relaxes to that of the bath in the long-time limit.

Naomichi Hatano introduced exceptional points in quantum mechanics using a classical analogue. He presented a first principle derivation of the Lindblad equation based on projection operators and applied it to a two-level system in an external electric field. The spectrum of the Liouvillian displays exceptional points: the second-order ones are located on lines in the electric field-dissipation rate parameter space, while the third-order one is at a point.

Abraham Nitzan discussed the quantum thermodynamics of strongly coupled and driven resonant level models. In particular, he discussed an approximate approach based on a truncated expansion of the full system-bath density matrix that is written as a power series in the driving modulation rate, from which work, heat, and entropy production rates can be obtained. A complementary description was also developed, expressing the density matrix in terms of the asymptotic eigenstates of the system using Møller transition operators, which yields a host of results that are consistent with the standard NEGF results for this problem.

Roman Krems explored the possibility of using machine learning to build physical models for open quantum systems based on very restricted available information, and showed how Bayesian machine learning could be used to address the inverse problem of inferring the Hamiltonian of a system from knowledge of a few dynamical observables. He illustrated these methods using two applications, (i) constructing accurate potential energy surfaces from gas-phase reactive scattering data, and (ii) the model selection problem aiming to derive the particular lattice model Hamiltonian that gives to rise to specific quantum transport properties for particles in a phonon field.

Giuseppe Luca Celardo discussed electronic states with macroscopic excitonic coherence lengths as an emergent property of the nanotubular structures found in natural light harvesting systems like the chlorosome. This coherence arises due to the interplay between geometry and cooperativity observed in processes such as superradiance and super-transfer. Due to this interplay, an energy gap between the excitonic ground state and the first excited state emerges which, counterintuitively, increases with the length of the nanotube up to a critical system size which is close to the length of the natural complexes considered.

Géraldine Haack introduced the reset master equation evolution equation, which describes the interaction of a quantum system with an environment in a probabilistic and phenomenological way. The use and validity of this reset equation with respect to the laws of thermodynamics were discussed, with a focus on local detailed balance and entropy balance. She discussed how this approach can be applied in understanding how to generate or maintain entanglement in open quantum systems, which is a central challenge in quantum information science.

Andrew Kent Harter discussed Floquet edge state protection in non-Hermitian topological systems. He mapped out the re-entrant PT phase diagram for a two-level system with time periodic PT-symmetric gain and loss, that features a PT unbroken phase. As the driving frequency nears resonance the system enters a PT-broken phase, and when the driving frequency is increased further, the system re-enters the PT-symmetric phase. This analysis was extended to the spatially extended (periodic) one-dimensional Su-Schrieffer-Heeger model.

Jean-Bernard Bru discussed the dynamics of fermions and quantum spin systems with long range or mean field interactions, with the strong-coupling BCS-Hubbard model serving as an example. He argued that long-range dynamics in such models is in general equivalent to a nontrivial combination of quantum and classical dynamics, the solution of a self-consistent equation.

Michael Thorwart discussed the question of whether or not, and on what time-scale, the dynamics of molecular excitons in biological light harvesting networks is quantum coherent. Despite over a decade of debate, and contradictory experimental results, there seems to be some convergence in the field on aspects of this issue in terms of the nature of the observed coherence (vibrational), and on the time-scale of the electronic coherence involved in the process (approximately 10 fs).

David Coker presented how signatures of vibronic energy transfer emerge in nonlinear spectroscopic signals. Semi-classical methods based on a new hybrid partial linearized and coherent state density matrix dynamics approach were outlined, and applied to compute the time-resolved two-dimensional electronic spectra to elucidate these signatures in models for natural light harvesting systems.

Aaron Kelly discussed a selection of recently developed approaches for simulating nonequilibrium quantum dynamics based on ensembles of classical-like trajectories. The performance of selected techniques of this type was investigated in a variety of nonadiabatic charge and energy transfer processes, including cavity-bound spontaneous emission, charge separation and polaron formation, and heat transport through molecular junctions.

Paul Brumer discussed how processes induced by natural light display properties distinct from those studied in the laboratory using pulsed lasers. He showed that studying the dichotomy of these situations helps address the presence or absence of stationary coherences, and reveals new tests for the range of validity of secular versus nonsecular treatments of driven dynamics.

Qiang Shi spoke about applications of the non-perturbative hierarchical equations of motion approach in simulating charge and energy transfer dynamics in condensed phase systems. A new approach to calculate the exact time non-local and time-local memory kernels and their high order perturbative expansions were discussed, along applications of the HEOM method to charge separation dynamics at the donor/acceptor interface in organic photovoltaic devices, excitation energy transfer in the Fenna-Matthews-Olson complex, and electron transport in molecular junctions.

Dvira Segal discussed full counting statistics for charge and energy transport, in terms of methods and applications to study the steady state transport of particles and energy in open quantum systems. She described numerous benefits of the FCS approach, and explained in more details recent analysis of experimental data of anomalous electronic shot noise, which revealed fundamental information on the conducting junction.

Bonus Tutorial Talks: **Naomichi Hatano** A non-Markovian Analysis of Quantum Otto Engine, **Jianshu Cao** Stochastic Formalism and Simulation of Quantum Dissipative Dynamics.

Outcome of the Meeting

The meeting involved scientists that study complementing aspects of open quantum system dynamics: mathematical foundations of the equations of motion, chemical dynamics in real systems, principles of quantum thermodynamics, and method development. While the community is diverse, questions over the validity of techniques, approaching the strong coupling limit, and applications to real systems unified the different presentations. All the attendees commented that through the workshop they met new people, learned about new fields, and expanded their scientific network. Several of the participants initiated collaborations based on interactions at the meeting. The meeting provided mathematicians with an appreciation of the complexity of real systems, and the fact that simplifying approximations that are favourable mathematically are not justified in complex environments. The Chemistry and Physics communities were exposed to the process of rigorously assessing the validity of approximate techniques. Altogether, attendees felt that similar meetings aiming to consolidate the diverse communities involved in studies of open quantum systems should be organized in the near future. In particular, it was repeatedly suggested to the organizers to try and arrange for another BIRS event in the coming years...

Participants

Anders, Janet (University of Exeter)
Aoki, Takaaki (The University of Tokyo, AIST)
Bru, Jean-Bernard (University of the Basque Country & BCAM & Ikerbasque)
Brumer, Paul (University of Toronto)
Cao, Jianshu (Massachusetts Institute of Technology)
Celardo, Giuseppe Luca (IFUAP-BUAP Puebla)
Cerrillo, Javier (Technical University Berlin)
Coker, David (Boston University)
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Haack, Géraldine (University of Geneva)
Hanna, Gabriel (University of Alberta)
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Koch, Christiane (University of Kassel)
Kosloff, Ronnie (Hebrew University of Jerusalem)
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Limmer, David (UC Berkeley)
Merkli, Marco (Memorial University of Newfoundland)
Nazir, Ahsan (University of Manchester)
Nitzan, Abraham (University of Pennsylvania)
Petruccione, Francesco (Stellenbosch University)
Plenio, Martin (Ulm University)
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non-equilibrium - multiple baths unitary ¡–¿ dissipative dynamics Criteria for the accuracy

Chapter 18

Workshop on Probabilistic and Extremal Combinatorics (19w5009)

September 1-6, 2019

Organizer(s): Penny Haxell (University of Waterloo), Michael Krivelevich (Tel Aviv University), Benny Sudakov (ETH Zurich)

Overview of the Field

Combinatorics, also known as Discrete Mathematics, is a fundamental mathematical discipline which studies the nature of discrete mathematical objects, such as permutations, graphs and set-families. Encompassing some of the most basic and natural mathematical questions, Combinatorics is probably as old as the human ability to count. During the twentieth century and the first two decades of the present century, the field has experienced remarkable growth, transitioning from a collection of mostly isolated results relying on ad hoc arguments, to a major branch of mathematics with its own theory, problems and techniques. Modern Combinatorics has well-established and fruitful connections to numerous scientific fields, including Number Theory, Discrete Geometry, Statistical Physics, Evolutionary Biology and, most notably, Theoretical Computer Science, with which it is intimatively intertwined. Combinatorial methods and ideas have been exported to many of the above disciplines, in some cases leading to outstanding results.

The workshop focused on two major branches of Combinatorics: Extremal Combinatorics and Probabilistic Combinatorics. These two highly-related fields have flourished in recent decades, producing several breakthroughs and many fascinating results, and leading to the creation of a vibrant community comprising both senior and young researchers. We now briefly overview each of these two disciplines.

Extremal Combinatorics encompasses several important areas of research, such as Extremal Graph (and Hypergraph) Theory, Extremal Set Theory, and Ramsey Theory. Extremal Graph Theory typically asks to maximize/minimize some graph parameter over all graphs satisfying a given property. This field originated in the classical theorems of Mantel (1907) and Turán (1941), which determined the maximum possible number of edges of an n-vertex graph containing no clique of a given size. Since then, questions of this type have been studied for other natural combinatorial objects, such as uniform hypergraphs, tournaments and matrices. As a testament to the field's importance, it suffices to say that the study of extremal-(hyper)graph-theoretic questions has lead to major developments in Combinatorics, like the Regularity Method.

Ramsey Theory is the branch of Combinatorics dealing with the fundamental phenomenon, perhaps best described by Motzkin's famous quote, that "complete disorder is impossible". In other words, every large enough system, chaotic as it may be, must contain relatively large structured subsystems. Concrete manifestations of this idea have been studied in many settings, starting with F. Ramsey's original theorem which states that no matter how one colors the edges of a large enough complete uniform hypergraph, one is always guaranteed to find a large monochromatic complete subhypergraph (which constitutes the structured subsystem). Due to the fundamental nature of such questions, they have found uses in many combinatorial studies, as well as in other branches of mathematics.

Probabilistic Combinatorics studies probability spaces of discrete structures. This field originated in the 1940s with the revolutionary realization that probabilistic reasoning can be applied to deterministic problems. A key example of this is a so-called existence proof, which goes as follows. In order to prove the existence of a combinatorial structure of a given type having some desirable properties, one can define a suitable probability distribution over objects of the given type, and show that the probability that a randomly drawn object possesses the prescribed properties is strictly larger than zero. Such a proof guarantees the existence of a certain object without explicitly describing it. This Probabilistic Method, as it came to be known, has been successfully used to find examples and counterexamples to multiple longstanding conjectures, and has since become a standard tool in the combinatorialist's toolkit. This success has in turn led to the study of the typical properties of various combinatorial objects, such as random graphs and matrices. Probabilistic Combinatorics has also had a profound impact on Computer Science, serving as the mathematical foundation for the design of randomized algorithms and the study of randomness in computation, and inspiring such fundamental notions as quasi-randomness and graph expansion. Finally, the combination of probabilistic techniques with other sophisticated tools has recently led to striking results, like Keevash's celebrated resolution of the 150-year old problem on the existence of designs.

Ramsey theory

Jacob Fox *Hypergraph Ramsey numbers*
In this talk, we solve a longstanding open problem of Erdős and Hajnal on off-diagonal hypergraph Ramsey numbers, and discuss a variety of related problems.

A k-uniform hypergraph, or simply k-graph, $G = (V, E)$ consists of a vertex set V and an edge set $E \subseteq \binom{V}{k}$. Ramsey's theorem states that for any k-graphs H_1 and H_2, there is a positive integer N such that any k-graph G of order N contains H_1 (as a subgraph) or its complement $\overline{G}$ contains H_2. The Ramsey number $r(H_1, H_2)$ is the smallest such N, and the main goal of graph Ramsey theory is to estimate $r(H_1, H_2)$, especially when one or both of H_i is a complete graph K_n.

In 1972, Erdős and Hajnal [19] posed the problem of determining the minimum independence number of a 3-graph on N vertices in which there are at most two edges among any four vertices, and showed that the answer is between $\Omega(\log N/\log\log N)$ and $O(\log N)$. In the language of Ramsey numbers, this is equivalent to

$$2^{\Omega(n)} \leq r(K_4^{(3)} \setminus e, K_n^{(3)}) \leq n^{O(n)}, \tag{0.1}$$

where $K_4^{(3)} \setminus e$ is the 3-graph on four vertices and three edges. This problem has received considerable attention during the half-century since it was posed, see, e.g., [17]. We solve this Erdős-Hajnal problem and show that the upper bound in (0.1) is tight. That is, $r(K_4^{(3)} \setminus e, K_n^{(3)}) = n^{\Theta(n)}$. We prove this result with a carefully designed probabilistic construction, and entropy inequalities are used in the analysis. We further extend this result to prove similarly tight bounds for off-diagonal 3-uniform Ramsey numbers of link hypergraphs versus complete hypergraphs. For details, see [21].

based on joint work with Xiaoyu He.

Dhruv Mubayi *Polynomial to exponential transition in Ramsey theory*
We give two new results in Ramsey theory, one for graphs and one for hypergraphs.

Graphs. For fixed $s \geq 3$, we prove that if optimal K_s-free pseudorandom graphs exist, then the Ramsey number $r(s,t) = t^{s-1+o(1)}$ as $t \to \infty$. Our method also improves the best lower bounds for $r(C_\ell, t)$ obtained by Bohman and Keevash [9] from the random C_ℓ-free process by polylogarithmic factors for all odd $\ell \geq 5$ and $\ell \in \{6, 10\}$. For $\ell = 4$ it matches their lower bound from the C_4-free process. These results all follow from the following theorem.

Theorem 18.0.1 ([34])**.** *Let F be a graph, n, d, λ be positive integers with $d \geq 1$ and $\lambda > 1/2$ and let $t = \lceil 2n \log^2 n/d \rceil$. If there exists an F-free (n, d, λ)-graph, then*

$$r(F, t) > \frac{n}{20\lambda} \log^2 n. \tag{0.2}$$

We also prove, via a different approach, that $r(C_5, t) > (1 + o(1))t^{11/8}$ and $r(C_7, t) > (1 + o(1))t^{11/9}$. These improve the exponent of t in the previous best results and appear to be the first examples of graphs F with cycles for which such an improvement of the exponent for $r(F, t)$ is shown over the bounds given by the random F-free process and random graphs. This is a joint work with Jacques Verstraëte.

Hypergraphs. Given $s \geq k \geq 3$, let $h^{(k)}(s)$ be the minimum t such that there exist arbitrarily large k-uniform hypergraphs H whose independence number is at most polylogarithmic in the number of vertices and in which every s vertices span at most t edges. Erdős and Hajnal [19] conjectured (1972) that $h^{(k)}(s)$ can be calculated precisely using a recursive formula and Erdős offered \$500 for a proof of this. For $k = 3$ this has been settled for many values of s including powers of three but it was not known for any $k \geq 4$ and $s \geq k + 2$. We settle the conjecture for all $s \geq k \geq 4$ [26]. This is a joint work with Alexander Razborov.

Geometric combinatorics

Hao Huang ***Covering cubes by hyperplanes***

Note that the vertices of the n-dimensional cube $\{0, 1\}^n$ can be covered by two affine hyperplanes $x_1 = 1$ and $x_1 = 0$. However if we leave one vertex uncovered, then suddenly at least n affine hyperplanes are needed. This was a classical result of Alon and Füredi [3], followed from the Combinatorial Nullstellensatz. To see that n planes suffice, one can just take all $x_i = 1$ for $i = 1, \cdots, n$.

In this talk, we consider the following natural generalization of the Alon–Füredi theorem: what is the minimum number of affine hyperplanes such that the vertices in $\{0, 1\}^n \setminus \{\vec{0}\}$ are covered at least k times, and $\vec{0}$ is uncovered? We conjecture that for fixed integer k, and sufficiently large n, the minimum number of affine hyperplanes needed is $n + \binom{k}{2}$. We prove this conjecture for $k \leq 3$, using a punctured version of the Combinatorial Nullstellensatz.

We also develop an analogue of the Lubell–Yamamoto–Meshalkin inequality for subset sums, and solve the problem asymptotically for fixed n and $k \to \infty$. We show that in this setting, the minimum number of affine hyperplanes needed is $(1 + \frac{1}{2} + \cdots + \frac{1}{n} + o(1))k$, solving the fractional version of the cube covering problem.

Joint work with [16] with Alexander Clifton (Emory University)

Peter Keevash ***Isoperimetric stability***

A prominent open problem at the interface of Geometry, Analysis and Combinatorics is to understand the stability of isoperimetric problems. The meta-problem is to characterise sets whose boundary is close to the minimum possible given their volume; there are many specific problems obtained by giving this a precise meaning. For the discrete cube, the two natural notions are vertex boundary and edge boundary; the descriptions of the minimisers for both notions are classical results of Extremal Combinatorics. In joint work with Eoin Long, we have recently obtained corresponding stability results, namely that approximate minimisers for the edge boundary are close to disjoint unions of cubes, and approximate minimisers for the vertex boundary are close to generalised Hamming balls.

There is a large prior literature on the edge boundary, including earlier work of Ellis and of Ellis, Keller and Lifshitz that gives much more precise stability results for families that are very close to minimising the edge boundary. Also, Keller and Lifshitz independently used very different methods to prove a somewhat stronger version of my result with Long. In the setting of the vertex boundary, nothing was known prior to our work, no doubt due to the apparent intractability of extracting structural information from the only known proof method (compression, which alters the structure). Remarkably, we were able to obtain structural information via local stability arguments that keep tight control of structure over a long process of decompression. Independently, Przykucki and Roberts recently gave a very different argument and obtained another stability result that complements ours (it is applicable to a different range of parameters).

A much wider context for the edge boundary is its interpretation (in the setting of biased measures on the cube) as the influence of Boolean functions and its connection (via the Margulis-Russo formula) to the sharp threshold phenomenon, which has led to fundamental insights and applications spanning a variety of areas of Mathematics (Gaussian Geometry and Isoperimetry), Computer Science (Computational Complexity) and Economics (Social Choice). One fundamental question addressed by a conjecture of Kahn and Kalai is to characterise properties with coarse thresholds / functions of small influence. Results of Friedgut, Bourgain and Hatami say (roughly) that such properties / functions exhibit some kind of 'junta-like' behaviour, meaning that one can get a significant density increase by fixing the values of a small set of coordinates. However, all of these results only apply to the 'dense setting' where the initial density is bounded away from 0 and 1. In joint work with Lifshitz, Long and Minzer, we prove such results in the 'sparse setting' (i.e. any initial density) that establish a variant of the Kahn-Kalai Conjecture and a sharp form of Bourgain's Theorem. Our main tool is a new hypercontractive inequality for quasirandom boolean functions. We also give applications of our sharp threshold result to Extremal Combinatorics (via the 'junta method'), including proofs of two conjectures in a range of parameters that is within a constant factor of being optimal, namely the Huang-Loh-Sudakov Conjecture on cross matchings and the Furedi-Jiang-Seiver Conjecture on the Turán numbers of linear paths in hypergraphs.

Joint work with Noam Lifshitz, Eoin Long and Dor Minzer

Lisa Sauermann ***On the size of subsets of $\mathbb{F}_p^n$ without p distinct elements summing to zero***

For given positive integers m and n, what is the minimum integer s such that among any s points in the integer lattice $\mathbb{Z}^n$ there are m points whose centroid is also a lattice point in $\mathbb{Z}^n$? This problem is called the Erdős-Ginzburg-Ziv problem, because its answer can be interpreted as the so-called Erdős-Ginzburg-Ziv constant $\mathfrak{s}(\mathbb{Z}_m^n)$ of $\mathbb{Z}_m^n$. In 1961, Erdős, Ginzburg and Ziv [18] proved a result essentially stating that $\mathfrak{s}(\mathbb{Z}_m^1) = 2m - 1$, and since then Erdős-Ginzburg-Ziv constants have been studied intensively.

Alon and Dubiner [2] showed that for a fixed dimension n, the quantity $\mathfrak{s}(\mathbb{Z}_m^n)$ grows linearly with m. On the other hand, they raised the question of finding good upper bounds for $\mathfrak{s}(\mathbb{Z}_m^n)$ when m is fixed and n is large. The most interesting case here is when $m = p \geq 3$ is a prime (since this case implies bounds for general m).

This problem of bounding $\mathfrak{s}(\mathbb{F}_p^n)$ for a fixed prime $p \geq 3$ and large n is essentially equivalent to bounding the maximum size of a subset of $\mathbb{F}_p^n$ that does not contain p distinct elements summing to zero. Asking about this maximum size is also a natural question in itself, and the special case of $p = 3$ is actually equivalent to the famous cap-set problem (which asks for the maximum size of a subset of $\mathbb{F}_p^n$ without a three-term arithmetic progression).

The main result discussed in this talk is the following new upper bound for the maximum size of a subset of $\mathbb{F}_p^n$ without p distinct elements summing to zero for any fixed prime $p \geq 5$ and large n. For p and n going to infinity, this bound is of the form $p^{(1/2)\cdot(1+o(1))n}$, whereas all previously known upper bounds were of the form $p^{(1-o(1))n}$ (with p^n being a trivial bound). Hence this new bound is a qualitative improvement over the previous bounds.

Theorem 18.0.2. *Let $p \geq 5$ be a fixed prime. Then for any positive integer n and any subset $A \subseteq \mathbb{F}_p^n$ which does not contain p distinct elements $x_1, \ldots, x_p \in A$ with $x_1 + \cdots + x_p = 0$, we have*

$$|A| < C_p \cdot (2\sqrt{p})^n .$$

Here, C_p is a constant only depending on p.

The proof of Theorem 18.0.2 uses the so-called multi-colored sum-free theorem which is a consequence of the Croot-Lev-Pach polynomial method. This method and its consequences were already applied by several authors to prove bounds for the maximum size of a subset of $\mathbb{F}_p^n$ without p distinct elements summing to zero. However, using some new combinatorial ideas, we significantly improve their bounds.

Yufei Zhao ***Equiangular lines with a fixed angle***
Solving a longstanding problem on equiangular lines, we determine, for each given fixed angle and in all sufficiently large dimensions, the maximum number of lines pairwise separated by the given angle.

Theorem 18.0.3. *Fix $\alpha \in (0, 1)$. Let k be the minimum number of vertices of a graph whose adjacency matrix has spectrial radius exactly $(1 - \alpha)/(2\alpha)$, and set $k = \infty$ if no such graph exists.*
The maximum number $N_\alpha(d)$ of equiangular lines in $\mathbb{R}^d$ with common angle $\arccos \alpha$ satisfies

(a) $N_\alpha(d) = \lfloor k(d - 1)/(k - 1) \rfloor$ *for all sufficiently large $d > d_0(\alpha)$ if $k < \infty$.*

(b) $N_\alpha(d) = d + o(d)$ *as $d \to \infty$ if $k = \infty$.*

Significant progress on made recently on the this problem in [7], where the following key step of the solution was introduced.

Theorem 18.0.4. *For every $\alpha \in (0, 1)$, there exists some $\Delta = \Delta(\alpha)$ so that for every set of equiangular lines in $\mathbb{R}^d$ with common angle $\arccos \alpha$, one can choose a set S of unit vectors, with one unit vector in the direction of each line in the equiangular set, so that each unit vector in S has inner product $-\alpha$ with at most Δ other vectors in S.*

Our key new insight is a new result in spectral graph theory, which shows that the multiplicity of the second largest eigenvalue of the adjacency matrix of a connected bounded degree graph is sublinear.

Joint work with Zilin Jiang, Jonathan Tidor, Yuan Yao, and Shengtong Zhang.

Extremal Set Theory

Shoham Letzter ***Minimum saturated families***
We call a family $\mathcal{F}$ of subsets of $[n]$ s-saturated if it contains no s pairwise disjoint sets, and moreover no subset of $[n]$ can be added to $\mathcal{F}$ while preserving this property.

More than 40 years ago, Erdős and Kleitman [20] conjectured that an s-saturated family of subsets of $[n]$ has size at least $(1 - 2^{-(s-1)}) \cdot 2^n$. It is easy to show that every s-saturated family has size at least $\frac{1}{2} \cdot 2^n$, but, as was mentioned by Frankl and Tokushige [22], even obtaining a slightly better bound of $(1/2 + \varepsilon) \cdot 2^n$, for some fixed $\varepsilon > 0$, seems difficult. In [12], we proved such a result, showing that every s-saturated family of subsets of $[n]$ has size at least $(1 - 1/s) \cdot 2^n$.

This lower bound is a consequence of a multipartite version of the problem, in which we seek a lower bound on $|\mathcal{F}_1| + \ldots + |\mathcal{F}s|$ where $\mathcal{F}_1, \ldots, \mathcal{F}_s$ are families of subsets of $[n]$, such that there are no s pairwise disjoint sets, one from each family $\mathcal{F}_i$, and furthermore no subset of $[n]$ can be added to any of the families while preserving this property. We show that $|\mathcal{F}_1| + \ldots + |\mathcal{F}_s| \geq (s - 1) \cdot 2^n$, which is tight, as can be seen, for example, by taking $\mathcal{F}_1$ to be empty, and letting the remaining families be the families of all subsets of $[n]$.

We give two short proofs of this result, one using algebraic methods, and one based on correlation inequalities.

Extremal graph theory

Matija Bucić ***Nearly-linear monotone paths in edge-ordered graphs***
How long a monotone path can one always find in any edge-ordering of the complete graph K_n? This appealing question was first asked by Chvátal and Komlós [15] in 1971, and has since attracted the attention of many researchers, inspiring a variety of related problems. The prevailing conjecture is that one can always find a monotone path of linear length, but until now the best known lower bound was $n^{2/3-o(1)}$ due to Milans [32]. We almost close this gap, proving that any edge-ordering of the complete graph contains a monotone path of length $n^{1-o(1)}$. Our main results are the following.

Theorem. In any edge-ordering of the complete graph K_n, there is a monotone path of length

$$f(K_n) \geq \frac{n}{2^{O\left(\sqrt{\log n \log\log n}\right)}} = n^{1-o(1)}.$$

The altitude $f(G)$ of a graph G is defined as the maximum k such that every edge-ordering of G has a monotone path of length k.

Theorem. Let G be a graph with n vertices and average degree $d \geq 2$. Then

$$f(G) \geq \frac{d}{2^{O\left(\sqrt{\log d \log\log n}\right)}}.$$

This is a joint work with Matthew Kwan, Alexey Pokrovskiy, Benny Sudakov, Tuan Tran, and Adam Zsolt Wagner.

Shagnik Das ***How redundant is Mantel's Theorem?***

One of the all-time combinatorial classics, Mantel's Theorem [30] asserts that if one forbids an n-vertex graph G from containing any triangle, then G can have at most $\frac{n^2}{4}$ edges. This fundamental theorem has inspired a great deal of research, including the foundational work of Turán. Turán's Theorem [43] describes the largest K_r-free graphs, in particular showing that they have $(1 - \frac{1}{r-1} + o(1))\binom{n}{2}$ edges.

In this talk we explored an extension of these theorem suggested by Gil Kalai. In the above results, we forbidded any of the potential r-cliques from appearing in our graph G. Suppose instead that our resources are somewhat more limited, in the sense that, for some $0 \leq m \leq \binom{n}{r}$, we can only forbid m of the r-cliques from appearing in G. What choice of forbidden cliques then minimises the maximum number of edges G can have? In particular, how many cliques need to be forbidden to recover the bounds from Mantel's and Turán's Theorems?

Some asymptotic bounds in this direction, showing that a cubic number of forbidden cliques are necessary and sufficient to recover the classic extremal bounds, were earlier obtained by Allen, Böttcher, Hladký and Piguet [1]. Focussing on the case $r = 3$, we presented some precise results beyond this initial range, determining how many additional edges can be achieved when fewer triangles are forbidden. At the other end of the spectrum, when there are only quadratically many forbidden triangles, we discussed the connection of this problem to combinatorial designs, explaining how Steiner Triple Systems can be used to construct sets of forbidden triangles that are hard to avoid.

This is a joint work with Ander Lamaison and Tuan Tran.

Daniel Král ***Extremal problems concerning cycles in tournaments***

The conjecture of Linial and Morgenstern [28] asserts that, among all tournaments with a given density d of cycles of length three, the density of cycles of length four is minimized by a random blow-up of a transitive tournament with all but one parts of equal sizes, i.e., a tournament with the structure similar to graphs appearing in the Erdős-Rademacher problem on triangles in graphs with a given edge density. We prove this conjecture for $d \geq 1/36$ using methods from spectral graph theory, and demonstrate that the structure of extremal examples is more complex than expected and give its full description for $d \geq 1/16$.

The talk was based on the paper [14].

Tibor Szabó ***On the quasirandomness of the projective norm graph***

The projective norm graphs $NG(q,t)$ provide tight constructions in the Turán problem for complete bipartite graphs $K_{t,s}$ when $s > (t-1)!$ ([5]). The $K_{t,s}$-freeness of $NG(q,t)$ is a very much atypical property: in a random graph with the same edge density a positive fraction of t-tuples are involved in a copy of $K_{t,s}$. Yet, projective norm graphs are random-like in various other senses. Most notably their second eigenvalue is of the order of the square root of the degree, which, through the Expander Mixing Lemma, implies further quasirandom properties concerning the density of small enough subgraphs. In our papers [8, 31] we explore how far this quasirandomness goes. In particular we make progress on what subgraphs it must contain, beyond the eigenvalue methods of the Expander Mixing Lemma. Our results extend those of Alon and Shikelman [6] and Ma et al [29] on generalized

Turán numbers, moreover imply that the $K_{4,7}$-free projective norm graph $NG(q,4)$ does contain $K_{4,6}$ for every prime power $q \geq 5$.

The main contribution of our proof is the estimation, and sometimes determination, of the number of solutions $X \in \mathbb{F}_{q^t}$ of the norm equation system $N_t(X + A_i) = a_i,\ (i = 1, \ldots, r)$, for various constants $A_i \in \mathbb{F}_{q^t}$ and $a_i \in \mathbb{F}_q^*$, where $N_t : \mathbb{F}_{q^t} \to \mathbb{F}_q$ denotes the norm function, defined by $N_t(A) = A^{q^{t-1}+q^{t-2}+\cdots q+1}$. In connection with norm graphs it has been proved before [25] that for $r = t$ and arbitrary prime power q, the number of solutions is at most $t!$. Here we investigate this problem for arbitrary t when $r \leq 3$. We find that for $r = 2$ and arbitrary $t \geq 3$, the number of solutions is the expected $(1+o(1))q^{t-2}$, except in a very special case of $t = 3$, when it is two times that. We characterize the solutions in this special case via a surprising connection to classic planar Singer difference sets [41]. This connection can then be utilized to show that for the critical case of $r = 3 = t$, there do exist parameters with $6 = 3!$ solutions. Finally for $r = 3$ and arbitrary t we use elementary methods to bound the number of solutions by $6q^{t-3}$, which was only known for $t = 3$, using algebraic geometry.

Joint work with Tomas Bayer, Tamás Mészáros, and Lajos Rónyai.

Extremal hypergraph theory

Noga Alon ***Traces of Hypergraphs***

What is the largest number of distinct projections (traces) onto k coordinates guaranteed in every family of m binary vectors of length n ?

This fundamental combinatorial question received a considerable amount of attention, has applications in theoretical Computer Science, Geometry, Machine Learning, Probability and more, and is wide open for most settings of the parameters.

In joint work with Moshkovitz and Solomon [1] we found an asymptotic solution of the question for linear k and sub-exponential m, greatly improving earlier estimates.

In particular, for every constants $r > 1$ and $0 < a < 1$, when n is large, every family of $m = n^r$ binary vectors of length n has at least $\tilde{\Theta}(n^C)$ projections on some set of $k = an$ coordiantes, where $C = \frac{r+1-\log(1+a)}{2-\log(1+a)}$. This is tight up to the hidden polylogarithmic term in the $\tilde{\Theta}$ notation.

David Conlon ***Improved bounds for the Brown–Erdős–Sós problem***

Let $f_r(n, v, e)$ be the maximum number of edges in an r-uniform hypergraph on n vertices which contains no induced subgraph with v vertices and at least e edges. The Brown–Erdős–Sós problem [10, 11] of determining $f_r(n, v, e)$ is a central question in extremal combinatorics, with surprising connections to a number of seemingly unrelated areas. For example, the result of Ruzsa and Szemerédi [38] that $f_3(n, 6, 3) = o(n^2)$ implies Roth's theorem on the existence of 3-term arithmetic progressions in dense subsets of the integers. As a generalisation of this result, it is conjectured that

$$f_r(n, e(r-k) + k + 1, e) = o(n^k)$$

for any fixed $r > k \geq 2$ and $e \geq 3$. The best progress towards this conjecture, due to Sárközy and Selkow [39, 40], says that

$$f_r(n, e(r-k) + k + \lfloor \log e \rfloor, e) = o(n^k),$$

where the log is taken base two. Building on an idea of Solymosi and Solymosi [42], we improve the Sárközy–Selkow bound, showing that $\lfloor \log e \rfloor$ can be replaced with $O(\log e / \log \log e)$. Even for the special case where $r = 3$ and $k = 2$, the proof relies on applying the hypergraph removal lemma at all uniformities.

Joint work with Lior Gishboliner, Yevgeny Levanzov and Asaf Shapira

Asaf Ferber ***Resilience for perfect matchings in random hypergraphs***

Let $m_d(k, n)$ be the smallest integer m for which every k-uniform hypergraph on n vertices and with minimum d-degree at least m contain a perfect matching (we always assume that n is divisible by k). The problem of determining $m_d(k, n)$ has attracted a lot of attention in the last few decades. Quite surprisingly, this problem is still wide open, and have led to the development of many techniques and interesting connections with other areas (see, e.g., the surveys [37, 44] and the references therein).

Recently, there has been interest in extending extremal theorems to random environments. In our setting, we are interested in finding minimum degree conditions for the existence of a perfect matching in subgraphs of a typical random hypergraph $H^k_{n,p}$. We prove that for $p \geq C\max\{n^{-k/2+\varepsilon}, n^{-k+d+1}\}$, a typical $H^k_{n,p}$ is such that every subgraph $G \subseteq H$ with minimum d-degree at least $(1+o(1))m_d(k,n)$ contains a perfect matching. Note that this holds for all d, k even in cases when the exact value of $m_d(k,n)$ is unknown. Our proof is based on a new "non-constructive" absorbers technique which we believe is of independent interest.

Joint work with Matthew Kwan.

Alexandr Kostochka ***Super-pancyclic hypergraphs and bipartite graphs***

We find Dirac-type sufficient conditions for a hypergraph H with few edges to be hamiltonian. It is convenient to use the language of the bipartite graphs that are the incidence graphs of hypergraphs. For integers n, m, and δ with $\delta \leq m$, we denote by $\mathcal{G}(n,m,\delta)$ the set of all bipartite graphs with partition (X,Y) such that $|X| = n \geq 2, |Y| = m$ and for every $x \in X$, $d(x) \geq \delta$. In 1981 Jackson proved that if a graph $G \in \mathcal{G}(n,m,\delta)$ satisfies $n \leq \delta$ and $m \leq 2\delta - 2$, then it contains a cycle that covers X. He also conjectured that if $G \in \mathcal{G}(n,m,\delta)$ is 2-connected, $m \leq 3\delta - 5$ and $n \leq \delta$, then the same conclusion holds.

We prove this conjecture and describe the extremal graphs for Jackson's Theorem. We also show that under the conditions of Jackson's Theorem, the significantly stronger conclusion holds: G is X-super-pancyclic, i.e., for every $A \subset X$ with $|A| \geq 3$, G has a cycle C_A such that $V(C) \cap X = A$. We also find necessary conditions for a graph in $\mathcal{G}(n,m,\delta)$ to be super-pancyclic that are often sufficient for it. We conjecture that these conditions are equivalent for a graph in $\mathcal{G}(n,m,\delta)$ to be super-pancyclic.

Joint work with Ruth Luo and Dara Zirlin

Mykhaylo Tyomkyn ***When Ramsey met Brown, Erdős and Sós***

Brown, Erdős and Sós [10] conjectured that for every $c > 0$ and $k \geq 3$ any r-uniform hypergraph with n vertices and cn^2 edges contains k edges spanned by at most $(r-2)k+3$ vertices – an $((r-2)k+3,k)$-configuration, for short. It is well known that this question reduces to linear hypergraphs, that is hypergraphs with no two edges sharing more than one vertex. A complete linear r-graph (also known as r-Steiner System) is a linear hypergraph corresponding to an edge-decomposition of a complete graph K_n into copies of K_r. We prove the following Ramsey version of the Brown-Erdős-Sós conjecture.

Theorem 18.0.5. *For every integer c there exists $r_0 = r_0(c)$ such that for every $r \geq r_0$ and integer $k \geq 3$ there exists $n_0 = n_0(c,r,k)$ such that every c-colouring of a complete linear r-graph on $n > n_0$ vertices contains a monochromatic $((r-2)k+3,k)$-configuration.*

In the important special case of $c = 2$ we show that r_0 can be chosen as small as 4.

Theorem 18.0.6. *For any integers $r \geq 4$ and $k \geq 3$ there exists $n_0 = n_0(r,k)$ such that every 2-colouring of a complete linear r-graph on $n > n_0$ vertices contains a monochromatic $((r-2)k+3,k)$-configuration.*

This is a joint work with Asaf Shapira.

Jacques Verstraete ***Ordered graphs and hypergraphs: new results and open problems***

There has been substantial recent interest in extremal problems for ordered graphs, with the recent breakthrough of Marcus and Tardos on excluded permutations and the Stanley-Wilf and Furedi-Hajnal conjectures.

We give a survey of selected results, techniques and applications, as well as new results and techniques for ordered hypergraphs, with applications to ordered trees in graphs, tight paths in hypergraphs, and directed paths in eulerian digraphs, amongst others.

Joint work with Z. Furedi, T.Jiang, A. Kostochka, D. Mubayi

Design Theory

Adam Wagner ***Completion and deficiency problems***

Given a partial Steiner triple system (STS) of order n, what is the order of the smallest complete STS it can be embedded into? The study of this question goes back more than 40 years. In this talk we answer it for relatively sparse STSs, showing that given a partial STS of order n with at most $r \leq \varepsilon n^2$ triples, it can always be embedded into a complete STS of order $n + O(\sqrt{r})$, which is asymptotically optimal. We also obtain similar results for completions of Latin squares and other designs.

This suggests a new, natural class of questions, called deficiency problems. Given a global spanning property $\mathcal{P}$ and a graph G, we define the deficiency $\mathrm{defi}(G)$ of the graph G with respect to the property $\mathcal{P}$ to be the smallest positive integer t such that the join $G * K_t$ has property $\mathcal{P}$. To illustrate this concept we consider deficiency versions of some well-studied properties, such as having a K_k-decomposition, Hamiltonicity, having a triangle-factor and having a perfect matching in hypergraphs [35].

The main goal of this talk is to propose a systematic study of these problems; thus several future research directions are also given.

This is a joint work with Rajko Nenadov and Benny Sudakov.

Probability theory

Omer Angel ***Pairwise optimal coupling of multiple random variables***

A **coupling** of a collection of random variables $(X_i)_{i\in I}$ is a set of variables $(X'_i)_{i\in I}$ on some common probability space with the given marginals, i.e. X_i and X'_i have the same law. We omit the primes when there is no risk of confusion. The **total variation distance** between two random variables X and Y is defined as

$$d_{TV}(X,Y) = \sup_A \left\{ |\mathbb{P}(X \in A) - \mathbb{P}(Y \in A)| \right\},$$

where the supremum is over all (measurable) sets A. The fundamental, classical theorem relating the total variation distance to coupling is the following folklore theorem.

Theorem 18.0.7. *For any two random variables X and Y, there exists a coupling such that $\mathbb{P}(X \neq Y) = d_{TV}(X,Y)$. Moreover, this is the smallest possible value of $\mathbb{P}(X \neq Y)$ for any coupling.*

When coupling more than two random variables, the total variation bound cannot be achieved simultaneously for all pairs even in very simple cases. For example, there are 3 random variables with pairwise total variation distance 1/2, but in any coupling some pair disagrees with probability at least 2/3. We prove a generalization of Theorem 18.0.7 with a slightly higher probability of disagreement, based on two different constructions.

Theorem 18.0.8. *For any countable collection $\mathcal{S}$ of real random variables, there exists a coupling such that, for any $X, Y \in \mathcal{S}$,*

$$\mathbb{P}(X \neq Y) \leq f(d_{TV}(X,Y)),$$

where $f(x) = \frac{2x}{1+x}$.

For rational values of x, proving that $f(x)$ is optimal is equivalent to a certain extremal combinatorial problem, which we can solve for some but not all values of x.

Joint work Yinon Spinka.

Expander graphs

Nati Linial ***Expander Graphs – Both Local and Global***

Let $G = (V, E)$ be a finite graph. For $v \in V$ we denote by G_v the subgraph of G that is induced by v's neighbor set. We say that G is (a, b)-regular for $a > b > 0$ integers, if G is a-regular and G_v is b-regular for every $v \in V$.

Recent advances in PCP theory call for the construction of infinitely many (a, b)-regular expander graphs G that are expanders also locally. Namely, all the graphs $\{G_v | v \in V\}$ should be expanders as well. While random regular graphs are expanders with high probability, they almost surely fail to expand locally. Here we construct two families of (a, b)-regular graphs that expand both locally and globally. We also analyze the possible local and global spectral gaps of (a, b)-regular graphs. In addition, we examine our constructions vis-a-vis properties which are considered characteristic of high-dimensional expanders.

It is hard to overstate the significance of expander graphs in theoretical computer science and the impact their study has had on a number of mathematical areas. A particularly fascinating example of such an application is Dinur's proof of the PCP Theorem. However, in recent advances in PCP theory more specialized expander graphs are required. If v is a vertex in a graph G we denote by G_v the subgraph of G that is induced by v's neighbors and call it the link of v in G. We seek large regular expanders G such that G_v is an expander for every $v \in V(G)$.

One of the first discoveries in the study of expanders is that for every $d \geq 3$ asymptotically almost every d-regular graph is a very good expander. However, it is easy to verify that almost every d-regular graph is very far from satisfying the above requirement, as G_v is typically an anticlique. So, here is our basic question: Given positive integers $a > b$ do there exist arbitrarily large (a, b)-expanders? Namely, a-regular expander graphs G such that every G_v is a b-regular expander. If so, how good can the expansion properties (edge expansion, spectral gap) of G and the graphs G_v be?

These investigations are closely related to the recently emerging field of high-dimensional expanders. Vertex-expansion, edge-expansion, spectral gaps and the speed of convergence of the simple random walk on the graph are key ingredients in the theory of expander graphs. While these parameters need not perfectly coincide, they mutually control each other quite tightly. In contrast, the high-dimensional theory suggests a number of inherently different ways to quantify expansion. Namely, the connections between these concepts are nowhere as tight as in the one-dimensional case of expander graphs. It is very suggestive to explore families of (a, b)-expanders in light of this array of quantitative measures of high-dimensional expansion.

Let G be a graph and $v \in V(G)$. The link of v denoted G_v is the subgraph of G that is induced by the vertex set $\{u \in V \mid uv \in E\}$.

Definition 18.0.9. *Let $a > b \geq 0$ be integers. An (a, b)-regular graph G is an a-regular graph, where for every vertex $v \in V(G)$ the link G_v is b-regular.*

It is natural to ask how large the spectral gaps can be in an (a, b)-regular graph. We prove an optimal Alon-Boppana type bound which makes no reference to the graph's local expansion:

Theorem 18.0.10. *The second eigenvalue of an (a, b)-regular graph satisfies*

$$\lambda_2 \geq b + 2\sqrt{a - b - 1} - o_n(1).$$

The bound is tight.

In the graphs that we construct to prove the tightness of the bound in Theorem 18.0.10, all the links are disconnected. So, the next obvious question is whether the same bound can be attained by graphs whose links are all expanders, or at least connected. The following theorem shows that the answer is negative, by describing some tradeoff between local and global expansion.

Theorem 18.0.11. *Consider an (a, b)-regular graph each of whose links has edge expansion at least $\delta > 0$. Then there exists some $\varepsilon = \varepsilon(a, b, \delta) > 0$ such that the second eigenvalue of the graph satisfies:*

$$\lambda_2 \geq \left(b + 2\sqrt{a - b - 1}\right)(1 + \varepsilon) - o_n(1).$$

For fixed a and b with $a \geq b^2 + O(b)$, ε strictly increases with δ. For any other fixed values of a and b, ε increases for small enough δ.

The main new construction that we introduce here is the Polygraph. It can be viewed as a family of new graph products which transform a high-girth regular expander into an (a, b)-expander. To illustrate this idea, let $q > p \geq 0$ be integers, let G be a graph with distance function ρ and girth larger then $3p + 3q$. The vertex set of the polygraph G_S is $V(G)^3$ and (x_1, x_2, x_3) is a neighbor of (y_1, y_2, y_3) iff the multiset of three distances $[\rho(x_i, y_i)|i = 1, 2, 3]$ coincides with the multiset $[p, q, p + q]$.

For illustration, here is a way of viewing the Polygraph corresponding to $p = 0$ and $q = 1$. Take three copies of a d-regular triangle-free graph G and have a token move on each of them. At every step two of the tokens move to a neighboring vertex and the third token stays put. Any configuration of tokens is a vertex of the graph and the above process defines its adjacency relation.

Theorem 18.0.12. *Let $q > p \geq 0$ be even integers. If G is connected, non-bipartite and its girth is bigger than $3p + 3q$, then G_S is an (a, b)-regular local ε-spectral expander and global ε'-spectral expander. Here a, b and ε depend only on p and q, while ε' depends also on the spectral gap of G.*

Joint work with Michael Chapman and Yuval Peled.

Matroid theory

Alexey Pokrovskiy ***Halfway to Rota's basis conjecture***

In 1989, Rota made the following conjecture. Given n bases $B_1, ..., B_n$ in an n-dimensional vector space V, one can always find n disjoint bases of V, each containing exactly one element from each B_i (we call such bases rainbow bases). Rota's basis conjecture remains open despite its apparent simplicity and the efforts of many researchers (for example, the conjecture was recently the subject of the collaborative "Polymath" project). In this talk, it was discussed how to find $(0.5 - o(1))n$ disjoint rainbow bases, improving the previously best known bound of $n/logn$.

Theorem 18.0.13 (Bucić, Kwan, Pokrovskiy, and Sudakov, [13])**.** *For any $\varepsilon > 0$, the following holds for sufficiently large n. Given bases $B_1, \ldots, B_n$ of a rank-n matroid, there are at least $(1/2 - \varepsilon)\, n$ disjoint rainbow bases.*

See [13] for the full details. In order to simplify the presentation, the talk focused on proving the following weaker result:

Proposition *In any family of n-edge trees $T_1, \ldots, T_n$ on the same vertex set, it is possible to find $\sqrt{n}$ edge-disjoint rainbow forests of size $n - 1$ (here a rainbow forest is one which contains at most one edge from each $T_1, \ldots, T_n$).*

This proposition is easier than the full theorem from [13] in three different ways:

- It is about graphic matroids rather than general matroids. This doesn't affect the proof strategy, but makes the matroids easier to visualise.
- If only finds rainbow forests of size $n - 1$ (rather than $n - 1$ like Rota's Conjecture would predict). This is a convenient simplification because it means that every rainbow forest we consider misses some colour.
- It finds only $\sqrt{n}$ rainbow forests. This is an illuminating because the full proof of Theorem 18.0.13 uses an iterative argument to find $(1/2 - \varepsilon)\, n$ disjoint rainbow bases. When one performs only one step of the iteration, then one naturally obtains $\sqrt{n}$ rainbow objects.

Joint work with Bucić, Kwan, and Sudakov.

Other subjects

Matthew Kwan ***An algebraic inverse theorem for the quadratic Littlewood–Offord problem***
Consider a quadratic polynomial $f(\xi_1, \ldots, \xi_n)$ of independent Bernoulli random variables. What can be said about the concentration of f on any single value? This generalises the classical Littlewood–Offord problem, which asks the same question for linear polynomials. As in the linear case, it is known that the point probabilities of f can be as large as about $1/\sqrt{n}$, but still poorly understood is the "inverse" question of characterising the algebraic and arithmetic features f must have if it has point probabilities comparable to this bound (see [36]).

In this talk we discuss some results joint with Lisa Sauermann [26] of an algebraic flavour, showing that if f has point probabilities much larger than $1/n$ then it must be close to a quadratic form with low rank. We also give an application to Ramsey graphs, asymptotically answering a question of Kwan, Sudakov and Tran [27].

Bhargav Narayanan ***Disproportionate division***
The cake-cutting problem, whose study was initiated by Banach and Steinhaus in 1949, is a classical measure partitioning problem concerned with the division of a 'cake', here the unit interval $[0, 1]$, amongst $n \geq 2$ agents each with their own 'utilities', here non-atomic Borel probability measures $\mu_1, \mu_2, \ldots, \mu_n$ on $[0, 1]$. Given non-negative demands $\alpha_1, \alpha_2, \ldots, \alpha_n$ summing to 1, a disproportionate division for these demands is a partition $X_1 \cup X_2 \cdots \cup X_n$ of $[0, 1]$ with $\mu_i(X_i) \geq \alpha_i$ for all $1 \leq i \leq n$. Folklore arguments from algebraic topology show that a disproportionate division for n agents with arbitrary demands may always be found with $O(n^2)$ cuts, and a more efficient rendition of this argument, recently discovered by Segal-Halevi, shows that in fact $O(n \log n)$ cuts always suffice. Our main result improves on these decades-old topological arguments as follows.

Theorem 18.0.14. *For all $n \geq 2$, given non-atomic probability measures $\mu_1, \mu_2, \ldots, \mu_n$ on $[0, 1]$ and non-negative reals $\alpha_1, \alpha_2, \ldots, \alpha_n$ summing to 1, there exists a disproportionate division for these demands with at most $3n - 4$ cuts.*

It is clear that $n - 1$ cuts are always necessary for n agents, so this result is tight up to multiplicative constants. Our proof of Theorem 18.0.14 is combinatorial as opposed to topological; an attractive byproduct of this approach is that the proof is constructive, yielding an effective procedure for disproportionate division. While Theorem 18.0.14 determines the optimal number of cuts for disproportionate division with n agents up to multiplicative constants, the problem of pinning down this extremal number still remains. Unlike with fair division, it turns out that $n-1$ cuts do not always suffice; there is a construction demonstrating that $2n-2$ cuts may be necessary in general. We suspect that this construction, not Theorem 18.0.14, reflects the truth, and that the tightness of this construction should follow from topological considerations: to this end, we present the following conjecture.

Conjecture 1. *For any $n \geq 2$ non-atomic probability measures $\mu_1, \mu_2, \ldots, \mu_n$ on the unit circle S^1 and non-negative reals $\alpha_1, \alpha_2, \ldots, \alpha_n$ summing to 1, there exists a partition of the set $[n] = P \cup Q$ into two nonempty sets and a partition of the circle $S^1 = X \cup X^c$ into two intervals such that*

$$\min_{i \in P} \mu_i(X) = \sum_{j \in P} \alpha_j \text{ and } \min_{i \in Q} \mu_i(X^c) = \sum_{j \in Q} \alpha_j.$$

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Chapter 19

Topology and Measure in Dynamics and Operator Algebras (19w5073)

September 9-13, 2019

Organizer(s): George Elliott (University of Toronto), Thierry Giordano (University of Ottawa), David Kerr (Texas A&M University), Xin Li (Queen Mary University of London)

It is not a coincidence that ergodic theory and the theory of operator algebras were both born as formal disciplines under the pioneering vision of von Neumann, and indeed the two subjects have enjoyed a venerable history of interaction dating back to the seminal papers of Murray and von Neumann in the 1930s and 40s. This interaction largely respects the two distinct but interrelated streams into which each of the subjects principally branches, the one measure-theoretic (von Neumann algebras and measurable dynamics) and the other topological (C^*-algebras and topological dynamics). In the early years both ergodic theory and operator algebras benefitted both separately and together from a common viewpoint of operators on Hilbert space, but the eventual development in dynamics of combinatorial and probabilistic methods, in conjunction with an emphasis on asymptotic over local structural phenomena, seemed at a certain point to cause the two to drift apart. It is certainly true that dynamics has never ceased to provide a rich source of examples and inspiration in operator algebras, but it is only the last few decades that operator algebra theory has really been able to repay its debts through the promotion of a certain kind of abstract structural viewpoint that links it up with the theory of orbit equivalence and questions of rigidity, finite approximation, and tileability in the study of general groups and their actions (what is often nowadays compiled under the rubric "measured group theory").

One of the major themes that has long guided progress in both ergodic theory and operator algebra theory is the linkage between measure and topology, not only at the direct technical level (as one can see for example in the variational principle in dynamics and in the study of traces on C^*-algebras) but also at the level of analogy. This latter kind of connection, involving the identification of fruitful conceptual correspondences, has played out with spectacular consequences in the classification theory of amenable operator algebras. Indeed the celebrated work of Connes and Haagerup on the von Neumann algebra side not only gave us a classification of amenable (i.e., injective) factors that paralleled the work of Elliott on AF C^*-algebras, but has also served as an invaluable resource of techniques and ideas in the much more ambitious classification program that evolved out of the AF framework, a program which in its simple unital form has now essentially been consummated, after many years of research by many hands, through a felicitous combination of papers by Gong–Lin–Niu [8], Elliott–Gong–Lin–Niu [6], and Tikuisis–White–Winter [17] (these treat the stably finite case, with the purely infinite case having been handled earlier by Kirchberg and Phillips in the 1990s).

In the C*-algebra world, counterexamples of Toms and Rørdam based on work of Villadsen showed that amenability (or, as it is more commonly known in this setting, nuclearity) by itself is insufficient for classifiability by standard invariants (K-theory and traces), and a major goal of the Elliott program has been to formulate the right abstract regularity property that for the purposes of classification would replace amenability. We now know this role to be fulfilled by the nuclear dimension of Winter and Zacharias. The idea of such a dimensional invariant based on completely positive approximation and order-zero maps was a driving force in the novel approach to classification that Winter developed in the 2000s, and an influential part of this project has been the Toms–Winter conjecture postulating the equivalence of finite nuclear dimension, $\mathcal{Z}$-stability, and strict comparison for simple separable unital nuclear C*-algebras. In addition to its technical utility in classification arguments, the property of $\mathcal{Z}$-stability, itself a kind of finite-dimensional embeddability via order-zero maps, has turned out be a considerably more flexible condition to verify in C*-crossed products on the basis of underlying dynamical data.

It is the breakthroughs of Matui and Sato on the Toms–Winter conjecture [10, 11] that bring us to the defining theme of the workshop. In this work Matui and Sato brought von Neumann algebra techniques to bear in a surprisingly direct way on problems of a C*-algebraic nature, announcing a new phase in the interplay between measure and topology within operator algebra theory. These methods and ideas have been widely influential, and in particular have paved the way to further advances on the Toms–Winter conjecture leading to the recent full confirmation of its hypothesized equivalence between finite nuclear dimension and $\mathcal{Z}$-stability in the simple separable unital nuclear case [2]. In the domain of topological dynamics, with completely independent motivation coming from problems in entropy theory, Downarowicz and Zhang showed that amenable groups can be exactly tiled using finitely many Følner shapes, yielding a refinement of the Ornstein–Weiss tileability that can be viewed as a hybridization of topological and measure-theoretic perspectives [5]. These apparently disparate developments were soon discovered to be closely related through the fulcrum of $\mathcal{Z}$-stability, with the Toms–Winter conjecture now coming to serve as the passport to classifiability for a large swath of crossed products. The aim of the workshop was to consolidate and promote all of these ideas operating at the intersection of measure and topology, and in particular to explore how they play out within the classification theory of C*-algebras and in the study of dynamical and discrete structures that represent its basic source of examples and applications.

One of the unusual and very timely opportunities that the workshop afforded was an in-depth exposition of a new approach to the stably finite classification due to José Carrión, Jorge Castillejos, Samuel Evington, James Gabe, Christopher Schafhauser, Aaron Tikuisis, and Stuart White. This work traces its origins to a prior BIRS workshop and combines von Neumann algebra methods inspired by Connes and Haagerup with the powerful KK-theoretic methodology recently developed by Schafhauser, very much exemplifying the theme of the meeting and providing a striking illustration of the simplifying power of the measure-theoretic perspective in the analysis of topological structure. The entire constellation of ideas was presented in a series of four lectures, the first by Carrión on the classification of *-homomorphisms, the second by Evington on complemented partitions of unity and uniform property Gamma (the latter being the crucial tool in [2] for establishing the equivalence of of finite nuclear dimension and $\mathcal{Z}$-stability in the Toms–Winter conjecture), the third by Gabe highlighting the similarities with the purely infinite classification and speculating on the possibility of a truly unified theory, and the fourth by Castillejos on applications of complemented partitions of unity and uniform property Gamma. Talks on nuclear dimension were delivered by Stuart White and Wilhelm Winter, the first on obtaining estimates in the presence of $\mathcal{O}_\infty$-stability and the second on a relativization to sub-C*-algebras. In the non-unital domain, Huaxin Lin reported on classification and range results in the non-unital case obtained in collaboration with George Elliott, Guihua Gong, and Zhuang Niu [7] and with Guihua Gong.

These presentations on classification were augmented by a discussion of some of the ramifications of uniform property Gamma for the study of crossed products in the talks of Hung-Chang Liao on the small boundary property and almost finiteness and of Zhuang Niu on radius of comparison and mean dimension for actions of $\mathbb{Z}^d$ and groups of subexponential growth [12, 13]. These represent two approaches to the question of deciding when a free minimal action of an amenable group on a compact metrizable space yields a classifiable crossed product, a problem which can be traced back to the early days of classification theory as one of its principal sources of motivation and about which there is now some optimism of finally being able to attain a more or less general conclusion. In a complementary direction, Karen Strung showed us how many classifiable C*-algebras that may not be expressible as crossed products can nevertheless be realized dynamically by using the equivalence relation that naturally arises from the breaking of orbits in a $\mathbb{Z}$-action [14]. This brings us more into line with the measure-theoretic perspective of von Neumann algebras, where orbit breaking is already directly built into the structure of the crossed product, and opens up a wellspring in the search for model algebras in classification. Viewing actions on C*-algebras as objects in their own right, Gábor Szabó presented a categorical framework, anchored in the relation of cocycle conjugacy, for establishing equivariant versions of the core components and statements of the Elliott classification program [16]. Coming back to the question of how discrete data transfers into C*-algebra structure, but now in the context of k-graph C*-algebras, Elizabeth Gillaspy discussed the relation between Morita equivalence and moves on the graph, with an eye towards a longer-term effort to establish the kind of classification theorem that Eilers, Restorff, Ruiz, and Sørensen obtained in the ordinary graph framework. On the groupoid front, Charles Starling presented an equivalent set of conditions for the simplicity of a C*-algebra associated to an étale groupoid, resolving a question about the simplicity of a non-Hausdorff example coming from the Grigorchuk group [3], while Volodymyr Nekrashevych demonstrated that the dynamic asymptotic dimension of the groupoid of germs associated to a locally expanding self-covering of a compact space is equal to the covering dimension of the space, and in particular is finite, which brings these specimens under the compass of classification.

We also obtained a glimpse into rigidity phenomena, a topic which looks to be one of the next major horizons in C*-algebra theory following a long and impressive line of development over the last two decades in the domains of von Neumann algebras and measure-preserving dynamics. In this direction we heard talks by Hanfeng Li on entropy and Shannon orbit equivalence [9], by Yuhei Suzuki on “tight” inclusions of C*-algebras [15], and by Mehrdad Kalantar on representation rigidity for groups. The representation theme was also taken up by Kristin Courtney, who spoke on amalgamated free products of residually finite-dimensional C*-algebras [4], and Rufus Willett, who spoke on stability questions connected to index theory and on their relevance to classification theory.

All in all, the workshop gave us a vivid picture of C*-algebra theory at a historic crossroads, on the crest of spectacular advances which have not only resulted in definitive classification theorems but also delivered powerful new tools that promise to usher in new chapters in the study of regularity, homogeneity, and rigidity in dynamics and operator algebras, both within and beyond the realm of amenability.

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Chapter 20

Random Matrix Products and Anderson Localization (19w5086)

September 15 - 20, 2019

Organizer(s): David Damanik (Rice University), Anton Gorodetski (University of California Irvine)

In 1977 Philip Anderson shared the Nobel Prize in Physics with his doctoral thesis advisor John van Vleck and his collaborator Nevill Mott. The Nobel Prize was awarded “for their fundamental theoretical investigations of the electronic structure of magnetic and disordered systems”, or, in other words, for the discovery of what is nowadays called *Anderson localization*. In condensed matter physics, Anderson localization is the absence of diffusion of waves in a random (disordered) medium. A popular, though not quite equivalent, mathematical justification of (spectral) Anderson localization is pure point spectrum of the corresponding Schrödinger operator with random potential, along with exponentially decaying eigenfunctions.

Many random models aside from Schrödinger operators with potentials given by iid random variables at each site of a finite-dimensional lattice have been considered, for example sparse random potentials, decaying random potentials, the “trimmed” Anderson model, and the Anderson model on regular trees. But most of the existing methods of proof either require some form of absolute continuity of the randomness (e.g., the Kunz-Souillard method, the fractional moment method, or spectral averaging), or use a highly involved and technically challenging machinery (e.g. multiscale analysis). At the same time, recently it became clear that theory of random matrix products can be used to provide more geometrical and transparent proofs of Anderson Localization, at least in 1D case (see the extended abstracts of talks by Jake Fillman, Victor Kleptsyn, Tom VandenBoom, and Xiaowen Zhu below). New results were obtained in higher dimensional case as well, see the extended abstract of Charles Smart below.

The workshop was organized to bring together people who contributed to the recent progress in the field, as well as both experts and graduate students specializing in the areas that are directly related to random matrix products and/or Anderson Localization.

The report consists of two sections. In the first one we collected some of the open problems that were presented at the problem sessions that were organized during the workshop. Also, the participants were requested to provide the extended abstracts of the talks, that would contain the formal statements of the main results that were presented, and would be useful as an ”entry point” to the subject. The second one consists of the extended abstracts that were provided by the participants.

Open Problems

Here we provide the list of open problems that were presented during the problem sessions organized at the workshop. The participants were encouraged to share open problems related to the topic of the workshop that they are familiar with and find interesting, even if a problem is well known to the community and was initially formulated long time ago.

Problems presented by Jake Fillman (Texas State University)

Given an irrational $\alpha \in \mathbb{R}$, the skew-shift is a dynamical system that takes place on the 2-torus $\mathbb{T}^2 := \mathbb{R}^2/\mathbb{Z}^2$. The dynamics are given by $T = T_\alpha$:

$$T(\theta_1, \theta_2) := (\theta_1 + \alpha, \theta_1 + \theta_2), \quad (\theta_1, \theta_2) \in \mathbb{T}^2.$$

For each $\boldsymbol{\theta} = (\theta_1, \theta_2) \in \mathbb{T}^2$, one defines a potential $V_{\boldsymbol{\theta}} \in \ell^\infty(\mathbb{Z})$ via

$$V_{\boldsymbol{\theta}}(n) = 2\cos(2\pi(P_2(T^n\boldsymbol{\theta}))), \quad n \in \mathbb{Z},$$

where $P_2(\theta_1, \theta_2) = \theta_2$. Then, for each $\boldsymbol{\theta} \in \mathbb{T}^2$, and $\lambda \in \mathbb{R}$, one has a Schrödinger operator $H_{\boldsymbol{\theta},\lambda}$ given by

$$[H_{\boldsymbol{\theta},\lambda}\psi](n) = \psi(n-1) + \lambda V_{\boldsymbol{\theta}}(n)\psi(n) + \psi_{n+1}.$$

By standard arguments, there is a fixed set Σ_λ such that $\Sigma_\lambda = \sigma(H_{\boldsymbol{\theta},\lambda})$ for all $\boldsymbol{\theta} \in \mathbb{T}^2$. We proposed the following open problems:

1. Prove or disprove that Σ_λ is an interval or has at most finitely many gaps for all $\lambda > 0$.
2. Prove or disprove that the Lyapunov exponent of $H_{\boldsymbol{\theta},\lambda}$ is positive for all $\lambda \neq 0$.
3. Prove or disprove that the family $\{H_{\boldsymbol{\theta},\lambda}\}_{\boldsymbol{\theta}\in\mathbb{T}^2}$ enjoys Anderson localization for any $\lambda \neq 0$.

We note that Problem 2 is easily solved for $|\lambda| > 1$ by Herman's estimate; the open problem is then for $\lambda \in [-1, 1] \setminus \{0\}$.

Problems presented by Anton Gorodetski (University of California, Irvine)

One of the most basic results in the theory of the 1D ergodic Schrödinger operators is the theorem by Pastur that claims that the spectrum is a compact set that is the same for almost every initial condition (i.e. for almost all phases). In particular, in the case of a potential given by iid random variables, it is known that the almost sure spectrum is a finite union of intervals. The statement certainly cannot hold in general in the non-stationary setting, i.e. for a potential given by independent but not identically distributed variables. At the same time, due to Kolmogorov zero-one law, the almost sure essential spectrum is well defined in this case. *Is it possible to give a description of the essential spectrum (as a set) in this case?* It is known that the essential spectrum does not have to be a finite union of intervals, see the extended abstract of the talk by A.Gorodetski below. *Is it true that in the case of the potential given by independent random variables with variation uniformly bounded away from zero the essential spectrum must contain an interval?*

An attempt to construct a counterexample that would answer the latter question we were trying to consider a potential given by $V_1(n) + V_2(n)$, where $\{V_1(n)\}$ is a Fibonacci potential with large coupling, and $\{V_2(n)\}$ is an Anderson-Bernoulli potential. *What is the spectrum (as a set) of the corresponding Schrödinger operator? Is it a Cantor set? Cantorval? Does it contain an interval?*

Problems presented by Nishant Rangamani (University of California, Irvine)

We begin with the set-up of the problem. Let I be a compact interval and suppose for each $E \in I$ we have a family of independent and identically distributed random matrices (i.i.d.) $Y_1^E, \ldots, Y_n^E, \ldots$ in $SL_2(\mathbb{R})$. Suppose further that the smallest closed subgroup generated by the matrices is strongly irreducible and contracting and $\mathbb{E}[\log^+ ||Y_i^E||] < \infty$. Under these conditions, Kingman's subadditive ergodic theorem together with Furstenberg's theorem imply that the Lyapunov exponent which can be defined (for fixed E) as $\lim_{n\to\infty} \frac{1}{n} \log ||Y_n^E \cdots Y_1^E||$ exists almost surely and is strictly positive.

The next development along these lines revolved around obtaining further analogs of results for i.i.d. real random variables (e.g. central limit theorem, large deviations, etc.). These developments built around the work of Furstenberg and was carried out by Guivarc'h, Goldsheid, Le Page, and Raugi (among many other authors as well).

In particular, in 1982, Le Page proved analogs of both central limit theorem and large deviation theorems for products of i.i.d. matrices (under appropriate moment condition and a condition on the smallest closed subgroup of $SL_2(\mathbb{R})$ generated by the matrices - strong irreducibility and contracting). These results were later extended to the matrix elements of such products by Tsay. However, these results are all obtained under a moment condition. In particular, it is required that $\mathbb{E}[\exp(\log^+ ||M||)] < \infty$. This is known as having a finite exponential moment. We note that this material and additional background is well covered in the monograph by Bougerol and Lacroix[1].

Thus, it is natural to ask what happens in the absence of such a moment condition.

In particular, can estimates be made as to the speed of the convergence of the products (and their matrix elements) when there is no exponential moment? Towards this end, there has been recent work by Cagri Sert[2] which identifies a convex rate function (under no moment condition) through which a weak large deviation principle can be stated. However, the specifics of the rate function can only be identified in the regime of an exponential moment and it remains desirable to obtain results which link the strength of the moment to the rate at which the random products deviate from their mean.

We state Tsay's theorem for large deviations of the matrix elements below in order to illustrate what types of estimates are available with an exponential moment. We note that it is likely that the rate at which the matrix elements converge to the mean reflects the strength of the moment and in the absence of an exponential moment, one should in turn expect slower convergence to 1 in the probabilities below.

Theorem.[3] *Suppose I is a compact interval and for each $E \in I$, $Y_1^E, \ldots, Y_n^E, \ldots$ are i.i.d. random matrices such that the smallest closed subgroup of $SL_2(\mathbb{R})$ generated by the matrices is strongly irreducible and contracting. In addition, suppose $\mathbb{E}[\exp(\log^+ ||Y_1^E||)] < \infty$. Then, for any $\varepsilon > 0$, there is an $\eta > 0$ and an N such that for any $E \in I$, any unit vectors u, v, and $n > N$,*

$$\mathbb{P}[e^{(\gamma(E)-\varepsilon)n} \leq |\langle Y_n^E \cdots Y_1^E u, v\rangle| \leq e^{(\gamma(E)+\varepsilon)n}] \geq 1 - e^{-\eta n}. \tag{0.1}$$

Problems presented by Xiaowen Zhu (University of California, Irvine)

Open problem: Prove strong dynamical localization w.r.t. uniform distance in multi-particle model.

The multi-particle model can be defined as follows:

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Let $H_\omega : l^2(\mathbb{Z}^{nd}) \to l^2(\mathbb{Z}^{nd})$, where n is the number of the particles and d is the dimension of the space.
Let $\mathbf{x} = (x_1, x_2, \cdots, x_n) \in \mathbb{Z}^{nd}$ where each $x_i \in \mathbb{Z}^d$ will denote the position of the i-th particle. For future convenience, denote $x_i = (x_i^1, \cdots, x_i^d)$, where $x_i^j \in \mathbb{Z}$.
Let $V_\omega(x_i) = \omega_{x_i}$ be i.i.d random variables with single-site distribution μ supported on $\mathbb{R}$ that is bounded and non-trivial (supported on more than one point).
Define

$$(H_\omega\psi)(\mathbf{x}) = (\triangle_{nd}\psi)(\mathbf{x}) + \sum_i V_\omega(x_i) + \sum_{1\le i<j\le n} U(x_i - x_j),$$

where $\triangle_{nd}$ is discrete Laplacian on $l^2(\mathbb{Z}^{nd})$, $U : l^2(\mathbb{Z}^d) \to l^2(\mathbb{Z}^d)$ is the short-range interaction, so we require $U(x) = U(-x)$ and $U(x) = 0$ if $|x| > r$ for some constant $r > 0$.

In order to introduce that, we need definition of two different distance for $\mathbf{x}, \mathbf{y} \in \mathbb{Z}^{nd}$, that is the uniform distance $||\mathbf{x}-\mathbf{y}||_\infty$ and Hausdorff distance $d_H(\mathbf{x}, \mathbf{y})$:

$$||\mathbf{x}-\mathbf{y}||_\infty = \max_i \max_j |x_i^j - y_i^j|$$

$$d_H(\mathbf{x}, \mathbf{y}) = \max\{\max_i \min_k ||x_i - y_k||, \max_i \min_k ||y_i - x_k||\}$$

where $||x_i - y_k|| = \max_{1\le j\le n} |x_i^j - y_k^j|$.
Note that $d_H(\mathbf{x}, \mathbf{y}) \le ||\mathbf{x}-\mathbf{y}||_\infty$. And with this notation, $d_H(\mathbf{x}, \mathbf{y}) < L$ if and only if $\forall x_i$, $\exists y_k$ such that $||x_i - y_k|| < L$, and $\forall y_i$, $\exists x_k$ such that $||y_i - x_k|| < L$.

What we know about this model is Anderson localization and strong dynamical localization w.r.t. Hausdorff distance, i.e.

$$\mathbb{E}(\sup_{t\in\mathbb{R}} | < \delta_{\mathbf{x}}, e^{-itH_\omega}\delta_{\mathbf{y}} > |) \le e^{-Cd_H(\mathbf{x},\mathbf{y})}$$

What is unknown is strong dynamical localization w.r.t. infinity distance, i.e.

$$\mathbb{E}(\sup_{t\in\mathbb{R}} | < \delta_{\mathbf{x}}, e^{-itH_\omega}\delta_{\mathbf{y}} > |) \le e^{-C||\mathbf{x}-\mathbf{y}||_\infty}$$

This problem is interesting because of the physics interpretation: We know in the random system in $\mathbb{Z}^d$, if there are only one particle in low energy, the probability that it escapes to some point far away decay exponentially by the strong dynamical localization. Now consider n particles, if one starts with the intial state where all n particals are gathered at the same position, say 0, and wondered what's the probability of one of them escaping to some point far away, according to strong dynamical localization w.r.t. uniform distance, you get no information since the Hausdorf distance of this two states of positions are 0. But since even for just one particle, the probability of escape is exponentially small, it makes sense to guess that in this case, the probability of escape is exponentially small, which will be implied by strong dynamical localization w.r.t. uniform distance. One could also think about the case you start with all particles gathered together and all except one has escaped to some where far away, which should be even smaller. This can't be recognized through dynamical localization w.r.t. Hausdorff distance as well.

Presentation Highlights

Here we provide the extended abstracts of the talks that were given by the participants of the workshop.

Random matrix products and random dynamical systems

by Peter Baxendale (University of Southern California)

This tutorial and historical survey was in two parts. The first part considered the connection between random matrix products and random dynamical systems. The random matrices are assumed to form a stationary sequence of $d \times d$ matrices; the restriction to $SL(d, \mathbb{R})$ is unnecessary and is not applicable to dissipative stochastic systems. The concept of multiplication of random matrices extends to composition of random mappings, and hence to random dynamical systems. An important concept is that of the associated skew-product flow. It is in this setting that the multiplicative ergodic theorem (giving rise to the Lyapunov spectrum) and the associated local stable manifold theorem (justifying the use of the linearized system to approximate the underlying non-linear system) can be applied. See [1, 4].

The second part showed how some of these ideas can be used in the analysis of a stochastic bifurcation scenario for a damped and random excited non-linear harmonic oscillator. The linearized system is a 2-dimensional linear stochastic differential equation with top Lyapunov exponent $\lambda = \lambda(\beta, \sigma)$ depending on the coefficient of linear dissipation β and the noise intensity σ. The calculation of λ using the Fursteberg-Khas'minskii formula will be discussed. When $\lambda < 0$ it is shown that both the linearization and the underlying non-linear system are almost-surely stable. However when $\lambda > 0$ the non-linear effects become significant, and the behavior of the non-linear system for small positive λ will be determined using information from the moment Lyapunov function. The scenario when the parameters (β, σ) are varied in such a way that λ passes through 0 is a stochastic version of the deterministic Hopf bifurcation. See [2, 3].

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Random perturbations of hyperbolic dynamics

by Florian Dorsch (Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)

We consider a random dynamical system on an L-dimensional sphere $\mathbb{S}^{\mathsf{L}}$, $\mathsf{L} \geq 2$, given by

$$v_n \;=\; \mathcal{T}_n \cdot v_{n-1}\,, \qquad n \in \mathbb{N}\,, \tag{0.2}$$

where the action $\cdot\;: \mathrm{GL}(\mathsf{L}+1,\mathbb{R}) \times \mathbb{S}^{\mathsf{L}} \to \mathbb{S}^{\mathsf{L}}$ of the general linear group is

$$\mathcal{T} \cdot v \;=\; \mathcal{T}v\|\mathcal{T}v\|^{-1}\,, \tag{0.3}$$

and the random matrices $\mathcal{T}_n$ are of the form

$$\mathcal{T}_n \;=\; \mathcal{R}\,(\mathbf{1} \,+\, \lambda r_n U_n)\,, \qquad n \in \mathbb{N}\,. \tag{0.4}$$

Here, the matrix $\mathcal{R}$ is supposed to be deterministic and hyperbolic, *i.e.*, it is of the form

$$\mathcal{R} = \mathrm{diag}(\kappa_{\mathsf{L}+1}, \ldots, \kappa_1)\,, \qquad\qquad \kappa_1 \geq \cdots \geq \kappa_{\mathsf{L}+1} > 0 \tag{0.5}$$

and $\{r_n\}_{n\in\mathbb{N}}$ and $\{U_n\}_{n\in\mathbb{N}}$ are assumed to be sequences of independent and identically distributed random variables taking on values in $[0,1]$ and $\mathrm{O}(\mathsf{L}+1)$, respectively. Moreover, we assume that $r_n \not\equiv 0$ and that the U_n are distributed according to the Haar measure on $\mathrm{O}(\mathsf{L}+1)$.

Each vector $v = (v_1, \ldots, v_{\mathsf{L}+1})^{\mathsf{T}} \in \mathbb{R}^{\mathsf{L}+1}$ is split into its upper part $\mathfrak{a}(v) \in \mathbb{R}^{\mathsf{L}_\mathfrak{a}}$, middle part $\mathfrak{b}(v) \in \mathbb{R}^{\mathsf{L}_\mathfrak{b}}$ and lower part $\mathfrak{c}(v) \in \mathbb{R}^{\mathsf{L}_\mathfrak{c}}$ via

$$\mathfrak{a}(v) \;=\; (v_1, \ldots, v_{\mathsf{L}_\mathfrak{a}})^{\mathsf{T}}\,, \qquad \mathfrak{b}(v) \;=\; (v_{\mathsf{L}_\mathfrak{a}+1}, \ldots, v_{\mathsf{L}_\mathfrak{a}+\mathsf{L}_\mathfrak{b}})^{\mathsf{T}}\,, \qquad \mathfrak{c}(v) \;=\; (v_{\mathsf{L}_\mathfrak{a}+\mathsf{L}_\mathfrak{b}+1}, \ldots, v_{\mathsf{L}+1})^{\mathsf{T}}\,,$$

where $(\mathsf{L}_\mathfrak{a}, \mathsf{L}_\mathfrak{b}, \mathsf{L}_\mathfrak{c}) \in \mathbb{N}\times\mathbb{N}\times\mathbb{N}$ are such that $\mathsf{L}_\mathfrak{a} + \mathsf{L}_\mathfrak{b} + \mathsf{L}_\mathfrak{c} = \mathsf{L}+1$. Associated to that partition, let us introduce the *macroscopic gap* $\gamma = \gamma\,(\mathcal{R}, \mathsf{L}_\mathfrak{b}, \mathsf{L}_\mathfrak{c})$ between the upper and lower parts by

$$\gamma \;=\; \min\left\{1\,,\; \frac{\kappa_{\mathsf{L}_\mathfrak{c}}^2}{\kappa_{\mathsf{L}_\mathfrak{b}+\mathsf{L}_\mathfrak{c}+1}^2} \,-\, 1\right\} \;\in\; [0,1]\;.$$

If the macroscopic gap γ is positive, the entries of the upper part $\mathfrak{a}$ can be seen as the repulsive entries of the hyperbolic action. Therefore, the deviation of the random path $\{v_n\}_{n\in\mathbb{N}}$ from the attractive part of the phase space can be measured as the norm of the upper part $\|\mathfrak{a}(v_n)\|$. The main result provides a quantitative bound on the expectation value of $\|\mathfrak{a}(v_N)\|^2$ for sufficiently large N.

Theorem [1]. *Suppose that* $(\mathsf{L}_\mathfrak{a}, \mathsf{L}_\mathfrak{b}) \neq (1,1)$ *and* $\gamma > 0$*. Then, for all* $0 < \lambda \leq \frac{1}{4}$ *there exist* $N_0 = N_0(\mathsf{L}, \mathsf{L}_\mathfrak{c}, \lambda) \in \mathbb{N}$ *such that*

$$\mathbb{E}\,\|\mathfrak{a}(v_N)\|^2 \;\leq\; 2\left(\frac{\mathsf{L}+1}{\mathsf{L}_\mathfrak{a}+\mathsf{L}_\mathfrak{b}}\right)^{\frac{\mathsf{L}_\mathfrak{a}+\mathsf{L}_\mathfrak{b}-2}{\mathsf{L}_\mathfrak{c}+2}} \left(\frac{6}{\gamma}\,\frac{\mathsf{L}_\mathfrak{a}}{\mathsf{L}_\mathfrak{c}}\,\lambda^2\right)^{\frac{\mathsf{L}_\mathfrak{c}}{2+\mathsf{L}_\mathfrak{c}}} \tag{0.6}$$

for all $N \geq N_0$ *and* $v_0 \in \mathbb{S}^{\mathsf{L}}$.

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Sufficient criteria for the application of Fürstenberg's theorem

by Jake Fillman (Texas State University)

The talk describes simple sufficient criteria that enable one to apply the classical theorem of H. Fürstenberg on products of random matrices to deduce positive Lyapunov exponents. To begin, let us recall a few relevant definitions. A subgroup $G \subseteq \mathrm{SL}(2,\mathbb{R})$ is called strongly irreducible if there does not exist a finite set $\emptyset \neq \Lambda \subseteq \mathbb{RP}^1$ such that $g\Lambda = \Lambda$ for every $g \in G$. We call G a type-F subgroup if G is closed, non-compact, and strongly irreducible.

Given a Borel probability measure ν supported in $\mathrm{SL}(2,\mathbb{R})$, consider a sequence $A_1, A_2, \ldots$ of iid random variables with common distribution ν. One is interested in the Lyapunov exponent:

$$L(\nu) = \lim_{n\to\infty} \frac{1}{n} \int_{\mathrm{SL}(2,\mathbb{R})^n} \log \|A_n A_{n-1} \cdots A_1\| \, d\nu^n.$$

In essentially all proofs of localization in the 1D Anderson model, positivity of the Lyapunov exponent supplies the key input to begin a localization proof, although there are notable exceptions, (e.g. [9, 10]). Classically, one used multi-scale analysis to prove localization [3], but there have been several modern approaches using one-dimensional tools (hence yielding simpler proofs) [1, 7, 8].

Theorem 20.0.1 (Fürstenberg [6])**.** *Let ν be a probability measure supported in $\mathrm{SL}(2,\mathbb{R})$ with $\mathbb{E}(\log\|g\|) < \infty$ and let G_ν denote the smallest closed subgroup of $\mathrm{SL}(2,\mathbb{R})$ containing $\mathrm{supp}\nu$. If G_ν is a type-F subgroup of $\mathrm{SL}(2,\mathbb{R})$, then $L(\nu) > 0$.*

The main theorem of [2] gives simple criteria to check whether one may apply Theorem 20.0.1 for analytic one-paramter families.

Theorem 20.0.2 (Bucaj, Damanik, F., Gerbuz, VandenBoom, Wang, Zhang [2])**.** *Let $A, B : \mathbb{C} \to \mathrm{SL}(2,\mathbb{C})$ be entire functions such that:*

(i) *If $z \in \mathbb{R}$, then $A(z), B(z) \in \mathrm{SL}(2,\mathbb{R})$,*

(ii) $\mathrm{Tr}\, A(z)$ *and* $\mathrm{Tr}\, B(z)$ *are non-constant,*

(iii) *if* $\mathrm{Tr}\, A(z) \in [-2,2]$ *or* $\mathrm{Tr}\, B(z) \in [-2,2]$*, then $z \in \mathbb{R}$, and*

(iv) $[A(z), B(z)] := A(z)B(z) - B(z)A(z) \neq 0$ *for at least one $z \in \mathbb{C}$.*

Then, there is a discrete set $D \subseteq \mathbb{R}$ *with the property that the closed subgroup generated by* $A(x)$ *and* $B(x)$ *is a type-F subgroup of* $\mathrm{SL}(2, \mathbb{R})$ *for any* $x \in \mathbb{R} \setminus D$.

The key observation is that one can encode the failure of the hypotheses of Fürstenberg's theorem by the vanishing of analytic quantities. Namely, if $\mathrm{Tr}\, A$, $\mathrm{Tr}\, B$, and $\det[A, B]$ are all nonzero, then one can show that the closed group generated by A and B is of type F.

Critically, hypotheses (i)–(iii) are automatically satisfied in essentially any model based on Schrödinger operators, leaving (iv) as the relevant "nontriviality condition". One can use Theorem 20.0.2 to easily verify positivity of the Lyapunov exponent in several models, such as the continuum Anderson model [2], Schrödinger operators arising from a decomposition of radial metric tree graphs [4], and 1D Schrödinger operators with random point interactions [5]. [Joint work with V. Bucaj, D. Damanik, V. Gerbuz, T. VandenBoom, F. Wang, Z. Zhang]

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Exponential growth of products of non-stationary Markov-dependent matricest

by Ilya Goldsheid (Queen Mary, University of London)

1. Introduction

Let $(g_n)_{n\geq 1}$ be a sequence of matrices, $g_n \in SL(m,\mathbb{R})$ and set

$$S_n = g_n ... g_1 \tag{0.7}$$

In the seminal 1963 paper [2], H. Furstenberg proved, among others, the following fact.

Theorem 20.0.3. *Suppose that:*

(a) $(g_n)_{n\geq 1}$ is a sequence of independent identically distributed (i.i.d.) random matrices with distribution μ.

(b) The group $\bar{G}_\mu$ generated by the support of μ does not preserve any probability measure on the unit sphere in $\mathbb{R}^m$. (The relevant definitions can be found below.)

Then the following limit (called the top Lyapunov exponent of the product S_n) exists with probability 1 and is strictly positive:

$$\lim_{n\to\infty} \frac{1}{n} \ln \|S_n\| = \gamma > 0. \tag{0.8}$$

In 1980 A. Virtser [36] extended this result result to the case of stationary Markov chains.

The purpose of this work is to establish sufficient conditions for exponential growth of products of Markov-dependent matrices in the case when the underlying Markov chain is non-stationary.

Remark. *In fact, Furstenberg proved, under the additional condition of strong irreducibility of $\bar{G}_\mu$, that for any unit vector x a.s. $\lim_{n\to\infty} \frac{1}{n} \ln \|S_n x\| = \gamma$. We don't discuss this aspect of Furstenberg's result here.*

Products of *independent* non-identically distributed matrices were considered in the past. Here are some references.

Paper [1] by Delyon-Simon-Souillard deals with matrices arising in the theory of localization for Anderson model in dimension one with a potential decaying at infinity. These matrices are of the form

$$g_n = \begin{pmatrix} \lambda a_n q_n & -1 \\ 1 & 0 \end{pmatrix}, \tag{0.9}$$

where q_n are i.i.d. random variables, $\lambda > 0$ is a constant, and a_n satisfy $C_1|n|^{-\alpha} < |a_n| < C_2|n|^{-\alpha}$ for some positive constants $C_1,\ C_2,\ \alpha$ $(n \neq 0)$. The technique of [1] depends heavily on q_n being i.i.d. with a 'good' probability density function.

An earlier paper [3] by Simon, even though it does not explicitly consider products of matrices, easily implies interesting estimates for the speed of growth for products of matrices (0.9) with $\alpha = \frac{1}{2} - \varepsilon$ $(\varepsilon > 0)$. The independence of q_n's and the existence of their densities are extensively used in the proofs in this paper while the fact that the densities are the same is not that important (see remarks in [3, page 254]).

Finally, the results of papers by Shubin-Vakilian-Wolff [4], Wolff-Shubin [6], and Wolff [7] are perhaps most closely related to the results of this work. Paper [4] provides constructive estimates for the norm of an operator which is the average of a certain representation of $SL(2,\mathbb{R})$, where the average is computed over the distribution of the matrices. In tern, this result implies a constructive estimate for the rate of growth of products of matrices (0.9) with $\lambda = 1$, $a_n = 1$ and the distribution of q_n's being non-trivial (not concentrated at one point). We note that the exponential growth of such products follows from Furstenberg's theorem. However, the constructive estimates established in [4] imply more than that. Namely, they imply, under natural conditions, the exponential growth of the product of independent non-identically distributed matrices. The situation with the proof of localization is similar: formally speaking, the proof in [4] is given for the case of i.i.d. potentials; in fact, their proof works also for non-identically distributed potentials (see comments in [4, page 943]).

It is yet to be established which results from [1] can be extended to the case when the q_n's do not have a density function by using the estimates from [4].

In summary, the exponential growth of products of $m \times m$ matrices which are independent but not necessarily identically distributed can be deduced from the results obtained in [4], [6], and especially [7] (we shall comment on this statement later).

The non-stationary Markov-dependent sequences of matrices form a new class of matrices for which exponential growth of their products can be established. They include independent matrices as a particular case. In the case of independent matrices, our proofs are simpler than those in [7].

2. Statement of the main result

Our setting is as follows.

The Markov chain. Let $(X, \mathcal{B})$ be a measurable set (with $\mathcal{B}$ being the sigma-algebra of measurable subsets of the set X). Consider a Markov chain ξ_n, $n \geq 1$, with phase space X and initial distribution μ_1. For any $B \in \mathcal{B}$, set

$$k_n(x, B) = \mathbb{P}(\xi_{n+1} \in B \,|\, \xi_n = x).$$

We write $k_n(x, dy)$ for the corresponding transition kernel of the chain ξ_n.

Let μ_n be the distribution of ξ_n. As usual, for $n \geq 2$ and $B \in \mathcal{B}$ we have

$$\mu_n(B) = \mathbb{P}(\xi_n \in B) = \int_X \mu_{n-1}(dx) k_n(x, B).$$

We thus have a sequence of 'Markov related' measure spaces $(X, \mathcal{B}, \mu_n)$. Denote H_n the Hilbert space of μ_n-square integrable complex valued functions,

$$H_n = \{f : \; f : X \mapsto \mathbb{C}, \; \int_X |f(x)|^2 \mu_n(dx) < \infty\}$$

with the standard inner product: if f, $h \in H_n$ then

$$< f, h >_{H_n} = \int_X f(x) \bar{h}(x) \mu_n(dx).$$

Set

$$H_n^{(0)} = \{f \in H_n : \; \int_X f(x) \mu_n(dx) = 0\}.$$

The integral with respect μ_n will be denote $\mathbb{E}_n : \mathbb{E}_n(f) \equiv \int_X f(x)\mu_n(dx)$

Let $K_n : H_{n+1} \mapsto H_n$ be the operator defined by

$$(K_n f)(x) = \int_X k_n(x, dy) f(y).$$

Note that the operator K_n 'computes' the conditional expectation of $f(\xi_{n+1})$ conditioned on $\xi_n = x$ and it is easy to see that if $f \in H_{n+1}$ then $K_n f \in H_n$.

Denote K_n^0 the restriction of K_n to H_{n+1}^0. Note that if $\mathbb{E}_{n+1}(f) = 0$ then $\mathbb{E}_n(K_n f) = 0$, that is $K_n^0 : H_{n+1}^0 \mapsto H_n^0$.

The matrices. Let $g : X \mapsto SL(m, \mathbb{R})$ be a matrix-valued $\mathcal{B}$-measurable function on X. Define a sequence of random matrices g_j by setting $g_j = g(\xi_j), \; j \geq 1$. Let ν_j be the distribution of g_j, that is for a Borel subset Γ, $\Gamma \subset SL(m, \mathbb{R})$, we set

$$\nu_j(\Gamma) = \mathbb{P}(g(\xi_j) \in \Gamma).$$

By $\mathrm{supp}(\nu_j) \subset SL(m, \mathbb{R})$ we denote the support of ν_j.

For a distribution ν on $SL(m, \mathbb{R})$ we define a group G_ν as follows:

$$G_\nu = \text{ closed group generated by the set } \{g\bar{g}^{-1} \; : \; g, \, \bar{g} \in \mathrm{supp}(\nu)\}. \tag{0.10}$$

By $\mathcal{S}$ we denote the unit sphere in $\mathbb{R}^m$.

Definition. *For $g \in SL(m, \mathbb{R})$ and $u \in \mathcal{S}$ we define $g.u = gu/||gu||$. The induced action of g the set of probability measures on $\mathcal{S}$ is defined by $g\kappa(B) = \kappa(g.^{-1}B)$, where κ is a probability measure on $\mathcal{S}$ and B is a Borel subset of $\mathcal{S}$. We say that a probability measure κ on $\mathcal{S}$ is preserved by g if $\kappa(B) = (g\kappa)(B)$ for any Borel B. A group G preserves the measure κ on $\mathcal{S}$ if every $g \in G$ preserves κ.*

We suppose that the Markov chain ξ and the function g satisfy the following assumptions:

I. For some c, $0 \le c < 1$, for all $n \ge 1$

$$\|K_n^0\| \le c.$$

II. There is a set M of probability measures on $SL(m,\mathbb{R})$ which is compact with respect to weak convergence and such that:

(a) all ν_n belong to M,

(b) for any measure $\nu \in M$ the group G_ν does not preserve any probability measure on $\mathcal{S}$.

We are now in a position to state our main result:

Theorem 20.0.4. *Suppose that assumptions I, II are satisfied. Then there is a $\lambda > 0$ such that with probability 1*

$$\liminf_{n\to\infty} \frac{1}{n} \ln \|g_n \dots g_1\| \ge \lambda. \tag{0.11}$$

Remark. With a slight abuse of notation, we use $\|\cdot\|$ to denote the norm of matrices, functions, and operators. This makes many formulae look less cumbersome while their meaning is always obvious from the context.

3. The idea of the proof explained in a simplified setting

Suppose that matrices $g_n,\ n \ge 1$ are independent, μ_n is the distribution of g_n, $\mu_n \in M$. In this setting, $X = \mathcal{S}$ and therefore $\mu_n = \nu_n$. Our probability space is $\left(\mathcal{S}^{\mathbb{N}}, \prod_{j=1}^{\infty}\mu_j\right)$, where $\prod_{j=1}^{\infty}\mu_j = \mu_1 \times \mu_2 \times$ ..... The abbreviation a.s. means almost surely with respect to this product measure.

As before, we suppose that M is a compact set of probability measures on $SL(m,\mathbb{R})$ and that for any $\mu \in M$ the group G_μ does not preserve any probability measure on the unit sphere $\mathcal{S}$.

In this simplified setting, we prove Theorem 1 in three steps.

Step 1. Note that in order to prove (0.11) it suffices to show that there is a $c > 0$ such that

$$\mathbb{E}(\|S_n\|^{-\frac{m}{2}}) \le e^{-cn}. \tag{0.12}$$

Indeed, by the Markov inequality for any $\varepsilon > 0$

$$\mathbb{P}(\|S_n\| \le e^{\varepsilon n}) = \mathbb{P}(\|S_n\|^{-\frac{m}{2}} \ge e^{-\frac{m}{2}\varepsilon n}) \le e^{\varepsilon\frac{m}{2}n}\mathbb{E}(\|S_n\|^{-\frac{m}{2}}) \le e^{(\varepsilon\frac{m}{2}-c)n}.$$

If $\varepsilon < 2c/m$ the the Borel-Cantelli lemma implies that the set $\{n : \|S_n\| \le e^{\varepsilon n}\}$ is a.s. finite. This means that (0.11) holds a.s. for any $\gamma < 2c/m$.

Step 2. Let $L_2(\mathcal{S}, dx)$ be the Hilbert space of complex valued functions on $\mathcal{S}$ equipped with the Lebesgue measure dx which is normalized to 1. The inner product of $f,\ h \in L_2(\mathcal{S}, dx)$ is given by

$$< f, h >= \int_{\mathcal{S}} f(x)\bar{h}(x)dx.$$

Let $\mathbb{V}$ be the set of unitary operators in $L_2(\mathcal{S})$. Consider a unitary 'representation' $\rho : SL(m,\mathbb{R}) \mapsto \mathbb{V}$: the unitary operator $\rho(g) \equiv V_g$ acts on $f \in L_2(\mathcal{S})$ as follows:

$$V_g f(x) = f(g.x)||gx||^{-\frac{m}{2}}. \tag{0.13}$$

It is easy to verify that

$$||f|| = ||V_g f|| \quad \text{and that} \quad V_{g_1 g_2} = V_{g_2} V_{g_1}. \tag{0.14}$$

For $\mu \in M$, put

$$W_\mu = \int_{SL(m,\mathbb{R})} V_g d\mu(g).$$

Theorem 20.0.5. *If no probability measure on $\mathcal{S}$ is preserved by G_μ then $||W_\mu|| < 1$.*

Idea of the proof. We shall show that if $||W_\mu|| = 1$, then there is a probability measure on $\mathcal{S}$ which is preserved by G_μ.

The idea of the proof becomes particularly transparent if there is a function $f \in L_2(\mathcal{S}, dx)$ with $||f|| = 1$ and such that $||W_\mu f|| = 1$. So, let this be the case. Define $f_g = V_g f$ and $\varphi = W_\mu f = \int_{SL(m,\mathbb{R})} f_g d\mu(g)$. Then

$$1 = ||W_\mu f|| = \left|\left|\int_{SL(m,\mathbb{R})} f_g d\mu(g)\right|\right| \leq \int_{SL(m,\mathbb{R})} ||f_g|| d\mu(g) = 1$$

and hence

$$\left|\left|\int_{SL(m,\mathbb{R})} f_g d\mu(g)\right|\right| = 1.$$

Since the space $L_2(\mathcal{S}, dx)$ is uniformly convex, this equality takes place if and only if $f_g = \text{const}$ for μ-almost all $g \in SL(m, \mathbb{R})$. For instance, if we put

$$\varphi(x) = W_\mu f(x) = \int_{SL(m,\mathbb{R})} f_g(x) d\mu(g) \tag{0.15}$$

then for μ-almost all $g \in SL(m, \mathbb{R})$ and almost all $x \in \mathcal{S}$

$$\varphi(x) = f_g(x). \tag{0.16}$$

Equality (0.16) implies equality of measures with densities $|\varphi(x)|^2$ and $|f(g.x)|^2||gx||^{-m}$ respectively:

$$\int_{\mathcal{S}} \psi(x)|\varphi(x)|^2 dx = \int_{\mathcal{S}} \psi(x)|f(g.x)|^2||gx||^{-m} dx, \tag{0.17}$$

where ψ is any continuous function on $\mathcal{S}$. But then $\varphi = f_g$ for μ-almost all g (where once again the equality means the that the corresponding measures are equal). Since for any probability measure κ the measure $g\kappa$ is weakly continuous in g, we have that $f_{g_1} = f_{g_2}$ for any g_1 and g_2 from the support of μ and hence $f_{g_2 g_1^{-1}} = f$, which means that a measure with the density $|f|^2$ is preserved by any $g_2 g_1^{-1}$ with $g_1,\ g_2 \in \text{supp}\mu$.

If $\|W_\mu f\| < 1$ for every $f \in L_2(\mathcal{S}, dx)$ but $\|W_\mu\| = 1$ then there is a sequence of functions $f_n \in L_2(\mathcal{S}, dx)$ with $\|f_n\| = 1$ and such that $\lim_{n\to\infty} \|W_\mu f_n\| = 1$. We shall view the functions $|f_n|^2$ as densities of measures κ_n on $\mathcal{S}$, $d\kappa_n(x) = |f_n(x)|^2 dx$. Since $\mathcal{S}$ is a compact set, any such sequence has a weakly converging subsequence. So, we shall suppose from now on that $\lim_{n\to\infty} \kappa_n = \kappa$. The equalities which were used above would now hold only in the limit $n \to \infty$ and one concludes that $g_1\kappa = g_2\kappa$. This completes the proof of Theorem 20.0.5. □

Step 3. Since $\|S_n\| \geq \|S_n x\|$, $x \in \mathcal{S}$, (0.12) would follow from

$$\int_{\mathcal{S}} \mathbb{E}(\|S_n x\|^{-\frac{m}{2}}) dx \leq e^{-cn}. \tag{0.18}$$

Note next that

$$\|g_n ... g_1 x\|^{-\frac{m}{2}} = (V_{g_n ... g_1}\mathbf{1})(x) = (V_{g_1} ... V_{g_n}\mathbf{1})(x),$$

where $\mathbf{1}$ is the function on $\mathcal{S}$ which takes value 1 at every $x \in \mathcal{S}$. Therefore

$$\int_{\mathcal{S}} \mathbb{E}(\|S_n x\|^{-\frac{m}{2}}) dx = \mathbb{E}\left(\int_{\mathcal{S}} \|g_n ... g_1 x\|^{-\frac{m}{2}} dx\right)$$
$$= \mathbb{E}\left(\int_{\mathcal{S}} (V_{g_1} ... V_{g_n}\mathbf{1})(x) dx\right) = \mathbb{E}\left(< V_{g_1} ... V_{g_n}\mathbf{1}, \mathbf{1} >\right) =< \mathbb{E}\left(V_{g_1} ... V_{g_n}\right)\mathbf{1}, \mathbf{1} > .$$

Since the operators $V_{g_1},...,V_{g_n}$ are independent we obtain

$$\mathbb{E}\left(V_{g_1}...V_{g_n}\right)=\mathbb{E}\left(V_{g_1}\right)...\mathbb{E}\left(V_{g_n}\right)=W_{\mu_1}...W_{\mu_n}$$

Finally,

$$\int_{\mathcal{S}}\mathbb{E}(\|S_nx\|^{-\frac{m}{2}})dx=< W_{\mu_1}...W_{\mu_n}\mathbf{1},\mathbf{1}>\leq\|W_{\mu_1}\|...\|W_{\mu_n}\|\leq e^{-cn}, \tag{0.19}$$

where $c=\inf_{\mu\in M}(-\ln\|W_\mu\|)$. $\Box$

4. Additional comments

1. Theorem 20.0.5 is the main ingredient of the above proof. We could, instead of proving it, use a more general result from [7] (see Theorem 1 in this paper). However, our goal is to prove the exponential growth and for that we have to control the single concrete mapping (0.13) from $SL(m,\mathbb{R})$ into the space V which has properties (0.14) (and which is not quite a representation - though the difference is trivial). Our reliance on the general representation theory is almost non-existent and this, together with the simplicity of the above proof and the fact that it makes this work more self-contained justifies our approach.

2. In the context of products of matrices, operators W_μ were first explicitly defined in [36] where it was proved that the spectral radius of W_μ is less than 1. In the case of identically distributed independent g_n this fact implies Theorem 20.0.4. In fact, [36] starts with a more complicated version of this operator which allows one to control products of stationary Markov dependent matrices and, once again, the positivity of the Lyapounov exponent follows from the fact that the corresponding spectral radius is less than 1.

The full proof of our Theorem 20.0.4 requires an approach which makes use of a simplified version of constructions introduced and is more geometric than in that in this paper.

3. For matrices g_j of the form (0.9), important constructive estimates of $||W_\mu W_{\tilde{\mu}}||$ were obtained in [4]. They are seem to be optimal in some natural sense.

With a little more work, one could obtain constructive estimates also for $||W_\mu||$.

4. Furstenberg's theorem for the i.i.d. case follows from Theorem 20.0.4. If the identity matrix I is in the support $\mathrm{supp}\mu$ then our G_μ and the $\bar{G}_\mu$ from Theorem 20.0.3 are the same group. If $I\notin\mathrm{supp}(\mu)$, then we can apply our theorem to the measure $\tilde{\mu}=\frac{1}{2}\mu+\frac{1}{2}\delta_I$. It is easy to see that the Lyapunov exponent for $\tilde{\mu}$ is positive if and only if the Lyapunov exponent for μ is positive. This observation completes the proof of Furstenberg's theorem.

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Sums of Cantor sets and non-stationary Anderson-Bernoulli Model

by Anton Gorodetski (University of California, Irvine)

Questions on the structure of Sums of Cantor sets appear naturally in many areas of dynamical systems, number theory, and spectral theory. One can use the known machinery to give an example of a non-stationary Anderson-Bernoulli potential such that the almost sure essential spectrum of the corresponding discrete Schrödinger operator $H : l^2(\mathbb{Z}) \to l^2(\mathbb{Z})$ intersects an open interval at a Cantor set of zero measure. Construction is very explicit. Namely, choose any sequence $\{n_k\}_{k\in\mathbb{N}}$ of integers such that

$$n_k \to \infty \ \text{ and } \quad n_{k+1} - n_k \to \infty \quad \text{as} \quad k \to \infty.$$

We define the random potential in the following way:

$$V(n) = \begin{cases} 0 \text{ or } 1 \text{ with probability } 1/2, & \text{if } n \notin \{n_k\}; \\ 0 \text{ or } 100 \text{ with probability } 1/2, & \text{if } n \in \{n_k\}. \end{cases}$$

Theorem 20.0.6. *Almost sure essential spectrum of the operator H with the potential $\{V(n)\}$ defined above is a union of the interval $[-2, 3]$ and a Cantor set contained in the interval $[98, 102]$.*

To characterize the spectrum of an operator it will be convenient to use the following criterion:

Proposition 1. *Let $\{V(n)\}_{n\in\mathbb{Z}}$ be a bounded potential of the discrete Schrödinger operator H acting on $\ell^2(\mathbb{Z})$ via*

$$[Hu](n) = u(n+1) + u(n-1) + V(n)u(n). \tag{0.20}$$

Then we have the following:

1) Energy $E \in \mathbb{R}$ belongs to the spectrum of the operator H if and only if there exists $K > 0$ such that for any $N \in \mathbb{N}$ there is $m \in \mathbb{Z}$ and a unit vector $\bar{u}$, $|\bar{u}| = 1$, such that $|T_{[m,m+i],E}\,\bar{u}| \le K$ for all $|i| \le N$, where $T_{[m,m+i],E}$ is the product of transfer matrices given by

$$T_{[m,m+i],E} = \begin{cases} \Pi_{m+i-1,E}\dots\Pi_{m,E}, & \text{if } i>0;\\ \mathrm{Id}, & \text{if } i=0;\\ \Pi^{-1}_{m+i,E}\dots\Pi^{-1}_{m-1,E}, & \text{if } i<0,\end{cases}$$

and $\Pi_{n,E} = \begin{pmatrix} E-V(n) & -1 \\ 1 & 0 \end{pmatrix}$.

2) Energy $E \in \mathbb{R}$ belongs to the essential spectrum of the operator H if and only if there exists $K > 0$ such that for any $N \in \mathbb{N}$ there is a sequence $\{m_j\}_{j\in\mathbb{N}}, m_j \in \mathbb{Z}$, with $|m_j - m_{j'}| > 2N$ if $j \neq j'$, and unit vectors $\bar{u}_j$, $|\bar{u}_j| = 1$, such that $|T_{[m_j,m_j+i],E}\,\bar{u}_j| \le K$ for all $|i| \le N$ and all $j \in \mathbb{N}$.

For each $\omega \in \{0,1\}^{\mathbb{Z}}$ consider an operator $H_\omega : l^2(\mathbb{Z}) \to l^2(\mathbb{Z})$ given by the potential

$$V_\omega(n) = \begin{cases} 100, & \text{if } n=0;\\ \omega_n, & \text{if } n\neq 0.\end{cases}$$

There are uncountably many operators of this form. Each of them has exactly one eigenvalue in the interval $[98, 102]$. Let us denote this eigenvalue by E_ω.

Intersection of the almost sure essential spectrum of the operator H given by the potential $\{V(n)\}$ with the interval $[98, 102]$ is exactly $\cup_{\omega\in\{0,1\}^{\mathbb{Z}}} E_\omega$.

Notice that if $A > 2$, then the matrix of the form $\begin{pmatrix} A & 1 \\ -1 & 0 \end{pmatrix}$ has two eigenvalues, namely $\frac{A+\sqrt{A^2-4}}{2} > 1$ and $\frac{A\sqrt{A^2-4}}{2} = \left(\frac{A+\sqrt{A^2-4}}{2}\right)^{-1} < 1$. Let us denote the proectivizations of the corresponding eigenvectors by $x_1(A)$ and $x_2(A)$.

For an operator H_ω each transfer matrix $\Pi_{n,E}$, $n \neq 0$, must be either $\begin{pmatrix} E & 1 \\ -1 & 0 \end{pmatrix}$, or $\begin{pmatrix} E-1 & 1 \\ -1 & 0 \end{pmatrix}$, and we are interested in the regime where $E \in [98, 102]$. Let us denote by $I_1(E)$ the interval on S^1 between the points $x_1(E)$ and $x_1(E-1)$, and by $I_2(E)$ the interval between the points $x_2(E)$ and $x_2(E-1)$. Denote by $f_{n,E}$ the proectivization of the map $\Pi_{n,E}$. Then if $n \neq 0$, we have $f_{n,E}(I_1(E)) \subset I_1(E)$, and $f^{-1}_{n,E}(I_2(E)) \subset I_2(E)$. Moreover, $f_{n,E}|_{I_1(E)}$ and $f^{-1}_{n,E}|_{I_2(E)}$ are contractions for each $n \neq 0$. For a given $\omega \in \{0,1\}^{\mathbb{Z}}$ there exists exactly one point $z_\omega(E) \in I_1(E)$ such that

$$z_\omega(E) = \cap_{n\in\mathbb{N}} f_{-n,E} \circ \ldots \circ f_{-1,E}(I_1(E)).$$

Notice that if the vector $\bar{w} \in \mathbb{R}^2$, $|\bar{w}| = 1$, correspond to the direction defined by $z_\omega(E)$, then

$$\left(\Pi_{-n,E}\dots\Pi_{-1,E}\right)^{-1}(\bar{w}) \to 0 \ \text{ as } \ n \to \infty,$$

and for any vector $\bar{v} \nparallel \bar{w}$

$$\left|\left(\Pi_{-n,E}\dots\Pi_{-1,E}\right)^{-1}(\bar{v})\right| \to \infty$$

exponentially fast as $n \to \infty$. The set $K(E) = \cup_{\omega\in\{0,1\}^{\mathbb{Z}}} z\omega(E)$ is a dynamically defined Cantor set inside of $I_1(E)$. Notice that $\left|f'_{n,E}|_{I_1(E)}\right| \sim \frac{1}{E^2}$, and in our regime $E \sim 100$. Hence Hausdorff dimension of $K(E)$ is small, $\dim_H K(E) = \dim_B K(E) \ll 1/2$.

Similarly, the set

$$C(E) = \cup_{\omega\in\{0,1\}^{\mathbb{Z}}} \left(\cap_{n\in\mathbb{N}} f_{1,E}^{-1} \circ \ldots \circ f_{n,E}^{-1}(I_2(E))\right)$$

is a dynamically defined Cantor set, and $\dim_H C(E) = \dim_B C(E) \ll 1/2$.

A given point $E \in [98, 102]$ is an eigenvalue of an operator H_ω for some $\omega \in \{0,1\}^{\mathbb{Z}}$ if $f_{0,E}(K(E)) \cap C(E) \neq \emptyset$. Now Proposition 20.0.6 follows from the following statement:

Lemma 1. *Let $K(E)$ and $C(E)$ be two families of dynamically defined Cantor sets on $\mathbb{R}^1$, $E \in [0,1]$. Suppose that the following properties hold:*

1. *The Cantor set $K(E)$ is generated by two C^1-smooth (both in $x \in \mathbb{R}^1$ and $E \in [0,1]$) orientation preserving contractions $f_{1,E}, f_{2,E} : \mathbb{R}^1 \to \mathbb{R}^1$;*

2. *The Cantor set $C(E)$ is generated by two C^1-smooth (both in $x \in \mathbb{R}^1$ and $E \in [0,1]$) orientation preserving contractions $g_{1,E}, g_{2,E} : \mathbb{R}^1 \to \mathbb{R}^1$;*

3. $\max(K(0)) < \min(C(0))$ *and* $\min(K(1)) > \max(C(1))$*;*

4. *There exists $\delta > 0$ such that*
$$\frac{\partial f_{i,E}(x)}{\partial E} > \delta, \quad \frac{\partial g_{i,E}(x)}{\partial E} < -\delta$$
for all $E \in [0,1]$, $i = 1, 2$, and $x \in \mathbb{R}^1$;

5. *We have*
$$\max_{E\in[0,1]} \mathit{dim}_B\, C(E) + \max_{E\in[0,1]} \mathit{dim}_B\, K(E) < 1.$$

Then

$$\{E \in [0,1] \mid C(E) \cap K(E) \neq \emptyset\}$$

is a Cantor set of box counting dimension not greater than

$$\left(\max_{E\in[0,1]} \mathit{dim}_B\, C(E) + \max_{E\in[0,1]} \mathit{dim}_B\, K(E)\right).$$

Notice that the question on the structure of the set of translations of one Cantor set that have non-empty intersections with another is closely related to the questions about the structure of the difference of two Cantor sets. Sums (and differences) of dynamically defined Cantor sets were heavily studied, e.g. see [1] and references therein. But in our case we needed to work with two Cantor sets that depend on a parameter, so the question about the set of parameters that correspond to a non-empty intersection of the sets cannot be directly reduced to considering the difference of the Cantor sets, and therefore we need Lemma 1 above.

The reported results were obtained as a joint project with Victor Kleptsyn.

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Random Hamiltonians with Arbitrary Point Interactions: Positivity of the Lyapunov Exponent

by Mark Helman and Jacob Kesten (Rice University)

We consider disordered Hamiltonians with arbitrary point interactions under minimal assumptions on the randomness. Such operators are realized via self-adjoint vertex conditions imposed on a discrete set of points in the real line. However, contrary to all previously considered Kronig–Penney type random models, we make no assumptions on the regularity of the probability distribution of the i.i.d. random variables in question, which is essential in the study of several random quantum graph models.

In our model, the disordered Hamiltonians are given by the Laplace operator subject to arbitrary random self-adjoint singular perturbations which are supported on a random discrete subset of the real line. Here, the underlying one-step transfer matrix takes a much more general form than in the previous studies. In this setting, we managed to prove the following dichotomy: Either every realization of the random operator has purely absolutely continuous spectrum or spectral and exponential dynamical localization hold. The core of such proof of Anderson Localization for those operators is our new result of the positivity of the Lyapunov exponent for all energies outside of a discrete set.

In particular, we verify the assumptions of Theorem 2.1 in [1], with the matrices being the one step-transfer matrices from the above model, which are given by $\mathcal{M}^E(\ell, B) := B \begin{bmatrix} \cos\sqrt{E}\ell & \frac{\sin\sqrt{E}\ell}{\sqrt{E}} \\ -\sqrt{E}\sin\sqrt{E}\ell & \cos\sqrt{E}\ell \end{bmatrix}$, where $B \in \mathrm{SL}_2(\mathbb{R})$ and $\ell \in \mathbb{R}_{>0}$. This verification boiled down to showing that the commutator of 2 such transfer matrices, $\mathcal{M}^E(\ell_1, B_1)$ and $\mathcal{M}^E(\ell_2, B_2)$, is a non-identically zero function of the energy, E, over $\mathbb{C}$, except for the trivial cases when $\ell_1 = \ell_2$ and $B_1 = \pm B_2$, or $B_i = \pm I_2$ for $i = 1, 2$. Then, [1, Theorem 2.1] gives that the Lyapunov Exponent of the model is positive away from a discrete set of energies $E \in \mathbb{R}$, thus allowing us to conclude that spectral and exponential dynamical localization holds for all but a discrete set of energies, on which the spectrum of the operator will be purely absolutely continuous.

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Cantor Spectrum for CMV and Jacobi Matrices with Coefficients arising from Generalized Skew-Shifts

by Hyunkyu Jun (Rice University)

Let X be a compact metric space and let $T : X \to X$ be a strictly ergodic homeomorphism, which fibers over an almost periodic dynamical system (generalized skew-shifts). This means there exists an infinite compact abelian group $\mathbb{G}$ and an onto continuous map $h : X \to \mathbb{G}$ such that $h(T(x)) = h(x) + g$ for some $g \in \mathbb{G}$. We consider CMV matrices and Jacobi matrices whose Verblunsky coefficients and respectively, Jacobi coefficients are obtained by a continuous sampling map along an orbit of T.

Our interest is to investigate spectral properties of CMV and Jacobi matrices. Let $f \in C^0(X, \mathbb{D})$ where $\mathbb{D}$ is the unit disk in the complex plane. Define the bi-infinite Verblansky coefficients $\{\alpha_n\}_{n\in\mathbb{Z}}$ as $\alpha_n := f(T^n x)$ where $x \in X$. Let $\mathcal{C}_x$ be the associated bi-infinite CMV matrix. By minimality of T, there exists $\Sigma \subset \partial\mathbb{D}$ such that $\sigma(\mathcal{C}_x) = \Sigma$ for all $x \in X$. Moreover, in Damanik et al [2], the authors show

$$\partial\mathbb{D} \setminus \Sigma = \{z \in \partial\mathbb{D} : (T, \overline{A}_{f,z}) \text{ is uniformly hyperbolic}\}$$

where

$$\overline{A}_{f,z}(x) := \frac{1}{z^{-1/2}\sqrt{1 - |f(x)|^2}} \begin{bmatrix} z & -\bar{f}(x) \\ -f(x)z & 1 \end{bmatrix}.$$

One of our results states:

Theorem 1. *For a generic $f \in C^0(X, \mathbb{D})$, we have that $\partial\mathbb{D} \setminus \Sigma$ is dense; that is, the associated CMV operators have a Cantor spectrum.*

Here, by saying f is generic, this means f is an element of countable intersection of open dense subsets of $C^0(X, \mathbb{D})$.

For the Jacobi case, define the bi-infinite Jacobi coefficients $\{a_n\}_{n\in\mathbb{Z}}$ and $\{b_n\}_{n\in\mathbb{Z}}$ by $a_n = f_a(T^n(x))$ and $b_n = f_b(T^n x)$, respectively. Let $\mathcal{J}_x$ be the associated Jacobi matrix. By minimality of T, there exists $\Sigma' \subset \mathbb{R}$ such that $\sigma(\mathcal{J}_x) = \Sigma'$ for all $x \in X$. Moreover, in Marx [3], the author shows

$$\mathbb{R} \setminus \Sigma' = \{E \in \mathbb{R} | (T, A_{E,f_a,f_b}) \text{ is uniformly hyperbolic}\}$$

where

$$A_{E,f_a,f_b}(x) = \frac{1}{f_a(x)} \begin{bmatrix} E - f_b(x) & -1 \\ f_a(x)^2 & 0 \end{bmatrix}$$

The other major result states:

Theorem 2. *Let $f_a \in C^0(X, \mathbb{R})$ with $f_a(x) > 0$ for all $x \in X$. For generic $f_b \in C^0(X, \mathbb{R})$, we have that $\mathbb{R} \setminus \Sigma'$ is dense; that is, the associated Jacobi matrices have Cantor spectrum.*

Here, by saying f_b is generic, this means f_b is an element of a countable intersection of open dense subsets of $C^0(X, \mathbb{R})$.

The proofs heavily builds upon the results in Avila et al [1]. Moreover, the proof of Theorem 2 is a direct application of results in [1]. In Avila et al [1], the authors prove that an $SL(2, \mathbb{R})$-cocycle with a certain property can be perturbed so that it is uniformly hyperbolic. This implies that if a cocycle associated to a CMV matrix, $(T, \overline{A}_{f,z})$, is not uniformly hyperbolic, it can be perturbed so that it is a uniformly hyperbolic $SL(2, \mathbb{R})$-cocycle. Our proof converts this perturbed $SL(2, \mathbb{R})$-cocylce to one associated with a CMV matrix while the uniformly hyperbolicity is preserved.

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Furstenberg theorem: now with a parameter!

by Victor Kleptsyn (CNRS, Institut de Recherche Mathématique de Rennes)

Let (Ω, μ) be a probability space, $J \subset \mathbb{R}$ be a compact interval of parameters, and $F : \Omega \times J \to SL(2, \mathbb{R})$ be a bounded measurable (and continuous in second argument) map that to any $\omega \in \Omega$ puts in correspondence a matrix $F_a(\omega)$ that depends continuously on the parameter $a \in J$. One of the main application of our results is given by products of transfer matrices for 1D Anderson Model, where the role of the parameter is played by the value of energy E. For a given sequence $\bar{\omega} \in \Omega^{\mathbb{N}}, \bar{\omega} = \omega_1 \omega_2 \dots$ denote

$$T_{n,a,\bar{\omega}} = F_a(\omega_n) F_a(\omega_{n-1}) \dots F_a(\omega_1).$$

Furstenberg-Kesten Theorem [1] implies that for each value of the parameter $a \in J$ there is a subset $\Omega_a \subseteq \Omega^{\mathbb{N}}$ with $\mu^{\mathbb{N}}(\Omega_a) = 1$ such that for any $\bar{\omega} \in \Omega_a$ the limit

$$\lambda_F(a) := \lim_{n \to \infty} \frac{1}{n} \log \|T_{n,a,\bar{\omega}}\|$$

exists.

Is it possible to choose Ω_a uniformly in the parameter? In other words, is it true that $\mu^{\mathbb{N}}$-almost surely the limit above exists for all values of the parameter $a \in J$? It turns out that the answer to these questions is drastically different depending of presence or absence of uniform hyperbolicity.

Definition A collection of $SL(2, \mathbb{R})$ (or $SL(k, \mathbb{R})$) matrices $\{M_\alpha\}_{\alpha \in \mathcal{A}}$ is called uniformly hyperbolic if there exists a constant $\eta > 1$ such that for any finite sequence of matrices $M_{\alpha_1}, M_{\alpha_2}, \dots, M_{\alpha_n}$ we have $\|M_{\alpha_1} M_{\alpha_2} \dots M_{\alpha_n}\| > \eta^n$.

There is a number of equivalent ways to describe uniform hyperbolicity of $SL(2, \mathbb{R})$ (or $SL(k, \mathbb{R})$) cocycles, such as an invariant splitting into stable and unstable directions, or the absence of a Sacker-Sell solution. In particular, existence of invariant one-dimensional stable and unstable directions for uniformly hyperbolic $SL(2, \mathbb{R})$ cocycles combined with Birkhoff Ergodic Theorem immediately implies the following statement:

Proposition *In the setting above, assume that for each $a \in J$ the collection of matrices $\{F_a(\omega)\}_{\omega\in\Omega}$ is uniformly hyperbolic. Then, for $\mu^{\mathbb{N}}$-a.e. $\bar{\omega} \in \Omega^{\mathbb{N}}$ the limit*

$$\lim_{n\to\infty} \frac{1}{n} \log \|T_{n,a,\bar{\omega}}\| = \lambda_F(a) > 0$$

exists for all $a \in J$.

Remark *In the case of $SL(k,\mathbb{R})$, $k > 2$, even uniform hyperbolicity does not guarantee the convergence uniformly in parameter, or even pointwise convergence for all parameters. More restrictive assumptions (e.g. positivity of all entries of the matrices) are needed.*

The case of positive Lyapunov exponent in absence of uniform hyperbolicity is usually referred to as *non-uniformly hyperbolic case.*

From now on, we will proceed under the following standing assumptions:

(A1) **(Furstenberg condition)** Denote by μ_a the measure $\mu_a = (F_a)_*(\mu)$. We assume that for each $a \in J$ the measure μ_a on $SL(2,\mathbb{R})$ satisfies the (individual) Furstenberg non-degeneracy condition, that is, its support is not contained in any compact subgroup of $SL(2,\mathbb{R})$, and there is no $\operatorname{supp}\mu_a$-invariant finite union of proper subspaces of $\mathbb{R}^2$.

(A2) **(C^1-boundedness)** The maps $F_a(\omega)$ are C^1-smooth in the parameter $a \in J$, with uniformly bounded C^1-norm, i.e. there exists $M > 0$ such that for all $\omega \in \Omega$ and all $a \in J$

$$\|F_a(\omega)\|, \left\|\frac{d}{da} F_a(\omega)\right\| \leq M.$$

(A3) **(Non-uniform hyperbolicity)** For each $a \in J$ the collection of matrices $\{F_a(\omega)\}_{\omega\in\Omega}$ is not uniformly hyperbolic.

(A4) **(Monotonicity)** There exists $\delta > 0$ such that

$$\frac{d}{da} \arg(F_a(\omega)\bar{v}) > \delta > 0$$

for all $a \in J, \omega \in \Omega, \bar{v} \in \mathbb{R}^2\backslash\{0\}$. In other words, as we increase the parameter, the image of any given vector $\bar{v}$ spins in the positive direction with a speed that is bounded from below.

Our main result is the following theorem, describing the behaviour of the random parameter-dependent products of $SL(2,\mathbb{R})$ matrices:

Theorem 20.0.7 (Parametric version of Furstenberg Theorem)**.** *Under the assumptions $(A1) - (A4)$ above, for $\mu^{\mathbb{N}}$-almost every $\bar{\omega} \in \Omega^{\mathbb{N}}$ the following holds:*

- ***(Regular upper limit)*** *For every $a \in J$ we have*

$$\limsup_{n\to\infty} \frac{1}{n} \log \|T_{n,a,\bar{\omega}}\| = \lambda_F(a) > 0.$$

- ***(G_δ-vanishing)*** *The set*

$$S_0(\bar{\omega}) := \left\{ a \in J \mid \liminf_{n\to\infty} \frac{1}{n} \log \|T_{n,a,\bar{\omega}}\| = 0 \right\}$$

is a (random) dense G_δ-subset of the interval J.

- ***(Hausdorff dimension)*** *The (random) set of parameters with exceptional behaviour,*

$$S_e(\bar{\omega}) := \left\{ a \in J \mid \liminf_{n \to \infty} \frac{1}{n} \log \|T_{n,a,\bar{\omega}}\| < \lambda_F(a) \right\},$$

  has zero Hausdorff dimension:

$$\dim_H S_e(\bar{\omega}) = 0.$$

Notice that in this case existence of a dense subset of energies in the spectrum for which the limit that defines the Lyapunov exponent does not exist was shown in [2, Theorem 6.2].

Other related results as well as the complete proof of Theorem 1 can be found in [3].

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Non-stationary versions of Anderson Localization and Furstenberg Theorem on random matrix products

by Victor Kleptsyn (CNRS, Institut de Recherche Mathématique de Rennes)

The asymptotic behavior of sums of i.i.d. random variables is very well studied in the classical probability theory. Analogous questions on random products of matrix-valued i.i.d. random variables were initially formulated in the simplest case of 2×2 matrices with positive entries by Bellman. Later these questions attracted lots of attention due to the results by Furstenberg and Kesten [1] who showed that exponential rate of growth of the norms of the random products (aka Lyapunov exponent) is well defined almost surely, and Furstenberg [2, 3], where it was shown that under some non-degeneracy conditions Lyapunov exponent must be positive.

The most famous and classical result is the following Furstenberg Theorem:

Theorem 20.0.8. *Let $\{X_k, k \geq 1\}$ be independent and identically distributed random variables, taking values in $SL(d,\mathbb{R})$, the $d \times d$ matrices with determinant one, let G_X be the smallest closed subgroup of $SL(d,\mathbb{R})$ containing the support of the distribution of X_1, and assume that*

$$E[\log \|X_1\|] < \infty.$$

Also, assume that G_X is not compact, and there exists no G_X-invariant finite union of proper subspaces of $\mathbb{R}^d$. Then there exists a positive constant λ_F such that with probability one

$$\lim_{n\to\infty} \frac{1}{n} \log \|X_n \dots X_2 X_1\| = \lambda_F > 0.$$

In the first part of this paper we generalize Furstenberg Theorem to the case when the random variables $\{X_k, k \geq 1\}$ do not have to be identically distributed. Here is our setting:

Let $\{\nu_\alpha\}_{\alpha \in K}$, $\operatorname{supp} \nu_\alpha \subset SL(d,\mathbb{R})$, be a collection of compactly supported probability measures, indexed by a parameter α from a compact metric space K. We assume that dependence of ν_α on α is continuous (in weak-* topology). As a partial case, one can consider a finite collection $\{\nu_i\}_{i=1,\dots,k}$ of probability measures on $SL(d,\mathbb{R})$.

For any $A \in SL(d,\mathbb{R})$ we will denote by $f_A : \mathbb{RP}^{d-1} \to \mathbb{RP}^{d-1}$ the induced projective transformation. We make the following

Standing Assumption: *We assume that for any $\alpha \in K$ there are no Borel probability measures μ_1, μ_2 on $\mathbb{RP}^{d-1}$ such that $(f_A)_*\mu_1 = \mu_2$ for ν_α-almost every $A \in SL(d, \mathbb{R})$.*

Let us fix some sequence $\{\alpha_i\}_{i\in\mathbb{N}}$, $\alpha_i \in K$, and let $A_i \in SL(d, \mathbb{R})$ be chosen randomly with respect to distribution ν_{α_i}. Set $T_n = A_n A_{n-1} \dots A_1$, and denote

$$L_n = \mathbb{E} \log \|T_n\|, \tag{0.21}$$

where the expectation is taken over the distribution $\nu_{\alpha_1} \times \nu_{\alpha_2} \times \dots \times \nu_{\alpha_n}$.

Theorem 20.0.9. *Under the Standing Assumption above, for any fixed sequence $\{\alpha_i\}_{i\in\mathbb{N}} \in K^{\mathbb{N}}$ we have*

$$\liminf_{n\to\infty} \frac{1}{n} L_n > 0.$$

A statement similar to Theorems 20.0.9 was previously announced by I. Goldsheid, see the extended abstract of his talk above.

In the case of $SL(2, \mathbb{R})$ matrices one can actually say much more.

Theorem 20.0.10. *In the case $d = 2$ (i.e. in the case of random non-stationary products of $SL(2, \mathbb{R})$ matrices) almost surely additionally to the statement of Theorem 20.0.9 the following hold:*

1) $\lim_{n\to\infty} \frac{1}{n} (\log \|T_n\| - L_n) = 0$;

2) There exists a unit vector $\bar{v} \in \mathbb{R}^2$ such that $|T_n \bar{v}| \to 0$ as $n \to \infty$. Moreover,

$$\lim_{n\to\infty} \frac{1}{n} (\log |T_n \bar{v}| + L_n) = 0$$

The statement of Theorem 20.0.9 and the first part of Theorem 20.0.10 in the case of products of i.i.d. random matrices correspond to the classical Furstenberg Theorem.

We will prove Theorem 20.0.10 via Large Deviations Estimates Theorem, that is also of independent interest:

Theorem 20.0.11. *In the case $d = 2$, for any $\varepsilon > 0$ there exists $\delta > 0$ such that for all sufficiently large $n \in \mathbb{N}$ we have*

$$\mathbb{P} \{|\log \|T_n\| - L_n| > \varepsilon n\} < e^{-\delta n},$$

where $\mathbb{P} = \nu_{\alpha_1} \times \nu_{\alpha_2} \times \dots \times \nu_{\alpha_n}$. Moreover, the same estimate holds for the lengths of random images of any given initial unit vector v_0:

$$\forall v_0 \in \mathbb{R}^2,\ |v_0| = 1 \quad \mathbb{P} \{|\log \|T_n v_0\| - L_n| > \varepsilon n\} < e^{-\delta n}.$$

The reported results were obtained in collaboration with A. Gorodetski.

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Phase transition of capacity for uniform G_δ sets

by Fernando Quintino (University of California, Irvine)

In a joint work with Victor Kleptsyn, we consider a family of dense G_δ subsets of $[0,1]$, defined as intersections of unions of small uniformly distributed intervals, and study their capacity. That is, given a (sufficiently fast) decreasing sequence $r_n \to 0$, for every n we consider a union of n equally spaced intervals of length r_n:

$$V_n := \bigcup_{j=1}^{n} J_{k,n}, \tag{0.22}$$

where $J_{k,n}$ is an open interval of length r_n centered at $c_{k,n} = \frac{k+(1/2)}{n}$:

$$J_{k,n} := (c_{j,n} - \frac{r_n}{2}, c_{j,n} + \frac{r_n}{2}), \quad c_{j,n} = \frac{2j+1}{2n}, \quad j = 0, 1, \ldots, n-1. \tag{0.23}$$

Then we define the <u>uniform G_δ-set</u> S, corresponding to the sequence r_n, by

$$S := \bigcap_{m=1}^{\infty} \bigcup_{n=m}^{\infty} V_n; \tag{0.24}$$

it is immediate to see that S is indeed a G_δ-subset of $[0,1]$. Such an example is interesting for us for two reasons. First, in [2] we found that by considering different decrease speed for the lengths r_n, we observed a sharp phase transition: while for a fast decrease this set is of zero capacity, for a slower one it turns out to be of <u>full</u> capacity (that is, equal to the capacity of $[0,1]$ itself). Given a compactly supported measure μ on $\mathbb{C}$, one defines its (Coulomb) <u>energy</u> as a double integral:

$$I(\mu) := \iint -\log|z-w|\, d\mu(z) d\mu(w). \tag{0.25}$$

The logarithmic capacity of a bounded subset $X \subset \mathbb{C}$ is then defined by minimizing this energy:

Definition. Let $\mathcal{P}(X)$ be the space of probability measures, supported on a (bounded) set $X \subset \mathbb{C}$. The <u>logarithmic capacity</u> of this set is

$$\mathrm{Cap}(X) := \exp(-\inf\{I(\mu) \mid \mu \in \mathcal{P}(X)\}).$$

Theorem 20.0.12 (Phase transition, V. Kleptsyn, F. Quintino)**.** *For* $r_n = e^{-n^\alpha}$*,*

1. *if* $\alpha > 2$*, then* $\mathrm{Cap}(S) = 0$*,*
2. *if* $\alpha < 2$*, then* $\mathrm{Cap}(S) = \mathrm{Cap}([0,1])$*.*

Second, such a G_δ set can be considered as a toy model for the set of exceptional energies in the parametric version of the Furstenberg theorem on random matrix products[18]. A more general G_δ-sets can be constructed in the following way. Consider the set

$$\widetilde{S} = \bigcap_m \bigcup_{k \geq m} I_k,$$

where I_k are intervals of length r'_k. In this general setting a similar pattern seems to be at play.

Theorem 20.0.13 (V. Kleptsyn, F. Quintino)**.** *If the series* $\sum_n \frac{1}{|\log r'_n|}$ *converges, then the set* $\widetilde{S}$ *is of zero capacity.*

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Exponential Dynamical Localization for Random Word Models

by Nishant Rangamani (University of California, Irvine)

We give a new proof of spectral localization for the one-dimensional Schrodinger operators whose potentials arise by randomly concatenating words from an underlying set. We then show that once one has the existence of a complete orthonormal basis of eigenfunctions (with probability one), the same estimates used to prove it naturally lead to a proof of exponential dynamical localization in expectation (EDL) on any compact interval not containing a finite set of critical energies.

The random word models we consider are defined on $l^2(\mathbb{Z})$ and are given by

$$H_\omega\psi(n) = \psi(n+1) + \psi(n-1) + V_\omega(n)\psi(n).$$

The potential V is a family of random variables defined on a probability space Ω. To construct the potential V above, we consider words (vectors in $\mathbb{R}^n$ with $1 \le n \le m$), $\dots\omega_{-1}, \omega_0, \omega_1, \dots$, so that $V_\omega(0)$ corresponds to the kth entry in ω_0. A precise construction of the probability space Ω and the random variables $V_\omega(n)$ is carried out in [1]. In particular, the authors show that there is a finite set D so that the Lyapunov exponent is positive outside of D.

Motivated by recent proofs of spectral and dynamical localization given for the Anderson model in [2] and a proof of exponential dynamical localization in expectation given in [3], we demonstrate the application of these techniques in the random word case to obtain the two theorems listed at the end of this section.

We note that the proofs given in [2] and [3] use positivity and large deviations of the Lyapunov exponent to replace parts of the multi-scale analysis. The major improvement in this regard (aside from a shortening of the length and complexity of localization proofs in one-dimension) is that the complement of the event where the Green's function decays exponentially can be shown to have exponentially rather than sub-exponentially small probability. These estimates were implicit in the proofs of spectral and dynamical localization given in [2] and were made explicit in [3]. The authors in [3] then used these estimates to prove EDL for the Anderson model and we extend these techniques to the random word case.

There are several issues one encounters when adapting the techniques developed for the Anderson model in [2] and [3] to the random word case. Firstly, in the Anderson setting, a uniform large deviation estimate is immediately available using a theorem in [4]. Since random word models exhibit local correlations, there are additional steps that need to be taken in order to obtain suitable analogs of large deviation estimates used in [2] and [3]. Secondly, random word models may have a finite set of energies where the Lyapunov exponent vanishes and this phenomena demands some care in obtaining estimates on the Green's functions analogous to those in [2,3].

The aforementioned results are:

Theorem [5] The spectrum of H_ω is almost surely pure point with exponentially decaying eigenfunctions.

Theorem [5] *There is a finite* $D \subset \mathbb{R}$ *such that if* I *is a compact interval and* $D \cap I = \emptyset$*, then there are* $C > 0$ *and* $\alpha > 0$ *such that* $\mathbb{E}\left[\sup_{t\in\mathbb{R}} \left|\langle \delta_p, P_I(H_\omega)e^{-itH_\omega}\delta_q\rangle\right|\right] \leq Ce^{-\alpha|p-q|}$ *for any* $p, q \in \mathbb{Z}$.

Here P_I denotes the spectral projection onto the interval I.

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Unique continuation and localization on the planar lattice

by Charles Smart (University of Chicago)

Recall that the Anderson–Bernoulli model is a random linear operator on $\ell^2(\mathbb{Z}^d)$ given by

$$H = -\Delta + \beta V,$$

where Δ is the graph Laplacian, $\beta > 0$ is the noise strength, and $V : \mathbb{Z}^d \to \{0, 1\}$ is a Bernoulli potential. We discuss the following two results.

Theorem 20.0.14 (Ding–Smart)**.** *If $d = 2$, then H almost surely has pure-point spectrum in* $[0, \varepsilon]$.

Theorem 20.0.15 (Li–Zhang)**.** *If $d = 3$, then H almost surely has pure-point spectrum in* $[0, \varepsilon]$.

These results advance the state of the art by establishing localization for singular noise in dimensions larger than one. Following the program of Bourgain–Kenig, the key ingredients of these theorems are the following unique continuation results.

Theorem 20.0.16 (Ding–Smart)**.** *The following holds for all $\alpha > 1 > \varepsilon > 0$ and sufficiently large $L > 0$. If $d = 2$, $|\bar{\lambda}| < \alpha$, and $Q = [-L, L]^2 \cap \mathbb{Z}^2$, then*

$$\mathbb{P}[\mathcal{E}] \geq 1 - e^{-L^{1/4-\varepsilon}}$$

where $\mathcal{E}$ is the event that

$$H\psi = \lambda\psi \quad \text{in } Q \quad \text{and} \quad |\lambda - \bar{\lambda}| \leq e^{-L^{1/2+\varepsilon}}$$

implies

$$\#\{x \in Q : |\psi(x)| \geq e^{-L^{1+\varepsilon}} |\psi(0)|\} \geq L^{3/2-\varepsilon}.$$

Theorem 20.0.17 (Li–Zhang)**.** *There is a $p > 0$ such that, for all $\alpha > 1 > \varepsilon > 0$, the following holds for sufficiently large $L > 0$. If $d = 3$, $|\Delta\psi| \le \alpha|\psi|$ holds in $Q = [-L, L]^3 \cap \mathbb{Z}^3$, then*

$$\#\{x \in Q : |\psi(x)| \ge e^{-L^{1+\varepsilon}}|\psi(0)|\} \ge L^{3/2+p}.$$

Both of these unique continuation theorems use ideas from recent work of Buhovsky–Logunov–Malinnikova–Sodin.

Anderson localization for radial trees

by Selim Sukhtaiev (Rice University)

We establish spectral and dynamical localization for several Anderson–Bernoulli models on metric and discrete radial trees. The localization results are obtained on compact intervals contained in the complement of discrete sets of exceptional energies. All results are proved under the minimal hypothesis on the type of disorder: the random variables generating the trees assume at least two distinct values. This level of generality, in particular, allows us to treat radial trees with disordered geometry as well as Schrödinger operators with Bernoulli-type singular potentials. Our methods are based on an interplay between graph-theoretical properties of radial trees and spectral analysis of the associated random differential and difference operators on the half-line.

More specifically, let us denote the common distribution of single sites random variables by μ and the continuum Kirchhoff–Laplacian by H. Assume that suppμ is a bounded set containing at least two elements. Then there exists a discrete set of exceptional energies D such that:

(i) The operator H_ω exhibits Anderson localization at all energies outside of D. That is, almost surely, H_ω has pure point spectrum and any eigenfunction of H_ω corresponding to an energy $E \in R \setminus D$ enjoys an exponential decay estimate of the form

$$|f(x)| \le \frac{Ce^{-\lambda|x|}}{\sqrt{w_o(|x|)}}$$

with $C > 0$ and $\lambda > 0$, where $w_o(|x|)$ denotes the number of vertices in the generation of x, i.e., $w_o(|x|) = \#\{y \in \mathcal{V} : gen(y) = gen(x)\}$.

(ii) For every compact interval $I \in R \setminus D$ and every $p > 0$, there exists a set $\Omega^* \subset \Omega$ with $\mu(\Omega^*) = 1$ such that for every $\omega \in \Omega^*$ and every compact set $K \subset \Gamma_{b_\omega,\ell_\omega}$ one has

$$\sup_{t>0} \left\| |X|^p \chi_I(H_\omega) e^{-itH_\omega} \chi_K \right\|_{L^2(\Gamma_{b_\omega,\ell_\omega})} < \infty,$$

where $\chi_I(H_\omega)$ is the spectral projection corresponding to I, and $|X|^p$ denotes the operator of multiplication by the radial function $f(x) := |x|^p$, $x \in \Gamma_{b_\omega,\ell_\omega}$, where $|x|$ denotes the distance from x to the root o.

This result together with its discrete version is established in [1].

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Diophantine properties of matrices

by Yuki Takahashi (Tohoku University)

Let $d \geq 2$, and let $\mathcal{A} = \{A_i\}_{i \in \Lambda}$ be a finite collection of $GL_d(\mathbb{R})$ matrices. Write $A_{\mathbf{i}} = A_{i_1} \cdots A_{i_n}$ for $\mathbf{i} = i_1 \cdots i_n$. We say that the set $\mathcal{A}$ is Diophantine if there exists a constant $c > 0$ such that for every $n \in \mathbb{N}$, we have

$$\mathbf{i}, \mathbf{j} \in \Lambda^n, A_{\mathbf{i}} \neq A_{\mathbf{j}} \implies \|A_{\mathbf{i}} - A_{\mathbf{j}}\| > c^n.$$

The set $\mathcal{A}$ is strongly Diophantine if there exists $c > 0$ such that for all $n \in \mathbb{N}$,

$$\mathbf{i}, \mathbf{j} \in \Lambda^n, \mathbf{i} \neq \mathbf{j} \implies \|A_{\mathbf{i}} - A_{\mathbf{j}}\| > c^n.$$

Clearly, $\mathcal{A}$ is strongly Diophantine if and only if it is Diophantine and generates a free semigroup. For any collection of linearly independent vectors $v_1, \cdots, v_d$ in $\mathbb{R}^d$ consider the cone

$$\Sigma = \Sigma_{v_1, \cdots, v_d} = \{x_1 v_1 + \cdots x_d v_d : x_1, \cdots, x_d \geq 0\}.$$

If a matrix $A \in GL_d(\mathbb{R})$ satisfies

$$A(\Sigma \setminus \{0\}) \subset \Sigma^\circ,$$

we say that Σ is strictly invariant for A. Given a cone $\Sigma = \Sigma_{v_1, \cdots, v_d}$, denote by $\mathcal{X}_{\Sigma, m}$ the set of all $GL_d(\mathbb{R})$ m-tuples of matrices for which Σ is strictly invariant. We consider $\mathcal{X}_{\Sigma, m}$ as an open subset of $\mathbb{R}^{d^2 m}$.

Let $\Sigma = \Sigma_{v_1, \cdots, v_d}$ be a cone in $\mathbb{R}^d$ and $m \geq 2$. Together with B. Solomyak, the author proved the following in [1]: For a.e. $\mathcal{A} \in \mathcal{X}_{\Sigma, m}$, the m-tuple $\mathcal{A}$ is strongly Diophantine. In particular, a.e. m-tuple of positive $GL_d(\mathbb{R})$ matrices is strongly Diophantine.

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Localization for the one-dimensional Anderson model via positive Lyapunov exponents and a Large Deviation Theorem

by Tom VandenBoom (Yale University)

It is well-known that the one-dimensional Anderson model is almost-surely Anderson localized – that is to say, the operator

$$H_\omega = \Delta + \omega$$

almost surely (in $\omega = (\omega_n)_{n\in\mathbf{Z}}$) has pure point spectrum with exponentially decaying eigenfunctions provided the terms ω_n are sampled i.i.d. and randomly. However, proofs of this fact in one dimension have until recently (cf. [2, 7, 8]) utilized the sophisticated multi-dimensional machinery of Multi-Scale Analysis (MSA) to handle highly singular probability distributions [3, 9]. In this talk, we demonstrate a simplified proof of Lyapunov behavior for all generalized eigenfunctions of an almost-sure H_ω [2].

To state our result precisely, we require some notation: let $\tilde{\mu}$ be a probability measure with compact real support $A \subset \mathbf{R}$, and denote by $(\Omega, \mu) = (A^{\mathbf{Z}}, \tilde{\mu}^{\mathbf{Z}})$ the associated probability space on the full shift over A. Letting $\omega \in \Omega$ and $E \in \mathbf{C}$, define the Schrödinger transfer matrix $M_n(E,\omega)$ as the unique $SL(2,\mathbf{R})$ matrix such that $u \in \mathbf{C}^{\mathbf{Z}}$ solves $H_\omega u = Eu$ if and only if $[u_n \;\; u_{n-1}]^\top = M_n(E,\omega)[u_0 \;\; u_{-1}]^\top$. Then the Lyapunov exponent $L(E) = \lim_{n\to\infty} \frac{1}{n}\int_\Omega \log \|M_n(E,\omega)\| d\mu(\omega)$ exists and is positive for all $E \in \mathbf{R}$ by Furstenberg's theorem. Our result is that, for μ-almost every $\omega \in \Omega$, for any generalized eigenvalue $E(\omega)$ of H_ω, the norms of the transfer matrices $M_n(E(\omega),\omega)$ grow at precisely the Lyapunov rate:

$$\lim_{n\to\infty} \frac{1}{n} \log \|M_n(E(\omega),\omega)\| = L(E(\omega)).$$

Our proof can also be extended to prove dynamical localization via the standard SULE techniques [4].

Historically, proofs of Anderson localization in complete generality involved three key ingredients: first, an initial length-scale estimate coming from positivity of the Lyapunov exponent; second, a Wegner estimate on the density of states; and finally, the MSA machinery. Our proof has similar first ingredients; namely, we achieve an initial length-scale estimate using positive Lyapunov exponents from Furstenberg's Theorem [5, 6], and then prove a Large Deviation Theorem (LDT) (which serves the same role as the Wegner estimate). Where our proof differs significantly from previous proofs is in the final step, whereby we eliminate long-range "double resonances": distant pairs of intervals supporting simultaneous localization. We eliminate such pairs using our LDT and independence; this step is the focus of this talk. With the double resonances eliminated, one can apply an Avalanche Principle argument to the transfer matrices to conclude exponential decay of the generalized eigenfunctions. This strategy, initially observed by Bourgain and Schlag in application to strongly mixing potentials [1], is very general and applicable to a variety of one-dimensional models.

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A short proof of Anderson localization for the 1-d Anderson model

by Xiaowen Zhu (University of California, Irvine)

The proof of Anderson localization for 1D Anderson model with arbitrary (e.g. Bernoulli) disorder, originally given by Carmona-Klein-Martinelli in 1987, is based on the Furstenberg theorem and multi-scale analysis. This topic has received a renewed attention lately, with two recent new proofs, exploiting the one-dimensional nature of the model. At the same time, in the 90s it was realized that for one-dimensional models with positive Lyapunov exponents some parts of multi-scale analysis can be replaced by considerations involving subharmonicity and large deviation estimates for the corresponding cocycle, leading to nonperturbative proofs for 1D quasiperiodic models. Here we present a proof along these lines, for the Anderson model. It is a joint work with S. Jitomirskaya. Our entire proof of spectral localization fits in three pages and we expect to present almost complete detail during the talk. I will also present my proof of Anderson localization for the OPUC (Orthogonal polynomial on the unit circle) with any nontrivial i.i.d random Verblunsky coefficients, in the spirit of the work above. This proof was commissioned by Barry Simon for the new edition of his OPUC book.

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Chapter 21

Emerging Statistical Challenges and Methods for Analysis of Human Microbiome Data (19w5221)

September 15 - 20, 2019

Organizer(s): Toby Kenney (Dalhousie Univ.), Glen Satten (Emory Univ.), Greg Gloor (Univ. of Western Ontario), Rob Beiko (Dalhousie Univ), Natalie Knox (Bacterial Genomics for Public Health Agency of Canada), Shyamal Peddada (Univ. of Pitsburg), Michael Wu (Fred Hutch), Hong Gu (Dalhousie Univ.)

Overview of the Field

Recent developments in high-throughput sequencing have allowed almost all the microbes in a community to be identified through amplicon sequencing of the 16S rRNA ribosomal gene; further, bacterial genes can be identified through shotgun metagenomic sequencing. With many different types of omics data being collected, development of data analysis methods that are tailored towards these different types of data has lagged behind.

This workshop aimed to address some of the main challenges in dealing with the microbiome data. The topics of discussion can mostly be divided into four main categories: modelling, calibrating and correcting for measurement errors in microbiome data; using statistical tools to answer biological questions about the microbiome; integrating multiple types of omics data and applying microbiome data analysis in scientific and clinical contexts.

For the first category, each type of data is subject to its own measurement errors, caused by limitations in the technology. This has contributed to major replicability problems with published results in the field. Recent research has shed some light into some of the measurement bias and variance arising in microbiome data.

For the second category, there are a number of biological questions arising in the study of the microbiome, such as how the microbiome differs between patients and healthy controls, how the microbiome changes over time, and the organisation of microbial communities. There has been a large amount of work in this area from the bioinformatics community, but many of the methods used are ad-hoc, without sound statistical justification, and do not allow statistical inference.

For the third category, the majority of early microbiome studies were based on amplicon sequencing of 16S. However, there are many limitations to this type of data. Therefore, there has been increased interest in collecting more detailed data, such as whole genome sequencing, transcriptomics, metabolomics, etc. These data types could give a more complete picture of how the microbial community functions. However, each data type comes with its own limitations and structure. Therefore new statistical methods are needed to account for these limitations and structures.

For the fourth category, many of the invited researchers work in scientific and clinical settings, and have first-hand experience of the application of microbiome research for answering questions. A number of presentations at the workshop discussed some of the possible applications of microbiome research, and what statistical problems need to be solved before these applications could be realised.

Challenges raised in the workshop

The workshop brought together a number of investigators with different perspectives and different backgrounds that ranged from practitioners and users, to developers of statistical approaches for studying microbial communities. Topics and presentations ranged from highly theoretical to practical applications. The majority of tools presented were used to analyze Operational Taxonomic Unit (OTU) or higher level datasets.

There were several talks on benchmarking different tools for OTU level analysis, with a general conclusion that further work needs to be done. One challenge is that each tool is developed based on very different assumptions about how the data were generated, and what error processes were important or even realistic. There was a spirited discussion about the methodological, biological, and statistical assumptions of various approaches. Participants with deep knowledge of how the data were collected and generated made the point that high throughput sequencing data collection was much more complex and technically challenging than is apparent in many published datasets. One participant made the salient point that the error associated with microbiome datasets was nested, with different steps in the process generating error with different properties. The reality of nested error-generating processes is not currently taken into account appropriately by existing tools and this is a challenge and an opportunity for further development.

One presentation pointed out that microbiome datasets often lack a ground truth, and identified this as a major challenge in the field. This was a very important point, because many tools are developed with particular assumptions in mind. Tool development seems to follow a formula, where novel assumptions are made, tested in silico, and then benchmarked using a publicly-available dataset. The tool is “successful” if it has “more power” on an existing dataset than previous tools. This approach results in tools that identify false positive features, or that identify novel features that fit the particular assumptions, but that may not fit the actual process by which the data is generated. The microbiome field would be well served by datasets with known ground truths that are externally validated by other means.

Less attention was given to methods specifically designed to deal with Amplicon Sequence Variant (ASV), shotgun metagenomic or metatranscriptomic datasets (or the integration of these). Several presentations showed the potential increase in descriptive power by incorporating these approaches. One presentation showed how metagenomic data analysis, particularly the recovery of genomes from metagenome samples, can miss important features including those that relate directly to pathogenicity and antimicrobial resistance. Tools to properly examine these datasets are underdeveloped currently, and it was recommended that there be a major emphasis on tool development in these areas at the expense of OTU-level analysis. Several presentations were made showing that compositional-data based approaches showed promise, although the sentiment was not unanimous that approaches based on log-ratios were always superior.

In the end, the workshop achieved its goals of bringing diverse voices together for a robust discussion. It is rare to get biomedical scientists, practical and theoretical statisticians in a venue where they can have meaningful conversations. We need many more opportunities like this where frank conversations can be had in an environment that can build understanding and trust between all of the fields that need to be present to properly analyze and understand complex high-dimensional data, like that generated in the analysis of microbiomes.

Modelling and handling measurement error

Bias due to the microbiome experiment

Microbiome experiments are still in their infancy. One manifestation of this is that there are no agreed-on methods for standardizing microbiome measurements, or for using positive (external) control samples to adjust, calibrate, or normalize microbial count measurements. A few 'model community' samples with known composition, typically comprising around 10 OTUs, are available either commercially or from various consortia. However, even when these model community samples are run as positive controls in a microbiome experiment, there is no real way to use these results except to qualitatively claim a plate is 'in control.'

An exciting new development in microbiome studies is the development of a model for the biases that can occur in a microbiome experiment. This relatively simple mathematical model may eventually have a profound effect on how microbiome data are analyzed. If this model is correct, then it also provides a language to discuss bias, a framework to imagine how samples might be standardized, and even ideas on types of analysis that could give unbiased results even if individual OTU counts are all biased.

The microbiome bias model was developed by BIRS workshop participant Ben Callahan [15] and presented at the workshop by Ben Callahan. The model states that each OTU (or ASV) is subject to a multiplicative bias. Thus, if the 'true' count for OTU j in sample i was X^*_{ij}, we would instead observe counts X_{ij} given by

$$X_{ij} = X^*_{ij} e^{\beta_j}$$

where e^{β_j} is called the 'bias factor' for the jth OTU. This model further implies that the observed OTU proportions p_{ij} are related to true OTU proportions p^*_{ij} by

$$p_{ij} = \frac{p^*_{ij}}{\sum_{j'} p^*_{ij'}}. \tag{0.1}$$

Note that changing β_j to $\beta_j + b$, for every OTU j leaves p_{ij} unchanged, so that only relative bias factors can be defined (i.e., a sample is unbiased when $\beta_j = \beta$ for all j).

An important consequence of this model is that the shift in observed probabilities p_{ij} actually depends on the composition of the entire sample because of the denominator in (0.1). Thus, a sample with many OTUs having the same bias factors may have produce smaller shifts in observed OTU frequencies than a sample with OTUs having highly divergent bias factors. If the bias factors of two phylogenetically-related OTUs are more similar than the bias factors of two OTUs that are not phylogenetically close, this would imply that the sample with phylogenetically-related OTUs would have less biased observations than the sample with phylogenetically-distant OTUs. As a result, this model predicts it is not safe to compare the OTU frequencies of two samples with the hope that any bias 'cancels out.' Note this phenomenon occurs even if the bias factor for a fixed OTU is the same in every sample.

One new development reported at the BIRS workshop for the first time was a relatively simple log-linear modeling framework to estimate bias parameters in (0.1) using model community data. The original work of Callahan and colleagues did not provide this kind of simple but universal method for estimating bias parameters. BIRS workshop participant Glen Satten presented this model, along with two analyses of model community data.

In the first analysis, the bias factors of a commercially-available (Zymo) model community were compared when extracted under two conditions. In the first condition, the samples were analyzed as provided by Zymo; in the second condition, the samples were mixed with a smokeless tobacco product (Snus) from Sweden that was verified to be free of bacteria. The purpose of this experiment was to see if the biological matrix (i.e., the Snus) affected the bias factors. The experiment was repeated with four different extraction protocols. The analyses showed that the biological matrix had a significant effect on the bias factors for at least 3 of the four protocols (significance of the fourth protocol depends on whether we adjust for multiple comparisons).

The second analysis used the model community data of [2]. These data are unusual in that most samples had only two or three of the seven OTUs studied by Brooks et al [2]. This allowed a test of whether the bias factor of an OTU depended on the composition of the sample; a direct test of the model proposed by Callahan. The analysis showed no evidence of failure of the Callahan model (even while finding significant plate effects).

A final aspect of the bias model of Callahan is that it suggests how samples might be better analyzed in the future. Two approaches were discussed: bias adjustment and selection of models that are impervious to bias. Considering the first approach, it is unreasonable to think that bias factors for every observable OTU or ASV will be measured at some point. However, it is conceivable that the variability in bias factors can be explained by covariates. Some covariates would presumably be related to the physical organization of the bacterium, such as Gram status. Other covariates may be related to PCR, such as primer mismatch or GC content. Residual variability after accounting for important covariates may segregate according to the phylogenetic relationships among OTUs. If this is the case, it is possible to imagine a model-based bias adjustment as a way of normalizing microbiome data. Considering the second approach, it is easy to see that the denominator in (0.1) cancels out if a ratio of OTU frequencies within a sample are considered, e.g. if we pick one OTU (say, J) as a reference and only examine ratios $\frac{p_{ij}}{p_{iJ}}$. Similarly, the bias factors would cancel out if we only looked at ratios of ratios, i.e. if we compared the ratio of $\frac{p_{ij}}{p_{iJ}}$ to $\frac{p_{i'j}}{p_{i'J}}$. Compositional data analyses would satisfy these conditions, and so the bias model of Callahan provides an interesting reason to continue development of compositional data analysis methods for microbiome data.

Correction of Poisson measurement errors

Another important issue with microbiome data is the variance of the microbiome counts. Typically, for count data, the observed variance depends upon the total abundance. For rare OTUs, the relative error is much larger than for common OTUs, while the absolute error is much larger for common OTUs. This discrepancy can impact a number of data analysis methods. For example, principal component analysis (PCA) is a method that identifies the major directions in variation for multivariate data set, such as the microbiome.

A method for correcting PCA for Poisson measurement error was recently developed by workshop participants Hong Gu and Toby Kenney [11] and presented at the workshop by Hong Gu. The method estimates an unbiased variance covariance matrix estimator by correcting Poisson distributed measurement errors. The method can also estimate the principal components of log-transformed data, under Poisson noise. This offers the significant benefit of permitting a log-transformation of sparse data. Handling zero counts has been a challenge for methods based on log-transformation. The semiparametric Poisson model presented offers a method for dealing with these counts.

The talk precipitated in-depth discussion about the relative importance of Poisson error compared to other sources of error in the data, such as OTU bias, and amplification variance. On one hand, it was argued that microbiome data show evidence of large overdispersion, so that the Poisson noise is only a small fraction of the total noise in the data. On the other hand, it was argued that a lot of the overdispersion is in fact signal, so needs to not be removed, and while there is some overdispersion due to the data collection, it is challenging to separate it from the signal until more is know about the data collection. Meanwhile, microbiome data is sparse, and while the Poisson noise may be a small fraction of the noise for abundant OTUs, it is likely to play a significantly larger role for rare OTUs. Work is ongoing on extending the method to correct for overdispersed measurement error.

Particular microbiome analyses

Differential abundance

One of the key questions in microbiome research is how microbial communities from two environments differ, and one of the main approaches to this question is the identification of taxa which are differentially abundant in the two ecosystems. A number of methods for performing differential abundance analysis were discussed. Although simulation studies are often conducted to evaluate the performance of various procedures in terms of false discovery rates (FDR) and power, researchers at this meeting recognized that the following two issues are important to consider: (a) The parameter of interest in the statistical hypothesis. Some methods test for relative abundances and others test for absolute abundance. Both of these parameters are important, depending upon the scientific question of interest. Often researchers are not precise in what exactly they are testing. This leads to wrong analysis and misinterpretation of data. (b) Some statistical tests are specifically designed to test statistical hypotheses regarding relative abundances and others for absolute abundance. The simulation studies are often designed to generate the null data under one or the other type hypothesis, i.e. null hypothesis of no differential abundance or the null hypothesis of null differential relative abundance. However, researchers compare the FDR and power using these same simulated data but different hypotheses. Thus, a data are generated under the null hypothesis of equal relative abundance but are being used to test the null hypothesis of no differential absolute abundance. This will result in inflated FDR for methods designed for no differential abundance and vise-versa. For these reasons simulation studies need to be conducted carefully.

An important issue in differential abundance testing and other microbiome analyses is how to deal with the variation in sequencing depth. The traditional approach in microbiome data analysis is to consider proportions instead of counts. However, as was demonstrated in one presentation, variations in proportions can be caused by changes in the abundance of OTUs with large bias factors. Log-ratios can be used instead, and have been used in a number of compositional data analyses. However, the microbiome data is very sparse with many zero counts, which are problematic when computing log-ratios. Therefore substantial work is needed on developing methods for approximating log-ratios of sparse counts. Another approach is to treat the count correction as a parameter to be estimated in the model. The relative merits of these methods were presented in several talks. However, it is clear that this is a very challenging problem with no completely satisfactory solutions, and a lot of further work is ongoing in the field.

Kernel Methods

An alternative to analysis of individual taxa (OTUs) is to conduct community level analysis (also called β-diversity analysis) wherein the entire microbial profiles is collectively assessed for association with an outcome or variable of interest. By focusing on the overall profile, this mode of analysis can be more powerful when taxa show individually modest, yet concerted, shifts. Kernel methods represent a powerful approach for facilitating community level analyses by way of the Microbiome Regression-Based Kernel Association Test (MiRKAT) [**?**]. Focusing on a quantitative outcome (y_i), MiRKAT relates y_i to covariates C_i and microbiome profiles Z_i through the model

$$y_i = \beta_0 + C_i'\beta + h(Z_i) + \varepsilon_i,$$

where β_0 and β are coeffiecents for the intercept and covariate effects and ε_i follows a distribution with mean 0 and variance σ^2. $h(\cdot)$ is a generally specified function of the microbiome profiles sitting within a reproducing kernel Hilbert space generated by a positive definite kernel function $K(\cdot,\cdot)$. Then through the connections between kernel methods and linear mixed models, assessing the null hypothesis that $H_0 : h(Z_i) = 0$ can be done by constructing a variance component score statistic

$$Q = \frac{1}{\hat{\sigma}^2}\hat{\varepsilon}' K \hat{\varepsilon}$$

where $\hat{\sigma}$ and $\hat{\varepsilon}$ are estimated under H_0 and K is a matrix with $(i,j)^{th}$ element equal to $K(Z_i, Z_j)$. Q asymptotically follows a mixture of χ^2 distributions. Intuitively $K(\cdot,\cdot)$ measures similarity between pairs of individuals based on their microbiome profiles such that K is a similarity matrix. Then this analysis essentially compares similarity in microbiome profiles to similarity in outcomes. By constructing similarities via transformation of ecologically relevant distances and dissimilarities, this enables capture of key structure in microbiome data such as phylogeny and qualitative/quantitative relationships [13, 4, 19].

Kernel methods are a generalization of commonly used distanced-based permutation approaches [1], but allow for improved covariate adjustment and computational efficiency through use of asymptotic distributions. In addition, this allows investigators to harness the rich literature on kernel-based association test procedures, which are widely used within the genetics literature, to facilitate analysis within the context of more complicated microbiome studies such as those with multivariate, longitudinal, cluster correlated, or survival endpoints [23, 18, 24].

In the meeting several talks touched upon kernel methods. One talk focused fully on using kernel methods to conduct integrative analysis of microbiome and other types of genomic data. Specifically, the use of multiple omic technologies (host genetics, epigenetics, proteomics, metataxonomics, etc.) on the same cohort is rapidly increasing. However, investigating associations across complex multivariate outcomes with distinct data structures remains a challenge. One proposed method presented was the use of a dual kernel-based association test (DKAT) to evaluate the similarity between datasets [22]. Specifically, a kernel machine regression model, MiRKAT, may be used as a robust microbiome regression-based kernel association test to circumvent challenges associated with large omics multivariate datasets. This approach is tailored to capture data structure and their inherent characteristics (e.g. high dimensional data, non-normally distributed, zero-abundant). The utility of such a method was applied to identify associations between the gut microbiome and host gene expression of IBD patients[17]. The basic approach of DKAT is to first compute the pair-wise similarity in the microbiome profiles and that of the other datasets (e.g. host gene expression profiles). The similarities for each dataset are then compared to each other and assessed via kernels. The test for multivariate correlation between the kernelized data using a kernel RV coefficient. As multi-disciplinary research continues to expand, the number of outcomes measured per subject will invariably grow and increase in complexity. Sophisticated and computationally efficient statistical approaches that are amenable to large complex datasets will be necessary to enable intricate association testing between microbiome taxa and other measured outcomes.

Modelling temporal dynamics of microbial communities

Another topic raised was modelling of temporal dynamics of microbial communities. This is a very new topic in microbiome research. While some studies have collected time-series data on the microbiome, the analysis of these studies in terms of efforts to understand the temporal dynamics has been very limited. One talk presented new research into the use of stochastic differential equations for modelling the temporal dynamics. Two projects in this area were presented. The first looked at the dynamics of single genera, focussing on questions of whether there is evidence for temporal continuity and for mean reversion in microbial communities, looking particularly at data from the human gut microbiome from the moving picture dataset [3]. The evidence from the data suggests that there is temporal continuity, and strongly indicates that the system is subject to mean reversion. By analysing the Fisher information matrix for the models in question, it is possible to estimate the most informative sampling scheme for estimating temporal dynamics. For the level of mean reversion estimated from the gut, the best sampling frequency is found to be in the range of one sample every 0.8-3.2 days.

For the temporal interactions between multiple genera, a stochastic generalised Lotka-Volterra equation was used. The theory behind this equation has been developed, and the equation has a unique solution with a stationary ergodic distribution. The parameters of this equation can be estimated from real data using Approximate MLE estimators. These are shown to improve upon previous estimators based on deterministic differential equations with normal error. Using this model, it is possible to estimate the interactions between the most abundant genera. For the gut data from the moving picture data set [3], it was found that there is evidence that *Lachnospiraceae* inhibits both *Ruminococcaceae* and an unspecified genus from family Bacteroidales. *Ruminococcaceae* appears to inhibit *Bacteroidaceae*, which appears to inhibit another unspecified genus from family Bacteroidales. Meanwhile, evidence suggests that *Porphyromonadaceae* stimulates growth of the other genera, particularly *Ruminococcaceae*. This is consistent with what little is known biologically about these organisms, but paves the way for further biological insights into the functioning of microbial communities.

Metagenomic data and other Omics Data

Limitations of Metagenome-Assembled Genomes

Although the analysis of marker genes such as the 16S ribosomal RNA gene can provide insight into the taxonomic composition of microbial communities, these analyses convey little about the functional capabilities of the corresponding microorganisms. Assigning a name such as *Escherichia coli* or *Bacteroides thetaiotaomicron* to an OTU or ASV gives incomplete information due to the potential for considerable functional variation among members of a given species. Genome sequencing from culture can yield further insights, but culturing the entire repertoire of microorganisms from, for example, a stool sample cannot be done. Metagenomics, the shotgun sequencing of DNA extracted directly from a sample without culturing, can overcome this limitation, and we can search these metagenomes for important functions such as pathogenicity, metabolic functions, and antimicrobial resistance. However, the power of metagenomic analysis comes at the cost of tearing genomes into small DNA fragments that lose information about even their closest neighbouring sequence in the genome. Researchers have tried to overcome this last limitation by reassembling entire genomes from metagenomes. This procedure requires the assignment of reads from a potentially complex metagenome to a "bin" that hopefully corresponds to a single, real genome, and assembly of the reads in that bin to produce a "metagenome-assembled genome" or MAG. The problem is very challenging, and as with most problems in bioinformatics, multiple approaches have been developed to accomplish this task. A preliminary simulation study of three methods plus one meta-method showed that bin "purity" (i.e., the percentage of reads in a bin that belonged to the correct genome) and assembly completeness varied substantially by method and by genome, with closely related genomes often confounding MAG assembly. However, overall accuracy scores fail to address the question of what we are missing in MAG assemblies that are inevitably not perfect. A deeper analysis of the simulated dataset revealed that two types of genetic structures, plasmids and genomic islands, were recovered at extremely low ($< 40\%$ in the best case) levels of sensitivity. These structures are highly mobile and often bear genes that confer pathogenicity and antimicrobial resistance; thus it is important to recognize that MAG reconstruction alone should not be used to infer these traits. Future development should focus on incorporating reference-based assembly, better use of reads that do not assemble in the early stages of the algorithm, and long-read sequencing to augment the traditional short-read approaches.

Integration of Microbiome and other Omics Data

High throughput microbiome profiling studies have identified associations between microbiome composition and a wide range of human disease and traits including cancer, HIV, menopause, blood pressure, and others [20, 9, 16, 21]. Despite the plethora of findings, the specific mechanisms by which the microbiome influences these conditions and health outcomes remain unclear. To this end, many studies are now interested in integrating other types of genomic data such as metabolomics [14], gene expression [17], and DNA methylation [5] into microbiome studies. These other genomic markers can serve as intermediaries between microbiome composition and outcomes and may provide clues as to the specific manner by which microbes drive subsequent processes and disease. Conversely, guided by recent interest in microbiome studies and the potential impact, many large scale genomic studies, such as large genome wide association study cohorts [10], are also collecting microbiome data. The ability to integrate microbiome data with other types of genomic data promises comprehensive achievement of many biological, clinical and public health questions that have eluded researchers for decades.

Despite the promises of these data, statistical analysis of these data continue to present difficulties for researchers. Some of the central challenges sometimes include the standard problems for analyzing -omics data including high-dimensionality, nonlinear effects, interactions among data features, modest effect sizes, and limited availability of samples. However, in analyzing multiple data types, it is also necessary to accommodate the nature of the individual data types. For example, microbiome data are subject to zero inflation, over-dispersion, compositionality, and structural (e.g. phylogenetic and functional) constraints [12]. Other data types have their own personalities that present challenges. Finally, a major challenge lies in identifying the problem at hand: many researchers are conceptually interested in data integration yet do not have a specific problem that is well formed. The vagueness of the problem often prevents direct translation into mathematical and statistical terms. This last issue poses a particularly grand challenge for statisticians as it hinders development and application of relevant statistical tools.

Particular problems of interest are contextual, but within the context of multi-omics data, we borrow a recently presented taxonomy for describing studies involving multiple omics data types developed by Zhao [26]. In particular, Zhao classifies studies based on data structure and research questions. Data structure, here, is a simple dichotomization of whether the different types of omics are collected on the same sample or on different individuals (sampling unit). Research questions can be loosely broken down as synthesis questions and transfer questions. Synthesis questions essentially are questions wherein multiple -omics are aggregated to understand an outcome

Data Structure	Question Type Synthesis	 Transfer
Same Samples	Subtyping Prediction models Visualization	Correlation Mediation analysis Effect modification
Different samples	Understanding relationships between disease	Predicted metabolomics

Table 21.1: *Specific types of multi-omic studies conducted within the context of microbiome profiling fall into categories based on data structure and research question.*

better. Transfer questions are questions wherein one type of -omic data is used to better understand another -omic data type or to better analyze another (possibly with regard to outcome).

Some example studies are given in Table 21.1. For example, subtyping to identify enterotypes or clusters of microbial communities (individuals) can be done using just microbiome data, but could be improved by also including metabolomics data measured on the same individuals. That the metabolomics improves an already feasible analysis implies that the question is a synthesis question. Similarly, mediation analysis generally requires both data types to be collected on the same individuals. Moreover, mediation would not be feasible without both types of data. Therefore, the question in this case is a transfer question.

Application of microbiome data analysis in scientific and clinical contexts

Decreasing costs for next-generation sequencing have accelerated the availability of this sequencing technology to research labs, hospitals, public health labs, and other regulatory bodies. As such, many are embracing the use of metataxonomic and shotgun metagenomics approaches for a multitude of purposes including infectious disease detection, antimicrobial resistance prediction, and microbial community characterization across various sectors. Though many bioinformatics solutions are available for metataxonomic and shotgun metagenomics data processing, relatively few user-friendly statistical solutions are available. This is a critical gap given that many metagenomic and microbiome studies are being undertaken by biologists, clinicians, or research personnel with limited statistical expertise. In particular, the application of clinical metagenomics – shotgun sequencing of a clinical specimen for unknown infectious disease detection – is rapidly being embraced by frontline laboratories in cases where conventional microbiological testing has failed to identify the infectious agent [7, 8]. Unlike microbial community characterization studies, the goal of a clinical metagenomics approach is to identify and report the causative agent with an interpretation criterion supported by a confidence threshold. To date, no such statistical method or interpretation criterion exists. In this regard, there is a need for infectious disease experts and statisticians to work together towards the development of an approach for reporting of clinical metagenomics findings.

Microbiome methodologies are frequently applied in many studies to identify key taxonomic features that are differentially abundant. As reported during this workshop, many statistical methods have been developed for differential abundance testing, however, random forest classification, a machine learning approach, can also be used to identify key taxa of importance in microbiome studies. In one study presented [6], a random forest classifier approach was used to classify Crohn's disease and healthy control subjects. The model performed well and important features for classification were consistent with taxa identified using differential abundance testing. This approach may be useful to identify biomarkers highly associated with disease.

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Chapter 22

Classification Problems in Von Neumann Algebras (19w5134)

September 29 - October 4, 2019

Organizer(s): Adrian Ioana (University of California, San Diego), Jesse Peterson (Vanderbilt University)

Overview of the Field

Overview of the topic of the workshop

Von Neumann algebras are algebras of bounded operators on a Hilbert space that are closed under taking the adjoint and in the weak operator topology. If their center consists only of multiples of the identity, they are called factors. Since its early development in the 1930's, the subject has been closely connected to ergodic theory and group theory, via a seminal construction which associates von Neumann algebras to countable groups and their actions on measure spaces. A major theme in the area remains to classify such group and group measure space von Neumann algebras. This problem is typically studied when the von Neumann algebras are II_1 factors, which corresponds to the groups being infinite conjugacy class (icc) and respectively the actions being free, ergodic and probability measure preserving. Early work, concentrating on the amenable case, culminated with Connes' celebrated classification of amenable factors in the 1970's [8]. By contrast, the non-amenable case turned out to be extremely difficult, in large part remaining intractable.

In recent years, there have been spectacular advances in the classification of von Neumann algebras, generated largely by Popa's discovery of deformation/rigidity theory in the early 2000s [31]. Much of this progress has been stimulated by the reemerging connections to ergodic theory and group theory, as well as recent newly developed connections to measured group theory and logic. We next overview some of the recent breakthroughs made on classification problems within von Neumann algebras as well as on problems at the interface with measured group theory and model theory.

Group von Neumann algebras

First, remarkable progress has been made in the study of structural properties and the classification of group von Neumann algebras. By using deformation/rigidity theory, Ozawa and Popa (2007) proved that the free group factors $\mathrm{L}(\mathbb{F}_n)$, with $n \geq 2$, satisfy a structural property called strong solidity [27]. This considerably strengthened the absence of Cartan subalgebras for such factors obtained by Voiculescu in the mid 1990s using free probability theory [34]. A surprising result of Guionnet and Shlyahtenko (2012) shows that for small q and a fixed number of generators, the q-deformed free group factors are all isomorphic [19]. Despite this progress in understanding the structure of the free group factors, it is a longstanding open problem whether II_1 factors arising from non-abelian free groups of different ranks are isomorphic or not.

Another outstanding problem asks to prove that the arithmetic groups $\mathrm{PSL}_k(\mathbb{Z})$ give rise to non-isomorphic II_1 factors, for different values of k. More generally, a far-reaching rigidity conjecture of Connes from 1980 predicts that property (T) groups having isomorphic von Neumann factors must be isomorphic. Since property (T) passes from groups to their von Neumann algebras, the conjecture is equivalent to a superrigidity statement: the von Neumann algebra of a property (T) group completely determines the group. A breakthrough in this direction was made by Ioana, Popa and Vaes who discovered the first examples of superrigid groups [23]. However, these groups do not have property (T), leaving open the problem of a finding even a single example of an icc superrigid group with property (T). In 2018, using a new notion for groups called proper proximality, the first structural results for the von Neumann algebras of $\mathrm{PSL}_k(\mathbb{Z})$ with $k \geq 3$ were obtained in [6]. This opens up a promising angle of attack on the isomorphism problem for $\mathrm{L}(\mathrm{PSL}_k(\mathbb{Z}))$.

Group measure space von Neumann algebras

Secondly, some of most striking recent developments in the theory of von Neumann algebras concern the classification of group measure space von Neumann algebras. These include the discovery by Peterson [28], Popa and Vaes [32], and Ioana [21] of the first families of group actions which are W^*-superrigid, in the sense that the group and action can be entirely recovered from their von Neumann algebras. Another major accomplishment is due to Popa and Vaes (2012) who showed that group measure space factors arising from arbitrary free actions of free groups have a unique Cartan subalgebra [33] up to unitary conjugacy. In combination with work of Gaboriau ([16],[17]), they deduced that factors associated to actions of free groups of different ranks are never isomorphic. This settled the group measure space version of the free group factor problem. More generally, a well-known conjecture predicts that if a group G has a positive first L^2-Betti number, then any II_1 factor associated to a free action of G must have a unique Cartan subalgebra, up to unitary conjugacy. If true, it would follow that the first L^2-Betti number of the group is an isomorphism invariant of the group measure space factor.

Von Neumann algebras and measured group theory

Thirdly, recently there have been important advances on several classification problems at the interface of von Neumann algebras and measured group theory. The latter studies groups by looking at the orbit structure of their measure preserving actions on probability spaces. A central theme is to classify such actions up to orbit equivalence. This is closely related to the classification of group measure space von Neumann algebras. Much of the recent progress on these classification problems has been achieved hand-in-hand. For instance, ideas from the theory of von Neumann algebras were used to show that any non-amenable group admits uncountably many free ergodic actions that are not orbit equivalent [11] (see also [20] and [18]). Using his deformation/rigidity theory, Popa famously proved that Bernoulli actions of property (T) groups are superrigid with respect to orbit equivalence [30]. Another theme in measured group theory which has received considerable attention in the last few years is the classification of conjugation invariant positive definite functions (in short, characters) of a given group. This is equivalent to classifying all II_1 factor representations of the group. In 2007, Bekka proved that $\mathrm{PSL}_k(\mathbb{Z})$ with $k \geq 3$ has only one such representation, the left regular representation [3]. In 2015, Peterson obtained a far-reaching generalization which shows the same holds for all lattices in higher rank simple Lie groups [29]. This confirmed a conjecture of Connes from the 1980s, and extended Margulis' celebrated normal subgroup theorem.

Von Neumann algebras and model theory

Finally, there has been significant interest recently in the model theory of von Neumann algebras initiated by Farah, Hart and Sherman ([13], [14], [15]). A primary goal here is to classify II_1 factors up to elementary equivalence. Two II_1 factors are elementarily equivalent if and only if they admit isomorphic ultrapowers, with respect to some, possibly very large, ultrafilters. Until recently, only three distinct elementary classes of II_1 factors have been known, similar to the isomorphism situation for separable II_1 factors in the 1940s-1960s. However, Boutonnet, Chifan and Ioana succeeded in providing a continuum of non-elementarily equivalent II_1 factors [2]. Elementary equivalence of II_1 factors still remains largely mysterious. A basic question is to find non-elementary II_1 factors that are not McDuff, or perhaps do not even have property Gamma.

Objectives and structure of the workshop

The principal aim of this workshop was to further research on the classification of von Neumann algebras, by capitalizing on the recent advances described above and taking advantage of newly developed connections to other areas. The workshop brought together leading experts and young researchers working in von Neumann algebras and interacting areas, such as measured group theory, logic, C^*-algebras and free probability.

The workshop had 37 participants in a very active area at the intersection of operator algebras with ergodic theory and logic. There were 25 talks, of 50 or 25 minutes each, about one third of which were given by promising young reseachers (seven postdoctoral researchers and one graduate student). The talks were generally of high quality and generated a lot of stimulating discussions and interactions among the participants.

Presentation highlights

In this section, we discuss some of the main results presented, divided into several thematic directions:

Structure and classification of von Neumann algebras

Several talks were devoted to problems concerning the structure and classification of von Neumann algebras that arise intrinsically in the theory.

Marius Junge: q-Gaussian von Neumann algebras

Junge discussed a new class of von Neumann algebras, called q-Gaussian algebras with coefficients, which are q-Gaussian analogues of amalgamated free products. He presented a strong solidity theorem for such algebras inspired by Popa and Vaes' work [33] discussed in Section 22.

Yusuke Isono: Popa's intertwining theory for type III factors

A fundamental tool in deformation/rigidity theory is Popa's intertwining theorem. This provides a method to prove unitary conjugacy of subalgebras of a given II_1 factor. In order to apply deformation/rigidity theory to von Neumann algebras of type III, there have been several attempts to generalize the intertwining technique to this setting. Isono explained his very recent work which extends the intertwining technnique to general von Neumann algebras of type III [25].

Two of the talks were devoted to superrigidity phenomena for group algebras, see Section 22. We recall that a countable group Γ is called W^*-superrigid (respectively, C^*-superrigid) if it can be recovered from its group von Neumann algebra $\mathrm{L}(\Gamma)$ (respectively, reduced C^*-algebra $\mathrm{C}^*_r(\Gamma)$).

Sven Raum: Superrigidity for group operator algebras

Raum started with an excellent introduction to the state-of-art of the C^*-superrigidity problem for groups. He then presented a recent result showing that any torsion free 2-step nilpotent group is C^*-superrigid [12].

Ionut Chifan: Some rigidity aspects in von Neumann algebras and C^*-algebras arising from groups.

In a related talk, Chifan explained how techniques used to establish W^*-superrigidity results in [23] can be employed to provide a new class of groups which are C^*-superrigid. These groups appear as wreath products with non-amenable core. In particular, they are non-amenable and thus different than the groups considered by Raum. Moreover, for these groups one can calculate the automorphism group of their reduced C^*-algebras.

Ben Hayes: Maximal rigid subalgebras of deformations and L^2-cohomology, I, and
Rolando de Santiago: Maximal rigid subalgebras of deformations and L^2-cohomology, II

Hayes and de Santiago gave two back-to-back talks on their recent joint work with Hoff and Sinclair [10]. Hayes presented a theorem which implies that if G is a group with positive first L^2-Betti number, then its von Neumann algebra $\mathrm{L}(G)$ cannot be generated by two subalgebras with property (T) with diffuse intersection. This is a consequence of a conceptul result showing that if a diffuse subalgebra Q is rigid (in the sense of Popa) with respect to a mixing malleable deformation of M, then it is contained in a unique maximal rigid subalgebra of M. In the second talk, de Santiago presented additional consequences of these techniques, including a result asserting that the quasi-normalizer of a rigid diffuse subalgebra generates a rigid subalgebra.

Lauren Ruth: Von Neumann equivalence and properly proximal groups.
Ruth explained an interesting new notion of equivalence for countable groups, called von Neumann equivalence, which generalizes both W^*-equivalence and measure equivalence. Solving a poblem posed in [6], Ruth and co-authors proved that proper proximality is invariant under von Neumann equivalence, and thus under measure equivalence [22].

David Jekel: Free complementation of certain MASAs in $\mathrm{L}(\mathbb{F}_d)$ via conditional transport of measure
Jekel discussed recent exciting work in which he establishes a "triangular" version of the free transport phenomenon pioneered by Guionnet and Shlyakhtenko in [19] (see Section 22). This has striking applications to the structure of the free groups factors $\mathrm{L}(\mathbb{F}_d)$ which can be realized as the von Neumann algebra $\mathrm{W}^*(S_1, ..., S_d)$ generated by d freely independent semicircular elements. Specifically, Jekel shows that if P is any non-commutative polynomial, then for every small enough $\varepsilon > 0$, the von Neumann algebra generated by $S_1 + \varepsilon \cdot \mathrm{P}(S_1, ..., S_d)$ is freely complemented, and thus maximal amenable, in $\mathrm{L}(\mathbb{F}_d)$.

Von Neumann algebras and measured group theory
Several talks were focused on the topics at the intersection of von Neumann algebras and measured group theory discussed in Section 22. First, three talks were devoted the study of orbit equivalence relations associated to probability measure preserving actions of countable groups.

Yoshikata Kida: Groups with infinite FC-center have the Schmidt property
A countable group is said to have the Schmidt property if it admits an ergodic free probability measure preserving action such that the full group of the associated orbit equivalence relation contains a non-trivial central sequence. Klaus Schmidt asked whether any inner amenable group has this property. Kida explained a recent result showing that any countable group with infinite FC-center has the Schmidt property [26].

Pieter Spaas: The Jones-Schmidt property and central sequence algebras
Spaas presented examples of countable equivalence relations that do not have the Jones-Schmidt property, answering a question of Vaughan Jones and Klaus Schmidt from 1985 [24]. He also discussed connections with structural properties of central sequence algebras, and implications for unique McDuff decompositions.

Daniel Drimbe: Orbit equivalence rigidity for product actions
Drimbe presented a new type of a rigidity phenomenon in orbit equivalence: for a large class of product actions $\Gamma = \Gamma_1 \times ... \times \Gamma_n$ on $X = X_1 \times ... \times X_n$, the orbit equivalence relation remembers the product structure of the group action [9]. More precisely, if a free ergodic action of a group Λ on Y is orbit equivalent to Γ on X, then essentially Λ is a product of n groups such that its action on Y is a product of n actions.

Secondly, we also had two talks devoted to character rigidity.

Bachir Bekka: Characters of algebraic groups
Bekka discussed the characters of the group $G(k)$ of k-points of an algebraic group G defined over a field k. Under the assumption that $G(k)$ is generated by its unipotent elements, he presented a complete classification of $\mathrm{Char}(G(k))$ in two cases: 1) G is k-simple and k is an arbitrary infinite field; 2) G is an arbitrary algebraic group and k is a number field [4].

Remi Boutonnet: Stationary characters on lattices in semi-simple groups
A positive definite function ϕ on a countable group G is called a stationary character with respect to a probability measure μ on G if it satsfies $\mu * \phi = \phi$. Boutonnet presented a recent breakthrough joint with Houdayer in which

they show that stationary characters of higher-rank lattices G are genuine characters [5]. He presented several applications of this result to representation theory, operator algebras and topological dynamics. In particular, he explained a striking consequence which is new even for $G = \mathrm{SL}_k(\mathbb{Z})$ with $k \geq 3$: any weakly mixing unitary representation of G weakly contains the left regular representation. He also explained how this work allows to recover Peterson's character rigidity theorem discussed in Section 22.

Von Neumann algebras, the Connes Embedding Problem and Model Theory

The Connes Embedding Problem (CEP) is a major open problem in operator algebras which asks whether any separable II_1 factor M can be embedded into the ultrapower R^ω of the hyperfinite II_1 factor R. While originally formulated in terms of von Neumann algebras, this problem has equivalent formulations in many different areas, including C^*-algebras, quantum information theory and model theory.

Isaac Goldbring: Playing games with II_1 factors

Goldbring introduced several games that one can play with II_1 factors and the connection between these games and other active areas of research, including the Connes Embedding Problem and the study of elementarily equivalent II_1 factors. Towards the end of the talk, he mentioned an open question asking whether the hyperfinite II_1 factor R is infinitely generic, and pointed out that a negative answer would lead to the first example of two non-elementarily equivalent existentially closed II_1 factors.

Scott Atkinson: Ultraproduct embeddings and amenability for tracial von Neumann algebras

Atkinson discussed a recent result joint with S.Kunnawalkam Elayavalli showing that for Connes embeddable tracial von Neumann algebras M amenability is characterized by the property that any two embeddings into an ultrapower of R are conjugate by unital completely positive maps [1]. He also explained a theorem, partially answering a question of Popa, which shows amenability of M is also equaivalent to the separability of the space of embeddings of M into any ultraproduct of II_1 factors.

Kate Juschenko: Representations of products of the free group, transport operators and Connes' embedding problem

Juschenko discussed several conjectures related to the Connes' embedding problem, in the spirit of Kirchberg's equivalent reformulation in terms of unitary representation of products of free groups.

Thomas Sinclair: Tensor products of matrix convex sets
Sinclair spoke on joint work with R. Araiza and A. Dor-On on the tensor theory of matrix convex sets. As an application, they obtain a new formulation of the Connes' embedding problem via noncommutative Choquet theory.

Ian Charlesworth: Matrix models for ε-independence
Charlesworth explained how to construct matrix models (in a certain tensor product of matrix algebras) for the notion of ε-independence, which is an interpolation of classical and free independence.

C^*-algebras
Tim de Laat: Exotic group C*-algebras of simple Lie groups with real rank one.
The reduced and full C^*-algebras of a locally compact group G concide exactly when G is amenable. In general, for non-amenable groups G, there can be many *exotic* C^*-algebras sitting between the reduced and full C^*-algebras. De Laat presented results on exotic C^*-algebras of Lie groups of rank of G which arise from L^p-integrable representations of G.

Claire Anantharaman-Delaroche: Weak containment vs amenability for group actions and groupoids
A groupoid or a group action on a C^*-algebra has the weak containment property if the associated reduced and full C^*-algebras coincide. For groups, this property is equivalent to amenability. Anatharaman Delaroche discussed the subtle question of whether in general the weak containment property implies amenability.

Alain Valette: Explicit Baum-Connes for $\mathbb{Z}^2 \rtimes \mathbb{F}_2$
Valette reported on an explicit calculation of the assembly map appearing in the Baum-Connes conjecture in the case of the semi-direct product $G = \mathbb{Z}^2 \rtimes \mathbb{F}_2$, where $\mathbb{F}_2 < \mathrm{SL}_2(\mathbb{Z})$ is a free subgroup on 2 generators.

Kristin Courtney: Amalgamated Products of Strongly RFD C^*-algebras arising from locally compact groups
Courtney's talk discussed joint work with T. Shulman giving new instances of when residual finite dimensionality of C^*-algebras is preserved under the amalgamated free product construction. This is proven to hold for pairs of "strongly residually finite dimensional" C^*-algebras amalgamated over a central subalgebra.

Other topics
Stefaan Vaes: Ergodicity and type of nonsingular Bernoulli actions
Vaes reported on a joint work with M. Björklund and Z. Kosloff on nonsingular Bernoulli actions. In this very impressive work, the authors prove in almost complete generality that a nonsingular Bernoulli action is either dissipative or weakly mixing, and determine its Krieger type.

Robin Tucker-Drob: Inner amenability and the location lemma
Tucker-Drob overviewed recent results on inner amenable groups, focusing on joint work with P. Wesolek and B. Duchesne, in which they obtained a complete characterization of inner amenability for generalized wreath product groups.

Andrew Marks: Measurable realizations of abstract systems of congruence
An abstract system of congruences describes a way of partitioning a space into finitely many pieces satisfying certain congruence relations. Marks discussed the question of when there are realizations of abstract systems of congruences satisfying various measurability constraints (e.g., requiring the pieces to be Borel). Marks presented a general result showing that, under certain assumptions, abstract systems of congruences can be realized by any hyperfinite action of $\mathbb{F}_2$ on a standard probability space using measurable pieces.

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Chapter 23

Spaces of Embeddings: Connections and Applications (19w5232)

October 13th - 18th, 2019

Organizer(s): Dev Sinha (University of Oregon), Ryan Budney (University of Victoria), Robin Koytcheff (University of Louisiana at Lafayette)

Background

Manifolds are basic objects of study in topology. They are "locally Euclidean" meaning that to one with limited eyesight, like an ant on a hill or a person looking at the horizon, they seem like an unlimited, uniform expanse. They arise throughout mathematics, first studied as they arose in solving equations but from there touching on virtually every subfield.

An embedding is essentially a copy of one manifold in another. Thus studying all embeddings captures relationships between two instances of these basic objects. The subject is akin in this way to representation theory in algebra. Because of its basic nature, the study of embeddings was a primary focus in the mid twentieth century, with an initial flowering through the work of Whitney, Morse and Haefliger. After a relatively quiet period, the study of embeddings has enjoyed a renaissance since roughly the turn of the century for two reasons. First, a combination of new techniques have both proven successful at resolving long-standing questions and opening up new lines of inquiry. Also, astonishing connections with topics such as field theory have increased interest from and fostered fruitful exchanges with a wide range of mathematicians.

Early work on spaces of embeddings

Haefliger is perhaps the most prominent pioneer in moving from considering just a single embedding to the collection of all embeddings from one manifold to another, which we refer to as a *space of embeddings* and denote $\mathrm{Emb}(M, N)$. The space of immersions – maps for which the domain manifold can intersect itself globally but still must be locally an embedding – has been well understood since the 1950's by work of Smale, so topologists often start with the question of "promoting" immersions to be embeddings. A main technique Haefliger developed was a parametrized double-point elimination process. These were successful to a point, but became difficult to manage computationally and had clear "hard" limitations on the extent to which they could capture the homotopy type of embedding spaces. Meanwhile, nearby branches of mathematics experienced wonderful developments: 3-manifold theory and 4-manifold theory were being rewritten via Thurston's work on geometrization and Donaldson's use of gauge theory respectively. The rich connections these subfields have with other areas of mathematics were not apparent in the techniques initially developed to study embeddings.

Interest in the subject of embedding spaces was renewed starting in the 1980's by the work of Vassiliev [69], Birman and Lin [6], and Jones [35]. The Jones polynomial, a new invariant of knots (that is, embeddings of circles in $\mathbb{R}^3$), was inspired by statistical mechanics and interpreted field-theoretically by Witten [76]. The mystery of how the Jones polynomial fits into the rest of low-dimensional topology, and mathematics more generally, inspired much interest. Vassiliev made a major contribution shortly thereafter. The coefficients of the Jones polynomial, after a simple change of variables were shown to be *finite-type invariants*. These are numerical invariants of knots that satisfy simple crossing-change formula. Vassiliev found the source of all such invariants in his study of the cohomology of the space of knots. His technique was to view the space of knots as the complement of a discriminant space in a contractible mapping space, inspired in part by the study of complements of linear arrangements from algebraic geometry. Via a duality argument, this converted the study of the space of embeddings, which is homogeneous, with a readily stratified discriminant space. Such a stratification allowed for employment of spectral sequences.

Independently, in the 1980's Tom Goodwillie made a beautiful observation about the homotopy type of pseudo-isotopy embedding spaces [25]. These embedding spaces by design fit into fiber bundles relating the homotopy type of other embedding spaces, so they are useful for induction arguments. The Morlet Disjunction Lemma described the relative homotopy groups of pairs of pseudo-isotopy embedding spaces. Goodwillie's observation was that these pseudo-isotopy embedding spaces satisfy an even more revealing multiple disjunction lemma. This framework for describing the effects of multiple disjunctions through the language of categories and functors evolved into what is now known as the Goodwillie–Klein–Weiss calculus of embeddings [75, 11, 18]. Moreover, Goodwillie recognized and developed a similar framework in algebraic topology. These frameworks and others inspired by them are know generally as *functor calculus*. The embedding calculus gave useful models for the homotopy types of embedding spaces and was shown to be the natural extension of Haefliger's approach. Embedding calculus provides a sequence of approximations, denoted $T_n\mathrm{Emb}(M, N)$ to the homotopy-type of the embedding space $\mathrm{Emb}(M, N)$. These approximations were proven to be "sharp" as $n \to \infty$ provided the co-dimension of the embeddings was at least three, and thus the relevance to case of co-dimension-two classical knots remained a mystery.

While classical knot theory primarily focuses on whether knots can be deformed to one another, spaces of knots were of interest because of their close connection to the space of diffeomorphisms of a three-sphere, $\mathrm{Diff}(S^3)$. Allen Hatcher's theorem from 1983 that $\mathrm{Diff}(S^3)$ is homotopy equivalent to its subspace of linear diffeomorphisms [31] has as a consequence that the unknot component of $\mathrm{Emb}(S^1, S^3)$ has the homotopy type of the subspace of great circles, i.e. the Stiefel manifold $V_{4,2} \simeq S^3 \times S^2$. Hatcher went on to describe what could be said about the homotopy type of the other components of $\mathrm{Emb}(S^1, S^3)$, combining everything that was known about 3-manifolds at the time, such as the work of Haken, Waldhausen, Mostow, Prasad, Thurston and himself. This allowed an iterated fiber bundle description of the homotopy type of all the components of $\mathrm{Emb}(S^1, S^3)$ that he wrote up in an unpublished draft [32]. These results are complementary to those of Goodwillie, Klein, and Weiss, and these authors and Hatcher all expressed interest in the relationship between their techniques and the work of Vassiliev.

A final important precursor to the current state of embedding theory is the work by Bott and Taubes [7] and others on configuration space integrals, starting in the early 1990's. These integrals arise in field theory, in particular Chern–Simons theory, and require compactifications as defined by Axelrod and Singer [4]. Such integrals can be used to define knot and link invariants which generalize the Gauss linking integral. By celebrated work of Kontsevich, they produce all Vassiliev (i.e. finite-type) knot invariants [37]. A key insight was that the combinatorics of the integrals which are isotopy invariant are governed by a (co)chain complex of graphs, which because of the roots in perturbative Chern–Simons theory are sometimes called Feynman diagrams. In the 1990's, Kontsevich pioneered the use of these integrals and graph (co)homology in a number of settings [38, 39, 40], such as the cohomology of $\mathrm{Emb}(S^1, \mathbb{R}^n)$, 3-manifold invariants, characteristic classes of manifold bundles, outer space, mapping class groups, deformation quantization of Poisson manifolds, and formality of the little disks operad – topics which played a prominent role in his Fields Medal citation. These areas continue to be developed by multiple communities of mathematicians to this day. Kontsevich's graph complexes are now seen to encode a variety of previously understood structures, including Haefliger's calculation of isotopy classes of higher-dimensional links in the 1960's; the cohomology of configuration space, calculated by Arnold [1] and F. Cohen [16] independently around 1970; the (Koszul dual) Yang–Baxter relations in work of Kohno on braids [36] in the 1980's; and the 4T relations in Bar-Natan's combinatorial formulation of Vassiliev invariants [5] in the 1990's.

Further developments, and the current state of the field

Recent work on embedding spaces has brought together these historical precedents.

In the 2000's, two important connections between Vassiliev invariants and embedding calculus were established. Budney, Conant, Scannell, and Sinha [11] showed that the integral type-2 invariant appears quite explicitly as the only invariant defined through the third embedding calculus approximation. Building on work of Scannell and Sinha [61], Volić showed that Bott–Taubes integrals can be defined on $T_n\mathrm{Emb}(S^1, \mathbb{R}^3)$ [71] and thus a homology analogue of the Taylor tower is a universal Vassiliev invariant over $\mathbb{R}$ [70]. This led to the conjecture that the embedding calculus tower is the universal integer-coefficient finite-type invariant of knots. To this day, the only universal Vassiliev invariants that are understood explicitly rather than formally are those defined with coefficients in the real numbers.

Budney developed an action of the operad of little cubes on embedding spaces and showed the space of classical long knots is freely generated by this action on the space of prime knots [8]. This is a space-level generalization of Schubert's connect-sum decomposition of knots, whose commutativity is at the heart of this action, and a partial resolution of the extension problem for the homotopy types of $Emb(S^1, S^3)$ described by Hatcher.

Shortly thereafter, Sinha [62] and Salvatore [59] followed with actions of the 2-cubes and framed 2-discs operads on embedding calculus approximations to long knot spaces, bringing some clues towards bridging our understandings of the high co-dimension and classical settings. We now have a multitude of operad actions on embedding spaces, but the significant question of how these actions compare to each other remains to be resolved. The 2-cubes action implies the existence of a second binary operation on homology, called a graded Poisson or Gerstenhaber bracket. Sakai used Budney's operad action together with Bott–Taubes integrals to show certain bracket homology classes are non-trivial [57].

Later, Budney described a new topological operad that acts on embedding spaces, called the splicing operad [10]. This operad encodes the full decomposition of knot exteriors coming from their geometrization. The proof of the geometrization conjecture [53] allows for an operadic description of the homotopy type of the splicing operad, together with a full description of the homotopy type of the space of classical knots. Roughly speaking, the splicing operad solves Hatcher's extension problem. However, the splicing operad exacerbates the problem of a multitude of operads acting on embedding spaces and the embedding calculus tower. An appealing unresolved question is if the splicing operad act on the stages of the embedding calculus tower $T_n\mathrm{Emb}(S^1, \mathbb{R}^3)$. An affirmative answer to this would be a major step towards unifying Hatcher's 3-manifold techniques with the embedding calculus.

Back in the direct study of embedding spaces, global understanding of computations in the higher co-dimension setting have come through application of rational homotopy theory, and in particular formality of configuration spaces through integrals. Motivated by a conjecture of Kontsevich, Sinha initiated the development of models for $T_k\mathrm{Emb}(\mathbb{R}^1, \mathbb{R}^n)$ through spaces of natural transformations from the 1-disks operad ("balls" in the circle) to the n-disks operad (balls in Euclidean space). These gave rise to the actions of (different) operads above. After developing a substantial amount of machinery (e.g. the deRham theory of piecewise algebraic forms, which required new results in analysis), Lambrechts, Turchin, and Volić [45] carried through a program of Kontsevich to show that these operads are formal, including in relationship to one another. This result is a triumph, whose main consequence is that the calculation of the rational homology of spaces of knots reduces to a calculation in combinatorics and algebra that is easy to formulate, though difficult to understand. Turchin later put this in the context of homotopical algebra, allowing the possibility of more sophisticated algebra being brought to bear. A corollary in turn is that Vassiliev's original approximations with rational coefficients are "sharp," but only because they coincide with the answers given by embedding calculus techniques. Arone and Turchin have similarly reduced the calculation of rational homotopy groups to combinatorics [3].

Parallel to these developments, configuration space integrals and graph cohomology have been developed in a number of directions. Extending Bott-Taubes field-theoretic integrals, Cattaneo, Cotta-Ramussino and Longoni constructed real-valued cohomology classes in spaces of knots [14]. Turchin has shown that the chain complexes defining these have the same homology as the corresponding knot spaces, but logically this could be a coincidence with most of the field theory classes being zero, presenting another question which needs to be resolved. These integrals have similarly been used for example by Watanabe [72], Koytcheff, Munson, and Volić [42] and Pelatt and Sinha [55] to generate elements of cohomology of embedding spaces. Following Kontsevich [39], various researchers also used them to define invariants of rational homology spheres [46, 43, 48]. Conant and Vogtman studied graph cohomology in connection to outer automorphisms of free groups and mapping class groups [19, 20]. More recently, Idrissi [34] and independently Campos and Willwacher [15] used such integrals to produce rational homotopy models for general configuration spaces. *** Should go through resources such as Willwacher's ICM talk to flesh this out just a touch more.***

Following these developments we have the following perspective. In co-dimension three and higher one can view the embedding calculus as a universal framework, building information about embeddings from the study of configuration spaces. This framework is bolstered by ideas coming field theory and singularity theory. In dimensions two and three, geometrization and other 2- and 3-manifold techniques, as demonstrated by Hatcher, are the appropriate framework. For diffeomorphisms in higher dimensions, it seems that a combination of techniques could be relevant in different ranges. But fleshing out these frameworks, applying them for maximal impact, and understanding their connections with other areas will occupy mathematicians in this area for some time to come. In particular, our recent work showed [12] that the n-th stage of the Taylor tower produces additive, order-$(n-1)$ finite-type invariants of classical knots, and it gave substantial spectral-sequence evidence for the the enticing conjecture that it produces all such abelian-group-valued invariants.

Presentation Highlights

In this section, we divide the content into three areas: graphs and geometric topology, functor calculus and operads.

Graphs and geometric topology

A significant portion of the results presented at our workshop involve connections between combinatorial data and differential topology, in particular the construction of nontrivial (co)homology classes in spaces of embeddings using (co)cycles in graph complexes.

The most prominent of these is **Tadayuki Watanabe**'s disproof of the Smale Conjecture in dimension 4, which appeared in his 2018 preprint [74]. This result builds on his earlier work [73] on Kontsevich's characteristic classes in the cohomology of $B\mathrm{Diff}(D^n;\partial D^n)$, coming from configuration space integrals. Watanabe had previously used a generalization of Habiro's clasper surgery [30], originally defined to study for knots and links, to construct dual homology classes in $B\mathrm{Diff}(D^n;\partial D^n)$ which pair nontrivially with the Kontsevich cohomology classes, for odd $n \geq 5$. His recent work on the Smale conjecture adapts the construction of homology classes to the case $n = 4$. In that paper, he uses work of Fukaya on graphs embedded along Morse flows – an extension of the theory of configuration space integrals – to construct the dual cohomology classes. Watanabe's result is an unexpected one that will very likely have significant consequences in 4-manifold theory.

Another striking result using some similar methods is forthcoming work of **Danica Kosanović**, who presented a proof that the map from the space $\mathcal{K} = \mathrm{Emb}(\mathbb{R}, \mathbb{R}^3)$ of long knots in $\mathbb{R}^3$ to the n-th stage $T_n\mathcal{K}$ of its Taylor tower is surjective on path components. The group $\pi_0(T_n\mathcal{K})$ already had a known combinatorial description in terms of trivalent graphs. Kosanović's method is to use gropes, as developed in this setting by Conant and Teichner [18], to construct embeddings realizing this combinatorial data. Another key aspect of her proof is to use the model for $T_n\mathcal{K}$ given by spaces of punctured knots. She used clasper surgery as a heuristic way to explain the methods, which thus bear some resemblance to Watanabe's work. Kosanović's techniques could be described as a very careful refinement of [12]. Her result uses the monoidal structure introduced therein and a beautiful relationship between gropes in finite-type invariants and the layers of the Taylor tower. It also relates to work of Conant, Schneiderman, and Teichner [21] on link invariants via 4-dimensional topology.

The study of embeddings using combinatorial data also appeared in presentations of **Michael Polyak** and **Christine Lescop**. They described configuration space invariants of knots and links in $\mathbb{R}^3$ [56, 29, 47] and of rational homology 3-spheres [48]. In their talks and informal sessions, both also shared recent results including Polyak's new combinatorial formulae for Milnor invariants of string links and David Leturcq's study of knotted S^n's in S^{n+2} [50]. Those ideas are a bridge from linking numbers via configuration spaces to the more nuanced settings of knot invariants and cohomology of diffeomorphism groups. Indeed, the Kontsevich characteristic classes are a higher-dimensional generalization of finite-type invariants of homology 3-spheres. Moreover, Lescop's work (partly with Greg Kuperberg) on Morse propagators [49] appears closely related to the techniques used in Watanabe's disproof of the 4-dimensional Smale conjecture.

Also fitting into this theme is work presented by **Keiichi Sakai** on configuration space integrals for isotopy classes of higher-dimensional knots [58]. **Arnaud Mortier** has begun to study the cohomology of the space of knots in $\mathbb{R}^3$ that arises from graphs with valence greater than 3 [52]. His work proceeds via the "Knizhnik–Zamolodchikov" approach to Vassiliev invariants rather than the "Chern–Simons" approach (topologically, by generalizing the winding number for braids rather than the linking number for closed links).

Functor calculus

As the state-of-the-art framework for studying embeddings in high co-dimension, the calculus of embeddings featured prominently in the workshop. **Tom Goodwillie** himself presented new directions for functor calculus starting "from the ground up," that is, from the perspective in his Ph.D. thesis, where the subject originated. He conjectures that spaces of maps from graphs into a manifold can be used to understand pseudoisotopy and hence the algebraic K-theory of a space. These spaces bear some resemblance to the Morse homotopy invariant of Fukaya used in Watanabe's recent work.

Pascal Lambrechts presented a definitive result with Boavida de Brito, Pryor, and Songhafouo Tsopméné, which provides a cosimplicial model for spaces of embeddings, given a simplicial model for the source manifold. This considerably generalizes Sinha's cosimplicial model for $T_n\mathrm{Emb}(\mathbb{R}, \mathbb{R}^n)$. **Don Stanley** presented joint work with Songhafouo Tsopméné on functor calculus in the setting of more general model categories, continuing their earlier work [64, 65].

Ben Knudsen gave a presentation describing the extent to which the Taylor tower sees the difference between smooth structures and formal smooth structures on manifolds. In all dimensions other than four, formal smooth structures are known to coincide with smooth structures. In dimension 4, formal diffeomorphism coincides with homeomorphism. Knudsen's result in joint work with Kupers is that the embedding calculus tower does not see the difference. Thus the space of 1-dimensional knots cannot be used to distinguish 4-manifolds which are homeomorphic but not diffeomorphic. This extends a recent line of inquiry by Arone and Szymik [2] and answers a question posed by Viro. In the positive, Knudsen and Kupers show that the embedding calculus tower can be used to distinguish exotic spheres, starting in dimension sixteen. The conjecture is that such techniques should give invariants in any dimension in which exotic spheres exist.

Apurva Nakade presented work which applies functor calculus to symplectic topology [54]. Similarly to the result of Knudsen and Kupers, he showed that various spaces of formal embeddings are equivalent to the limits of their embedding calculus towers. In other words, the tower sees the "flexible side" of symplectic geometry/topology. There is a growing group of people interested in applications of functor calculus to symplectic topology, such as Francisco Presas (Madrid) and Tamas Kalman (Tokyo Tech).

Sander Kupers gave a presentation of some results of on spaces of diffeomorphisms. This included his Ph.D. thesis work [44], where he proved some finite generation results for $B\mathrm{Diff}_\partial(D^n)$, thus resolving some long-standing open problems in high-dimensional manifold theory. Though the result is about the space of diffeomorphisms itself, the proof uses work of Weiss on embedding calculus. He mentioned a result with Randal-Williams on $\pi_*(B\mathrm{Diff}_\partial(D^n)) \otimes \mathbb{Q}$, which nicely complements Watanabe's work on the graph homology classes, and which was obtained by playing embedding calculus and the theory of Galatius, Madsen, Tillmann, and Weiss against each other.

Operads

A final important topic appearing in multiple talks was the theory of operads, especially those equivalent to the little disks operad. Such results are of central importance for application to spaces of embeddings: viewing configuration spaces as modules over disks operads is central to both the embedding calculus and the study of field-theoretic integrals.

An example of how deeper understanding of configurations leads to deeper understanding of embeddings was given by the recent work of **Geoffroy Horel** and **Pedro Boavida de Brito**. Horel described actions of the Grothendieck–Teichmüller group (and thus the absolute Galois group) on localizations of the embedding calculus tower for the space of long knots, as well as an embedding of the absolute Galois group in the profinite completion of the tower. A key ingredient appeared to be the homotopy theory of E_n operads, including previous noteworthy work of Horel [33]. As a consequence, they show that at each prime p, the spectral sequence for homotopy of the tower collapses in a range of bidegrees that depends on p. This result is related to Kosanović's result and is similarly remarkable, providing further evidence for the universality conjecture from [12].

Paolo Salvatore presented his cell decomposition of the Fulton–Macpherson operad [60], which answered a question of Kontsevich and Soibelman from 2000. This decomposition involves trees with vertices labeled by cells of the cactus operad, which themselves correspond to graphs. Though the result is not explicitly about embedding theory, this operad has been heavily used in recent work on embedding spaces.

Victor Turchin's presentation culminated in a forthcoming result with Benoît Fresse and Thomas Willwacher in which they describe the path components of quite general spaces of high-dimensional string link. In particular, the source manifold need not even be a union of Euclidean spaces. Their result is remarkable not only for its definitive and far reaching statement but also because it ties together several of the key methods in the field. The description is in terms of a certain graph complex, which is an $\mathcal{L}_\infty$-algebra (roughly, a Lie algebra up to higher homotopies). The path components then correspond to the Maurer–Cartan elements in this graph complex, modulo gauge equivalence. They proceed through Willwacher's thorough understanding of the rational homotopy type of spaces of configurations in manifolds, as a module over the disks operad. Their work uses not only such physics-inspired homotopical algebra, but also the functor calculus and operads. It recovers and generalizes the classical work of Haefliger on isotopy of high-dimensional knots, as first pointed out by Songhafouo Tsopméné and Turchin [66, 67].

Scientific Progress Made

As is typical in mathematical meetings, progress is primarily through the generation of new lines of attack on standing questions and of new conjectures. While we organizers cannot be aware of all of these, we share a few that seem particularly promising.

Budney suggested a renewed attack on his problem [9] of the non-triviality of the unknotting map

$$K_{n,1} \to \Omega K_{n+1,1}.$$

If the map can be shown to extend $K_{n,1} \to \Omega^2 K_{n+1,1}$, inducing an isomorphism on the lowest-dimensional homology group, Lambrechts mentioned it could offer insight into Turchin's *Hodge decomposition*.

Budney and Salvatore outlined an idea to generate numerous inequivalent actions of the framed discs operad on $K_{n,1}$ for all n.

Lambrechts sought explanation for the degree-mixing isomorphisms of rational cohomology of embedding spaces across dimensions. For configuration spaces themselves, one can use S^1-equivariant cohomology to produce a chain of isomorphisms which relate cohomology across dimensions. Along with Horel's results presented at the workshop related to cyclic actions and previous work of Arone and Turchin which combined embedding calculus and orthogonal calculus, Sinha has been inspired to explore how equivariant cohomology could be used to establish collapse results.

Sakai would like to use Koytcheff's recent work [41] on $\mathbb{Z}$- and $\mathbb{Z}/p$-valued cohomology classes in spaces of knots and links to study torsion invariants of higher-dimensional knots and links.

Koytcheff, Kupers, and Turchin discussed the possibility of Kupers's conjecture that one can detect a nontrivial Browder operation on $B\mathrm{Diff}(D^n; \partial D^n)$.

Sinha proposed to use Kosanović's techniques to detect the isotopy classes of higher-dimensional knots and links described by Turchin. More precisely, he proposed constructing embeddings out of trees corresponding to homotopy classes and then detecting them via the Lie-coalgebraic Hopf invariants in his joint work with Ben Walter. The use of Hopf invariants to study components of the embedding calculus tower has already produced a new perspective on formulae of Polyak for Milnor invariants, and he and Koytcheff along with Nir Gadish are turning attention to the knot setting for an attack on the main conjecture.

Knudsen mentioned in his talk a broad conjecture of Kupers that spaces of embeddings or diffeomorphisms can be decomposed via a fiber sequence into a formally smooth part, detected by configuration space integrals, and a second part detected by gauge theory.

Another conjecture expressed by many participants is that configuration space integral cohomology classes for all spaces of embeddings, including diffeomorphisms, factor through the embedding calculus tower. In particular, the Kontsevich characteristic classes studied by Watanabe would factor through the tower. This result was proven for the case of classical knots in Ismar Volić's PhD thesis [70], under the supervision of Goodwillie. In this case, the simplicity of the source manifold was exploited, and it is not immediately obvious how those methods would generalize to say the cohomology of $B\mathrm{Diff}_\partial(D^n)$. A first case which many (including Willwacher) have said is worth pursing is showing the configuration space integrals of Cattaneo and his coauthors give the real cohomology of knot spaces, as has been calculated through the embedding calculus tower.

Both this workshop and the subsequent workshop on Unifying 4-Dimensional Knot Theory (19w5118) supported the collaboration between Budney and Gabai [11]. This result extends the work of Dax and Haefliger, showing that the unknotted S^2 in S^4 is the boundary of many distinct (up to isotopy) embedded 3-discs $D^3 \to S^4$. The result follows from a sequence of deductions, starting with the work of Dax and that of Arone and Szymik [2] that $\pi_1 Emb(S^1, S^1 \times S^3)$ is not finitely generated (for all components). A key step in is the observation of a strong connection between the unknot component of $\mathcal{K}_{n+1,n-1}$ and the classifying space of the space of embeddings of D^n into $S^1 \times D^n$ that agree with the map $p \longmapsto (1, p)$ on the boundary. This allows the deduction that the component of the unknot in the embedding space $Emb(S^{n-1}, S^{n+1})$ does *not* have the homotopy-type of the subspace of great $(n-1)$-spheres, provided $n > 2$.

Outcomes of the Meeting

The outcomes of the meeting are, happily, strongly in line with the goals coming in to the meeting. The meeting was structured with these goals in mind, and the outcomes generally exceeded expectations. We discuss both design and desired outcomes.

Cross-pollinate between geometric and algebraic topologists

Participants' backgrounds varied. While many have worked in embedding calculus, with its particular blend of algebraic and differential topology, some were geometric topologists (e.g. Lescop and Polyak), some were more homotopy theoretic (e.g. Stanley and Horel) and some have worked with different blends of geometric and algebraic topology (e.g. Budney, Kosanovic, and Kupers). To accommodate the different backgrounds, we took the suggestion of some participants and had two introductory sessions: one on embedding calculus and one on configuration space techniques and claspers in geometric topology. We alternated algebraic and geometric series of talks, and sequenced them carefully so that participants would be able to follow even if they were unfamiliar with an area.

Participants seemed very happy with the ability to expand mathematical knowledge outside their area of expertise. Algebraic topologists appreciated learning about new techniques related to configuration spaces, in particular Morse propagators, which are so central to the current application of algebraic topology to differential topology, as well as clasper surgery, which gives geometric structures analogous to the lower central series in algebra. Geometric topologists greatly appreciated the opportunity to get up to speed about an adjacent area, the calculus of embeddings, which was new to some participants. Those already working at the interface appreciated learning and exchanging on all sides. Some collaborations were initiated, and more broadly the ground was prepared for fruitful collaboration at this interface for years to come.

Disseminate top recent results, while fostering collaboration

The organizers polled participants ahead of the workshop for their priorities, and there was a strong expression of interest in time for collaboration. Nonetheless, at such a meeting of leaders from a number of fields, sharing recent breakthroughs is a priority. The organizers balanced these needs by having a large amount of time set aside for collaboration, in particular on Thursday, as well as having the aforementioned introductory sessions to aid collaboration across specialties. To help make the most of the relatively limited lecture time, talks with different speakers were nonetheless planned to build so that later speakers could rely on background from earlier in the program.

We benefited from having breakthrough results established relatively recently. Diffeomorphism groups are a central subject in topology, but little progress has been made in dimensions four and higher for forty years. Kupers and Watanabe presented breakthrough results, the former producing calculations of rational homotopy groups of diffeomorphisms which dwarfs previous knowledge and the latter disproving the Smale Conjecture in dimension four. Also, Kosanović used a blend of algebraic and geometric topology to resolve the last case of Goodwillie–Klein excision estimates, namely for classical knots. This could be a key step in showing the embedding calculus is a universal finite-type invariant. As for collaboration, participants clearly appreciated and made great use of the time. Informal talking at meals often resulted in a brief exchange of "we should talk more", and then finding time among the breaks and other free periods provided. It seems that desired meetings were always able to be scheduled.

Support and highlight contributions by mathematicians from underrepresented backgrounds

Some of the greatest contributions to the program were by mathematicians from underrepresented groups. As mentioned already, Kosanovic's result, part of her thesis work, resolves a longstanding key open question. Lescop led multiple sessions for algebraic topologists to learn about topics in geometric topology relevant to this area. Songhafouo Tsopméné was not able to attend (because of the birth of a child) but had his work prominently featured in three different talks.

Participants

Bauer, Kristine (University of Calgary)
Boavida de Brito, Pedro (Universidade de Lisboa)
Budney, Ryan (University of Victoria)
Goodwillie, Tom (Brown University)
Horel, Geoffroy (Université Paris 13)
Knudsen, Ben (Northeastern University)

Kosanovic, Danica (ETH Zurich)
Koytcheff, Robin (University of Louisiana at Lafayette)
Kupers, Alexander (Harvard University)
Lambrechts, Pascal (Universite de Louvain)
Lescop, Christine (CNRS)
Mortier, Arnaud (University of Caen Normandy)
Nakade, Apurva (University of Western Ontario)
Pelatt, Kristine (St. Catherine University)
Polyak, Michael (Technion)
Sakai, Keiichi (Shinshu University)
Salvatore, Paolo (Univ. of Rome Tor Vergata)
Sinha, Dev (University of Oregon)
Stanley, Donald (University of Regina)
Turchin, Victor (Kansas State University)

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Chapter 24

Report on the Workshop for Women in Commutative Algebra (19w5104)

October 20 - 25, 2019

Organizer(s): Karen Smith (University of Michigan), Sandra Spiroff (University of Mississippi), Irena Swanson (Reed College), Emily Witt (University of Kansas)

This is a report on the first-ever workshop for Women in Commutative Algebra. We organized and promoted the workshop around six working groups, each with two group leaders who are experts in very active research subareas. The group leaders and the topics of their groups were:

1. Combinatorics and differential operators, leaders Christine Berkesch, University of Minnesota, and Laura Matusevich, Texas A&M Univesity.
2. Methods in prime characteristic, leaders Karen Smith, University of Michigan, and Emily Witt, University of Kansas.
3. Combinatorial commutative algebra, leaders Sara Faridi, Dalhousie University, and Susan Morey, Texas State University.
4. Rees algebra, leaders Elisa Gorla, University of Neuchatel, Switzerland, and Claudia Polini, Notre Dame University.
5. Finite resolutions and complexes, leaders Claudia Miller, Syracuse University, and Alexandra Seceleanu, University of Nebraska.
6. Tropical commutative algebra, leaders Diane Maclagan, University of Warwick, United Kingdom, and Josephine Yu, Georgia Tech University.

We advertised the workshop on the AWM website and `commalg.org`. The application website asked for the year of Ph.D., current affiliation and position, ranked preferences for the groups, and any further relevant information. We had 98 candidates for the available 42 slots and we had to make some tough choices in selecting the participants. Depending on the preferences we divided the participants into the six groups so that each group would have about seven participants. We had a few cancellations, some of which we were able to replace, but due to late cancellations we were unable to replace two of the slots.

The main focus of the workshop was group work. On the morning of the first day the group leaders briefly presented the topics to all participants, and we met again in late afternoon to summarize the day's work. While the day's reports were interesting and informative, most groups felt that the afternoon meeting disturbed the work. Thus we did not have an all-participant meeting on Tuesday, but we did do brief summaries on Wednesday evening and longer summaries on Friday morning. On Thursday evening we had a group discussion/general panel long into the night in the social room on careers, professional climate, teaching advice, Ph.D. advising, and so on.

We received a favorable report from the AWM ADVANCE evaluation team. Some excerpts from that report are:

Logistics: "Participants who responded to the survey were very happy with the workshop logistics. Most respondents (97%) agreed that the application process was convenient or agreed that accommodations were satisfactory (98%). Every participant (100%) thought the conference facilities were adequate,.."

Group Size & Effectiveness: "Most respondents (69%) thought their group size was just right, but a substantial minority (28%) thought their groups were too large and one person thought her group was too small. .... Most respondents (94% to 100%) expressed broad support for their workshop group, were favorably disposed toward their workshop project, and expected to continue collaborating with their group members..."

Conference Expectations and Future Intentions: "The majority of respondents (97%) would attend this conference again as a member and almost every participant (97%) would recommend this workshop to a friend. Three quarters (75%) of respondents indicated that they would attend this workshop again in the future as a workshop leader."

Productivity: "The women who attended the workshop and responded to the survey are very productive in terms of research, despite having so many junior scholars.... All participants (100%) had presented their research in the past two years and more than two-thirds (70%) had received external funding."

Collaborative Experience and Attitudes: "Most WICA participants (97%) have experience collaborating on a project for publication....As the research literature suggests, there are trade-offs to collaborating;....While most participants claimed that collaboration requires more communication (59%) and coordination (66%), no one (0%) thought that it slowed their career advancement."

Summary: "Based on this report, the WICA RCCW appears to have been very successful. As one participant wrote in her open-ended comments, 'It was so fantastic an environment. The people were so nice, so good to work with, so smart. It felt so different and so relaxing to work with and talk to women all week long.' "

A last comment regarding the AWM is that, through their ADVANCE grant NSF-HRD 1500481, they provided the WICA workshop with $4000 in travel funding for some of the participants. For those at US institutions, additional travel funding was obtained from the National Science Foundation, DMS-1934391. Organizer Spiroff was the PI on the grant, with organizers Smith, Swanson, and Witt providing support of the proposal as Senior Personnel.

All working groups reported substantial progress in research and concrete plans to continue working on the started projects. Below are the summaries of the mathematical content of the six groups.

Combinatorics and differential operators

Group leaders: Christine Berkesch and Laura Matusevich.

Group members: Jean Chan, Patricia Klein, Janet Page, Janet Vassilev.

Overview

The ring of $\Bbbk$-linear differential operators ($\Bbbk$ a field) over a commutative $\Bbbk$-algebra R is defined as $D(R) = \cup_{n=0}^{\infty} D_{\Bbbk}^{n}(R)$, where $D_{\Bbbk}^{0}(R) = R$ and $D_{\Bbbk}^{n}(R) = \{P \in \mathrm{End}_{\Bbbk}(R) \mid Pf - fP \in D_{\Bbbk}^{n-1}(R) \text{ for all } f \in R\}$. It is a fact that $D_{\Bbbk}^{1}(R) = R + \mathrm{Der}_{\Bbbk}(R)$, where $\mathrm{Der}_{\Bbbk}(R)$ is the space of $\Bbbk$-linear derivations on R, but we point out that in general, the derivations are not enough to generate $D(R)$ as a $\Bbbk$-algebra.

When R is the polynomial ring over a field of characteristic zero, $D(R)$ is the well-known Weyl algebra, the ring of linear differential operators with polynomial coefficients. When $\mathrm{char}(\Bbbk) > 0$, $D(R)$ is the divided powers Weyl algebra, which is also well understood.

Rings of differential operators were introduced by Grothendieck [18] and Sweedler [32]. It is known that $D(R)$ can shed light on $\mathrm{Spec}(R)$, and the study of differential operators is of wide interest in commutative algebra and algebraic geometry. For example, the theory of Bernstein–Sato polynomials [6, 29], which is of much relevance for studying singularities in algebraic geometry [37, 23, 22, 14, 11] relies on an explicit understanding of $D(R)$. Also, an explicit description of $D(R)$ in the case where R is a reduced monomial ring of characteristic $p > 0$, is used in [34, Corollary 5.5] to prove that tight closure commutes with localization in that setting.

While differential operators are both intrinsically interesting and useful once an explicit description is given, providing such characterizations for specific (classes of) varieties is not easy. Due to this inherent challenge, we aim to compute rings of differential operators in combinatorial settings, where the additional structure gives rise to specialized tools that are not available in general.

When R is a Stanley–Reisner ring, $D(R)$ has a combinatorial description [34] in terms of the associated simplicial complex. This description applies over any base field $\Bbbk$, regardless of the characteristic. Affine toric varieties and their coordinate rings (semigroup rings) form another fundamental class of examples. In this case, the ring of differential operators is known when the base field $\Bbbk$ is algebraically closed of characteristic zero [21, 27, 30, 31].

The Group Members

The members of this working group represent a broad cross-section of commutative algebra. In order to study rings of differential operators in combinatorial contexts, our participants bring expertise in combinatorial aspects of algebra and geometry, including toric geometry, convex geometry, Stanley–Reisner theory, D-modules, characteristic p methods, singularity theory, homological algebra, and affine semigroup rings.

Given our very different areas of specialization, this is a collaboration that could only have been developed during an event such as this. The group chemistry has been exceptional, and all participants are strongly committed to the success of this project. We are deeply grateful to the workshop organizers and BIRS, for making this possible for us.

Our Results and Future Directions

During the Workshop, we focused on computing rings of differential operators over quotients of semigroup rings by radical monomial ideals (the base field is assumed to be of characteristic zero). We have a working conjecture in this case, and are in the process of proving it. This result could be an article on its own, but we believe that our ideas can be applied in more general contexts. Future plans also involve considering the case when the base field has positive characteristic. In this case, even the differential operators over semigroup rings are not known.

Methods in prime characteristic

Group leaders: Karen Smith and Emily Witt.

Group members: Eloisa Grifo, Zhibek Kadyrsizova, Jenny Kenkel, Jyoti Singh, Adela Vraciu.

We began an investigation of the moduli space of Frobenius split (or globally F-regular) projective varieties.

For a ring of prime characteristic, F-purity and F-regularity are nice-ness assumptions defined using the p-th power (or Frobenius) map. Their study was pioneered by Hochster, in collaboration first with Roberts and later with Huneke. Important contributions were made in the early stages also by several Indian mathematicians, notably Mehta and Ramanathan (who used the term "Frobenius split" for what is usually known as "F-purity" among commutative algebraists).

The conditions of F-purity and F-regularity on R place strong algebraic conditions on R such as various local cohomology modules vanishing. They also place strong geometric restrictions on the projective variety whose homogeneous coordinate ring is R (called "log Calabi-Yau" and "log Fano", respectively) by a theorem of Schwede and Smith. These conditions are important in algebraic geometry. The study of the moduli spaces (parameter spaces) of such varieties is quite active.

We approached this from an algebraic point of view. Although moduli of smooth cubics has been studied in prime characteristic, and moduli of log Fanos have been studied in characteristic zero, no systematic classification, up to isomorphism, of the set of all finitely generated graded algebras (of fixed characteristic p) that are F-pure (or F-regular) has been completed.

At Banff, we focused on finding a moduli space for F-pure cubic surfaces of characteristic two. For various reasons, cubic surfaces of characteristic two are especially interesting. It is important to note that even for smooth cubics in this case, very little was understood until recently (for example, there is a 2018 preprint of Dolgachec and Duncan).

What we accomplished at WICA: Let f be a homogeneous polynomial of degree d in n variables. We assume f is non-degenerate in the sense that the projective scheme in defines in $\mathbb{P}^{n-1}$ is not contained in a hyperplane. This is what we accomplished:

1. When $d = 2$ and n is arbitrary, we used the theory of quadratic forms to observe that there are only finitely many isomorphism types of quadric hypersurfaces in every charcteristic, though the story is a bit different in characteristic 2. Among these, we saw that all are F-pure, except the completely degenerate "double hyperplanes."

2. When $d = 3$, we may have finished the classification of **non-F-pure** cubics in characteristic 2. It appears there are finitely many and we can enumerate representatives of each isomorphism class.

3. When $d = 3$, we developed a program to prove that the **F-pure** cubics hypersurfaces in characteristic 2 are parameterized by the punctured four space $\mathbb{A}^4$ modulo a finite group action. Some details remain to be checked.

We intend to write the results of items (1) and (2) into a paper sometime soon and get together, hopefully this summer, to complete the work in (3).

Many open-ended areas of exploration remain and we hope to pursue them together in the future.

Combinatorial Commutative Algebra

Group leaders: Sara Faridi and Susan Morey.

Group members: Susan Cooper, Sabine El Khoury, Sarah Mayes-Tang, Liana Sega, and Sandra Spiroff.

None of the participants in this project had collaborated previously and the team involved participants at a variety of stages of their careers, resulting in beneficial new mentoring and research relationships.

The main question they worked on was: given an ideal I generated by monomials in a polynomial ring, if we know I has a free resolution supported on a simplicial complex Δ, can one find, from Δ, another simplicial complex supporting a free resolution of I^2? What about I^r for any r?

A free resolution of an ideal is a way to encode the relationships between the generators of the ideal into a sequence of free modules and maps between them. The smallest free resolution of I (in terms of the ranks of the modules involved) is unique up to isomorphism of complexes, and is called a minimal free resolution of I. If K is a field and I an ideal in the polynomial ring $S = K[x_1, \ldots, x_n]$, then the minimal free resolution is an exact sequence of free S-modules

$$0 \longrightarrow S^{\beta_p} \longrightarrow \ldots \longrightarrow S^{\beta_1} \longrightarrow S^{\beta_0} \longrightarrow I \longrightarrow 0,$$

where for each i, the non-negative integer β_i is called the i-th betti number of I. In the specific case of a monomial ideal, the betti numbers can be refined further into multigraded betti numbers, which are indexed by monomials in I.

The idea of supporting a resolution on a simplicial complex was initiated by Diane Taylor, who in her thesis [33] introduced a multigraded free resolution of a monomial ideal using the simplicial chain complex of a simplex whose vertices are labeled with the monomial generators of the ideal. Taylor's resolution always exists for any monomial ideal, but it is usually far from minimal. Taylor's work was extended in the decades to follow by discovering criteria for subcomplexes of the Taylor complex to support free resolutions of a monomial ideals [5, 4] and then further to cell complexes [5] and CW complexes [3, 20]. But it is shown by Velasco [36] that even CW complexes do no support all minimal resolutions.

The study of the behavior of powers of a fixed ideal is a classical problem. The powers of an ideal are used via the Rees algebra and related blowup algebras to understand resolutions of singularities, and are also of interest in their own right. For example, in [25], the depth function $\operatorname{depth} R/I^s$ is defined as a function of s. While this function is known to stabilize and the limiting behavior is known, finding the depths of the early powers of an ideal is an active area of research. Other invariants that are often studied for powers of ideals include regularity and associated primes. Having resolutions of the powers of an ideal that were close to minimal would provide a useful tool to advance all of these areas of study.

A second approach to studying powers of ideals is to understand their asymptotic behavior; often, there is uniformity in the limit that is not seen when studying individual members of the ideal. One direction of asymptotic relationships relates to the *graded betti numbers* of all powers of a monomial ideal, which are usually summarized in a two-dimensional *betti table* of the ideal. Recent research has demonstrated strong patterns in the sequence of betti tables of powers of a fixed ideal, both in cases where the tables eventually stabilize [16] and in cases where they continue to grow without bound [2].

The investigations of this group would tell us more about the graded betti numbers of powers of monomial rings, and could allow us to discern asymptotic patterns. It could also give new effective bounds for betti numbers of powers of monomial ideals.

For the purpose of a more concrete class of resolutions, the group began investigations at the recent Banff workshop by focusing on a special class of ideals whose resolutions are better-known, namely, those ideals that have resolution of length ("projective dimension") at most one [15], whose resolutions are supported on graphs. They were able to identify a structure that conjecturally supports a resolution of I^r for this class in general and prove that when the number of generators of the ideal is small, the conjecture holds for low powers, particularly $r = 2$. Along the way, they adapted an algorithm from [1] that prunes a Taylor resolution and produces a cellular one for a given monomial ideal to one that works in their setting.

The members of this research group came from varying areas of commutative algebra. Their differing mathematical backgrounds brought strength to the project, but the project also allowed each woman to expand her knowledge in the field. This area of research lies in the intersection of homological algebra and discrete topology. The field of combinatorial homotopy theory is rich with tools that, once found, any commutative algebraist could find indispensable (see [7] for a catalogue of some such tools). The expertise that the participants each brought (powers of ideals, combinatorial resolutions, homological methods, graph theory) allowed the group to produce a unique line of research and provides an opportunity of cross pollination by learning from the expertise of one another.

Since the conclusion of the Banff workshop, the group has agreed on how to advance the project given their disparate locations and the group's relatively large size. Their research is on-going. They have created a Dropbox for their project and have uploaded and shared various documents. Likewise, they have organized regular Skype meetings and intermittent visits of subgroups of the women and they have started applying for 1-2 week residential research opportunities, with an application to MSRI already submitted. In addition, face-to-face meetings are scheduled over the next several months at various locations.

Rees algebras

Group leaders: Elisa Gorla and Claudia Polini.

Group members: Ela Celikbas, Emilie Dufresne, Louiza Fouli, Kuei-Nuan Lin, Irena Swanson.

Let X be an $m \times n$ matrix whose entries are either zeros or distinct variables. A matrix X is *generic* if its entries are distinct variables, it is *sparse generic* if its entries are either zeros or distinct variables. Let $R = K[X]$ be the polynomial ring over a field K with variables the entries of X. Let I be the ideal of R generated by the maximal minors of X, I is called a *(sparse) determinantal* ideal. The study of rings and more generally of varieties that are defined by determinantal ideals of generic matrices has been a central topic of commutative algebra and algebraic geometry, see for example [9]. Sparse determinantal ideals were first studied by Giusti and Merle [17]. Recently, Boocher [8] determined their minimal free resolutions.

During the week at Banff, we studied the blowup algebras of sparse determinantal ideals, precisely their Rees algebras and special fiber rings. The Rees algebra of an ideal $J \subseteq R$ is the graded algebra $\mathcal{R}(J) = \oplus_{i=1}^{\infty} J^i t^i \subset R[t]$, where t is an indeterminate over R, and the *special fiber ring* $\mathcal{F}(J)$ is $\mathcal{R}(J)/\mathfrak{m}\mathcal{R}(J)$, where $\mathfrak{m}$ is the maximal (homogeneous) ideal of a local or graded ring R. The Rees algebra encodes many of the analytic properties of the variety defined by J and is the algebraic realization of the blowup of a variety along a subvariety. It plays a crucial role in the resolution of singularities of an algebraic variety. From the algebraic point of view the Rees algebra facilitates the study of the asymptotic behavior of the ideal and it is an essential tool for the computation of the integral closure of powers of ideals. Both the Rees algebra and the special fiber ring can be realized as quotients of polynomial rings. In particular, if J has n generators then $\mathcal{R}(J)$ is of the form $R[T_1, \ldots, T_n]/L$, where $L \subseteq R[T_1, \ldots, T_n]$ is the *defining ideal* of the algebra. The generators of L are the *defining equations* of $\mathcal{R}(J)$. Although blowing up is a fundamental operation, an explicit understanding of this process remains an open problem – for instance it is difficult in general to describe the generators of L. When J is generated by forms of the same degree, as in the case of sparse determinantal ideals, the problem of computing L explicitly is a classical problem in elimination theory. This question has been addressed in well over one hundred articles by commutative algebraists, algebraic geometers, and applied mathematicians. The problem is difficult and each class of ideals (or rational maps) seems to require different techniques. During the week at Banff, we studied this problem using techniques coming from SAGBI and Gröbner basis theory.

In the special case when I is the ideal generated by the maximal minors of a generic matrix, the Plücker relations among the minors are quadratic equations and they are the generators of the defining ideal of the special fiber ring. Together with the defining equations of the symmetric algebra, they are the defining equations of the Rees algebra.

We focused on the case when I is the ideal of maximal minors of a $2 \times n$ sparse matrix X. Our first goal was showing that $\mathrm{in}(\mathcal{R}(I)) = \mathcal{R}(\mathrm{in}(I))$, where $\mathrm{in}(\mathcal{R}(I))$ denotes the initial algebra of the Rees algebra of I and $\mathcal{R}(\mathrm{in}(I))$ denotes the Rees algebra of the initial ideal of I, with respect to suitable term orders. In situation when such a theorem holds, one can study the monomial algebra $\mathrm{in}(\mathcal{R}(I))$, then use standard deformation techniques to deduce properties for $\mathcal{R}(I)$ from those of $\mathrm{in}(\mathcal{R}(I))$.

By [12] the equality $\mathrm{in}(\mathcal{R}(I)) = \mathcal{R}(\mathrm{in}(I))$ would follow if we showed that $\mathrm{in}(I^k) = (\mathrm{in}(I))^k$ for all $k \leq \mathrm{rt}(\mathrm{in}(I))$, where $\mathrm{rt}(\mathrm{in}(I))$ denotes the relation type of $\mathrm{in}(I)$. By Conca, De Negri, and Gorla [**?**], the maximal minors of X are a universal Gröbner basis for I. By selecting a suitable term order and using results of Corso and Nagel [13] and Villarreal [36], we were able to determine the defining equations of $\mathcal{R}(\mathrm{in}(I))$, in particular we obtained $\mathrm{rt}(\mathrm{in}(I)) = 2$. By comparing Hilbert functions we were able to show that $\mathrm{in}(I^2) = (\mathrm{in}(I))^2$. Coupling this result with [12] we concluded that $\mathrm{in}(\mathcal{R}(I)) = \mathcal{R}(\mathrm{in}(I))$. Following the approach outlined, we were able to prove the following.

Theorem. *[(a)]*

1. *$\mathcal{R}(I)$ is of fiber type and in particular, the defining ideal of $\mathcal{R}(I)$ is given by the relations of the symmetric algebra of I and by the Plücker relations on I.*

2. *$\mathcal{R}(I)$ and $\mathcal{F}(I)$ have rational singularities (or they are F-rational in the positive characteristic case).*

3. *$\mathcal{R}(I)$ and $\mathcal{F}(I)$ are Cohen-Macaulay normal domains.*

4. *The Plücker relations of I form a Gröbner basis for the defining ideal of $\mathcal{F}(I)$.*

5. *$\mathcal{R}(I)$ and $\mathcal{F}(I)$ are Koszul algebras.*

Next we plan to study the case of sparse generic matrices of arbitrary size. Furthermore, we would like to consider the case where the entries of the matrix are linear forms.

Canonical Resolutions using Koszul Algebras

Group leaders: Claudia Miller and Alexandra Seceleanu.

Group members: Faber Eleonore, Lindo Haydee, Martina Juhnke-Kubitzke, Rebecca R.G.

The project involves generalizing some canonical resolutions over polynomial rings to the setting of Koszul algebras. An algebra is Koszul if the residue field has a linear resolution, that is, has Castelnuovo-Mumford regularity equal to zero. A necessary condition is that its defining relations are quadratic, but not every quadratic algebra is Koszul.

Although the definition may seem specialized, in fact, Koszul algebras show up naturally in many places in algebra and topology. They were first introduced by the algebraic topologist Priddy in 1970 in [28] as algebras for which the bar resolution, which is far from minimal, can be reduced to a very small subcomplex. This explained ideas that had been floating around in the work of May on restricted Lie algebras and of Bousfield, Curtis, Kan, Quillen, Rector, and Schlesinger. Koszul algebras have since appeared naturally in many places, linked to fundamental concepts, and studied extensively in fields as diverse as topology, representation theory, commutative algebra, algebraic geometry, noncommutative geometry, and number theory.

Furthermore, the associated theory of Koszul duality is a generalization of the duality underlying the Bernstein-Gelfand-Gelfand correspondence describing coherent sheaves on projective space in terms of modules over the exterior algebra. This exemplifies the special relevance of the pair of Koszul dual algebras given by a polynomial ring and an exterior algebra, as well as the philosophy that facts relating these algebras often have Koszul duality counterparts.

Our project involves taking results that describe resolutions of various modules over a polynomial ring S constructed starting from the Koszul complex (exterior algebra) Λ and its generalizations and proving analogs of these results using any pair of Koszul dual algebras, A and $A^{\perp}$, instead of S and Λ.

The main first goal was to generalize the canonical resolutions over a polynomial ring for the powers of the homogeneous maximal ideal constructed by Buchsbaum and Eisenbud in [10] to obtain free resolutions for powers of the homogeneous maximal ideal of a Koszul algebra. As opposed to working over S, in general these would be infinite resolutions. We achieved this goal and wrote a complete proof over the first few days. We were aided in our endeavor by learning from another workshop participant (Şega) that these resolutions were linear. The next step will be to put a differential graded algebra structure on the resolutions we have constructed. Such a structure is enormously helpful in further homological explorations. For this, we have a clear method of building it based on a known technique if we can define an appropriate homotopy, for which we have some ideas.

Last, we wanted to extend the theory of Macaulay inverse systems from polynomial rings to Koszul algebras. For this extensive project, the first step would be to obtain some understanding of the injective hulls of the residue field over the Koszul algebra as well as its quotients. We made progress in understanding some of these, and realized that even an extension to one class of Koszul algebras would be a large step beyond the known theory over polynomial rings. For this we have a candidate that would give an important extension and have made progress in studying it.

If we successfully develop this theory, then we will be able to apply it to obtain a much large class of resolutions by expanding work of one of the co-leaders over polynomial rings [26] to this class of Koszul algebras.

The workshop was invaluable for us in forming research collaborations with women, when so many of us are in departments with almost all men. Indeed, most in our group had never worked with the others, and, even though we share common interests in homological commutative algebra, had never worked on the same topics before, and particularly not on Koszul algebras.

On the last half day of the workshop, we spent an hour of intensive discussions with another group (Berkesch and Matusevich) about a potential connection between our projects, more specifically about whether the same methods in our project could have some hope of providing an application to their topic of interest, and we hope to get in touch once we know better how our separate projects develop. This gives us even more connections for future collaborations with some of the best women in our field.

In the weeks since the workshop ended, our group has kept working regularly. We have started writing the result we obtained, and we have had some online meetings in subgroups to keep working and discuss issues issues arising from further explorations of the literature. We have a joint folder where we keep background literature and written summaries of the information from each meeting for those who could not make the meeting time.

Tropical commutative algebra

Group leaders: Diane Maclagan and Josephine Yu.

Group members: Francesca Gandini, Milena Hering, Fatemeh Mohammadi, Jenna Rajchgot, Ashley Wheeler.

One motivation of this group was to investigate whether the tropical Bertini theorem of [24] holds in characteristic p. This theorem states that when $X \subset (K^*)^n$ is an irreducible variety over an algebraically closed field K of characteristic zero, then the set of rational hyperplanes H for which $\mathrm{trop}(X) \cap H$ is the tropicalization of an irreducible variety is dense in $\mathbb{P}^n_{\mathbb{Q}}$. The characteristic assumption comes from the use in the proof of a toric Bertini theorem of Fuchs, Mantova, and Zannier [16], which has a characteristic zero requirement. While there are counterexamples in characteristic p to the method of proof of the toric Bertini theorem of [16], these do not immediately give a counterexample to the Bertini statement, and even such a counterexample would not necessarily give a counterexample to the tropical variant.

Some progress was made towards this goal, and the group has already begun follow-up meetings.

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Chapter 25

Bridging the Gap between Kähler and non-Kähler Complex Geometry (19w5051)

October 27 - November 1 2019

Organizer(s): Vestislav Apostolov (Université du Québec à Montréal, Canada), Anna Fino (University of Torino, Italy), D.H. Phong (Columbia University, New York, United States), Dan Popovici (Université Paul Sabatier, Toulouse, France)

This workshop brought together mathematicians from all over the world who work on a wide range of different but related topics. The nineteen talks and the many private mathematical discussions sprang mainly from three very active research directions:

- Complex Geometry;
- Symplectic Geometry;
- Mathematical Physics.

Stimulating a dialogue between these vast research areas was at the core of the organisers' and the participants' preoccupations. We believe that new bridges have been built and new contacts have been established. So, we are able to say that this workshop was a success.

One of the unifying themes spanning the three main research directions listed above is **Mirror Symmetry**. This is a conjecture that arose in physics in the 1980s and the 1990s (the work [COGP91] of Candelas-de la Ossa-Green-Parkes being thought of as pioneering) but is still not entirely understood mathematically in spite of significant recent progress. Put in a crude way, the Mirror Symmetry Conjecture predicts that Calabi-Yau manifolds (i.e. compact Kähler manifolds X whose canonical bundle K_X is trivial) come in pairs $(X, \widetilde{X})$ such that the *complex structures* supported by the smooth manifold underlying X (the complex moduli space of X, i.e. the universal family of local deformations of the original complex structure of X, called the *Kuranishi family* $\mathrm{Def}(X)$ of X) bear a certain relationship with the *Kähler structures* supported by the mirror dual $\widetilde{X}$ (in the form of the complexified Kähler cone of $\widetilde{X}$, also called the Kähler moduli space).

A tremendous amount of different mathematics goes into this issue, ranging from complex algebraic geometry (sheaves, vector bundles, toric varieties), complex analytic and differential geometry (deformations of complex structures, connections, special Hermitian metrics), symplectic geometry (Lagrangian fibrations), Hodge Theory (variations of Hodge structure, spectral sequences), mathematical physics and pluripotential theory (Monge-Ampère-type equations and other geometric PDEs). All these research topics were represented in the talks and the participants' discussions in this workshop.

The study of Calabi-Yau manifolds can be seen in the context of the study of compact Riemannian 7-manifolds with holonomy G_2 and that of compact Riemannian 8-manifolds with holonomy $\mathrm{Spin}(7)$. Three possible models for the universe have been proposed as based on these three types of manifolds. Our workshop brought together experts from all these three areas.

Another unifying theme for the three main research directions mentioned above is the link between the existence of **Kähler-Einstein metrics** on certain classes of compact complex manifolds and the various notions of **stability**. Significant progress was accomplished recently by Chen-Donaldson-Sun and Tian and the many geometric flows have found a wide array of applications, some of which were reported during this workshop.

Overview of the Field

The classification of compact complex, not necessarily projective or even Kähler, manifolds is a major undertaking in modern mathematics. It involves the interplay between several kinds of structures (complex, metric, cohomological, topological, etc) that such a manifold supports. Hermitian metrics (defined as C^∞, positive definite, differential forms ω of bidegree $(1,\,1)$) exist on any compact complex manifold, but if they are required to satisfy d-closedness or $\partial\bar\partial$-closedness conditions, they need not exist. When they do, they impose a certain type of geometry on the underlying manifold and become a powerful tool in the classification theory.

Kähler metrics ω (i.e. those Hermitian metrics ω such that $d\omega = 0$) exist only rarely on compact complex manifolds X of complex dimension $n \geq 3$. However, related but weaker properties of either a metric nature (e.g. the balanced and the strongly Gauduchon conditions) or a cohomological nature (e.g. the $\partial\bar\partial$-property requiring the validity of the $\partial\bar\partial$-lemma) have emerged recently as powerful criteria for classification. They allow for large classes of possibly non-Kähler manifolds to behave in certains respects as Kähler manifolds and thus enable researchers to build virtually from scratch a classification theory of non-Kähler manifolds that share metric or cohomological properties with their Kähler counterparts.

Here is a brief description of some of the recent advances in this fast growing area.

(A) The metric side of the theory

A spectacular use of Kähler metrics and of possibly singular Hermitian metrics on the fibres of holomorphic line bundles was made by Siu in his proof of the **invariance of the plurigenera** conjecture for projective families of compact complex manifolds.

Theorem (Siu 1998 and 2000) *Let $\pi : \mathcal{X} \longrightarrow \Delta$ be a* **projective** *holomorphic family of compact complex manifolds over the unit disc $\Delta \subset \mathbb{C}$. Then, for every $m \in \mathbb{N}^\star$, the m-genus $\dim_{\mathbb{C}} H^0(X_t,\, mK_{X_t})$ is independent of the fibre $X_t := \pi^{-1}(t)$, $t \in \Delta$.*

By K_{X_t} one means the canonical line bundle of the fibre X_t, mK_{X_t} stands for its m^{th} tensor power (in additive notation in the Picard group), while H^0 denotes the space of global holomorphic sections. This was a major success of transcendental (mainly analytical) methods in algebraic geometry. Except for the case where the fibres X_t are assumed of general type, no algebraic proof of this result is known. The invariance of the plurigenera plays a major role in the **Minimal Model Program (MMP)** where projective (or merely compact Kähler) manifolds are to be classified up to birational equivalence.

The use of transcendental methods (e.g. special Hermitian metrics, non-rational cohomology classes, currents, pluripotential theory, geometric PDEs) becomes inevitable on general compact Kähler and non-Kähler manifolds since most of them contain no other complex submanifolds than the points. Thus, the familiar apparatus of curves, divisors and global holomorphic sections of line bundles used in algebraic geometry is often unavailable.

A major purely transcendental result was the following characterisation of the Kähler cone (= the open convex cone of all Kähler cohomology classes) of an arbitrary compact Kähler manifold.

Theorem(Demailly-Paun 2004) *Let X be a compact Kähler manifold with $dim_{\mathbb{C}} X = n$. The Kähler cone $\mathcal{K}_X$ of X is one of the connected components of the cone $\mathcal{P}_X$ consisting of the real $(1, 1)$-cohomology classes $\{\alpha\}$ such that $\int_Y \alpha^p > 0$ for every irreducible analytic subset $Y \subset X$ of dimension p and for every $p \in \{1, \dots, n\}$.*

This important result has had a major impact in complex geometry, including in the development of an MMP theory for Kähler 3-folds and in Mirror Symmetry.

Another example where special Hermitian metrics were instrumental in the resolution of a long-standing algebro-geometric problem for which purely algebraic methods had failed is the following **deformation closedness** property of a class of algebraic manifolds. The **Moishezon manifolds** are the compact complex manifolds that are bimeromorphically equivalent to projective manifolds.

Theorem (Popovici 2013) *Let $\pi : \mathcal{X} \longrightarrow \Delta$ be a holomorphic family of compact complex manifolds over the unit disc $\Delta \subset \mathbb{C}$. Suppose that the fibre X_t is* **projective** *for every $t \in \Delta \setminus \{0\}$ and that the fibre X_0 is a* **strongly Gauduchon** *manifold. Then X_0 is Moishezon.*

A Hermitian metric ω is said to be *strongly Gauduchon* if $\partial\omega^{n-1}$ is $\bar\partial$-exact. Manifolds carrying such a metric are called *strongly Gauduchon manifolds*.

(B) The cohomological side of the theory

The prototype of this endeavour is the notion of Kähler class on a Kähler manifold and the search for a canonical Kähler metric representing it, known as the *Calabi program*.

The notion of *strongly Gauduchon metrics* led to a generalisation in the non-Kähler context and in bidegree $(n-1,\, n-1)$ of the notion of Kähler class and of Yau's celebrated resolution of the Calabi conjecture. The idea of considering a Monge-Ampère-type equation in bidegree $(n-1,\, n-1)$ was first suggested by Demailly in discussions (2009) with Popovici about strongly Gauduchon metrics.

Theorem (Popovici–Tosatti–Weinkove–Szekelyhidi 2013, 2015) *Given an arbitrary* **Gauduchon metric** *ω on X (i.e. such that $\partial\bar\partial\omega^{n-1} = 0$), the following equation*

$$\left[\left(\omega^{n-1} + i\partial\bar\partial\varphi\wedge\omega^{n-2} + \frac{i}{2}\left(\partial\varphi\wedge\bar\partial\omega^{n-2} - \bar\partial\varphi\wedge\partial\omega^{n-2}\right)\right)^{\frac{1}{n-1}}\right]^n = e^{f+c}\,\omega^n \quad (\star)$$

subject to the positivity and normalisation conditions

$$\Omega_\varphi := \omega^{n-1} + i\partial\bar\partial\varphi\wedge\omega^{n-2} + \frac{i}{2}\,(\partial\varphi\wedge\bar\partial\omega^{n-2} - \bar\partial\varphi\wedge\partial\omega^{n-2}) > 0 \quad \textit{and} \quad \sup_X \varphi = 0, \tag{25.0.1}$$

has a unique C^∞ solution $\varphi : X \to \mathbb{R}$ for any given C^∞ real-valued function f and a unique constant $c \in \mathbb{R}$ depending on f.

This equation produces, in the **Aeppli cohomology** class $[\omega^{n-1}]_A$ of each Gauduchon metric ω on X, a unique Gauduchon metric ω_φ (the $(n-1)^{st}$ root of Ω_φ) depending on ω such that the volume form of ω_φ has been prescribed. (Recall that the Aeppli cohomology groups of X are defined as $H^{p,\,q}_A(X,\,\mathbb{C}) := \mathrm{Ker}(\partial\bar\partial)/\mathrm{Im}\,(\partial\bar\partial)$ in every bidegree $(p,\,q)$, where the operators ∂ and $\bar\partial$ act on either smooth differential forms or currents.) This relates to a natural object on the given compact complex manifold X, the so-called **Gauduchon cone** $\mathcal{G}_X$ (Popovici 2013) consisting of the Aeppli cohomology classes of all the Gauduchon metrics. It is an open convex cone in the Aeppli cohomology space $H^{n-1,\,n-1}_A(X,\,\mathbb{R})$ and is dual to Demailly's pseudo-effective cone of Bott-Chern cohomology classes of all the d-closed positive $(1,\,1)$-currents on X. It plays a growing role as a possible substitute of the classical Kähler cone (even on Kähler manifolds), including in a new approach to Mirror Symmetry, extended to possibly non-Kähler Calabi-Yau (i.e. whose canonical bundle is trivial) manifolds, very recently proposed by Popovici.

We end this brief overview with a reminder of the important class of **$\partial\bar\partial$-manifolds**, a key link between Kähler and non-Kähler geometries. These are the compact complex manifolds X such that for every bidegree $(p,\,q)$ and every d-closed $(p,\,q)$-form (or current) u on X, the following exactness properties are equivalent:

$$u\in\mathrm{Im}\,\partial \iff u\in\mathrm{Im}\,\bar\partial \iff u\in\mathrm{Im}\,d \iff u\in\mathrm{Im}\,(\partial\bar\partial).$$

All compact Kähler manifolds are $\partial\bar\partial$-manifolds, by the classical $\partial\bar\partial$-lemma, but there exist many important classes of $\partial\bar\partial$-manifolds that are not Kähler. Examples of non-Kähler Calabi-Yau $\partial\bar\partial$-manifolds include some 3-dimensional solvmanifolds (Fino-Otal-Ugarte 2014) and the Clemens manifolds (Friedman 2017). The $\partial\bar\partial$-condition implies the existence of a canonical (i.e. depending only on the complex structure) Hodge Decomposition and Symmetry, so $\partial\bar\partial$-manifolds behave cohomologically like Kähler manifolds.

Recent Developments and Open Problems

(A) Let us mention at least two alternative and more recent approaches to the **Mirror Symmetry Conjecture**.

• The SYZ approach to Mirror Symmetry

Another approach to Mirror Symmetry centred around the so-called Strominger-Yau-Zaslov (SYZ) conjecture. It predicts the existence of dual special Lagrangian T^n-fibrations in a mirror pair of Calabi-Yau manifolds. The existence of topological T^n-fibrations for non-singular Calabi-Yau hypersurfaces in toric varieties was proved by Zharkov in 1998, while Ruan proved in 1999 the existence of a Lagrangian torus fibration for the quintic threefold.

The underlying idea is to use the SYZ conjecture to construct the mirror manifold of a given Calabi-Yau manifold. This involves dualising and compactifying torus fibrations, i.e. fibrations $\pi : \mathcal{X} \to B$ whose general fibre is a torus. There are cases where it is known that the SYZ conjecture explains mirror symmetry from a topological point of view.

A significant result is the following

Theorem 25.0.1. (Gross 1999) The quintic threefold $X \subset \mathbb{P}^4$ has a well-behaved T^3-fibration with semistable fibres $f : X \to B$.

Moreover, f has a well-behaved dual $\check{f} : \check{X} \to B$ and $\check{X}$ is diffeomorphic to a specific non-singular minimal model of the mirror quintic.

Shortly after the above result, Ruan proved the existence of Lagrangian T^3-fibrations on the quintic and the mirror quintic that are probably dual to each other as can be seen by comparing their monodromies.

• The Gauduchon cone and Frölicher spectral sequence approach to Mirror Symmetry

This approach was proposed recently in [Pop18] in the general context of possibly non-Kähler Calabi-Yau manifolds (i.e. compact complex manifolds X whose canonical bundle K_X is trivial). Thus, it extends the Mirror Symmetry Conjecture to the possibly non-Kähler context.

As is well known, there is an obvious cohomological obstruction to some Kähler C-Y threefolds X having Kähler mirror duals $\widetilde{X}$. The Kuranishi family $(X)_{t\in\Delta}$ of a given Kähler C-Y manifold $X = X_0$ is unobstructed (i.e. its base space Δ is **smooth**, hence can be viewed as an open ball in the classifying space $H^{0,\,1}(X,\, T^{1,\,0}X)$) by the Bogomolov-Tian-Todorov theorem ([Bog78], [Tia87], [Tod89]). The triviality of the canonical bundle K_X implies the isomorphism $H^{0,\,1}(X,\, T^{1,\,0}X) \simeq H^{n-1,\,1}(X,\, \mathbb{C}) = H^{2,\,1}(X,\, \mathbb{C})$, where the last identity follows from the assumption $\dim_{\mathbb{C}} X := n = 3$. On the other hand, the complexified Kähler cone $\widetilde{\mathcal{K}}_{\widetilde{X}}$ of $\widetilde{X}$ is an open subset of $H^{1,\,1}(\widetilde{X},\, \mathbb{C})$. So a necessary condition for X and $\widetilde{X}$ to be mirror dual is that the tangent space to Δ at 0 (i.e. $H^{2,\,1}(X,\, \mathbb{C})$) be isomorphic to the tangent space to the complexified Kähler cone $\widetilde{\mathcal{K}}_{\widetilde{X}}$ at some point (i.e. $H^{1,\,1}(\widetilde{X},\, \mathbb{C})$), and vice-versa. It is thus necessary to have

$$h^{2,\,1}(X) = h^{1,\,1}(\widetilde{X}) \quad \text{and} \quad h^{2,\,1}(\widetilde{X}) = h^{1,\,1}(X).$$

However, there exist Kähler C-Y threefolds X such that $h^{2,\,1}(X) = 0$ (the so-called *rigid* such threefolds, those that do not deform). Consequently, the mirror dual $\widetilde{X}$, if it exists, cannot be Kähler since $h^{1,\,1}(\widetilde{X}) = 0$.

The idea of investigating the possible existence of a mirror symmetry phenomenon beyond the Kähler world was loosely suggested by Reid in 1987 and received attention recently in 2015 in a work by Lau-Tseng-Yau. However, the methods and point of view adopted in [Pop18] are very different from those of Lau-Tseng-Yau.

The standard approach to the study of the Kähler side of the mirror is to use Gromov-Witten invariants attached to pseudo-holomorphic curves and to count rational curves. However, on many non-Kähler compact complex threefolds with trivial canonical bundle, there exist no rational curves.

The work [Pop18] proposed a new approach to mirror symmetry by means of transcendental methods in the general, possibly non-Kähler context of compact complex manifolds whose canonical bundle is trivial. By extension of the classical definition, we shall still call them **Calabi-Yau (C-Y) manifolds**. This new point of view was then tested on the Iwasawa manifold, a well-known non-Kähler compact complex C-Y manifold, where one can take full advantage of the explicit nature of extensive computations for this particular manifold found in the works [Nak75], [Ang11] and [Ang14] of Nakamura and Angella.

We hope that the methods introduced in [Pop18] will apply to larger classes of C-Y manifolds in the future and that this article is the first in a series. One of the new ideas it introduces is the notion of local universal family of *essential deformations*, viewed as a subfamily of the Kuranishi family, of the Iwasawa manifold X. Three equivalent definitions are given: by removing the complex parallelisable small deformations from the Kuranishi family; by selecting the small deformations that have a kind of *polarisation* by the holomorphic non-closed 1-form γ associated with X; and by selecting the vector subspace of the Dolbeault cohomology space $H^{n-1,\,1}(X,\,\mathbb{C})$ (known to parametrise all the small deformations of a C-Y manifold X, while the complex dimension of X is $n=3$ here) that is naturally isomorphic to the vector space $E_2^{n-1,\,1}(X)$ featuring in bidegree $(n-1,\,1)$ on the second page of the Frölicher spectral sequence of X.

Looking ahead beyond the special case of the Iwasawa manifold treated in this paper, we come up against the question of what makes a deformation of a general, possibly non-Kähler, C-Y manifold *essential*. Our hunch is that a definition in terms of the Frölicher spectral sequence, that will yield a replacement for the Hodge decomposition in middle degree n, is the best bet in a general pattern that will hopefully emerge in the future after further examples of C-Y manifolds have been investigated.

One of the main ideas in this work was to overcome the double whammy of a possible non-existence of both Kähler metrics and rational curves by using the Gauduchon cone of the given non-Kähler C-Y manifold X. This furnishes both an alternative to the classical Kähler cone (that is empty on a non-Kähler manifold) and a transcendental substitute for cohomology classes of (currents of integration on) curves (e.g. by virtue of its elements' bidegree $(n-1,\,n-1)$, but also in a far deeper sense). We stress that the Gauduchon cone is relevant even on projective and on Kähler non-projective manifolds where it might be preferable to the Kähler cone in certain circumstances (for example, when it is strictly bigger, allowing for more flexibility).

The compact complex manifolds X on which every Gauduchon metric is strongly Gauduchon were introduced under the name of **sGG manifolds** and studied in a 2014 paper by Popovici and Ugarte. They contain the Iwasawa manifold and all its small deformations.

The main object of study in [Pop18] was the standard *Iwasawa manifold* $X=G/\Gamma$, defined as the quotient of the Heisenberg group

$$G:=\left\{\begin{pmatrix}1 & z_1 & z_3\\ 0 & 1 & z_2\\ 0 & 0 & 1\end{pmatrix}\ ;\ z_1,z_2,z_3\in\mathbb{C}\right\}\subset GL_3(\mathbb{C})$$

by its discrete subgroup $\Gamma\subset G$ of matrices with entries $z_1,z_2,z_3\in\mathcal{Z}[i]$.

The map $(z_1,z_2,z_3)\mapsto(z_1,z_2)$ factors through the action of Γ to a (holomorphically locally trivial) proper holomorphic submersion

$$\pi:X\to B,$$

where the base $B=\mathbb{C}^2/\mathcal{Z}[i]\oplus\mathcal{Z}[i]=\mathbb{C}/\mathcal{Z}[i]\times\mathbb{C}/\mathcal{Z}[i]$ is a two-dimensional Abelian variety (the product of two elliptic curves) and where all the fibres are isomorphic to the Gauss elliptic curve $\mathbb{C}/\mathcal{Z}[i]$.

Since G is a connected, simply connected, *nilpotent* complex Lie group, X is a *nilmanifold*. Furthermore, X is a *complex parallelisable* compact complex manifold (i.e. its holomorphic tangent bundle $T^{1,\,0}X$ is trivial) of complex dimension 3. In particular, its canonical bundle K_X is trivial, so X is a Calabi-Yau manifold in our generalised sense.

It is well known that X is not a $\partial\bar\partial$-manifold (in particular, it is not Kähler). In fact, its Frölicher spectral sequence does not even degenerate at E_1, so there is no Hodge decomposition either canonical or non-canonical on X.

However, despite X lacking the $\partial\bar\partial$ property, Nakamura showed in 1975 that the Kuranishi family $(X_t)_{t\in\Delta}$ of $X=X_0$ is *unobstructed*, so its base Δ is smooth and can be identified with an open ball in $H^{0,\,1}(X,\,T^{1,\,0}X)\simeq$

$H^{2,1}_{\bar\partial}(X, \mathbb{C})$. It can be easily checked that there is no Hodge decomposition of weight 3 since the Dolbeault cohomology group $H^{2,1}_{\bar\partial}(X, \mathbb{C})$ does not inject canonically into $H^3_{DR}(X, \mathbb{C})$. In fact, $b_3 = 10$ while $h^{3,0} = h^{0,3} = 1$ and $h^{2,1} = h^{1,2} = 6$, so in a sense the vector space $H^{2,1}_{\bar\partial}(X, \mathbb{C})$ is "too large" to fit into $H^3_{DR}(X, \mathbb{C})$.

The main result of [Pop18] can be loosely stated as follows.

Theorem 25.0.2. The Iwasawa manifold is its own mirror dual in the sense that its local universal family of essential deformations corresponds to its complexified Gauduchon cone.

The meaning of "corresponds" was made precise in the paper. Loosely speaking, it means that there exists a local biholomorphism between the local universal family of essential deformations and the complexified Gauduchon cone of the Iwasawa manifold and there exists an induced C^∞ isomorphism of variations of Hodge structures (VHS) that exist on either side of the mirror. Moreover, this isomorphism is holomorphic at the level of the rank-1 components and anti-holomorphic at the level of the rank-4 components of these VHS.

(B) The study of holomorphic families of compact complex, possibly non-Kähler, manifolds, that plays a key role in Mirror Symmetry, was recently given a different treatment from the point of view of Riemann-Roch-type theorems via a key use of the Bott-Chern cohomology that is often better suited to the non-Kähler context than the more familiar Dolbeault cohomology.

• A Riemann-Roch theorem in Bott-Chern cohomology

J.-M. Bismut, who participated in this workshop and gave a far-reaching talk with implications in complex, algebraic and arithmetic geometry, described a geometric problem on families of elliptic operators. He had solved this problem via a deformation to a family of non self-adjoint Fredholm operators.

Specifically, let $p : M \to S$ be a proper holomorphic projection of complex manifolds and let F be a holomorphic vector bundle on M. It is assumed that the vector spaces $H^{(0,p)}(Xs, F|X_s)$ have locally constant dimension. They are the fibers of a holomorphic vector bundle on S.

The problem that was addressed in this work is the computation of characteristic classes associated with the above vector bundle in a refinement of the ordinary de Rham cohomology of S, its Bott-Chern cohomology, and the proof of a corresponding theorem of Riemann-Roch-Grothendieck. When M is not Kähler, none of the existing techniques to prove such a result using the fiberwise Dolbeault Laplacians can be used. The solution is obtained via a proper deformation of the corresponding Dolbeault Laplacians to a family of **hypoelliptic Laplacians**, for which the corresponding result can be proved. This deformation is made to destroy the geometric obstructions which exist in the elliptic theory, like the fact that the metric is Kähler, namely the fact that the Kähler form is $\bar\partial\partial$-closed.

• A conjecture on deformation limits of Moishezon manifolds

In 2019, the resolution of a conjecture dating back to the 1970s about limits under holomorphic deformations of Moishezon manifolds was announced in [Pop19]. A *Moishezon manifold* is a compact complex manifold Y for which there exists a projective manifold $\widetilde{Y}$ and a holomorphic bimeromorphic map $\mu : \widetilde{Y} \longrightarrow Y$. By a classical result of Moishezon (1967), a Moishezon manifold is not Kähler unless it is projective.

The context is the following. We consider a complex analytic (or holomorphic) family of compact complex manifolds. This is a *proper holomorphic submersion* $\pi : \mathcal{X} \to B$ between two complex manifolds $\mathcal{X}$ and B. In particular, the fibres $X_t := \pi^{-1}(t)$ are compact complex manifolds of the same dimension. By a classical theorem of Ehresmann (1947), any such family is locally (hence also globally if the base B is contractible) C^∞ trivial. Thus, all the fibres X_t have the same underlying C^∞ manifold X (hence also the same De Rham cohomology groups $H^k_{DR}(X, \mathbb{C})$ for all $k = 0, \dots, 2n$), but the complex structure J_t of X_t depends, in general, on $t \in B$.

The statement below is a closedness result under deformations of complex structures: any deformation limit of a family of Moishezon manifolds is Moishezon. Indeed, the fibre X_0 can be regarded as the limit of the fibres X_t when $t \in B$ tends to $0 \in B$. We can, of course, suppose that B is an open disc about the origin in $\mathbb{C}$.

Theorem 25.0.3. ([Pop19]) Let $\pi : \mathcal{X} \to B$ be a complex analytic family of compact complex manifolds over an open ball $B \subset \mathbb{C}^N$ about the origin such that the fibre $X_t := \pi^{-1}(t)$ is a **Moishezon manifold** for every $t \in B \setminus \{0\}$. Then $X_0 := \pi^{-1}(0)$ is again a **Moishezon manifold**.

One of the major open problems in this direction is the transcendental version of the above result about deformation limits of *Fujiki class $\mathcal{C}$ manifolds*. Recall that a *Fujiki class $\mathcal{C}$ manifold* is a compact complex manifold Y for which there exists a compact Kähler manifold $\widetilde{Y}$ and a holomorphic bimeromorphic map $\mu : \widetilde{Y} \longrightarrow Y$.

Conjecture 25.0.4. Let $\pi : \mathcal{X} \to B$ be a complex analytic family of compact complex manifolds over an open ball $B \subset \mathbb{C}^N$ about the origin such that the fibre $X_t := \pi^{-1}(t)$ is a **Fujiki class $\mathcal{C}$ manifold** for every $t \in B \setminus \{0\}$. Then $X_0 := \pi^{-1}(0)$ is again a **Fujiki class $\mathcal{C}$ manifold**.

A two-step strategy for tackling this conjecture was outlined in a work by Popovici and Ugarte (2014):

Step 1: *prove that a compact complex manifold X belongs to the class $\mathcal{C}$ if and only if there are "many" closed positive $(1,\,1)$-currents on X.*

Step 2: *prove that there can only be "more" closed positive $(1,\,1)$-currents on X_0 than on the generic fibre X_t.*

The notion of *sGG manifold* was introduced there for this purpose by requiring the Gauduchon cone of the manifold to be as small as possible (i.e. equal to the a priori smaller strongly gauduchon cone). This is a way of saying that the given compact complex manifold X carries "many" closed positive $(1,\,1)$-currents since the closed convex cone of cohomology classes of such currents (called the *pseudo-effective cone*) is dual, under the duality between the Bott-Chern cohomology of bidegree $(1,\,1)$ and the Aeppli cohomology of bidegree $(n-1,\,n-1)$, to the closure of the *Gauduchon cone* introduced by Popovici in 2013 and also used in his new approach to Mirror Symmetry.

(C) Another very active area of research at the moment is the theory of geometric flows. The idea goes back to Hamilton and was used spectacularly by Perelman in his resolution of the Poincaré Conjecture. The Ricci flow, the Kähler-Ricci flow and the much more recent Anomaly flow have been staples of complex geometry and geometric analysis for the past fifteen years. Several interesting talks given in this workshop focused on some of these flows and their geometric applications.

Presentation Highlights

We will organise the presentation highlights according to the themes outlined above.

Mirror Symmetry and related issues

• **T. Collins** reported on some substantial progress on the SYZ appproach to Mirror Symmetry in joint work with A. Jacob and Y.-S. Lin. He discussed the existence of special Lagrangian torus fibrations on log Calabi-Yau manifolds constructed from del Pezzo surfaces, and some progress towards establishing SYZ mirror symmetry for these non-compact Calabi-Yau manifolds.

• In a similar but more gauge-theoretical vein, **M. Garcia Fernandez** reported on joint work with Rubio, Tipler, and Shahbazi centred on the *Hull-Strominger system and holomorphic string algebroids*. Specificallly, he gave an overview of a new gauge-theoretical approach to the Hull-Strominger system using holomorphic string algebroids.

In the smooth setup, a string algebroid provides an infinitesimal version of a principal bundle for the string group. The main focus of his talk was on the consequences of this approach for the existence and uniqueness problem, as well as for the moduli space metric. The discussion was illustrated by a key example.

Geometric flows and related issues

• There was a very interesting talk by **T. Fei** lying at the interface between geometric flows and mirror symmetry. It reported on some recent progress on the *anomaly flow* in joint work with Z.-J. Huang, D.H. Phong and S. Picard.

Specifically, the Hull-Strominger system describes the geometry of compactifications of heterotic superstrings with flux, which can be viewed as a generalization of Ricci-flat Kähler metrics on non-Kähler Calabi-Yau manifolds.

To overcome the difficulty of lacking the $\partial\bar{\partial}$-lemma, Phong, Picard and Zhang initiated the *Anomaly Flow* programme in a bid to understand the Hull-Strominger system. It has been proved in many cases that the Anomaly Flow serves as an effective way to investigate the Hull-Strominger system and in general canonical metrics on complex manifolds, such as giving new proofs of the Calabi-Yau theorem and the existence of a Fu-Yau solution.

In this talk, T. Fei presented some new progress on the Anomaly Flow, including its behavior on generalized Calabi-Gray manifolds and a unification of the Anomaly Flow with vanishing slope parameter and the Kähler-Ricci flow, which further allows one to generalise the notion of the Anomaly Flow to arbitrary complex manifolds.

• Another interesting talk was given by **L. Vezzoni** about the many links between the various geometric flows and several kinds pf special Hermitian metrics on compact complex manifolds.

Specifically, his talk centred on a *geometric flow of balanced metrics*. Recall that balanced metrics ω, introduced by Gauduchon in 1977, are a kind of dual of Kähler metrics. They are defined by the requirement that $d\omega^{n-1} = 0$ (where n is the dimension of the compact complex manifold), or equivalently that $d^\star_\omega \omega = 0$ (i.e. ω is required to be *co-closed*). Like Kähler metrics, they need not exist, but they exist in far more general situations than Kähler metrics, including on all Kähler manifolds.

Typical examples of balanced manifolds include modifications of Kähler manifolds, twistor spaces over anti-self-dual oriented Riemannian 4-manifolds and nilmanifolds. In his talk, L. Vezzoni discussed a geometric flow of balanced metrics that he had co-introduced with L. Bedulli in 2017. This flow is a generalisation of the Calabi flow to the balanced context. It preserves the Bott-Chern cohomology class of the initial metric and in the Kähler case reduces to the classical Calabi flow.

It was explained in the talk that this flow is well-posed and that its stability around Ricci flat Kähler metrics was emphasized. The talk also focused on a rencent problem in balanced geometry proposed Fino and Vezzoni.

Complex surfaces

The theory of complex surfaces holds a special place in complex geometry and differs in many respects from the geometry of compact complex manifolds of dimension ≥ 3. Compact complex surfaces were classified by Kodaira long ago, but the class VII in Kodaira's classification is still not entirely understood and a lot of effort has been going since at least the early 1980s into trying to complete Kodaira's classification. A whole array of different methods, coming from complex and algebraic geometry, differential geometry, the topology of 4-manifolds and, more recently, the various theories of geometric flows, have been used.

• An interesting talk that provided a link between this theme and the previous one was given by **J. Streets**. It reported on joint work with Y. Ustinovskiy on *generalised Kähler-Ricci solitons on complex surfaces*.

Specifically, generalised Kähler-Ricci solitons are canonical geometric structures on complex, non-Kähler manifolds. In his talk, J. Streets gave a complete classification of such structures on complex surfaces.

• This talk can be compared with the one given by **G. Dloussky** on *smooth rational deformations of singular contractions of class VII surfaces*.

Specifically, he considered normal compact surfaces Y obtained from a minimal class VII surface X by contraction of a cycle C of r rational curves with $c_2 < 0$. Dloussky's main result states that, if the obtained cusp is smoothable, then Y is globally smoothable. The proof is based on a vanishing theorem for $H^2(Y, \Theta)$, where Θ is the dual the sheaf of Kähler forms.

If $r \leq b_2(X)$ any smooth small deformation of Y is rational, and if $r = b_2(X)$ (i.e. when X is a half-Inoue surface), any smooth small deformation of Y is an Enriques surface.

Locally conformally Kähler (lck) geometry

This is another active area of research that was represented by several internationally recognised experts in this workshop.

• **A. Moroianu** lectured on *locally conformally Kähler manifolds with holomorphic Lee field*.

Specifically, a locally conformally K̈hler (lck) manifold is a compact Hermitian manifold (M, g, J) whose fundamental 2-form $\omega := g(J\cdot, \cdot)$ verifies the condition $d\omega = \theta \wedge \omega$ for a certain closed 1-form θ called the Lee form. This talk, based on joint work with F. Madani, S. Moroianu, L. Ornea and M. Pilca, focused on lck manifolds whose Lee vector field (the metric dual of θ) is holomorphic. It was shown that if its norm is constant or if its divergence vanishes, then the metric is Vaisman, i.e. the Lee form is parallel with respect to the Levi-Civita connection of g.

The talk went on to give examples of non-Vaisman lck manifolds with holomorphic Lee field and to explain how all such structures on manifolds of Vaisman type are classified.

• A link between the theory of complex surfaces and lck manifolds was provided by **A. Otiman** who lectured on *a class of Kato manifolds*.

Specifically, she described Kato manifolds, also known as manifolds with a global spherical shell. She revisited Brunella's proof of the fact that Kato surfaces admit locally conformally Kähler metrics and went on to show that this holds for a large class of higher-dimensional complex manifolds containing a global spherical shell.

On the other hand, she explained the construction of manifolds containing a global spherical shell which admit no locally conformally Kähler metric.

She went on to consider a specific class, which can be seen as a higher-dimensional analogue of the Inoue-Hirzebruch surfaces, and to study several of their analytical properties. In particular, she gave new examples, in any complex dimension $n \geq 3$, of compact non-exact locally conformally Kähler manifolds with algebraic dimension $n-2$, algebraic reduction bimeromorphic to $\mathbb{C}\mathscr{P}^{n-2}$ and admitting non-trivialholomorphic vector fields.

Hodge theory

This is another major research theme that featured prominently in this workshop. Among other things, it is related to Mirror Symmetry.

• **M. Verbitsky** lectured on the *deformation theory of non-Kähler holomorphically symplectic manifolds*, based on joint work with N. Kurnosov.

Specifically, in 1995, D. Guan constructed examples of non-Kähler, simply-connected holomorphically symplectic manifolds. An alternative construction, using the Hilbert scheme of Kodaira-Thurston surface, was given by F. Bogomolov.

Verbitsky and his co-author prove the *Local Torelli Theorem*, showing that holomorphically symplectic deformations of BG-manifolds are unobstructed, and the corresponding period map is locally a diffeomorphism.

Subsequently, using the local Torelli theorem, the authors prove the Fujiki formula for a BG-manifold, showing that there exists a symmetric form q on the second cohomology with the same properties as the Beauville-Bogomolov-Fujiki form for hyperkahler manifolds.

Verbitsky's talk tied in with both Stelzig's talk on a new computation method of various types of cohomology and Rollenske's talk on $\partial\bar{\partial}$ Calabi-Yau manifolds. All these three talks fall into the realm of possibly non-Kähler complex geometry.

• Specifically, **J. Stelzig** lectured on *zigzags and the cohomology of complex manifolds*. Deligne, Griffiths, Morgan and Sullivan famously characterised the $\partial\bar{\partial}$-property of compact complex manifolds by the following property:

The double complex of forms decomposes as a direct sum of two kinds of irreducible subcomplexes: 'squares' and 'dots', where only the latter contribute to cohomology.

In his talk, the author explored the implications of the following folklore generalisation of this:

Every (suitably bounded) double complex decomposes into irreducible complexes and these are 'squares' and 'zigzags', with a dot being a zigzag of length 1.

This affords insight into the structure of and relation between the various cohomology groups. When applied to complex manifolds, this yields, among other things, the analogue of the Serre duality for all the pages of the Frölicher spectral sequence, a three-space decomposition on the middle cohomology and new bimeromorphic invariants.

The talk ended with several open questions.

• **S. Rollenske**'s talk, based on joint work with B. Anthes, A. Cattaneo and A. Tomassini, was about *$\partial\bar{\partial}$-complex symplectic and Calabi–Yau manifolds: Albanese map, deformations and period maps*.

Specifically, let X be a compact complex $\partial\bar{\partial}$- manifold with trivial canonical bundle. The $\partial\bar{\partial}$-assumption means that the $\partial\bar{\partial}$-lemma is satisfied by X.

If X is Kähler then, up to a finite cover, X is the product of a simply connected manifold with its Albanese Torus $Alb(X)$, by the Beauville-Bogomolov decomposition theorem. The authors showed that in their more general setting, the Albanese map is still a holomorphic submersion but, in general, does not split after finite pullback.

The authors also showed that the Kuranishi space of X is a smooth universal deformation and that small deformations enjoy the same properties as X. If, in addition, X admits a complex symplectic form, then the local Torelli theorem holds and we obtain some information about the period map. It is in this last part of the talk that a direct link was established to Verbitsky's talk.

Conclusions

This workshop was rich in stimulating discussions and enlightening presentations. This report only scratches the surface of what was discussed. We greatly appreciated this opportunity of bringing together mathematicians from diverse backgrounds and the new ideas that arose from their discussions and presentations.

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Chapter 26

Unifying 4-Dimensional Knot Theory (19w5118)

November 4 - 8, 2019

Organizer(s): Scott Carter (University of South Alabama), Jeffrey Meier (Western Washington University), Alexander Zupan (University of Nebraska–Lincoln)

Overview of the Field

Our workshop focused on an exciting facet of smooth 4–manifold topology: the theory of knotted surfaces. Topology in dimension three has seen an explosion of activity over the last 30 years, reaching a peak with Perelman's proof of the Poincaré Conjecture in 2003 [40]. Other notable highlights include the groundbreaking discovery of the Jones Polynomial in knot theory [27] and the chain reaction Jones' work set off in quantum topology, algebra, and physics, including Witten's work connecting the Jones Polynomial to Chern-Simons theory [45]. In stark contrast, our understanding of 4–dimensional topology has many prominent gaps, including the intractable Smooth 4–dimensional Poincaré Conjecture, and breakthroughs have been more difficult to attain.

In 4–dimensional spaces, the interesting knotted objects are not loops but rather surfaces, and the first step in studying these objects is to find appropriate geometric representations, in the sense that these pictures should be easily manipulated and lend themselves to performing computations. Classical approaches to the theory of knotted surfaces include movies [14], broken surface diagrams [46] (defined below), and marked vertex diagrams [31, 47]. For example, whereas a classical knot diagram is the projection of a loop in $\mathbb{R}^3$ to an immersed curve in $\mathbb{R}^2$ equipped with crossing information, a broken surface diagram is the projection of a surface in $\mathbb{R}^4$ to generic surface in $\mathbb{R}^3$, which has also been equipped with "crossing information," suitably defined. Carter, Kamada, Roseman, Saito, and many others have made an industry out of developing this diagrammatic and combinatorial theory [5, 41], notably using quandles, an algebraic structure generalizing Fox's notion of n–colorability [6].

People study knotted surfaces from through a variety of lenses. Some attempt to import 3–dimensional ideas to dimension four. Others emphasize aspects of 4–dimensional knot theory that fit coherently within the theory of codimension two embeddings in dimension four and higher. While these two groups often consider surfaces in S^4, yet another active area of research draws from classical results in 4-manifold topology, considering the broader class of surfaces in arbitrary 4-manifolds. Some utilize the additional structure afforded by symplectic and complex manifolds. Researchers study geometric, algebraic, and combinatorial aspects of knotted surfaces. The purpose of our workshop was to encourage a dialogue among this wide variety of researchers, with a central goal of better understanding knotted surfaces. We wanted participants to share their most interesting tools and problems so that the entire field could benefit from novel, multi-faceted approaches to both new and old challenges. Overall, we were impressed by the engagement of everyone involved, and based on the feedback that reached us, the workshop was universally considered a success.

Recent Developments and Open Problems

One of the most important breakthroughs in the theory of knotted surfacers over the last couple of years was Gabai's surprising proof of the 4-dimensional Light Bulb Theorem, an incredible triumph of 3–dimensional techniques applied novelly and elegantly in a brand new setting [17]. The classical version of this theorem in dimension three states that any knot in $S^1 \times S^2$ that meets $\{pt\} \times S^2$ in a single point is isotopic to $S^1 \times \{pt\}$. In its full generality, Gabai's theorem asserts that if S and T are homotopic, smoothly embedded 2-spheres in a smooth 4-manifold X with a common dual (square-zero sphere meeting each of S and T in a single point), and in addition $\pi_1(X)$ has no 2-torsion, then S and T are smoothly ambient isotopic in X. An ongoing and popular trend in 4-dimensional research is to develop new invariants to prove that spaces are different; Gabai's theorem stands out as remarkable in that it shows instead that a vast collection of surfaces are the same. His work also elegantly generalizes an elementary result from one dimension lower.

Another recent development in knotted surface theory also connects ideas from dimensions three and four. In 2012, David Gay and Robion Kirby introduced trisections of smooth 4-manifolds, decompositions of 4-manifolds into three simple pieces, as an analogue of 3-dimensional Heegaard splittings in dimension four [18]. Following their work, Meier and Zupan adapted bridge splittings of classical knots to develop the theory of bridge trisections, decompositions of embedded surfaces in 4-manifolds into trivial disks and trivial tangles within the components of a 4-manifold trisection [38, 39]. Bridge trisections also yield a new structure called tri-plane diagrams. Tri-plane diagrams encode knotted surfaces in a novel way, and this area is ripe for the same types of advances obtained in the theory of broken surface diagrams.

A third area that has seen an explosion of activity over the last two decades is knot concordance. Two classical knots K_1 and K_2 in S^3 are (smoothly) concordant if there exists a (smoothly) embedded annulus $A \subset S^3 \times I$ connecting $K_1 \subset S^3 \times \{0\}$ to $K_2 \subset S^3 \times \{1\}$. As such, knot concordance occurs at the nexus of 3–manifold and 4–manifold topology, often employing tools from both areas. The theory of concordance also interacts with several specialized topics in geometric topology, including contact/symplectic topology, and the powerful Heegaard Floer and Khovanov homology theories [36]. Through these and other avenues, many researchers have made great gains in studying knot concordance by developing an arsenal of invariants to obstruct two knots from being concordant.

Our workshop connected researchers studying these related but somewhat disparate areas of knotted surface theory for the mutual benefit of all parties. By encouraging a dialogue, we brought together subject-matter experts in all of these sub-fields for the purpose of developing a more unified theory of knotted surfaces in dimension four.

In the view of the organizers, the most important open problems in knotted surfaces theory involve drawing out differences (if they exist) between the topological and smooth categories. The Smooth 4-dimensional Poincaré Conjecture (S4PC), which asserts that every smooth 4-manifold homeomorphic to S^4 is also diffeomorphic to S^4, is the last remaining case of the Generalized Poincaré Conjecture. The relative version of the S4PC is an important open problem in 2-knot theory, the Unknotting Conjecture, positing that if $K \subset S^4$ is a smoothly embedded 2-sphere such that $\pi_1(S^4 \setminus K) = \mathbb{Z}$, then K is isotopic to the unknotted 2-sphere. Also related to the S4PC is the classification of unit 2-knots in $\mathbb{CP}^2$: Suppose that K is a smoothly embedded 2-sphere in $\mathbb{CP}^2$ with square one.

Conjecturally, K is isotopic to the standard unit 2-knot, $\mathbb{CP}^1 \subset \mathbb{CP}^2$. Proving this conjecture is equivalent to showing that all Gluck twists in S^4 produce standard smooth S^4, which would be an incredible step toward a proof of the S4PC.

Presentation Highlights

Before discussing the content of some of the presentations, we wish to discuss the manner in which they were selected and organized. One of our goals was to organize an inclusive and open workshop, and to do so, we decided that instead of inviting particular speakers to give talks, we would ask every one of our 45 registered participants to submit an abstract if they wished to speak. In addition, when we solicited abstracts, we emphasized the varied areas of expertise among participants, expressing a desire for survey talks or at least some survey material in each talk. As a result of this process, we ended up with 23 talks, which we scheduled in 45 minute time slots for our allotted five days. The totality of topics covered by these talks was both broader and more representative than we could have achieved by selecting the talks ourselves, including diverse representation in terms of gender, career stage, and geographic location. We believe that going forward, this talk selection model is a fantastic one. Despite knowing how talks were "chosen," several participants commented that we did a great job creating the conference program (for which we deserved little credit).

Once we had our finalized list of talks, we set out to develop the schedule. The talks were split into rough categories, with similar talks grouped in morning or afternoon blocks. For example, the majority of the Tuesday talks centered on surfaces in manifolds other than S^4, and the three Wednesday talks focused on understanding differences between the smooth and topological categories. The talks that more closely resembled survey talks were planned for earlier in the week, while more technical results came later. We also ensured that each day's list of speakers was balanced by gender. In the following paragraphs, we highlight a few of the presentations that were a part of the workshop, but this list is by no means complete. We received considerable feedback about the quality of the entire program, and in all honesty, we could include any one of the 23 talks that were given as a highlight of the workshop.

The workshop commenced with a terrific talk from Cameron Gordon surveying known, mostly classical, results about knot groups in dimension four and other dimensions. Gordon's talk provided substantial historical context and set an excellent tone for a convivial and productive meeting. Following Gordon, Masahico Saito delivered an excellent survey about applications of quandle co-cycle invariants, a familiar topic for one cadre of participants and esoteric for another, well serving the workshop goal of unifying participants around common themes. The third talk of the first day, delivered by Shin Satoh, presented a surprising and important result related to the triple point number of knotted surfaces. In spirit, the triple point number is meant to be an analogue of crossing number. However, despite the fact that for each n there are finitely many classical knots with crossing number at most n, there are infinitely many 2-knots with triple point number zero (namely, ribbon 2-knots). Satoh demonstrated that the three-dimensional finiteness may be able to be recovered by passing to ribbon concordance classes of 2-knots, in the sense that every 2-knot with triple point number at most n might be ribbon concordant to a finite family of 2-knots, with some fairly convincing evidence.

The second day of the workshop opened with a comprehensive survey talk by Laura Starkston about the extra structure afforded by examining the symplectic topology of certain surfaces in 4-manifolds, including a variety of open problems, which are incorporated into the problem list below. As mentioned elsewhere in this report, Gabai used his Tuesday afternoon talk to announce his surprising, fundamental theorem proved jointly with Budney, that spanning 3-balls for the unknotted 2-sphere in S^4 are not unique up to isotopy [4]. This development is discussed in greater detail below.

The third day opened with Arunima Ray's talk about a piece of Freedman and Quinn's disk embedding theorem [16]. Over the last ten years, a group has researchers has pushed for a more modern treatment of Freedman's pioneering work underlying his now nearly 40-year-old proof of the topological Poincaré conjecture in dimension four. Ray is a leader of a group of low-dimensional topologists writing a new exposition and expansion of Freedman's work, and her talk covered joint work giving some explicit constructions lacking in Freedman and Quinn's original work.

As mentioned above, the model of soliciting abstracts gave many graduate students speaking opportunities. Highlights from the graduate student talks included a pair of talks about concordance of knotted surfaces. On Tuesday afternoon, Maggie Miller presented of her work generalizing Gabai's Light Bulb Theorem to a broader result about in which concordance of 2-knots replaces isotopy. On Thursday afternoon, Jason Joseph discussed his dissertation research, in which he uses Alexander modules to obstruct concordance of 2-knots, obtaining an alternative answer to a recently solved Kirby problem, and giving the first proof certain elements of the concordance monoid do not have inverses, implying that it is indeed a monoid and not a group [28].

Scientific Progress Made

While the most important aspect of this workshop was the presentation of new results and the motivation of open problems, another secondary purpose was achieved. Namely, through the processes of socialization and shared values, the workshop was able to forge new relationships between several communities of 4-dimensional topologist that include an older and younger generation, people whose work focused on disparate areas (e.g., topological, smooth, and symplectic categories), people who are normally geographically isolated from each other (our participants represented four continents), and groups whose work embraces different styles of approach (e.g., traditional diagrammatic aspects vs. surgery-theoretic, say).

One noteworthy event related the conference was the inception of an important collaboration between Ryan Budney and David Gabai. Gabai had been working in earnest in the months leading up to the workshop on the question of the uniqueness up to isotopy of embeddings of B^3 in S^4 such that the boundary of the embedded ball is the standard S^2 in S^4. (Note, this is but one facet of the research, which touches upon multiple important aspects of 4-dimensional topology. See, for example, Problem 26.0.30 below.) What follows is a paraphrasing of Budney's description of the collaboration.

Budney and Gabai had been discussing the problem for about a month by email prior to the workshop. In the first two days of the workshop, they outlined the proof of a theorem that could be phrased in a variety of ways – a few of which were mentioned in Gabai's talk. From one perspective, the theorem shows that the exterior of the trivial knot in S^4 admits infinitely many distinct fiberings over S^1 (with fibre an B^3), up to isotopy.

The exterior is $S^1 \times B^3$, and all the fiberings developed by Budney and Gabai come from the orbit of $\pi_0(\text{Diff}(S^1 \times D^3))$ acting on the standard fibering. In other words, they show that the mapping class group of the unknot exterior (leaving the boundary fixed pointwise) is not finitely generated. Another way of stating the result is that the component of the unknot in the space of embeddings $\text{Emb}(S^2, S^3)$ has a non-finitely generated fundamental group. So this is a large contrast from Hatcher's result (using the Smale conjecture) that the component of the unknot in $\text{Emb}(S^1, S^3)$ has fundamental group $\mathbb{Z}/2\mathbb{Z}$. In general their argument extends to say that $\pi_{n-3}(\text{Diff}(S^1 \times D^n))$ is not finitely generated when $n \geq 3$.

Another notable development came from Bob Gompf's contributions. According to Gompf, who proved the existence of infinitely many exotic $\mathbb{R}^4$'s, as a direct result of the invitation to the workshop and the workshop's theme, he developed a relative theory of exotic planes in $\mathbb{R}^4$ [20]. In Gompf's words, this work is "the threshold of a whole new research area," motivated directly by his workshop participation, and it is the subject of a forthcoming paper he is in the process of writing. The theme of adapting results about manifold to the relative cases of knots (in dimension three) or surfaces (in dimension four) is pervasive, and Gompf's work is a terrific concrete example of this principle at work. Five contributed problems stemming from his work are included in the problem list below.

The collaboration of Budney and Gabai described above is the most prominent example of a number of new collaborations that were initiated or strengthened during the workshop. As another example, Meier, Thompson, and Zupan initiated a new collaboration as a direct result of discussions that took place during the coffee breaks at the workshop. They revisited a problem they had considered with little progress before: Every bridge trisection of a knotted surface induces a cell decomposition of the underlying surface whose 1-skeleton is a cubic graph. An open question is whether the reverse is true: Given an abstract cubic graph Γ with a 3-coloring of its edges, is there a bridge trisected surface $\mathcal{K}$ inducing Γ? Together, they proved that the answer is yes for bipartite graphs and have continued to collaborate about the non-orientable case following the workshop. They expect to write a joint paper in the near future.

Joseph, Meier, Miller, and Zupan also initiated a new collaboration resulting from the workshop. In shuttle to the Calgary airport, Miller and Zupan realized that altogether, the four of them had established sufficiently many new results relating bridge trisections to other aspects of 2-knot theory that these results should collected in a coherent manuscript to be shared with the community. In particular, they have developed a algorithm to produce Seifert solids, the punctured 3-manifolds bounded by 2-knots in S^4 using tri-plane diagrams, a procedure to convert a tri-plane diagram to a broken surface diagram, and an elegant computation of the normal Euler number of a surface knot. They expect to write a joint paper in the near future.

Of course, we are limited to describing the collaborations including ourselves and those that were communicated, but we also witnessed the continuation of existing collaborations, for instance between Bar-Natan and Dancsworkshopo and between Auckly and Ruberman.

Outcome of the Meeting

In our proposal, we listed a number of goals for the workshop. The manner in which the workshop and its participants addressed several of these is articulated.

1. **Raise awareness of the state-of-the-art within each sub-field.** While our original goal was to include expository talks primarily at the beginning of the conference, this was not always possible. Talks by Dave Auckly, Hans Boden, Scott Carter, Celeste Damiani, Zsuzsanna Dancso, Bob Gompf, Cameron Gordon, Mark Hughes, Sashka Kjuchukova, Laura Starkston, Arunima Ray, and Masahico Saito included introductory and background material that informed the participants of the scope of the results that were presented.

2. **Adapt machinery across different representations of knotted surfaces.** Talks by Jason Joseph, Seungwong Kim, Vince Longo, Maggie Miller, and Danny Ruberman helped describe relations among the various sub-genres of surfaces in 4-spaces. In general, we feel that the workshop did an excellent job of exposing researchers to approaches to knotted surface theory that might represent a departure from their usual techniques and skill sets.

3. **Develop new knotted surface invariants.** Talks of Hans Boden, Dave Gabai, Mark Hughes, Byeorhi Kim, Masahico Saito, and Laura Starkston addressed the development of invariants. The development of invariants remains an important goal of the field, broadly construed. One approach to finding invariants is sufficiently develop diagrammatic theories over which the invariants might be defined. The workshop greatly enabled the development of diagrammatic theories, both classical and more recent.

4. **Understand various representations of symplectic surfaces.** Informal discussions among presenters and non-presenters occurred in these regards. Talks of Dave Auckly, Maggie Miller, Arunima Ray, and Laura Starkston are also relevant.

5. **Explore the implications of the 4–dimensional Light Bulb Theorem.** This was one of our greatest successes of the workshop. Ryan Budney and Dave Gabai used Gabai's techniques to establish that there are non-unique smooth spanning 3-balls that are bounded by an unknotted sphere. Maggie Miller and Dave Gabai both gave excellent talks related to recent work that has grown out of Gabai's theorem.

6. **Compile a list of important problems.** Immediately following the workshop, speakers and other participants were asked to contribute one or more problems related to the contents of the workshop program. The organizers curated that list, and the resulting product was a comprehensive and wide-ranging list of problems that can help shape the directions of the theory of embedded surfaces in S^4 and in other 4-manifold in the future. That problem list is included as the next section.

In short, all of our stated objectives were addressed. Many were fully achieved, and others will shape the directions of research that occurs in the near future and beyond.

Problem List

After the workshop, we requested that all presenters (and anyone else interested) submit a problem or two related the their talk or to some conversation they had during the workshop. This problem list was then curated, distributed to conference participants, and posted online so that a broader audience could access some of the workshop developments. The problem list follows below.

Problems about knotted surfaces in S^4

Problem 26.0.1 (Cameron Gordon)**.** *Is there an algorithm to decide whether or not a (PL locally flat) 2-knot is (PL or TOP) unknotted?*

Problem 26.0.2 (Gordon)**.** *Is there a 2-knot whose group has unsolvable word problem?*

The reader is encouraged to refer to [21, Theorem 7.1], which shows that a positive answer to Problem 26.0.2 implies a negative answer to Problem 26.0.1.

Problem 26.0.3 (Masahico Saito)**.** *Find algebraic and diagrammatic interpretations of the quandle 3-cocycle invariant for knotted surfaces.*

For classical knots, the quandle 2-cocycle invariant has an algebraic interpretation as obstructions of extending colorings to extensions of quandles, and a diagrammatic aspect in relation to the fundamental quandle class. Such interpretations for knotted surfaces will be desirable both for computations and applications.

Problem 26.0.4 (Vincent Longo)**.** *Is the connected sum of an even twist spun knot and an unknotted projective plane is diffeomorphic to the connected sum of the spin of the same knot and the unknotted projective plane?*

Longo proved that up to the parity of an integer n, all connected sums of an n-twist spun knot and an unknotted projective plane become diffeomorphic after a single trivial 1 handle addition, assuming either n is odd or K is a 2 bridge knot [37]. The remaining case of n an even integer and the knot having bridge number at least 3 is still open. The version of this problem for n odd is Kirby Problem 4.58 [33].

The triple point number of an S^2-knot is the minimal number of triple points for all possible diagrams of the 2-knot. It is known that a 2-knot has triple point number 0 if and only if it is a ribbon 2-knot, and that there is no 2-knot of triple point number 1, 2, nor 3. Recently Satoh proved that a 2-knot has triple point number 4 if and only if it is ribbon concordant to the 2-twist-spun trefoil knot. The following question is still open.

Problem 26.0.5 (Shin Satoh)**.** *For any integer $n > 4$, is there a minimal "finite" set S_n of 2-knots such that any 2-knot of triple point number n is ribbon concordant to some 2-knot belonging to S_n? In particular, does it hold $S_n = \emptyset$ if n is odd and $S_6 = \{$the 3-twist-spun trefoil knot$\}$?*

Two 2-knots K and J are n-concordant if there is a smooth concordance joining them such that the regular level sets consist of surfaces of genus at most n. All 2-knots are concordant [32], so any two are n-concordant for some n. Melvin proved that 0-concordant 2-knots have diffeomorphic Gluck twists and asked if every 2-knot is 0-slice, i.e. 0-concordant to the unknot. Recently Sunukjian [44], Dai-Miller [7], and Joseph [28] have shown the existence of infinitely many 0-concordance classes, but there are still many unanswered questions. As in the classical case, ribbon 2-knots are clearly 0-slice, but there are no known examples of nonribbon, 0-slice 2-knots. Joseph has shown that any 2-knot with nonprincipal Alexander ideal is not invertible in the 0-concordance monoid. There are no known examples of 2-knots which do have an inverse under 0-concordance, i.e. K and J which are not 0-slice but so that $K\#J$ is.

Problem 26.0.6 (Jason Joseph)**.** *Is every 0-slice 2-knot ribbon?*

Problem 26.0.7 (Joseph)**.** *Is any nontrivial 0-concordance class invertible?*

Problem 26.0.8 (Joseph)**.** *Are all 2-knots 1-concordant to the unknot?*

Problem 26.0.9 (Zsuzsanna Dancso)**.** *Is the conjectured set of Reidemeister moves for ribbon 2-knots (see for example [2] for a description) complete? Is the same true for ribbon 2-tangles and w-foams (see [3])?*

Problem 26.0.10 (Robin Gaudreau)**.** *Generalize the index of a crossing to the double curves of the projection of a knotted sphere in a 4-manifold.*

The index of a crossing in an oriented knot diagram on a surface is the signed intersection number of the curves obtained by smoothing the crossing with the orientation. Definitions for other knot theories, when applicable, follow from that one.

In the following, $M(K)$ is the closed orientable 4-manifold obtained by elementary surgery on a 2-knot K in S^4.

Problem 26.0.11 (Hillman)**.** *Let π be a (high-dimensional) knot group with commutator subgroup free of rank r ($\pi' \cong F(r)$). Then π has a presentation of deficiency 1. Is such a group $\pi \cong F(r) \rtimes \mathbb{Z}$ the group of a (fibred) ribbon 2-knot?*

See [23, Chapter 17.6] for more on 2-knots with groups of cohomological dimension 2.

Problem 26.0.12 (Hillman)**.** *Is there a 2-knot K such that $M(K)$ is an orbifold bundle over a flat 2-orbifold with general fibre an hyperbolic surface?*

See [24] for what little is known about constraints on such knots.

Problem 26.0.13 (Jonathan Hillman)**.** *Let $L = \sqcup L_i$ be a surface link in S^4, with regular neighbourhood $N(L) \cong L \times D^2$ and exterior $X(L) = \overline{S^4 \setminus N(L)}$. If $X(L)$ fibres over S^1 then $\chi(X(L) = 0$, and so*

$$\Sigma\chi(L_i) = \chi(N(L)) = \chi(N(L)) + \chi(X(L)) = \chi(S^4) = 2.$$

It is easy to find examples with one component a 2-sphere and the rest tori. Are there any fibred surface links with at least one hyperbolic component?

Problem 26.0.14 (Hillman: An old question of Hosokawa and Kawauchi [26])**.** *Is there a surface knot of genus ≥ 1 with aspherical exterior? More specifically, is there a knotted torus with exterior a compact finite volume $\mathbb{H}^4$-manifold?*

(With recent constructions of cusped hyperbolic 4-manifolds of small volume, this might have a chance.). Finally, the issue of the topological unknotting theorem for surfaces in S^4 should be revisited.

Problem 26.0.15 (Hillman)**.** *If $\pi_1(S^4 \setminus F) \cong \mathbb{Z}$, is F isotopic into the equator $S^3 \subset S^4$?*

Problems about knotted surfaces in other 4-manifolds

Problem 26.0.16 (Laura Starkston)**.** *Is every smooth 2-sphere in $\mathbb{CP}^2$ in the homology class $[\mathbb{CP}^1]$ or $2[\mathbb{CP}^1]$ isotopic to a symplectic 2-sphere?*

These are the only two homology classes in $\mathbb{CP}^2$ that can be represented by symplectic spheres (higher multiples are represented by symplectic surfaces of higher genus). Gromov proved using pseudoholomorphic curves that there is a unique symplectic isotopy class of symplectic 2-spheres in each of these two classes [22]. Therefore if any such smooth 2-sphere was isotopic to a symplectic one, there would be a unique smooth isotopy class of spheres in these homology classes. By contrast, for surfaces of higher genus in homology class $d[\mathbb{CP}^1]$ for d greater than or equal to 3, examples of Finashin [10] and (independently) Hee Jung Kim [29] show that there are smooth surfaces in $\mathbb{CP}^2$ such that the fundamental group of the complement is the same as that of a standard algebraic curve in the same homology class, but which are not isotopic to a standard algebraic curve.

Problem 26.0.17 (Starkston)**.** *Are there symplectic surfaces in $\mathbb{CP}^2$ which are not isotopic to complex curves? (This problem is open in both the smooth and singular cases.)*

The version for smooth surfaces is a long standing open question, and it has been proven that every symplectic surface homologous to $d[\mathbb{CP}^1]$ (degree d) for d less than or equal to 17 is isotopic to a complex curve. There are a few examples of singular symplectic surfaces which have a collection of singularity types which cannot be realized by a complex curve–(see Ruberman-Starkston [42] for line arrangement examples and Golla-Starkston [19] section 8 for an irreducible example), but there is no clear explanation for when exactly symplectic surfaces align with complex algebraic curves. A key direction which is currently lacking is constructive techniques–how can we build interestingly embedded examples of smooth or singular symplectic surfaces? Another direction on this problem is to change from surfaces in $\mathbb{CP}^2$ to more general 4-manifolds. There are examples of exotic isotopy classes of symplectic surfaces in the same homology class in some 4-manifolds, starting with examples of tori in elliptic surfaces by Fintushel and Stern [13]. However, looking at $S^2 \times S^2$ or $\mathbb{CP}^2$ blown-up once, one can find similar interesting open problems.

An outstanding problem for surface bundles over surfaces is the following:

Problem 26.0.18 (Inanc Baykur)**.** *Geography of surface bundles: For which pairs of integers (g, h) are there genus–g surface bundles over genus–h surfaces with positive signatures?*

A necessary condition is $g \geq 3$ and $h \geq 2$, and there are many examples going back to pioneering works of Kodaira, Atiyah, Hirzebruch, and Endo et al. Recent progress suggests there are only a few such pairs of (g, h) (at most two dozen) for which there may be no positive signature examples. This realization problem is harder for holomorphic surface bundles.

A much more advanced geography problem is:

Problem 26.0.19 (Baykur)**.** *Topography of surface bundles: How high can the signature of a genus–g surface bundle over a genus–h surface be?*

Increasingly sharper upper bounds have been provided by the works of Taubes, Kotschick and Hamenstädt. For $g, h > 1$, let $m = \frac{3\sigma}{\chi}$ be the slope of a surface bundle, where σ and χ are the signature and the Euler characteristic of the bundle. A more tractable variant of the above problem is:

Problem 26.0.20 (Baykur)**.** *Slopes of surface bundles: What is the highest slope $m = \frac{3\sigma}{\chi}$ for a surface bundle over a surface, with fiber and base genera greater than one?*

The highest known slope known to date is $2/3$, realized by holomorphic surface bundles constructed by Catanese-Solenske. Can one get to $m = 1$? (This is not possible for holomorphic surface-bundles.)

For two smooth surfaces R_1 and R_2 in a 4-manifold X, $fq(R_1, R_2)$ denote the Freedman-Quinn invariant of R_1 and R_2 [43].

Problem 26.0.21 (Maggie Miller)**.** *Construct a smooth 4-manifold X and positive-genus surfaces R_1 and R_2 smoothly embedded in X that are homotopic with $fq(R_1, R_2) = 0$ so that there exists a 2-sphere $G \subset X$ with trivial normal bundle which intersects R_1 transversely in one point but:*

(a) R_2 also intersects G transversely in one point yet R_1 and R_2 are not smoothly isotopic,

(b) R_1 and R_2 are not smoothly concordant.

Gabai's light bulb theorem [17] doesn't apply to most positive genus surfaces – one has to assume that the fundamental group of the surface includes trivially. But there is no known example where the theorem actually fails (although probably it does). Thus, this problem is asking for counterexamples to the light bulb theorem and concordance analogue when considering surfaces whose fundamental group includes non-trivially into the ambient manifold.

Problem 26.0.22 (Seungwon Kim)**.** *Adapt the approaches of Lee and others to find a new isotopy invariant of knotted surfaces in a closed orientable 4-manifold and in particular, an isotopy invariant of knotted surfaces in $\mathbb{CP}^2$.*

Lee and his collaborators developed ambient isotopy invariants of knotted surfaces in S^4 [30, 34, 35]; these invariants are analogues of the Kauffman bracket polynomial of knots in S^3. Hence, it is reasonable to ask whether similar invariants can be constructed for knotted surfaces in closed orientable 4-manifold.

Topological vs. Smooth problems

Problem 26.0.23 (Bob Gompf). *Are there unsmoothable 2-knots in S^4? Distinct smooth 2-knots that are topologically isotopic? Is smooth isotopy of 2-knots different from pairwise diffeomorphism?*

Such phenomena are well-known in other 4-manifolds. There are exotically embedded nonorientable surfaces in S^4 [9, 11, 12].

In the proper setting, up to ambient isotopy, there are uncountably many exotic planes $\mathbb{R}^2 \hookrightarrow \mathbb{R}^4$ that are smoothly, but not topologically, isotopic to the standard plane. (There are also embeddings that are smooth except at one point and are topologically standard, but not smoothable by a compactly supported isotopy. Smooth isotopy is the same as orientation-preserving pairwise diffeomorphism since $\mathbb{R}^n$ has no exotic self-diffeomorphisms.) There is an explicit movie description of an exotic plane (with time given by the radius function in $\mathbb{R}^4$), and uncountably many others obtained by suitable ramification. These all have the property that they can be modified, working outside an arbitrarily large ball in $\mathbb{R}^4$, to obtain a sphere (in fact, an unknotted sphere). There are uncountably many exotic planes for which such modification can only produce higher genus surfaces, but the known examples seem intractable to describe by movies, requiring infinitely many 2-handles. (Their construction involves taking the complement of an infinite intersection of reimbedded Casson towers.)

Problem 26.0.24 (Gompf). *Give an explicit description (movie) of an exotic plane that cannot be modified to a sphere outside every preassigned ball.*

Problem 26.0.25 (Gompf). *Are there combinatorial invariants that can distinguish exotic planes?*

Such invariants could not be determined by the underlying topology, e.g., the knot group. The known examples are distinguished by their double branched covers, which are potentially exotic smoothings of $\mathbb{R}^4$, or by the potentially exotic smoothings of $D^2 \times \mathbb{R}^2$ obtained by using the annulus at infinity to add boundary. Are double (or higher degree) branched covers of exotic planes always exotic?

The general theory of smooth proper 2-knots $\mathbb{R}^2 \hookrightarrow \mathbb{R}^4$ (or more general proper knotted surfaces) splits in two directions, namely studying exotic planes and working modulo exotic planes: Call two proper 2-knots equivalent if they become the same after pairwise end sum with suitable exotic planes. Every compact, orientable surface embedded in B^4 with nonempty boundary in ∂B^4 generates an infinite equivalence class (through passing to the interior and end summing with exotic planes). There is a forgetful map from equivalence classes to topological isotopy classes.

Problem 26.0.26 (Gompf). *Is this map a bijection?*

Presumably not, but nothing concrete appears to be known.

Problem 26.0.27 (Gompf). *Are any exotic planes in $\mathbb{C}^2$ holomorphic? Symplectic? Lagrangian?*

The movies mentioned above seem unlikely to yield symplectic surfaces, since they have many antiparallel sheets.

Problem 26.0.28 (Danny Ruberman). *Does every simply connected 4-manifold with $H_2 = \mathbb{Z}$ have a topological spine?*

This problem could be interpreted as in Ruberman's workshop talk – i.e. the spine is a tamely (locally PL) 2-sphere whose inclusion map is a homotopy equivalence). Or it could have no restriction at all – i.e. the sphere could be wildly embedded with no restrictions on local behavior.

Problem 26.0.29 (Dave Auckly). *All of the following problems concern the notion of stabilization.*

(a) *Does every pair of homeomorphic, smooth 4-manifolds become diffeomorphic after taking the connected sum with *one* copy of $S^2 \times S^2$?*

(b) *Do any homotopy class in the diffeomorphism group Diff(Z, D) that is trivial in Homeo(Z, D) become trivial after one stabilization?*

(c) *It is known that there are surfaces that require several internal stabilizations, i.e., $\#(S^4, T^2)$ to become equivalent. Are there examples of topologically isotopic surfaces with this property so that the complement of the surface is simply-connected?*

Spaces of diffeomorphisms and embeddings

Problem 26.0.30 (David Gabai). *Is $\mathit{Diff}_0(S^3 \times S^1)/\mathit{Diff}_0(B^4, \partial)$ non trivial?*

The conjectured answer is "yes." Budney and Gabai proved (during the conference) that

$$\mathrm{Diff}_0(B^3 \times S^1, \partial)/\mathrm{Diff}_0(B^4, \partial)$$

is non-trivial, but by construction, all of their maps are isotopically trivial when extended to $S^3 \times S^1$ [4].

Given a knot in S^3, if you include the knot into S^4, it becomes trivial. But there are two ways to trivialize the knot, and this question concerns whether or not those two trivialization (processes) are distinct, in a homotopy-sense. Let K_n be the space of smooth embeddings of $\mathbb{R}$ into $\mathbb{R}^n$ which agree with the map $x \mapsto (x, 0)$ outside of the interval $[-1, 1]$.

The inclusion $K_3 \to K_4$ is null homotopic. Here are two null homotopies of that inclusion map. In the first one, once the knot is included into K_4, you perturb it slightly so that it increases rapidly (in the 4th dimension) near the "start" of the interval $[-1, 1]$, and have the 4th coordinate decrease slowly along the interval $[-1, 1]$. Now there is a straight line homotopy in the $\mathbb{R}^3$ coordinates. When you remove the bump in the 4th dimension, that gives one null homotopy of the inclusion $K_3 \to K_4$. Repeat the same process, but using a bump function that increases along the interval $[-1, 1]$.

Combining the two maps together yields a map: $K_3 \to \Omega K_4$

Problem 26.0.31 (Ryan Budney). *Is the map $K_3 \to \Omega K_4$ null-homotopic?*

It is known to be trivial on rational homology, and rational homotopy groups. Budney believes this map is null-homotopic as well, and conjectures that there exists a non-trivial map $K_3 \to \Omega^2 K_4$ which is non-trivial on rational homology.

Problem 26.0.32 (Auckly). *Forthcoming work of Auckly and Ruberman implies that for some manifolds*

$$\mathrm{Ker}(\pi_n(\mathit{Diff}(Z)) \to \pi_n(\mathit{Homeo}(Z)))$$

has high rank summands, and for some manifolds $\pi_n(\mathit{Diff}(Z)) \to \pi_n(\mathit{Homeo}(Z))$ has a large cokernel.

(a) *Are there manifolds for which the kernel has an infinite rank summand? (Conjecturally, the answer is yes.)*

(b) *Is it non-trivial for every manifold? (This is difficult with current technology.)*

(c) *Is there one manifold for which all of these groups are non-trivial? For which all of these groups have an infinite rank summand?*

(d) *Is there a manifold so that the kernel and cokernel are both non-trivial? Both large? Both very large (e.g., contain infinite rank summands)?*

(e) *Is (d) be true for all 4-manifolds?*

(f) *What about the analogous questions for spaces of embeddings? (Results about a space of diffeomorphsims seems to yield results about spaces of embeddings for free.)*

Additional problems

Let G be a group, and S a set of generators for G. Given $\beta \in G$, an S-band decomposition of β is a product of the form

$$\beta = w_1 s_1^{\pm 1} w_1^{-1} \cdots w_p s_p^{\pm 1} w_p^{-1}$$

where each $s_j \in S$ and $w_j \in G$. The S-rank of β, denoted $\mathrm{rk}_S(\beta)$, is defined to be the smallest p for which such an S-band decomposition exists.

Problem 26.0.33 (Mark Hughes)**.** *Let B_n be the n-strand braid group, and $\Sigma = \{\sigma_1, \ldots, \sigma_{n-1}\}$ the Artin generators. Given a braid $\beta \in B_n$, is there a finite group H and a homomorphism $\phi : B_n \to H$ such that* $\mathrm{rk}_{\phi(\Sigma)}(\phi(\beta)) = \mathrm{rk}_\Sigma(\beta)$*? Is there a procedure for producing such a group H given β?*

Problem 26.0.34 (Hughes)**.** *A braid β is called quasipositive if it can be written as*

$$\beta = w_1 \sigma_{i_1} w_1^{-1} \cdots w_p \sigma_{i_p} w_p^{-1}$$

for some $i_j \in \{1, 2, \ldots, n-1\}$ and $w_j \in B_n$. Is there a algorithm to determine whether or not a braid is quasipositive?

Problem 26.0.35 (Hans Boden)**.** *Is the Tait flyping conjecture true for links in thickened surfaces and/or virtual links?*

Problem 26.0.36 (Boden)**.** *Do the Tait conjectures hold for welded links?*

The following is a sub-problem of the previous one:

Problem 26.0.37 (Boden)**.** *Does a reduced alternating diagram of a welded knot have minimal crossing number?*

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Chapter 27

Interactions between Brauer Groups, Derived Categories and Birational Geometry of Projective Varieties (19w5164)

November 10 - 15, 2019

Organizer(s): Nathan Grieve (Michigan State University), Collin Ingalls (Carleton University)

The workshop Interactions between Brauer Groups, Derived Categories and Birational Geometry of Projective Varieties (19w5164) took place at the Banff International Research Station (BIRS) during the time period November 10–15, 2019. It was an international event and was attend by 35 participants. A total of 19 individuals gave 50-60 minute lectures on topics which were of interest to the proposed subject areas.

Overview of the Field

The workshop 19w5164 focused on three important areas of scientific research within algebraic and arithmetic geometry. These topics include:

(1) Brauer groups;

(2) Derived Categories; and

(3) Birational geometry.

Some of the initial sources of motivation for these proposed topics included the work of Clemens and Griffiths, [15], that of Artin and Mumford, [4], and work of Mukai [30] and [31]. A main goal of the works [15] and [4] was to construct algebraic varieties which are unirational but not rational. Recall, also, that the techniques of [15] are Hodge theoretic in nature whereas those of [4] are algebraic; they are largely based on using the theory of maximal orders to construct conic bundles over rational surfaces.

Two key results from [15] and [4], respectively, are summarized in the following way.

Theorem ([15]). The intermediate Jacobian $(J(X), \Theta)$, for X a complex rational threefold, is a product of Jacobians of curves

$$(J(X), \Theta) \simeq \prod_i (J(C_i), \Theta_i).$$

Theorem ([4]). If X is a projective non-singular complex variety, then the torsion subgroup of the third integral cohomology group $H^3(X, \mathbb{Z})$ is a birational invariant. In particular, $H^3(X, \mathbb{Z})$ is torsion free when X is rational.

In terms of bounded derived categories of coherent sheaves on projective varieties, an important question is the extent to which they are classification invariants. For instance, for the case of Abelian varieties, the question of isomorphism invariance was addressed in work of Mukai [30] and [31]. In those works, in addition to establishing many other important results, the concept of Fourier-Mukai transform was systematically developed and applied.

Theorem ([31]). Let $\mathcal{P}$ be the Poincaré line bundle on $A \times \hat{A}$, for A an Abelian variety with dual Abelian variety $\hat{A}$. Then, the Fourier-Mukai transform

$$\Phi_{\mathcal{P}} \colon \mathrm{D}^b_{\mathrm{coh}}(A) \to \mathrm{D}^b_{\mathrm{coh}}(\hat{A})$$

is an equivalence of categories.

The above theorem of Mukai motivates the question as to the extent to which the bounded derived category of sheaves on a given non-singular projective variety determines the variety up to isomorphism. For non-singular projective varieties with ample canonical or anticanonical class, this question has been addressed by Bondal and Orlov [9]. Their main result can be stated as:

Theorem ([9]). Let X and Y be non-singular projective varieties with ample canonical or anticanonical class. If $\mathrm{D}^b_{\mathrm{coh}}(X)$ and $\mathrm{D}^b_{\mathrm{coh}}(Y)$ are equivalent, then X and Y are isomorphic.

The standard expository introductory treatment of derived categories and Fourier-Mukai transforms is the text by Huybrechts [25]. The theory of Fourier-Mukai transforms within the context of orbifold Deligne-Mumford stacks was pursued by Kawamata [26].

Another significant application of Fourier-Mukai transform techniques, building on [30] and [31], is through the theory of generic vanishing theory which was pioneered by Green and Lazarsfeld [19]. That theory has been a tool for studying irregular varieties. Within the context of Abelian varieties, the use of derived categories is a means for further developing the generic vanishing theory of Green and Lazarsfeld. In particular, the Generic Vanishing Theorem for Abelian varieties was emphasized by Hacon [21].

Theorem ([21]). Let $\mathcal{F}$ be a coherent sheaf on a complex Abelian variety A and let $\hat{A}$ be the dual abelian variety. Then every irreducible component of the cohomological support locus

$$V^i(A, \mathcal{F} \otimes P) := \left\{ P \in \hat{A} : h^i(A, \mathcal{F} \otimes P) \neq 0 \right\}$$

has codimension at least i.

This generic vanishing theory for Abelian varieties was refined and significantly developed further in a series of articles by Pareschi and Poppa [34], [35], [36]. In more recent times, there has been significant further developments which pertain to these topics. As one such example, we mention the recent work of Lombardi and Popa, [29], which builds on earlier work of Popa [37] and Popa-Schnell [38].

Continuing with questions in Hodge theory and their relevance to the topics of the workshop, note that, for instance, similar to the case of cubic threefolds which was considered in [15], a natural question is the extent to which cubic fourfolds in $\mathbb{P}^5$ are rational. A Hodge theoretic approach for producing examples of rational cubic fourfolds was given by Hassett [22].

The work [1] is motivated by rationality questions for cubic fourfolds and builds on work of Kuznetsov [27]. It proves a number of results in the direction of derived categories of cubic fourfolds. Another feature of [1] is that the authors use results from [10] to express some of their Fourier-Mukai calculations in terms of Hodge theory.

In a compatible direction, the works of Ballard-Favero-Katzarkov, including [7], and Ballard-et-al, [6], have a number of implications for the bounded derived categories of coherent sheaves on projective hypersurfaces, and cubic fourfolds in particular. For example, in [7], the authors combine their [7, Theorem 1.2] with results of Orlov [33] and Hochschild-Kostant-Rosenberg, [23], to reprove Griffiths' description of the primitive cohomology of a projective hypersurface [20]. Indeed, the following theorem is established in [7].

Theorem ([7]). Let Z be a non-singular, complete projective hypersurface defined by a homogeneous degree d polynomial

$$F \in \mathbf{C}[x_1, \ldots, x_n].$$

Then for all p, with $0 \leq p \leq n/2 - 1$, Orlov's theorem, [33], combined with the Hochschild-Kostant-Rosenberg isomorphism, induces an isomorphism

$$H^{p,n-2-p}_{\mathrm{prim}}(Z) \simeq \mathrm{Jac}(F)_{d(n-1-p)-n}.$$

In general, the theory of Fourier-Mukai functors and the concept of semiorthogonal decompositions for derived categories continue to be topics of significant interest. They have important connections to rationality questions and Brauer groups. Some recent works related to the scope of the workshop include [5] and [3]. In what follows, we describe in some detail these interconnections.

In [5], the authors use Clifford algebras and semiorthogonal decompositions for the derived category of quartic Del Pezzo fibrations to characterize the condition that a given generic degree four Del Pezzo fibration $X \to \mathbb{P}^1$ is rational. On the other hand, the theory of Fourier-Mukai functors has recently been used to study Jacobian elliptic fibrations [3]. In [3, Theorem 1.5], for example, certain twisted derived equivalences, which arise from such elliptic fibrations, are related to cyclic subgroups of quotients of Brauer groups.

Returning to extensions of the work of Artin-Mumford, [4], it is of continued interest to use tools from birational algebraic geometry to study ramfication in Brauer groups of function fields of algebraic varieties. The more recent developments should be seen as extensions to earlier work of Chan-Ingalls, [12], as well as Chan-Kulkarni [14]. As one more specific example, we mention the following form of the classical Castelnuovo's contraction theorem which was obtained in [12].

Theorem ([12]). Let S be a non-singular complex projective surface with function field $\mathbf{K}$. Let $\alpha \in \mathrm{Br}(\mathbf{K})$ be a Brauer class with ramification divisor Δ_α. Suppose that the ramification of α along irreducible curves in S is terminal. Then, with these assumptions, if E is an irreducible curve in S which has the two properties that: (i) $E^2 < 0$; and (ii) $(\mathrm{K}_S + \Delta_\alpha) \cdot E < 0$, then E is a (-1)-curve.

Finally, fixing an algebraically closed characteristic zero base field, by [8], [16], and [11], for instance, our basic understanding of the main theorems from higher dimensional birational geometry of projective varieties, especially those results which are the foundations of the minimal model program, has been clarified a good deal. Indeed, it is now understood that the main theorems of the minimal model program can be established as consequences of finite generation of adjoint rings.

Theorem ([16]). Let X be a non-singular complex projective variety and A an ample $\mathbb{Q}$-divisor on X. Let Δ_i be a $\mathbb{Q}$-divisor on X such that $\lfloor \Delta_i \rfloor = 0$, for $i = 1, \ldots, r$, and such that the divisor $\Delta_1 + \cdots + \Delta_r$ has simple normal crossings support. Then the adjoint ring

$$R(X; K_X + \Delta_1 + A, \dots, K_X + \Delta_r + A)$$

is finitely generated.

By contrast, the abundance conjecture remains an extremely important open question.

The numerical abundance conjecture ([32]). If (X, Δ) is a complex projective klt $\mathbb{Q}$-Gorenstein pair, then the numerical and the Iitaka dimension of the log canonical divisor $K_X + \Delta$ coincide.

These concepts, tools and more recent developments, within the area of birational geometry, are foundational to the main topics and themes of the workshop. Indeed, as is apparent in all of the sections that follow, each of the workshop's lectures intersected on these themes in some form or another.

Recent Developments and Open Problems

The workshop identified the continued importance of three main research directions (see Section 27). While many of these topics have close ties to the specific subject areas of the workshop, some have important more tangential overlap. We refer to the workshop's lectures themselves for motivation, background and statements of many of these recent developments and open problems. We summarize these lectures in Section 27.

In this section, we content ourselves with motivating and stating some more specific problems from three more broad areas which we feel are especially important to the specific aims of the workshop. In more precise terms, we feel that the workshop identifies the following three topics as especially important to follow-up in more specific further details. We then include a discussion and justification for future research on these topics. These three themes include:

(1) Topological, arithmetic and Hodge theoretic aspects of derived equivalences for projective varieties;

(2) Variations of geometric invariant theory and higher dimensional birational geometry; and

(3) Effective and explicit methods for Brauer groups, ramification and related objects.

Indeed, the above three interrelated topics closely reflect the three main subject areas of the workshop. In terms of point (1), about a third of the workshop's lectures directly dealt with the subject of derived categories. Specifically, they focused on topics such as: (i) orthogonal decompositions for twists of varieties over non-algebraically closed fields; (ii) the extent to which rational points may be considered as derived category invariants; and (iii) Hodge theoretic topological aspects of derived equivalence.

One reoccurring theme throughout the workshop was the classical problem about derived invariance of Hodge numbers. While several of the workshop's lectures reported upon the recent progress which has been made towards a complete understanding of this problem, they also indicated that continued research on that topic remains to be of interest. This is evidenced, for instance, by the lectures which were given by Lieblich, Bragg, Frei, McFaddin, Duncan, Gulbrandsen, Lombardi and Doran.

We state the problem of derived invariance of Hodge numbers in more precise terms below. For the case of (non-singular complex projective) threefolds, for example, an affirmative answer to the problem about derived invariance of Hodge numbers is known by work of Popa and Schnell [38].

Problem (Derived invariance of Hodge numbers). Suppose that X and Y are non-singular complex projective varieties with equivalent bounded derived categories of coherent sheaves

$$\mathrm{D}^b_{\mathrm{coh}}(X) \simeq \mathrm{D}^b_{\mathrm{coh}}(Y).$$

Then, within this context, does it follow that X and Y have equal Hodge numbers

$$h^{p,q}(X) = h^{p,q}(Y)$$

for all p and q?

The above mentioned problem about derived invariance of Hodge numbers, motivates the more general problem as to the extent to which derived equivalences between non-singular projective varieties can be seen as classification invariants. Again, this topic was a recurring theme throughout the workshop. The following problem was stated during the lecture by Lieblich. It has since been discussed, in more detail, in the recent arXiv preprint [28].

Problem (M. Lieblich and M. Olsson). Let X and Y be non-singular complex projective varieties. If there exists a filtered equivalence

$$\Phi\colon \mathrm{D}(X) \xrightarrow{\sim} \mathrm{D}(Y),$$

between derived categories of perfect complexes, then are X and Y birationally equivalent?

Turing to arithmetic questions, another topic of interest was the extent to which fields of definition enter into the picture in terms of questions about derived equivalences between pairs of projective varieties. As one example, the following problem of Addington-et-al arose during the lecture of Frei.

Problem (Addington-et-al). Suppose that X and Y are derived equivalent non-singular projective varieties over a number field $\mathbf{k}$. Then under what additional hypothesis (if any) does it hold true that X and Y simultaneously contain $\mathbf{k}$-rational points?

In terms of fields of definitions and existence of full exceptional collections over a given base field, the following conjecture of Orlov was emphasized during the lecture of McFaddin.

Conjecture (Orlov). Let X be a non-singular projective variety with field of definition a number field $\mathbf{k}$. If X admits a full exceptional collection which is defined over the base number field $\mathbf{k}$, then X is in fact rational.

From the view point of item (2), it is now understood that the logical link between the three topics of the workshop is achieved through the question of birational classification for higher dimensional algebraic varieties. An important role is also played through concepts which have origins in Mumford's Geometric Invariant Theory. As some entry points to these extremely important topics, we mention work of Dolgachev and Hu [17], Hu and Keel [24] and Reid [39].

Returning to the subject of bounded derived categories of coherent sheaves on projective varieties, the manner in which they relate to the concept of Variation of Geometric Invariant Theory Quotients (VGIT) has been studied in detail by Ballard-Favero-Katzarkov, [7], and their school. On the other hand, much can still be done to clarify and pin-down, in more precise terms, the exact manner in which VGIT is reflected in the overall context of birational classification.

The workshop's lecture by Lesieutre, about numerical dimension, emphasized the continued importance for the study of measures of positivity, growth and singularities within the overall context of algebraic geometry. The workshop touched on topics that have motivation from concepts in string theory and mathematical physics. For instance, the subject of homological mirror symmetry and its relation to the concept Landau-Ginzberg models was emphasized in talks of Katzarkov, Doran, Favero and Ballard.

As one more recent development, here we state a conjecture of Doran-Harder-Thompson which was emphasized in the lecture of Doran. It is discussed in more detail in the arXiv preprint [18].

Conjecture (Doran-Harder-Thompson). Let X be a Calabi-Yau variety which arises as a non-singular fiber of some Tyurin degeneration $\mathcal{V} \to \Delta$. Let X_1 and X_2 be quasi-Fano varieties which meet normally with common intersection a non-singular Calabi-Yau divisor X_0. Then the corresponding Landau-Ginzberg models $W_i\colon X_i^\vee \to$

$\mathbb{C}$ of the pairs (X_i, X_0), for $i = 1, 2$, glue together to give a fibration $W\colon X^\vee \to \mathbb{P}^1$. Finally, the compact fibers of the Landau-Ginzburg models consist of Calabi-Yau manifolds which are mirror to the common anti-canonical divisor X_0.

Finally, in the direction of point (3), we mention that several of the workshop's lectures highlighted the need for effective and explicit methods for the study of Brauer groups, ramification and related objects. This is evidenced, for example, in the lectures which were given by Diaz, Dhillon, Gille, Grieve, Lewis, Parimala and Scully.

As one classical representative example, which was highlighted in the lecture by Parimala, the classical Milnor Conjecture, which is now a theorem of Voevodsky, continues to provide impetus for more recent developments which pertain to ramification and other invariants which may be associated to quadratic forms and Brauer groups. For the sake of completeness, we state this conjecture (theorem of Voevodsky) below.

The Milnor Conjecture (Theorem of Voevodsky). Let $\mathbf{k}$ be a field with characteristic not equal to 2. Let $W(\mathbf{k})$ be the Witt ring of equivalence classes of quadratic forms and $I(\mathbf{k}) \subset W(\mathbf{k})$ the ideal of even dimensional forms. Put $I^n(\mathbf{k}) = I(\mathbf{k})^n$. Recall, that the ideal $I^n(\mathbf{k})$ is additively generated by the n-fold Pfister forms $\langle\langle a_1, \ldots, a_n\rangle\rangle := \langle 1, -a_1\rangle \otimes \cdots \otimes \langle 1, -a_n\rangle$, for $a_i \in \mathbf{k}^\times$. Then, with these notations and conventions, the map

$$e_n(\langle\langle a_1, \ldots, a_n\rangle\rangle) := (a_1) \cdot \ldots \cdot (a_n)$$

extends to give a homomorphism

$$e_n\colon I^n(\mathbf{k}) \to H^n(\mathbf{k}, \mathbb{Z}/2\mathbb{Z}).$$

This morphism is onto and has kernel equal to $I^{n+1}(\mathbf{k})$.

As a more recent conjecture, which pertains to ramification and Brauer groups, we state a form of the Period-index conjecture (following [2]).

The Perod-index conjecture. Suppose that $\mathbf{k}$ is either an algebraically closed, a C_1, or a p-adic field and set $e = 0, 1, 2$ accordingly. Let $\mathbf{K}$ be a field of transcendence degree n over $\mathbf{k}$. Then, for all $\alpha \in \operatorname{Br}(\mathbf{K})$, it holds true that

$$\operatorname{ind}(\alpha) \,|\, \operatorname{per}(\alpha)^{n-1+e}.$$

As another more specific representative problem, we mention a question which has origins in the work of Artin and Mumford [4]. It complements earlier related work of Chan and Kulkarni [13]. Its specific relation to the topics of the workshop was emphasized in the lecture of Grieve. Briefly, it asks to characterize, and distinguish between, the concepts of Brauer and orbifold birational logarithmic pairs.

Problem (Compare with [13]). Let S be a non-singular projective surface and (S, Δ) an orbifold pair

$$\Delta = \sum_i (1 - 1/m_i) C_i,$$

for m_i positive integers and C_i irreducible nonsingular curves in S. Suppose that Δ has simple normal crossings support. Let $\mathbf{K} = \mathbf{k}(S)$ be the function field of S, for $\mathbf{k}$ an algebraically closed characteristic zero field. Give necessary and sufficient conditions for the boundary orbifold divisor Δ to have shape

$$\Delta = \mathbb{D}(\alpha)_S = \Delta_\alpha$$

for $\mathbb{D}(\alpha)_S$ the trace of the ramification birational divisor $\mathbb{D}(\alpha)$ which is determined by α an element of $\operatorname{Br}(\mathbf{K})$, the Brauer group of $\mathbf{K}$.

One other topic which pertains to item (3) concerns the manner in which unramified cohomology groups can be used to verify or disprove the conclusion of the integral Hodge conjecture. For more precise statements, let X

be a non-singular complex projective variety. The conclusion of the integral Hodge conjecture asserts that every class $\alpha \in H^{p,p}(X, \mathbb{Z})$ is algebraic. Recall, that when $p = 0$ or $p = \dim(X)$, the conclusion is indeed trivially true, while the case that $p = 1$ follows from the celebrated Lefschetz $(1, 1)$-theorem.

On the other hand, for other values of p, the conclusion of the integral Hodge conjecture is known not to hold true in general. Of particular interest, is the case that $n = \dim(X) = 3$ and $p = 2$. Within that context, various results (both positive and negative) are known. In general, the following problem remains open and of interest.

Problem (The integral Hodge conjecture). Let X be a non-singular complex projective threefold. Then, under what hypothesis is it true that every class $\alpha \in H^{2,2}(X, \mathbb{Z})$ is algebraic?

Presentation Highlights

In this section, we describe some aspects of the workshop's lectures themselves and place some emphasis on their especially important aspects. First of all, about 3-4 weeks prior to the workshop, the organizers sent invitations to selected participants asking if they would be interested in giving a talk at the workshop. This method of solicitation and selection of talks was effective. Indeed, as is evidenced in what follows, all of the talks had either direct relevance to the main themes of the workshop or important interconnections.

The workshop's lectures made for an attractive, exciting and fresh viewpoint to the topics of the proposed workshop. In the selection of talks, the organizers were also able to achieve a good balance between the overall demographics both in terms of the subject of the lectures as well as in terms of the speakers themselves. Indeed, the speaker list itself includes a good blend of junior and senior participants.

The full list of invited speakers and the title of their talks is summarized below. The abstracts and video recordings of the lectures are available on the workshop's webpage
`http://www.birs.ca/events/2019/5-day-workshops/19w5164`.

(1) Ludmil Katzarkov: D modules and Rationality

L. Katzarkov's talk was a great start to the workshop. In only fifty minutes he was able to give context and motivation for much of the rest of the workshop. The topics which he discussed were wide ranging and included many examples. For instance, he motivated the subject of homological mirror symmetry and its relation to the Landsberg-Ginzberg model through an introductory question about the birational geometry of the projective plane. In doing so, he touched on the subject of toric varieties, the Monge Ampère Equation and the subject of Gromov-Witten Invariants, within the context of Hodge theory, rationality questions and orthogonal decompositions. Finally, he was able to achieve the main aim of his talk which was to propose a new approach to nonrationality questions.

(2) Ajneet Dhillon: Essential dimension of stacks of bundles

A. Dhillon gave a nice survey of the concept of essential dimension for gerbes. He motivated the discussion with examples and explained some of the most important numerical invariants that one can associate to a central simple algebra—the period and the index. Before explaining his recent joint work with I. Biswas and N. Hoffmann, he described a related conjecture of J.-L. Colliot-Thélène, N. Karpenko and A. Merkurjev which relates the essential dimension of a gerbe to its period. He also explained related work of P. Brosnan, Z. Reichstein and A. Vistoli.

(3) Max Lieblich: Torelli theorems for derived categories

M. Lieblich reported on joint work with M. Olsson. A main question was to detect birationally at the level of derived categories through the concept of a filtered derived equivalence. The idea is that these tools will allow for a suitable formulation, within the context of derived categories of projective varieties, of analogues to the more traditional Torelli-type theorems which arise via Hodge theory. Before explaining some of the more technical details to this project, including the concept of filtered derived equivalence and the use of Hochshild cohomology, he first surveyed some more classical results which were of direct interest to the subject of the workshop. These topics included the classical statement of the Torelli theorem combined with the works of Mukai, Bondal-Orlov and Kawamata.

(4) Daniel Bragg: Derived invariants of varieties in positive characteristic

Through the partnership between MSRI and BIRS, we were able to obtain travel funding to host D. Bragg who is currently a postdoctoral fellow at the University of California Berkeley. He is a former Ph.D. student of M. Lieblich. He reported on joint work with N. Addington and B. Antieau which pertained to the question of the extent to which Hodge numbers of projective varieties over fields of positive characteristic can be detected at the level of the derived category. In particular, they construct an example of derived equivalent threefolds, which are defined over a characteristic three field, which have different Hodge numbers. In disseminating these results, he explained some important techniques for working with differential forms in positive characteristic; for example the use of de Rham and crystalline cohomology theories, Dieudonné modules, and the theory of the de Rham Witt complexes.

(5) Sarah Frei: Rational points and derived equivalence

S. Frei is currently a postdoctoral fellow at Rice University and is a former Ph.D. student of N. Addington. We were able to provide her with travel funding through the BIRS-MSRI travel funding program. Frei's talk centred around arithmetic questions for derived categories. A main goal was to describe her joint work with N. Addington, B. Antieau and K. Horing which, among other things, gives examples which show that the concept of rational point for varieties over non-algebraically closed fields, cannot, in general, be considered as derived category invariants. This principal is illustrated by two kinds of examples. One is given by a certain torsor over a certain given Abelian variety; the other is given by a pair that consists of certain hyperkähler fourfolds. She aimed her talk at a wide audience. In doing so, she surveyed a number of topics and examples about the nature of derived invariants for varieties over non-algebraically closed fields.

(6) Charles Doran: Gluing Periods for DHT Mirrors

C. Doran reported on very recent joint work with F. You and J. Kostink. At the same time he explained the DHT mirror symmetry conjecture, which he made jointly with A. Harder and A. Thompson. As some of the background and motivation for these topics had already been given earlier in the week, for example in the talk by Katzarkov, Doran was able to proceed immediately with an explanation of these more recent developments. In doing so, he gave a detailed explanation of the Tyurin degenerations for Calbai-Yau manifolds and related topics. The idea is that if a Calabi-Yau manifold X admits a Tyurin degeneration to the union of two quasi-Fano varieties X_1 and X_2 intersecting along a smooth anticanonical divisor D, then the Landau-Ginzburg mirrors of (X_1, D) and (X_2, D) can be glued together to obtain the mirror variety of X. The main focus of the talk was to discuss the manner in which the periods of (X_1, D) and (X_2, D) related to the mirror of X. Moreover, it was explained how these techniques allow for a classification and construction of certain mirror polarized K3-surfaces and fibered Calabi-Yau threefolds.

(7) Humberto Diaz: Unramified cohomology and the integral Hodge conjecture

H. Diaz described his recent result which establishes existence of a new type of example which violates the integral Hodge conjecture. In more precise terms, after surveying some earlier related work of J. L. Colliot-Thélène and C. Voisin, he showed how one can construct complex Kummer threefolds, defined over number fields, which possess non-algebraic non-torsion $(2, 2)$-cohomology classes. These results were of interest to many of the workshop's more senior participants.

(8) Stephen Scully: On an extension of the separation theorem for quadratic forms over fields

S. Scully's talk dealt with the concept of Witt index for p, q-antistropic nondegenerate quadratic forms. First he gave some general motivation from the theory of quadratic forms. This included, for example, the question of the extent to which an anisotropic quadratic form remains isotropic after extension to the function field of a quadric. He then discussed how one is able to determine constraints on the Witt index, as a function of discrete invariants which were determined by p and q, which give insight to this interesting problem. Finally, he stated and proved some of his own more recent results on this topic after having first provided additional context via earlier related results by D. Hoffman.

(9) Patrick McFaddin: Twisted forms of toric varieties, their derived categories, and their rationality

P. McFaddin discussed his joint work with M. Ballard, A. Duncan and A. Lamarche which deals with the concept of twisted forms for toric varieties and the question of the extent to which existence of full-exceptional collections, in the derived category, can be used to deduce rationality properties. As some motivation for his joint work, he surveyed topics that surround a conjecture of Orlov. The idea is that if a variety admits a full exceptional collection over the base ground field, then it should be rational.

(10) Matthew Ballard: From flips to functors

M. Ballard reported on joint work, with a number of individuals including some of his graduate students. To begin with, he gave context and motivation by explaining a conjecture of Bondal and Orlov. The conjecture asserts that flops of smooth projective varieties should induce an equivalence of derived categories. The he sketched a construction as to how one may construct an integral Fourier-Mukai kernel, essentially starting from a flip of normal projective varieties. In doing so, he explained aspects of his joint work with Diemer and Favero. Later in the week, during his talk, D. Favero developed these themes further.

(11) Raman Parimala: Quadratic forms and Brauer groups

R. Parimala's talk encompassed many topics that surround the question of obtaining uniform bounds for splittings of elements in Brauer groups with some emphasis on quadratic forms. One theme was the manner in which quadratic forms and Clifford algebras may be used as a tool for studying the Brauer group. Of particular interest was the question of period index bounds for the Brauer group, of a given field, and the u-invariant. She also discussed the period index problem within the context of the recent work of B. Antieau-et-al which contains period index results for surfaces over p-adic fields. Finally, she reported on her more recent joint results which are in the direction of local global principles for existence of points for certain hyperelliptic curves with genus at least equal to two.

(12) John Lesieutre: Numerical dimension revisited

J. Lesieutre's lecture had subject the concept of numerical dimension for $\mathbb{R}$-Cartier divisors on nonsingular projective varieties. After giving a self-contained introduction to this subject, he explained his recent example which shows that, in general, the numerical and Iitaka dimensions for $\mathbb{R}$-Cartier divisors need not hold in general. Finally, this example was illustrated via a computer animation which was worked out in conjunction with his undergraduate research students.

(13) Alexander Duncan: Indistinguishability and simple algebras

A. Duncan reported on his joint work with M. Ballard, A., Lamarche and P. McFaddin, which has subject étale forms for projective varieties over non-algebraically closed fields. There are analogous questions for separable algebras. Some more technical aspects for establishing these results include several constructions that surround certain kinds of coflasque resolutions for linear algebraic groups. Explaining these more technical details was of interest and occupied a good deal of the talk.

(14) James Lewis: Indecomposable K_1 classes on a Surface and Membrane Integrals

J. Lewis surveyed many topics that surrounded algebraic cycles and mixed Hodge structures. For instance, he first motivated and outlined the construction of the transcendental regulator map before stating the conjecture about this map which is due to Bloch and Griffiths. He then discussed topics that deal with his more recent joint results which aim to shed light on the Milnor-Beilinson-Hodge conjecture. Finally, he explained why the concept of membrane integrals should allow for a tool for detecting indecomposable classes in the first Milnor K-group of a given projective algebraic surface.

(15) Martin Gulbrandsen: Donaldson-Thomas theory for abelian threefolds

M. Gulbrandsen lectured about Donaldson Thomas invariants for Calabi-Yau and abelian threefolds. He first discussed the key concepts and related results, for example illustrating how these invariants provide virtual counts for the number of stable sheaves with given fixed numerical invariants. Then he focused on the case of Abelian threefolds with some emphasis on the interpretation in terms of derived categories. One idea was to illustrate the difference between the Calabi-Yau and the threefold case in general. Finally, he reported on results which are contained in his joints work with R. Moschetti including related results by Oberdieck-Shen and Oberdieck-Piyaratue-Toda.

(16) Nathan Grieve: Birational divisors and consequences for noncommutative algebra and arithmetic

The concept of birational divisor arises in different contexts; for example in work of V. V. Shokurov and, independently, P. Vojta. This lecture by N. Grieve reported on related recent developments. The main emphasis was to motivate and explain his joint work (with C. Ingalls) which deals with log pairs which are determined by ramification of classes in Brauer groups of function fields of algebraic varieties. A key point was to explain how to define and study a birationally invariant concept of Iitaka-Kodaira dimension. The other idea was to determine the nature of this invariant for suitable embeddings of division algebras. He was also able to briefly mention how the concept of birational divisor arises in his recent works which deal with complexity and distribution of rational points in projective varieties. Those results build on earlier work of M. Ru and P. Vojta (among others).

(17) David Favero: VGIT for CDGAs

D. Favero reported on his joint more recent works including those with M. Ballard and L. Katzarkov. Particular attention was given to the subject of Variation of Geometric Invariant Theory quotients within the context of differential graded algebras. He also motivated the topic of variation of geometric invariant theory quotients from the point of view of M. Reid as well as subsequent work by Dolgachev-Hu which built on earlier work of M. Thaddeus. Some other topics of interest were the many more recent results about orthogonal decompositions for Derived Categories of Moduli Spaces and Deligne Mumford stacks. More specifically, Favero explained related results of Kawamata, Orlov, Baytrev-Borisov including his joint work with Kelly and Doran. He also reported on a recent joint project with N. K. Chidambaram, whose is currently a graduate student at the University of Alberta . Finally, Favero followed-up, in some more detail, topics which were discussed earlier in the week by Ballard.

(18) Luigi Lombardi: Fibrations of algebraic varieties and derived equivalence

The purpose of L. Lombardi's lecture was to report on recent results that deal with special classes of fibrations, onto normal projective varieties, which admit a finite morphism to an abelian variety. Of particular interest is their behaviour under derived equivalence. One of his more specific aims was to explain applications of his earlier joint work with M. Popa. That work had subject the topic of derived invariance for the non-vanishing loci (attached to the canonical bundle) and the generic vanishing theory. For example, he explained how that work can be used to understand the manner in which derived equivalences for such fibrations can be used to understand isomorphism classes of fibrations onto smooth projective curves with genus at least equal to two. Finally, he explained how the conjectural derived invariance of Hodge numbers relates to the question of derived invariance for fibrations onto higher dimensional bases.

(19) Stefan Gille: A splitting principle for cohomological invariants of reflection groups

S. Gille's talk was an inspiring conclusion to the workshop. He spoke about various cohomological invariants that can be associated to Milnor K-groups and questions about ramification. The topics which he discussed complemented a number of lectures which took place earlier in the week including the lecture by Lewis. To begin with, he surveyed various background results with some emphasis on the treatment which was given in J.P. Serre's UCLA lectures. This allowed him to report on his joint work with C. Hirsch in some detail. Briefly, those results deal with generalizations of more classical splitting principals, for cohomological invariants of Weyl groups, so as to apply to the case of orthogonal reflection groups.

Scientific Progress Made

At the conclusion of the workshop, the organizers reached out to the workshop's participants to inquire about scientific research related activities and progress that may been seen as outputs to the workshop itself. Several participants mentioned to us that the blend of the three diverse yet overlapping topics of the workshop allowed for solid progress in terms of developing their interactions further. We received several enthusiastic responses some of which we describe here.

As one representative example, M. Ballard made mention of the fact that the subject mater of the workshop was diverse yet cohesive. He also said he enjoyed several discussions about these varying intersecting topics, which include, for instance, derived categories, birational geometry, noncommutative algebra and arithmetic. He also made mention of the fact that the workshop contained a sufficient amount of common core interests that enabled these interactions to be meaningful and productive.

While not all invited participants were able to attend, we have received evidence that the workshop has still been at least a tangential benefit to those individuals. For example, shortly after the conclusion of the workshop, we have been informed from such individuals that they have benefited from the reading of the workshop's abstracts and watching of the recorded lectures themselves.

As some further evidence of the workshop's immediate impact, A. Dhillon made explicit mention that the workshop lectures and discussions have inspired a collection possible future research projects. He was also able to meet new researchers and made some offers of invitations for seminar lecturers for seminars at his home institution.

The concept of numerical dimension was the main focus of the lecture by J. Lesieutre; it also arose in passing during the lecture of N. Grieve. At the conclusion of the workshop, we learned from T. Eckl that these lectures inspired a possible joint project between himself and Lesieutre.

Finally, at the conclusion of the workshop, J. Lewis wrote to say that he was very excited about having had participated and that the interdisciplinary aspect of this workshop provided stimulus for interaction among colleagues within the fields of algebraic geometry, algebra and K-theory. He also mentioned that the workshop assisted in his recruitment of two more junior participants for the thematic research semester which he is organizing at the Newton Institute during the 2020 Spring Semester.

Outcome of the Meeting

The workshop 19w5164 facilitated research collaborations amongst researchers with expertise in Brauer groups, derived categories, birational geometry and nearby areas. It was a success and will have a lasting impact on the participants and the mathematical community at large. In short, the overall broader impacts of this event will be felt by researchers near to its theme for several years to come.

The organizers made efforts to ensure participation by qualified Canadian and internationally based individuals, woman, junior researchers and other visible minorities. This is evidenced directly in the workshop's participant list. This success in attracting qualified personnel was made possible by a handful of factors. For example, the workshop dates were compatible with the fall reading break at the University of Alberta. This facilitated attendance by more junior participants (including graduate students).

The fact that the workshop was held in Banff was a contributing factor for the attraction of participants. Indeed, the workshop hosted a good collection of international participants (including researchers who are based in the United States, Norway, the United Kingdom, Italy and Germany). Many of these individuals indicated directly to us that the workshops of this kind, held in Banff, are attractive for them to participate in.

It remains challenging to ensure adequate travel funding for more junior participants. To facilitate this cause, prior to the workshop, the organizers reached out to selected junior participants at MSRI member US based institutions. In doing so, the workshop was able to take advantage of the MSRI-BIRS travel funding program. Via this program, two US based postdoctoral fellows received travel funding (S. Frei and D. Bragg).

When making the workshop schedule, the organizers made an effort to allow for informal interaction time amongst participants. Similarly, when formulating the participant and speaker list, some care was taken to ensure a good blend of junior, emerging and senior researchers. There was time for discussion before and after the talks. The first day of the workshop coincided with the Remembrance Day regional holiday and a minute of silence was observed by participants midway through one of the scheduled lectures.

The workshop's more senior participants played an important role in facilitating these interactions. They participated directly in the lectures and discussed research related topics during the other scheduled and unscheduled portions of the workshop. As one final indication of broader impacts, we mention that already within the 6-8 weeks following the workshop, a handful of the workshop's participants have posted to the arXiv preprint server works which intersect with their contributions to the workshop.

Participants

Ballard, Matthew (University of South Carolina)
Belmans, Pieter (University of Luxembourg)
Bragg, Daniel (University of California Berkeley)
Chidambaram, Nitin Kumar (Max Planck Institute for Mathematics)
Chinen, Minako (University of Alberta)
Dhillon, Ajneet (University of Western Ontario)
Diaz, Humberto (Washington University St Louis)
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Chapter 28

Dimers, Ising models and their interactions (19w5062)

November 17 - 19, 2019

Organizer(s): Hugo Duminil–Copin (Institut des Hautes Etudes Scientifiques), Julien Dubédat (Columbia University), Gourab Ray (University of Victoria)

Overview of the Field

Problems arising from statistical physics constituted one of the core research areas in probability theory over the past few decades. It was predicted by physicists a long time ago that in two dimensions, such models possess a particularly rich structure with large scale conformal symmetries. In recent years we have witnessed the resolution of several longstanding conjectures in this area, perhaps the most important ones being a proof of convergence of percolation and Ising interfaces to Schramm's SLE curves by Smirnov and that of Loop-erased Random Walks and Uniform Spanning Trees by Lawler, Schramm and Werner. Frequently, the new probabilistic tools seem to provide a completely fresh approach to even known theorems in this area, which shed new light to problems previously perceived intractable. It seems that most new ideas in this area stem from combining tools arising in combinatorics, algebra and complex analysis with exciting modern developments in probability theory. Therefore, exchange of ideas by bringing together mathematicians with expertise in these various facets of the subject should be very exciting and productive.

The focus of this workshop was on two particularly popular models: the dimer model, which is a model of perfect matching on graphs and lattice spin models, with a particular focus on the Ising model and the random cluster model.

Recent Developments and Open Problems

The dimer model has been a popular one particularly because of the integrable nature of the model for planar graph, which beautifully combines together analysis, combinatorics and algebra [**?**]. In particular, a lot of progress has been possible in the last few decades spearheaded by the work of Kenyon where he analyzed the dimer model fluctuations on lattices exhibiting some strict microscopic symmetry [**?**]. A plethora of work has been done since then analysing the fine details of the model in various setups [**?**, **?**, **?**, **?**, **?**]. A part of the workshop involved talks reporting recent progress on some of these questions, see for example the talks highlighted in Sections 28, 28, 28, 28, 28 and 28. There has been recent interest in establishing universality for the dimer model fluctuations in general planar graphs, and also for certain simple non-planar setting, for example on a Riemann surface (see Section 28). However, one big highlight of the workshop was the combination of talks by Ramassamy (Section 28), Laslier and Chelkak (Section 28) where they outlined a program to attack this problem using certain special embeddings called s-embeddings. This approach promises far-reaching conclusions and sparked a lot of interest and excitement in the community.

The other topic of interest in this workshop was various spin models on lattices, in particular the Ising model. As is known, there are various height models which do not exhibit strong integrability properties like the dimer model; the six vertex model being the most notable example. Michael Aizenman (Section 28) talked about quantum spin models and how it is related to something called the dimerization phenomenon. Various other talks were on topics related to the six-vertex model (Sections 28, 28, 28, 28, 28, 28, 28). Some of these talks expanded on the connection of these models with the Ising model and the more general Ashkin–Teller model.

We now outline some of the open problems which arose from the workshop.

Benjamin Young

Consider a finite bipartite graph G, with boundary vertices colored cyclically in red, then green, then blue. Consider double-dimer configurations such that the boundary vertices are endpoints of double-dimer paths, and such that the connection of boundary vertices is "tripartite" (there is only one such connection pattern). Let Z be the partition function of such configurations. Let a, b, c, d be boundary vertices that are pairwise connected in the connection pattern, and for any $I \subset \{a, b, c, d\}$ let Z_I be the partition function obtained by removing the boundary vertices in I. Then it has been proved by Jenne that:

$$ZZ_{abcd} = Z_{ab}Z_{cd} + Z_{ad}Z_{bc}.$$

This identity has interpretations in cluster algebras. Can one find a probabilistic application?

Scott Sheffield

Sheffield discussed two open problems.

- Are there some "nearly planar" maps for which dimer models can be analyzed (showing convergence of suitably defined height functions to the GFF, understanding double dimer paths, etc.)?
- Can one understand the different ways that weighting by a dimer partition function can change the law of the scaling limit of a random planar map model?

Richard Kenyon

For $n \geq 2$, let $\Delta_n = \{x_1, \dots, x_n \geq 0 \mid x_1 + \dots + x_n = 1\}$. Then one has

$$\int_{\Delta_n} \frac{(x_1 \dots x_n)^{n-2}}{(x_1 \dots x_{n-1} + \dots + x_2 \dots x_n)^n} \text{dvol} = \frac{1}{(n-1)!}.$$

There is a convoluted way of proving this, related to counting of acyclic orientations of a line. Does one have a more straightforward way of computing this integral?

Nathanaël Berestycki

In several settings, it is known that the dimer model's height function converges to a GFF. For a discrete GFF h_N in some domain, it is known that the maximum is of order

$$c \log N + c' \log \log N + \xi$$

where ξ is some random variable. Can one get even the first term for the maximum of the dimer model's height function?

Nishant Chandgotia

Consider a model for which there exists two locally uniform ergodic Gibbs measures μ_1, μ_2, whose entropy satisfy $h(\mu_1) < h(\mu_2)$. Under some assumptions on the model, can one prove that there is another locally uniform ergodic Gibbs measure μ_3 such that $h(\mu_1) < h(\mu_3) < h(\mu_2)$? An interesting example is the case of proper 4-colorings of $\mathbb{Z}^3$.

Presentation Highlights

Leonid Petrov: From Yang-Baxter equation to Markov maps

We obtain a new relation between the distributions μ_t at different times $t \geq 0$ of the continuous-time TASEP (Totally Asymmetric Simple Exclusion Process) started from the step initial configuration. Namely, we present a continuous-time Markov process with local interactions and particle-dependent rates which maps the TASEP distributions μ_t backwards in time. Under the backwards process, particles jump to the left, and the dynamics can be viewed as a version of the discrete-space Hammersley process. Combined with the forward TASEP evolution, this leads to a stationary Markov dynamics preserving μ_t which in turn brings new identities for expectations with respect to μ_t. The construction of the backwards dynamics is based on Markov maps interchanging parameters of Schur processes, and is motivated by bijectivizations of the Yang-Baxter equation. We also present a number of corollaries, extensions, and open questions arising from our constructions.

Michael Aizenman: A Quantum Dimerization Phenomenon and the self dual F-K Random Cluster Models

Unlike classical antiferromagnets, quantum antiferromagnetic systems exhibit ground state frustration effects even in one dimension. A case in point is a quantum spin chain with the interaction between neighboring S-spins given by the projection on the two-spins singlet state. This 1D quantum system's ground state bears a close analogy to the self dual 2D Fortuin-Kasteleyn random cluster model, at $Q = (2S + 1)^2$. The corresponding stochastic geometric representation has led to the dichotomy (Aiz-Nachtergale): for each S the ground state exhibits either (i) slow decay of spin-spin correlations (as in the Bethe solution of the Heisenberg $S = 1/2$ antiferromagnet) or (ii) dimerization, manifested in translation symmetry breaking. Drawing on the recent analysis of the phase transition of the FK models (by Duminil-Gagnebin-Harel-Manolescu-Tassion, and Ray-Spinka), we show that in the infinite volume limit for any $S > 1/2$ this $SU(2S+1)$ invariant quantum system has a pair of distinct ground states, each exhibiting spatial energy oscillations, and exponential decay of correlations.

(Joint work with H. Duminil-Copin and S. Warzel).

Vadim Gorin: Shift invariance for the six-vertex model and directed polymers

Based on joint work with Alexei Borodin and Michael Wheeler.

This work is about a simple-looking property of a variety of integrable probabilistic systems that includes stochastic vertex models, (1+1)d directed polymers in random media and last passage percolation with specific weights, as well as universal objects of the Kardar-Parisi-Zhang universality class – the KPZ equation and the

Airy sheet. The property says that joint distributions of certain multi-dimensional observables in the system are unchanged under a shift of a subset of observation points.

It can be thought of as a far reaching generalization of the following known feature of the Brownian bridge: Fix $a < b$ and let $B(t)$, $0 \le t \le 1$, be a Brownian bridge such that $B(0) = a$ and $B(1) = b$. Let $\mathcal{L}_c$ denote the local time that $B(t)$ spends at level c. Then as long as $a \le c \le b$, the distribution of $\mathcal{L}_c$ does not depend on the choice of c.

While the above property of the invariance of Brownian local times under the shifts of c admits a bijective proof, we have not been able to find anything similar for the more complicated systems that we deal with. Instead, our proofs rely on much more advanced machinery of Yang-Baxter integrable vertex models.

Beyond intrinsic interest, the shift-invariance property yields explicit formulas for certain multi-dimensional distributions that were not accessible before. The basic idea is that shifts sometimes allow to reduce complicated configurations of observation points to simpler ones, for which exact expressions are already known.

Alessandro Giuliani: Universal height fluctuations and scaling relations in interacting dimer models

In this talk I will review the results on the universality of height fluctuations in interacting dimer models, obtained in collaboration with F. Toninelli and V. Mastropietro in a recent series of papers. The class of models of interest are close-packed dimers on the square lattice, in the presence of small but extensive perturbations that make them non-determinantal. Examples include the 6-vertex model close to the free-fermion point and the dimer model with plaquette interaction. By tuning the edge weights, one can impose a non-zero average tilt for the height function, so that the considered models are in general not symmetric under discrete rotations and reflections. It is well known that, in the determinantal case, height fluctuations in the massless (or 'liquid') phase scale to a Gaussian log-correlated field and their amplitude is a universal constant, independent of the tilt. Our main result is the following: when the perturbation strength is sufficiently small, log-correlations survive, with amplitude A that, generically, depends non-trivially and non-universally on the perturbation strength and on the tilt. Moreover, the amplitude A satisfies a universal scaling relation ('Haldane' or 'Kadanoff' relation), saying that it equals the anomalous exponent of the dimer-dimer correlation. The main steps and ideas of the proof are the following:

- The interacting partition function and generating function for dimer correlations is written as a Grassmann integral analogous to ϕ^4 theory in 2D; such integral is invariant under a local gauge transformation, related to the local conservation law of dimer number
- Such a Grassmann ϕ^4 theory can be studied by multiscale methods (fermionic Renormalization Group); the iteration is convergent provided that the sequence of relevant and marginal coupling constants stays bounded in the infrared; there are 4 such constants, and we have at disposal only 3 counterterms (fixing the slope of the height and the anisotropy between horizontal and vertical dimers) in order to adjust their initial data - In order to control the flow of the fourth running coupling constant (the effective quartic interaction) we compare it with the flow of an exactly solvable model for interacting fermions in $d = 1 + 1$, known as the Luttinger model, whose infrared behavior is the same as the one of the fermionic representation of interacting dimers
- The Luttinger model is solvable in a strong sense: exact formulas for correlations and critical exponents are available; the comparison between the fermionic representation of dimers and Luttinger in the infrared regime allows us to write the asymptotic behavior of dimer correlations in terms of the density-density and mass-mass correlations of the Luttinger model
- The comparison between the lattice Ward Identities for the dimer correlation functions (associated with the local gauge transformation mentioned above) and those for the Luttinger model allows us to relate the bare

parameters of the Luttinger model with the dressed parameters of the dimer model; such a relation allows us to export some of the scaling relations known for the Luttinger model to the dimer context.

Amol Aggarwal: Universality for Lozenge Tiling Local Statistics

A salient feature of random tiling models is that the local densities of tiles can differ considerably in different regions of the domain, depending on the boundary data. Thus, a question of interest, originally mentioned by Kasteleyn in 1961 [4], is how the shape of the domain affects the local behavior of a random tiling. In this talk, we consider uniformly random lozenge tilings of essentially arbitrary domains. We outline a proof of the result from [1] that the local statistics of this model around any point in the liquid region of its limit shape are given by the infinite-volume, translation-invariant, extremal Gibbs measure of the appropriate slope. This was predicted by Cohn-Kenyon-Propp in 2001 [2].

Unlike many of the previous proofs applicable to special domains, our method does not make direct use of a Kasteleyn matrix. Instead, we proceed by locally comparing a uniformly random lozenge tiling of a given domain with an ensemble of Bernoulli random walks conditioned to never intersect. The benefit to the latter model is that its algebraic structure appears to be more amenable to asymptotic analysis than does the Kasteleyn matrix. In particular, under reasonably general initial data, its convergence of local statistics was recently analyzed by Gorin-Petrov [3]. We show that the tiling model and path model can be coupled locally around a vertex in the liquid region so that they coincide with high probability. The convergence of local statistics for the latter model then imply the same for the former.

Central to implementing this procedure is to establish a “local law” for the random tiling, which states that the associated height function is approximately linear on any mesoscopic scale. The proof of this local law proceeds through a multi-scale analysis, using an effective global law at each scale and deterministic estimates showing that the gradient of the global profile is approximately constant between scales.

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Richard Kenyon: Darboux integrability and gradient models

This is joint work with Istvan Prause and is based on previous work with Jan de Gier and Sam Watson.

The 5-vertex model is a special case of the 6-vertex model and a generalization of the lozenge dimer model. We show how to compute the surface tension and limit shapes in the 5-vertex model via an explicit computation using the Bethe Ansatz technique.

One feature of the five vertex model is that the Euler-Lagrange equation for the surface tension minimizers has an explicit solution in terms of arbitrary analytic function inputs. This is known as “Darboux integrability”.

We showed that in fact any gradient model (variational problem for a function in two variables whose surface tension only depends on the gradient) is Darboux integrable by the same technique, on condition that the determinant of the Hessian of sigma is the fourth power of a harmonic function (harmonic in the underlying conformal coordinate).

This allowed us to extend our results on the 5-vertex model to a staggered weight 5-vertex model in which the weights are of isoradial type.

Marcin Lis: Spins, percolation and height functions

To highlight certain similarities in combinatorial representations of several well known two-dimensional models of statistical mechanics, we introduce and study a new family of models which specializes to these cases after a proper tuning of the parameters. To be precise, our model consists of two independent standard Potts models, with possibly different numbers of spins and different coupling constants (the four parameters of the model), defined jointly on a graph embedded in a surface and its dual graph, and conditioned on the event that the primal and dual interfaces between spins of different value do not intersect. We also introduce naturally related height function and bond percolation models, and we discuss their basic properties and mutual relationship. As special cases we recover the standard Potts and random cluster model, the 6-vertex model and loop $O(n)$ model, the random current, double random current and XOR-Ising model.

Alexander Glazman: Six-vertex and Ashkin-Teller models: order/disorder phase transition

Ashkin-Teller model is a classical four-component spin model introduced in 1943. It can be viewed as a pair of Ising models τ and τ' with parameter J that are coupled by assigning parameter U for the interaction of the products $\tau\tau'$ at every two neighbouring vertices. On the self-dual curve $\sinh 2J = e^{-2U}$, the Ashkin-Teller model can be coupled with the six-vertex model with parameters $a = b = 1$, $c = \coth 2J$ and is conjectured to be conformally invariant. The latter model has a height-function representation. We show that the height at a given face diverges logarithmically in the size of the domain when $c = 2$ and remains uniformly bounded when $c > 2$. In the latter case we obtain a complete description of translation-invariant Gibbs states and deduce that the Ashkin-Teller model on the self-dual line exhibits the following symmetry-breaking whenever $J < U$: correlations of spins τ and τ' decay exponentially fast, while the product $\tau\tau'$ is ferromagnetically ordered. The proof uses the Baxter-Kelland-Wu coupling between the six-vertex and the random-cluster models, as well as the recent results establishing the order of the phase transition in the latter model. However, in the talk, we will focus mostly on other parts of the proof:

- description of the height-function Gibbs states via height-function mappings and T-circuits,
- coupling between the Ashkin-Teller and the six-vertex models via an FK-Ising-type representation of these two models.

(this is joint work with Ron Peled)

Yinon Spinka: Discontinuity of phase transition of the planar random cluster model for q larger than 4: a short proof

The random-cluster model is by now a well-known dependent percolation model, which is also closely related to the Potts model. We consider here the random-cluster model on the square lattice $\mathbb{Z}^2$. An important quantity of interest in this model is the probability $\theta^{\mathrm{f/w}}(p,q)$ that the origin belongs to an infinite cluster under the free/wired random-cluster measure. For any $q \geq 1$, the model undergoes a phase transition at $p_c = \frac{\sqrt{q}}{1+\sqrt{q}}$ in the sense that $\theta^{\mathrm{f}}(p,q) = \theta^{\mathrm{w}}(p,q) = 0$ for all $p < p_c$ and $\theta^{\mathrm{f}}(p,q) = \theta^{\mathrm{w}}(p,q)$ for all $p > p_c$. The behavior at the critical parameter p_c is of particular interest. For example, the two functions $\theta^{\mathrm{f/w}}(p,q)$ are always continuous at every $p \neq p_c$, whereas they are continuous at $p = p_c$ precisely when $\theta^{\mathrm{w}}(p_c,q) = 0$; in this case, the phase transition is said to be continuous.

Baxter [1] conjectured that the phase transition is continuous for $1 \leq q \leq 4$ and discontinuous for $q > 4$. This was recently verified in a combination of two beautiful papers: the regime $1 \leq q \leq 4$ was proved by Duminil-

Copin, Sidoravicius and Tassion [3] and the regime $q > 4$ by Duminil-Copin, Gagnebin, Harel, Manolescu and Tassion [2]. We reprove the latter discontinuity of phase transition when $q > 4$ via a short probabilistic proof.

The original proof of discontinuity given in [2] relies on an analysis of the so-called Bethe ansatz aimed at computing the eigenvalues of a transfer matrix for the six-vertex model. Such an approach has the advantage of yielding a precise expression for the exponential rate of decay of the probability (under the free random-cluster measure) that the origin is connected to a far away point.

Our proof, while also exploiting the connection with the six-vertex model, does not rely on the Bethe ansatz. Instead, our proof is based on softer arguments (in particular, it does not require a computation of the correlation length) and only uses very basic properties of the random-cluster model (for example, we do not even need the Russo–Seymour–Welsh machinery developed recently in [3]).

Joint work with Gourab Ray.

[1] Rodney James Baxter, *Solvable eight-vertex model on an arbitrary planar lattice*, Philosophical Transactions of the Royal Society of London. Series A, Mathematical and Physical Sciences **289** (1978), no. 1359, 315–346.

[2] Hugo Duminil-Copin, Maxime Gagnebin, Matan Harel, Ioan Manolescu, and Vincent Tassion, *Discontinuity of the phase transition for the planar random-cluster and Potts models with* $q > 4$, arXiv preprint arXiv:1611.09877 (2016).

[3] Hugo Duminil-Copin, Vladas Sidoravicius, and Vincent Tassion, *Continuity of the phase transition for planar random-cluster and Potts models with* $1 \leq q \leq 4$, Communications in Mathematical Physics **349** (2017), no. 1, 47–107.

Zhongyang Li: Limit shape and height fluctuations of perfect matchings on square-hexagon lattices

We study asymptotics of perfect matchings on a large class of graphs called the contracting square-hexagon lattice,which is constructed row by row from either a row of a square grid or a row of a hexagonal lattice. We assign the graph periodic edge weights with period $1 * n$, and consider the probability measure of perfect matchings in which the probability of each configuration is proportional to the product of edge weights. We show that the partition function of perfect matchings on such a graph can be computed explicitly by a Schur function depending on the edge weights. By analyzing the asymptotics of the Schur function, we then prove the Law of Large Numbers (limit shape) and the Central Limit Theorem (convergence to the Gaussian free field) for the corresponding height functions. We also show that the distribution of certain type of dimers near the turning corner is the same as the eigenvalues of Gaussian Unitary Ensemble,and explicitly study the curve separating the liquid region and the frozen region for certain boundary conditions.

Sanjay Ramassamy: Dimers and circle patterns

In joint work with R. Kenyon, W. Y. Lam and M. Russkikh, we establish a correspondence between dimer models on planar bipartite graphs and centers of circle patterns. Circle patterns are a class of objects coming from discrete differential geometry, where they serve as discrete conformal maps.

Let G be a planar bipartite graph which is realized as a circle pattern, meaning that every vertex is mapped to a point in the plane in such a way that every face admits a circumcircle. Assume additionally that the realization of the dual graph of G (induced by mapping every dual vertex to the center of the circle corresponding to that face) is an embedding. Then one can assign a complex number to every edge of the bipartite graph, this complex number being the vector connecting the two centers lying on each side of that edge, such that the black endpoint of the edge lies to the left of the vector. This assignment of complex numbers to edges satisfies the Kasteleyn condition, a condition required on the entries of the Kasteleyn matrix used to compute the partition function and the correlations of the dimer model on G. Such a construction generalizes the isoradial case (all the circles have the same radius) proposed by Kenyon in 2002.

Conversely, let G be a planar bipartite graph equipped with edge weights satisfying the Kasteleyn condition. We ask whether there exist gauge equivalent edge weights (meaning weights inducing the same Boltzmann probability measure on dimer coverings of G) coming from an embedding as circle centers. Such a choice of edge weights is called a Coulomb gauge, because of the fact that it has zero divergence (the sum of the edge weights around any given vertex of G vanishes). We provide a positive answer to that question in the cases of finite planar graphs with outer face of degree four and of infinite planar graphs which are periodic in two directions. Given a choice of boundary conditions, Boltzmann measures for the dimer model on an unweighted planar bipartite graphs with outer face of degree 4 are in one-to-two correspondence with Coulomb gauges. For an infinite periodic graph, Coulomb gauges are in one-to-one correspondence with liquid ergodic Gibbs measures.

One application of this correspondence is in the field of geometry and dynamics. This correspondence identifies a local move on circle patterns called the Miquel move to a local move on dimers models called the urban renewal. This enables us to identify Miquel dynamics, a discrete-time dynamical system on the space of square-grid circle patterns, to the Goncharov-Kenyon dynamics on dimer models, from which the integrability of Miquel dynamics follows.

One can also hope to apply this correspondence to statistical mechanics, namely to the study of scaling limits for the dimer model. It is expected that circle center embeddings provide the right geometric setting to study general dimer models. One indication of this comes from the fact that they generalize the Tutte embedding adapted to the study of spanning trees and Chelkak's s-embeddings adapted to the study of the Ising model. Another indication comes from a general framework proposed by Chelkak-Laslier-Russkikh for obtaining the fluctuations as a Gaussian free field from the embedding as circle centers, as was explained in the later talks by Laslier and Chelkak. To illustrate this general framework, in a ongoing joint project with D. Chelkak, we are attempting to rederive via this method the conformal structure used to the define the Gaussian free field in the case of the Aztec diamond, where exact computations can be made.

Benoit Laslier and Dmitry Chelkak: Perfect t-embeddings of bipartite planar graphs and the convergence to the GFF - I & II

We discuss a concept of 'perfect t-embeddings', or 'p-embeddings', of weighted bipartite planar graphs. (T-embeddings also appeared under the name Coulomb gauges in a recent work of Kenyon, Lam, Ramassamy and Russkikh.) We believe that these p-embeddings always exist and that they are good candidates to recover the complex structure of big bipartite planar graphs carrying a dimer model. To support this idea, we first develop a relevant theory of discrete holomorphic functions on t-embeddings; this theory unifies Kenyon's holomorphic functions on T-graphs and s-holomorphic functions coming from the Ising model.

Further, given a sequence of (abstract) planar graphs G_n and their p-embeddings T_n onto the unit disc D, assume that (i) the faces of T_n satisfy certain technical assumptions in the bulk of D; (ii) the size of the associated origami maps O_n tends to zero as n grows (again, on each compact subset of D). We prove that (i)+(ii) imply the convergence of the fluctuations of the dimer height functions on G_n (provided that these graphs are embedded by T_n), to the GFF on the unit disc D equipped with the standard complex structure. Though this is not fully clear at the moment, we conjecture that the origami maps O_n are always small in absence of frozen regions and gaseous bubbles, so our theorem can be eventually applied to all such cases. Moreover, the same techniques are applicable in the situation when the limit of the origami maps arising from a sequence of p-embeddings is a Lorenz-minimal surface, in this situation one eventually obtains the GFF in the conformal parametrization of this surface.

In a related joint work with Sanjay Ramassamy we argue that such a Lorenz-minimal surface indeed arises in the case of classical Aztec diamonds; a general conjecture is that this should 'always' be the case due to a link between p-embeddings and a representation of the dimer model in the Plücker quadric. Time permitting, we also indicate how the theory of t-holomorphic functions specifies to the Ising case and discuss related results on conformal invariance of the Ising model as well as a more general perspective.

Nathanael Berestycki: The dimer model on Riemann surfaces

Temperley's bijection is a powerful tool for the study of the dimer model in the simply connected setting. This bijection relates the behaviour of a pair of dual uniform spanning trees to the dimer model on the graph obtained by superposing the planar and dual graph together with medial vertices: more specifically the height differences in the dimer model on this graph is equal to the winding of branches in either dual or primal spanning trees. Using this connection and its powerful generalisation by Kenyon and Sheffield (to the setting of T-graphs), we were able in a previous work to derive robust proofs of convergence of the height function in the simply connected setting to the Gaussian free field (GFF): in the scaling limit, the branches of the spanning tree become the flow line of the GFF, in other words the GFF and continuum spanning trees are related through imaginary geometry.

In this work we consider the case of Riemann surfaces, which is much harder to study via determinantal methods than it is in the simply connected case. Our goal is to prove the existence, universality and conformal invariance of the scaling limit of the height one-form in the dimer model. Consider the superposition of a graph and its dual (as well as medial vertices) embedded on a given Riemann surface M with finitely many holes and handles. Removing the correct number of medial vertices (which can be computed via Euler's formula), we show that the resulting graph is dimerable. These removed medial vertices can be thought of as punctures in the surface. We can apply Temperley's bijection since it is locally defined, but the resulting object will not be a pair of dual spanning trees. Instead, there are global topological constraints and we call the resulting (locally tree-like) structure Temperleyan forests (and their dual). A Temperleyan forest may contain cycles but only nontrivial ones, so that they are reminiscent of a simpler object: the Cycle-Rooted Spanning Forest (CRSF). In fact, we show that a CRSF is Temperleyan if and only if the branches emanating from every puncture decompose the surface into disjoint annuli; on a torus or an annulus every CRSF is Temperleyan (up to a choice of orientation of each cycle).

Furthermore, the height-form of the dimer model is, as in the simply connected case, closely related to the behaviour of the Temperleyan forest. Indeed, adopting the Fuchsian point of view on Riemann surfaces (in which the surface is represented as a polygon with certain periodic boundary conditions), we show that height differences can be identified with the winding of branches of the Temperleyan forest (as in the simply connected setting) plus some global topological corrections, which correspond to the fact that two points may not belong to the same component of the forest (so that one needs to "jump" over components). Given this result, we can apply ideas from our earlier work to show that if the Temperleyan forest admits a scaling limit, then so does the height-form: this is because winding is in some sense well behaved, whereas the global topological correction terms are easily handled.

Finally, on a torus or an annulus, a Temperleyan forest is equivalent to a CRSF (up to a Radon-Nikodym factor proportional to $2^{\#\text{cycles}}$). Since a CRSF can be sampled through a version of Wilson's algorithm, we show that (on any surface) CRSFs have a universal and conformally invariant scaling limit. Consequently the same holds for Temperleyan forests. Putting these results together, we obtain the scaling limit of the dimer height-form on the torus and the annulus. (A generalisation of this result to arbitrary surfaces is ongoing work.) On the torus, Dubedat showed that in the double isoradial case the limit was a compactified GFF, so our universality result implies this is always the case (solving a conjecture of Dubedat-Gheissari).

Joint work with Benoit Laslier (Paris) and Gourab Ray (Victoria).

Kurt Johansson: On the rough-smooth interface in the two-periodic Aztec diamond

The two-periodic Aztec diamond is a certain random tiling model. It can also be thought of as a dimer model or perfect matching on a certain bipartite graph. In models of this type it is possible to have three types of local dimer patterns, or limiting Gibbs measures, called frozen (solid), rough (liquid) ot smooth (gas). The double Aztec diamond is probably the simplest model where we can get a coexistence of all three phases so that we have, asymptotically, interfaces between the frozen and rough phases, as well as between the rough and smooth phases. The purpose of the work I report on is to understand the (local) geometry of the rough-smooth interface.

At the frozen-rough interface we have a well-defined boundary path at the discrete the level which converges to the Airy process after appropriate rescaling. The Airy process is a universal stochastic process that appears in many contexts in particular in random matrix theory and in random growth models. It is conjectured that at a typically at the interface between a rough and a frozen phase in a large class of random tiling models, the boundary process converges to the Airy process.

At the rough-smooth smooth boundary the situation is more complicated although here also we expect to have an Airy process. It is not obvious which geometric structure actually converges to the Airy process. The frozen boundary is clear, it is the place where we first see a change from the regular pattern. It is less clear exactly how one should define the boundary at the discrete level at the rough-smooth interface. At this boundary we see both local and long range structures and looking just locally, we can not tell if we are encountering a long range path or just a local structure (a loop). In joint work with Sunil Chhita and Vincent Beffara, we define this boundary precisely. We are not able to show that there is actually a last path that converges to the Airy process, but we are able to define a certain (signed) counting measure which in a sense counts the number of paths between in prescribed intervals, and show that this random measure converges to the Airy kernel point process.

Patrik Ferrari: Time-time correlation for the North polar region of the Aztec diamond

This talk is based on the papers [1] with H. Spohn and [2] with A. Occelli. We consider the boundary of the North polar region of the Aztec diamond. The interface between the random region and the frozen one is what we call the height function. Due to the shuffling algorithm, our model is a discrete time Markov chain, where time equals the size of the Aztec diamond.

We are interested in the time correlations of the height function. In particular we determine the limiting behavior of the covariance of the height function. When the two times are macroscopically close, that is, we consider time τN and time N with $1-\tau$ small, the first order correction of the time-time covariance is universal and given in term of the variance of the Baik-Rains distribution function (which is the stationary limiting distribution in KPZ models).

The result is proven in [2] in the language of last passage percolation with exponential random variables. However, due to the well-known link between Aztec diamond and discrete time TASEP with parallel update, which in turns is equivalent to a last passage percolation with geometric random variables, the same result will holds also for the Aztec diamond case.

[1] P.L. Ferrari and H. Spohn, On time correlations for KPZ growth in one dimension, SIGMA 12 (2016), 074.

[2] P.L. Ferrari and A. Occelli, Time-time covariance for last passage percolation with generic initial profile, Math. Phys. Anal. Geom. 22 (2019), 1.

Beatrice De Tiliere: Elliptic dimers and genus 1 Harnack curves

We consider the dimer model on a bipartite periodic graph with elliptic weights introduced by Fock. The spectral curves of such models are in bijection with the set of all genus 1 Harnack curves. We prove an explicit and local expression for the two-parameter family of ergodic Gibbs measures and for the slope of the measures.

This is work in progress with Cédric Boutillier and David Cimasoni.

Martin Tassy: Uniqueness of the limiting profile for monotonic Lipschitz random surfaces

For dimers and other models of random surfaces, limit shapes appear when boundary conditions force a certain response of the system. The main mathematical tool to study these responses is a variational principle which states that the limiting profile of the system must maximizes the integral of an entropy function often named surface tension. As a consequence, the strict convexity of the surface tension plays a crucial role as it forces the asymptotic profile which maximizes this integral to be unique. In this talk we will show that all models of Lipschitz random surfaces which are stochastically monotonic must have a strictly convex surface tension (joint with Piet Lammers).

Scott Sheffield: Laplacian determinants and random surfaces

My talk explored the ways that dimer models and other statistical physics models are related to Laplacian determinants, both on the discrete level and on the continuum level.

In particular, I recalled the geometric meaning of the so-called zeta-regularized determinant of the Laplacian, as it is defined on a compact surface, with or without boundary. Using an appropriate regularization, we found that a Brownian loop soup of intensity c has a partition function described by the $(-c/2)^{\text{th}}$ power of the determinant of the Laplacian. In a certain sense, this means that decorating a random surface by a Brownian loop soup of intensity c corresponds to weighting the law of the surface by the $(-c/2)^{\text{th}}$ power of the determinant of the Laplacian.

I then introduced a method of regularizing a unit area LQG sphere, and showing that weighting the law of this random surface by the $(-c/2)^{\text{th}}$ power of the Laplacian determinant has precisely the effect of changing the matter central charge from c to c'. Taken together with the earlier results, this provided a way of interpreting an LQG surface of matter central charge c as a pure LQG surface decorated by a Brownian loop soup of intensity c.

This talk was based on joint work with Morris Ang, Minjae Park, and Joshua Pfeffer.

Paul Melotti: The eight-vertex model via dimers

The eight-vertex model is an ubiquitous description that generalizes several spin systems, "ice-type" six-vertex models, and is related to Ashkin-Teller model, XYZ spin chains, and others. In a special "free-fermion" regime, it is known since the work of Fan, Lin, Wu in the late 60s that the model can be mapped to non-bipartite dimers, while in the six-vertex case the graph becomes bipartite. In this talk I show a relation between these non-bipartite dimers and a couple of bipartite dimers, that correspond to two different free-fermion 6V-models. More precisely, for any free-fermion 8V-model on a quadrangulation whose faces are colored black and white, there exists two free-fermion 6V-models that are in relation with the original 8V-model. The relation takes several forms:

- at the level of characteristic polynomials, that of the 8V-model is the product of those of the 6V-ones. Hence the former is the union of two Harnack curves;
- at the level of partition functions, the square of the 8V-one is the product of the 6V-ones;
- at the probabilistic level, the symmetric difference of two independent (identically distributed) 8V-configuration has the same distribution as the symmetric difference of two independent (differently distributed) 6V-configurations;
- at the level of Kasteleyn matrices, there is a simple relation between the inverse operators of all these models.

These can be proved using the formalism of order-disorder variables in a framework close to that of Dubédat.

This construction can be applied in an isoradial, Z-invariant setting, i.e. a regime of the model on the dual of a lozenge graph such that the star-triangle transformation is automatically satisfied. The relation, in combination with works of Boutillier, de Tilière and Raschel, yields the existence of an ergodic Gibbs measure, and exact, local formulas for correlations.

Scientific Progress Made

This program and hospitality of BIRS made it possible for several fruitful discussions and collaborations. We highlight a few here.

One point of controversy arose from a question of Sheffield (Section 28). It is common knowledge that every statistical physics model has an inherent central charge associated with them which governs the universality class of the model. The question was: is there any natural such class for the dimer model? For example, it was known since the time of Fisher that the Ising model can be mapped to a dimer model. Later, Dubedat showed that two Ising models can be mapped to a dimer model, a phenomenon known as Bosonization. On the other hand, Temperley's bijection maps Uniform spanning trees to dimer model. All these models are supposed to have different central charges. This sparked some informal debate on what is a 'natural' central charge that can be associated to the dimer model, and the general consensus was that dimer model has certain non-universal nature which impedes the assignment of such a universality class to the model. Various aspects of this question remain a matter of speculation and debate.

Sheffield asked another question regarding the analysis of dimer models on simplest non-planar domains, for example, one can add some 'pipes' in $\mathbb{Z}^2$. This sparked some interest and several possible suggestions were made. In the end it was unclear if a non-trivial limit can be achieved which is away from the gaseous phase of the model.

Another highlight was regarding the question of Berestycki concerning the maxima of the height function of the dimer model. After the proposal of the question, several suggestions were made by experts on how to progress with this question. In some cases, dimer height differences have the same law as a sum of independent Bernoulli variables; Dubedat suggests this might be a good starting point to study dimer height maxima.

Outcome of the Meeting

It was a general feeling during the meet that all the talks were of very high standard and engaging. Some of the comments regarding the meet by the participants is that it is quite rare for so many experts in the field to congregate for a specialized workshop like the one made possible here. Overall, this opened the doorway for some fruitful collaborations, raised some pertinent questions, and opened up the possibilities for future research directions for many of the participants.

Participants

Aggarwal, Amol (Harvard)
Aizenman, Michael (Princeton University)
Angel, Omer (UBC)
Berestycki, Nathanael (University of Vienna)
Boutillier, Cédric (Sorbonne Université)
Budzinski, Thomas (University of British Columbia)
Chandgotia, Nishant (Tata Institute of Fundamental Research- Centre for Applicable Mathematics)
Chelkak, Dmitry (ENS-Mitsubishi Heavy Industries)
Chhita, Sunil (Durham University)
Dauvergne, Duncan (Princeton University)

De Tiliere, Béatrice (University Paris Dauphine)
Dubedat, Julien (Columbia University)
Duminil-Copin, Hugo (Institut des Hautes Études Scientifiques (IHÉS))
Ferrari, Patrik (University of Bonn)
Giuliani, Alessandro (Università degli Studi Roma Tre)
Glazman, Alexander (Tel Aviv University)
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Greenblatt, Rafael (Università Roma Tre)
Harel, Matan (Tel Aviv University)
Johansson, Kurt (KTH Royal Institute of Technology)
Kenyon, Richard (Yale University)
Lammers, Piet (University of Cambridge)
Laslier, Benoit (University Paris-Diderot)
Li, Zhongyang (University of Connecticut)
Lis, Marcin (University of Vienna)
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Musiker, Gregg (University of Minnesota)
Petrov, Leonid (University of Virginia)
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Russkikh, Marianna (Massachusetts Institute of Technology)
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Spinka, Yinon (University of British Columbia)
Tassy, Martin (Dartmouth College)
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Chapter 29

Discrete subgroups of Lie groups (19w5040)

December 9 -13, 2019

Organizer(s): Michael Kapovich (University of California, Davis), Gregory Margulis (Yale University), Gregory Soifer (Bar Ilan University), Dave Witte Morris (University of Lethbridge)

Overview of the Field

Recent years have seen a great deal of progress in our understanding of "thin" subgroups, which are discrete matrix groups that have infinite covolume in their Zariski closure. (The subgroups of finite covolume are called "lattices" and, generally speaking, are much better understood.) Traditionally, thin subgroups are required to be contained in arithmetic lattices, which is natural in the context of number-theoretic and algorithmic problems but, from the geometric or dynamical viewpoint, is not necessary. Thin subgroups have deep connections with number theory (see e.g. [6, 7, 8, 18, 22]), geometry (e.g. [1, 14, 16, 38]), and dynamics (e.g. [3, 11, 27, 29]).

The well-known "Tits Alternative" [44] (based on the classical "ping-pong argument" of Felix Klein) constructs free subgroups of any matrix group that is not virtually solvable. (In most cases, it is easy to arrange that the resulting free group is thin.) Sharpening and refining this classical construction is a very active and fruitful area of research that has settled numerous old problems. For instance, Breuillard and Gelander [11] proved a quantitative form of the Tits Alternative, which shows that the generators of a free subgroup can be chosen to have small word length, with respect to any generating set of the ambient group. Kapovich, Leeb and Porti [26] provided a coarse-geometric proof of the existence of free subgroups that are Anosov. In a somewhat different vein, Margulis and Soifer [32] proved that $SL(n,\mathbb{Z}), n \geq 4$, contains free products of the form $\mathbb{Z}^2 \star F_k$ (where F_k is the free group of rank k) for all $k \geq 1$. (Answering a question of Platonov and Prasad, this implies that $SL(n,\mathbb{Z})$ has maximal subgroups of infinite index that are not free groups.) Also, it has been shown that $SL(n,\mathbb{Z})$ contains Coxeter groups (and, hence, right-angled Artin groups) when n is sufficiently large. Ping-pong type constructions have also emerged as an important technical tool in other contexts, such as for disproving the invariable generation property (by constructing a thin subgroup that intersects every conjugacy class [19]) and for proving the expander property for Cayley graphs of finite quotients of thin groups [22].

Conversely, there are also obstructions to the existence of thin subgroups. For example, no thin, Zariski-dense subgroup of $SL(n,\mathbb{Z})$ contains $SL(3,\mathbb{Z})$ [45]. Similarly, it has been shown in certain situations that thin, discrete, Zariski-dense subgroups cannot contain a lattice in a maximal unipotent subgroup of the ambient group [5, 35, 46].

The study of certain natural (and properly discontinuous) actions of thin groups is another important line of research. The famous Auslander Conjecture concerns actions of thin groups on affine spaces. (Namely, it is conjectured that if a group acts properly discontinuously and cocompactly on an affine space $\mathbb{R}^n$, then the group is virtually solvable.) Actions on more general geometric spaces (such as flag varieties) are also important. While it seems that nothing of interest can be said about such actions in general, a great deal of progress has been made in recent years analyzing actions of thin subgroups that satisfy further restrictions. The Anosov property has been of particular interest (see, for example, [11], [27], and [49]), as well as other forms of strengthening of discreteness, e.g. regularity, which has its origin in [3], see also [27].

This conference brought together a range of specialists whose expertise in order to educate each other in the broad spectrum of techniques and problems in the theory of discrete subgroups of Lie groups. A number of young researchers, including graduate students, actively participated in the conference as well.

Open Problems

On the first day of the workshop we conducted a problem session in the theory of discrete subgroups of Lie groups. Below are problems collected during and after the workshop.

Proper actions on affine spaces

Let Γ be a finitely generated group, $\rho : \Gamma \to GL(n,\mathbb{R})$ be the given representation, $Z^1(\Gamma,\rho)$ be the space of ρ-cocycles with values in $\mathbb{R}^n$, i.e. maps

$$u : \Gamma \to \mathbb{R}^n, u(\alpha\beta) = u(\alpha) + \rho(\alpha)u(\beta), \alpha, \beta \in \Gamma.$$

Note that $Z^1(\Gamma,\rho)$ is a finite-dimensional real vector space. Each cocycle $u \in Z^1(\Gamma,\rho)$ determines an affine action ρ_u of Γ on $V = \mathbb{R}^n$:

$$\rho_u(\gamma) : \mathbf{x} \mapsto \rho(\gamma)\mathbf{x} + u(\gamma).$$

Let $C = C_\rho \subset Z^1(\Gamma,\rho)$ denote the subset consisting of cocycles such that the action ρ_u of Γ on $\mathbb{R}^n$ is properly discontinuous.

Question 29.0.1 (N. Tholozan)**.** Is C open in $Z^1(\Gamma,\rho)$? Is it convex?

Note that the answer is positive for $n = 3$, this follows from the results of [21].

Question 29.0.2 (N. Tholozan)**.** Does C_ρ depend continuously on ρ?

Here one has to be careful with the topology used on the set of subsets of $Z^1(\Gamma,\rho)$. For closed subsets one uses Shabauty topology. For instance, if the subsets C are open, their complements are closed and, hence, one can interpret the question as of the continuity of the complement with respect to ρ.

For a finitely generated group Γ, let $P(\Gamma,n)$ denote the subset of $Hom(\Gamma, Aff(\mathbb{R}^n))$ consisting of representations defining proper actions of Γ on $\mathbb{R}^n$. Let $PA(\Gamma,n) \subset P(\Gamma,n)$ denote the subset consisting of actions ρ_u with P-Anosov linear part ρ (for some parabolic subgroup $P < GL(n,\mathbb{R})$).

Question 29.0.3 (G. Soifer)**.** To which extent $P(\Gamma,n)$ is open?

Note that in general $P(\Gamma, n)$ is not open even for $n = 3$, for instance, one can take a rank 2 free group Γ and a representation $\rho_u \in P(\Gamma, 3)$ whose linear part ρ contains unipotent elements. A small perturbation of ρ_u will yield a representation (with linear part in $SO(2,1)$) with nondiscrete linear part, hence, a non-proper affine action. One can also perturb a representation so that the linear part is deformed to a Zariski dense subgroup of $SL(3, \mathbb{R})$, again resulting in a non-proper action.

It is known that

$$PA(\Gamma, 3) \cap Hom(\Gamma, SO(2,1) \ltimes \mathbb{R}^3)$$

is open in

$$Hom(\Gamma, SO(2,1) \ltimes \mathbb{R}^3)$$

(this follows from the results of [21] and stability of Anosov representations).

Question 29.0.4 (G. Soifer)**.** To which extent $P(\Gamma, n)$ is open in general?

Conjecture 29.0.5 (The Auslander conjecture)**.** If $\Gamma < \mathrm{Aff}(\mathbb{R}^n)$ is a subgroup which acts properly discontinuously and co-compactly on $\mathbb{R}^n$, then Γ is virtually solvable.

Abels, Margulis and Soifer proved the Auslander conjecture for the dimensions $n \leq 6$ and observed that the following problem is important for the further progress towards the Auslander conjecture:

Conjecture 29.0.6 (Abels, Margulis, Soifer)**.** Let $\Gamma < O(4,3) \ltimes \mathbb{R}^7 < \mathrm{Aff}(\mathbb{R}^7)$ be a subgroup acting properly discontinuously and co-compactly on $\mathbb{R}^7$. Then the linear part of Γ is not Zariski dense in $SO(4,3)$.

Question 29.0.7. Does there exist a properly discontinuous cocompact group of affine transformations isomorphic to the fundamental group of a closed hyperbolic manifold?

Partial progress towards a negative answer to this problem was described at the talk by Suhyoung Choi at the workshop: He proved that such an action cannot exist under certain assumptions on its linear part (strengthening the P-Anosov condition).

Question 29.0.8 (G. Mostow)**.** Suppose that $M = \mathbb{R}^n/\Gamma$ is an affine manifold, such that the linear part of Γ is in $SL_n(\mathbb{R})$. Thus, Γ preserves the standard volume form on $\mathbb{R}^n$ and, hence, M has a canonical volume form as well. Does $Vol(M) < \infty$ imply that M is compact?

This question is motivated by Mostow's theorem that lattices in solvable groups are cocompact.

Question 29.0.9 (G. Soifer)**.** Study subgroups $\Gamma < \mathrm{Aff}(\mathbb{C}^n)$ acting properly discontinuously on $\mathbb{C}^n$.

More specifically:

Question 29.0.10 (G. Soifer)**.** Does there exist a free nonabelian subgroup $\Gamma < \mathrm{Aff}(\mathbb{C}^3)$ acting properly discontinuously on $\mathbb{C}^3$? For instance, consider the adjoint action of $SL_2(\mathbb{C})$ on $\mathbb{C}^3$ (identified with the Lie algebra of $SL_2(\mathbb{C})$). Consider a generic representation $\rho : F_2 = \langle a, b\rangle \to SL(2, \mathbb{C})$. Does there exist a cocycle $u \in Z^1(F_2, \mathbb{C}^3)$ and $m > 0$ such that the action on $\mathbb{C}^3$ of $\langle a^m, b^m\rangle$ given by ρ_u is properly discontinuous?

Conjecture 29.0.11 (Markus Conjecture)**.** Suppose that M is a compact n-dimensional affine manifold whose linear holonomy is in $SL(n, \mathbb{R})$. Is M complete?

This conjecture is known when the linear holonomy of M has "discompacity 1" (Y. Carriere, [13]), e.g. when M is a flat Lorentzian manifold, and also for convex affine manifolds of dimension ≤ 5, [25].

Conjecture 29.0.12 (M. Kapovich)**.** Suppose that M is a compact n-dimensional affine manifold whose linear holonomy is contained in a rank one subgroup of $SL(n, \mathbb{R})$. Is M complete?

Discrete subgroups of $SL(3,\mathbb{R})$

Question 29.0.13 (M. Kapovich)**.** 1. Does there exist a discrete a subgroup $\Gamma < SL(3,\mathbb{R})$ isomorphic to $\mathbb{Z}^2 \star \mathbb{Z}$ and containing only regular diagonalizable elements?

2. Does there exist a discrete subgroup $\Gamma < SL(3,\mathbb{Z})$ isomorphic to $\mathbb{Z}^2 \star \mathbb{Z}$?

Note that there are known examples, [43], of discrete subgroups $\Gamma < SL(3,\mathbb{R})$ isomorphic to $\mathbb{Z}^2 \star \mathbb{Z}$ where $\mathbb{Z}^2$ is super-singular: It is generated by three singular diagonalizable matrices A, B, C satisfying $ABC = 1$.

Question 29.0.14 (K. Tsouvalas)**.** Does there exist a discrete a subgroup $\Gamma < SL(3,\mathbb{R})$ isomorphic to $\pi_1(S) \star \mathbb{Z}$, where S is a closed hyperbolic surface ?

Note that it is impossible to find an Anosov subgroup $\Gamma < SL(3,\mathbb{R})$ isomorphic to $\pi_1(S) \star \mathbb{Z}$ with this property, since every Anosov subgroup of $SL(3,\mathbb{R})$ is either virtually free or a virtually surface group. Note, furthermore, that $SL(4,\mathbb{Z})$ contains subgroups isomorphic to $\mathbb{Z}^2 \star \mathbb{Z}$ and $\pi_1(S) \star \mathbb{Z}$.

Subgroups of $SL(n,\mathbb{Z})$, $n \geq 3$

While many "exotic" finitely generated groups embed in $SL(n,\mathbb{Z})$ for large n, very few subgroups of $SL(3,\mathbb{Z})$ are known: All currently known finitely generated thin subgroups of $SL(3,\mathbb{Z})$ are either virtually free or are virtually isomorphic to surface groups.

Problem 29.0.15. Construct thin subgroups of $SL(3,\mathbb{Z})$ which are neither virtually free nor are virtually isomorphic to surface groups.

For the next questions, we will need some group-theoretic definitions:

Definition 29.0.1. A group Γ is called coherent if every finitely generated subgroup of Γ is finitely presented. A group Γ is said to have the Howson property if the intersection of any two finitely generated subgroup of Γ is again finitely generated.

It is known that $SL(2,\mathbb{Z})$ is coherent (and, moreover, every discrete subgroup of $SL(2,\mathbb{C})$ is coherent), while $SL(4,\mathbb{Z})$ is non-coherent. Every discrete subgroup of $SL(2,\mathbb{C})$ which is not a lattice has the Howson property. However, there are (even arithmetic) lattices in $SL(2,\mathbb{C})$ which do not have the Howson property. The reason for this is the existence of finitely generated geometrically infinite subgroups of such lattices.

Question 29.0.16 (J.-P. Serre)**.** Is $SL(3,\mathbb{Z})$ coherent?

The answer would be positive if every finitely generated thin subgroup of $SL(3,\mathbb{Z})$ were virtually isomorphic to either a free group or a surface group. While groups such as $\mathbb{Z}^2 \star \mathbb{Z}$ and $\pi_1(S) \star \mathbb{Z}$ (where S is a surface) are coherent, the existence of embeddings of such groups in $SL(3,\mathbb{Z})$ might help us to find embeddings of more complicated subgroups and, hopefully, address the coherence problem.

Problem 29.0.17 (J.-P. Serre)**.** Is there a profinitely dense non-free subgroup in $SL(3,\mathbb{Z})$?

Question 29.0.18 (A. Detinko)**.** Does $SL(3,\mathbb{Z})$ have the Howson property?

Question 29.0.19 (M. Kapovich)**.** Suppose that Γ_1, Γ_2 are Anosov subgroups of $SL(3,\mathbb{Z})$. Is $\Gamma_1 \cap \Gamma_2$ finitely generated?

Problem 29.0.20 (T. Gelander, C. Meiri)**.** An element $g \in SL(3,\mathbb{Z})$ is called complex if for every $m \geq 1$ the matrix g^m has a non-real eigenvalue. Is it possible for a thin subgroup of $SL(3,\mathbb{Z})$ to contain a complex element?

Algorithmic problems

Question 29.0.21 (A. Detinko)**.** Is freeness decidable for finitely generated subgroups of arithmetic groups (e.g. of $SL(n,\mathbb{Z}), n \geq 3$)?

Note that freeness is undecidable for subsemigroups. Freeness is decidable for subgroups of $SL(2,\mathbb{Z})$. It is also decidable for some special classes of subgroups of arithmetic groups:

(a) Anosov subgroups.

(b) Subgroups which admit finitely-sided Dirichlet domains in associated symmetric spaces.

Freeness is likely to be, at least effectively, undecidable. The reason is the existence of badly distorted finitely generated free subgroups of $SL(n,\mathbb{Z})$ for large n: These are free subgroups whose distortion function is comparable to the k-th Ackerman function (for any k), see [15, 10] for the description of embeddings of such free groups in free-by-cyclic groups and [24, 48] for embeddings to $SL(n,\mathbb{Z})$.

Question 29.0.22 (A. Detinko)**.** Is arithmeticity decidable? More precisely, is there an algorithm that decides if a finitely generated Zariski dense subgroup Λ of an irreducible arithmetic group Γ (say, $SL(n,\mathbb{Z})$, $n \geq 3$) has finite index in Γ?

Note that this problem is semidecidable: There is an algorithm which will terminate if $\Lambda < \Gamma$ has finite index. The problem is known to be decidable for subgroups of $SL(2,\mathbb{Z})$ and undecidable for subgroups of $SL(2,\mathbb{Z}) \times SL(2,\mathbb{Z})$.

Question 29.0.23 (M. Kapovich)**.** Is the membership problem in finitely generated subgroups of $SL(3,\mathbb{Z})$ decidable?

Note that all known finitely generated subgroups of $SL(3,\mathbb{Z})$ have at most exponential distortion, hence, have decidable membership problem. In contrast, the membership problem is undecidable for finitely generated subgroups of $SL(4,\mathbb{Z})$. The reason is that that group contains $SL(2,\mathbb{Z}) \times SL(2,\mathbb{Z})$, which, in turn, contains a direct product of two free groups of large ranks. The latter admits finitely generated normal subgroups with undecidable membership problem (Mikhailova subgroups, [33]). However, in this case, the ambient lattice is reducible.

Fact 29.0.24. There exist irreducible arithmetic groups Γ such that for Zariski dense subgroups in Γ the membership problem is undecidable.

Very likely, the subgroups Γ can be found in $SO(p,q)$ for suitable p,q. The existence of Γ is an application of the Rips construction of small cancellation groups with non-recursively distorted normal subgroups [42], combined with with the Cubulation Theorem of Dani Wise [47] and the embedability of cubulated groups in RACGs (Right-Angled Coxeter groups), see [48], which, in turn, admit Zariski dense representations in $O(p,q) \cap GL(p+q,\mathbb{Z})$, see [4].

Note that the membership problem is decidable for subgroups with recursive distortion function, e.g. for quasiisometrically embedded subgroups, such as Anosov subgroups.

Maximal subgroups

Recall that a subgroup M of a group Γ is said to be maximal if there is no proper subgroup $\Lambda < \Gamma$ containing M.

According to [32], every Zariski dense subgroup Γ in a semisimple Lie group G (of positive dimension) admits maximal subgroups of infinite index. However, very little is known about maximal subgroups in this setting. The construction of maximal subgroups in [32] is a two-step process: First, construct an infinite rank free profinitely dense subgroup $\Lambda < \Gamma$ (this step is essentially constructive) and then, use Zorn's Lemma to get a maximal subgroup M:

$$\Lambda < \mathrm{M} < \Gamma.$$

The second step is completely nonconstructive.

Question 29.0.25 (G. Margulis, G. Soifer)**.** Suppose that $\Gamma < G$ is as above.

1. Is it true that for every maximal subgroup $\mathrm{M} < \Gamma$ is not finitely generated?
2. Is it true that Γ contains a free maximal subgroup?

Note that M. Akka and T. Gelander proved that there exists a finitely generated profinitely dense subgroup Γ of $SL_n(\mathbb{Z})$ such that the number of generators of Γ does not depend on n.

Question 29.0.26 (G. Soifer)**.** Does there exist a profinitely dense subgroup of $SL_n(\mathbb{Z})$ generated by two elements?

Other problems on thin subgroups

Definition 29.0.2. For a finitely generated group Γ with a finite generating subset S the Kazhdan constant $\kappa(\Gamma, S)$ is defined as

$$\kappa(\Gamma, S) = \inf_{\pi, v} \max_{g \in S} \|v - \pi_g v\|,$$

where the infimum is taken over all unitary representations (H_π, π) of Γ without fixed unit vectors, and all unit vectors $v \in H_\pi$. Then Γ is said to have Property T iff $\kappa(\Gamma, S) > 0$ for some/every finite generating subset S. A group Γ is said to have uniform Property T, if $\inf_S \kappa(\Gamma, S) > 0$ where the infimum is taken over all finite generating subsets S.

The following question goes back to [31]:

Question 29.0.27 (A. Lubotzky)**.** Does $SL(n, \mathbb{Z}), n \geq 3$, have the uniform Property T?

Note that Lubotzky was asking the more general question whether Property T implies uniform Property T, which was answered in the negative independently by Gelander & Zuk [20], and Osin [36]. The problem is open for all n. In the case of many classes of higher rank uniform lattices, the answer is known to be negative.

Question 29.0.28 (Bekka, de la Harpe, Valette)**.** Are there thin subgroups of $SL(n, \mathbb{Z}), n \geq 3$, satisfying Property T?

The difficulty is that the known examples of (infinite discrete) groups satisfying Property T tend to be: (a) super-rigid arithmetic groups, or (b) some combinatorially defined groups for which all real-linear representations are nondiscrete or nonfaithful.

One can attempt to combine super-rigid lattices, but such combinations tend to destroy Property T. Alternatively, one can attempt to use polygons of groups where vertex groups have Property T, with suitable spectral conditions on links of vertices, but such constructions tend to produce relatively compact subgroups of $SL(n, \mathbb{R})$.

Note that the property τ (with respect to the family of finite index normal subgroups which are kernels of homomorphisms to $SL(n, \mathbb{Z}/q\mathbb{Z})$) holds for thin subgroups of $SL(n, \mathbb{Z}), n \geq 3$, see [9].

For the next question, recall that standard proofs of the Tits Alternative yield Zariski dense free subgroups of the given semisimple Lie group G.

Definition 29.0.3. A free subgroup $\Gamma < G$ is hereditarily Zariski dense (or strongly dense, see [12]) if every noncyclic subgroup of Γ is Zariski dense in G.

The following problem is raised in [12]:

Question 29.0.29 (Breuillard, Green, Guralnick, Tao)**.** Is it true that every Zariski dense subgroup of a real semisimple Lie group G contains a hereditarily Zariski dense free subgroup? If so, is there a quantitative version of this result?

It appears that the only case when the affirmative answer is known is when G is 3-dimensional (in which case it is an immediate corollary of the Tits Alternative).

Characterization of higher rank lattices

Definition 29.0.4 (Prasad–Raghunathan rank)**.** Let Γ be a group. Let A_i denote the subset of Γ that consists of those elements whose centralizer contains a free abelian group of rank at most i as a subgroup of finite index. Thus, $A_0 \subset A_1 \subset \ldots$. The Prasad–Raghunathan rank, $\mathrm{prank}(\Gamma)$, of Γ is the minimal number i such that $\Gamma = \gamma_1 A_i \cup \cdots \cup \gamma_m A_i$ for some $\gamma_1, \ldots, \gamma_m \in \Gamma$.

For instance, if Γ is a lattice in a semisimple Lie group of rank n, then $\mathrm{prank}(\Gamma) = n$. If M is a compact Riemannian manifold of nonpositive curvature with $\Gamma = \pi_1(M)$, then $\mathrm{prank}(\Gamma)$ equals the geometric rank of M, i.e. the largest n such that every geodesic in M is contained in an immersed n-dimensional flat.

Definition 29.0.5 (BGP, Bounded Generation Property)**.** A group Γ is said to have BGP if there exist elements $\gamma_1, ..., \gamma_k$ such that every $\gamma \in \Gamma$ can be written as a product

$$\gamma = \gamma_1^{n_1} \gamma_2^{n_2} \cdots \gamma_k^{n_k}$$

for some $n_1, ..., n_k \in \mathbb{Z}$. (Note that a power of each γ_i appears only once.)

Question 29.0.30 (G. Prasad)**.** Does there exist a discrete Zariski dense subgroup $\Gamma < G$ (with G a simple real algebraic group) such that Γ is not a lattice but $\mathrm{prank}(\Gamma) = rank_{\mathbb{R}}(G)$?

Question 29.0.31 (M. Kapovich)**.** What algebraic properties distinguish higher rank (irreducible uniform) lattices?

For instance, such groups Γ have Prasad–Raghunathan rank, $\mathrm{prank}(\Gamma) \geq 2$. Are there discrete linear groups Γ which are not virtually nontrivial direct products and are not lattices, satisfying $\mathrm{prank}(\Gamma) \geq 2$? In the case of groups Γ of integer points of split semisimple algebraic groups over $\mathbb{Z}$, a defining feature are the Serre relators. However, Serre relators are for unipotent elements, which do not exist in uniform lattices. Uniform higher rank lattices satisfy approximate Serre relators. Do these determine whether a discrete linear group is a higher rank lattice?

Notice that there are some indirect signs that an algebraic characterization of lattices is possible:

1. Higher rank lattices are quasiisometrically rigid (Kleiner & Leeb [28], Eskin [17]).
2. Higher rank lattices are rigid in the sense of the 1st order logic (Avni, Lubotzky, Mieri [2]).
3. Appearance of Serre relators in profinite completions, (Prasad, Rapinchuk [39]).

The situation is not entirely clear even for nonuniform lattices. Many classes of higher rank nonuniform lattices satisfy the BGP. Nonlinear groups that satisfy the BGP were constructed by A. Muranov [34].

Question 29.0.32 (M. Kapovich)**.** Suppose that Γ is an abstract (infinite) $\mathbb{R}$-linear group satisfying the BGP. Is it isomorphic to a lattice in a Lie group?

Problem 29.0.33 (M. Mj)**.** Does $SL(3, \mathbb{Z})$ have the bounded generation property with respect to semisimple elements? I.e., is there a collection of k semisimple elements $g_1, ..., g_k \in SL(3, \mathbb{Z})$ such that every element of $SL(3, \mathbb{Z})$ has the form

$$g = g_1^{n_1} ... g_k^{n_k}?$$

Conjecturally, the answer is negative (for dynamical reasons related to ping-pong arguments) which should pave the way to prove that uniform lattices do not have bounded generation property.

Why are higher rank lattices super-rigid?

One way to say that an abstract group Γ is super-rigid is to require that for every field F and $n \in \mathbb{N}$, there are only finitely many conjugacy classes of representations $\Gamma \to GL(n, F)$. Of course, some groups do not admit any nontrivial linear representations, so it makes sense to restrict the discussion to finitely generated linear groups Γ.

Loosely speaking, such a group is (super) rigid if it satisfies some peculiar relators. There are many proofs of rigidity and super-rigidity of (higher rank irreducible) lattices, but none of these proofs (in the setting of uniform lattices) use relators satisfied by lattices, likely because such relators are simply unknown (see previous section). In contrast, there are known proofs of super-rigidity of some classes of higher rank non-uniform lattices (see [41] and references therein).

Question 29.0.34 (M. Kapovich)**.** What are group-theoretic reasons that make higher rank uniform lattices (super)-rigid? Are the approximate Serre relators responsible for this? Or high Prasad-Raghunathan rank?

The only known result in this direction is that the BGP implies super-rigidity, see [37].

Presentation Highlights

Suhyoung Choi (KAIST, Daejeon, Korea)
"Closed affine manifolds with partially hyperbolic linear holonomy"

The overall goal to show that closed manifolds of negative curvature do not admit complete special affine structures whose linear parts are partially hyperbolic in the dynamical sense. Furthermore, they should not admit complete affine structures with semi-simple P-Anosov linear holonomy groups.

Jeff Danciger (University of Texas, Austin)
"Affine actions with Hitchin linear part"

Properly discontinuous actions of a surface group on $\mathbb{R}^d$ by affine transformations were shown to exist by Danciger–Gueritaud–Kassel. In the talk, representing a joint work with Tengren Zhang, it is shown, however, that if the linear part of an affine surface group action is in the Hitchin component, then the affine action is not properly discontinuous. The key case is that of linear part in $\mathrm{SO}(n, n-1)$, so that $\mathbb{R}^d = \mathbb{R}^{n,n-1}$ is the model for flat pseudo-Riemannian geometry of signature $(n, n-1)$. Here, the translational parts determine a deformation of the linear part into $\mathrm{SO}(n, n)$ Hitchin representations and the crucial step is to show that such representations are not Anosov in $\mathrm{SL}(2n, \mathbb{R})$ with respect to the stabilizer of an n-plane.

Alla Detinko (University of Hull, Hull, UK)
"Zariski density and computing with infinite linear groups"

This talk, presenting a joint work with Dane Flannery and Alexander Hulpke, describes recent developments in a novel domain of computational group theory: Computing with infinite linear groups. Special consideration is given to algorithms for Zariski dense subgroups. This includes a computer realization of the strong approximation theorem, and algorithms for arithmetic groups. These methods are then applied to the solution of problems further afield by computer experimentation.

Cornelia Drutu (Oxford University, Oxford, UK)
"Effective equidistribution of expanding horospheres"

The topic of the talk is a result of effective equidistribution of a special family of expanding horospheres (modulo $SL(d, \mathbb{Z})$) in the locally symmetric space of positive definite quadratic forms of determinant one on $\mathbb{R}^d$ modulo $SL(d, \mathbb{Z})$. The proof uses uniform lattice point asymptotics for compact sets of d-dimensional dilating ellipsoids.

Anna Felikson (Durham University, Durham, UK)
"Coxeter groups, quiver mutations and hyperbolic manifolds"

Mutations of quivers were introduced by Fomin and Zelevinsky in the beginning of 2000's in the context of cluster algebras. Since then, mutations appear (sometimes completely unexpectedly) in various domains of mathematics and physics. Using mutations of quivers, Barot and Marsh constructed a series of presentations of finite Coxeter groups as quotients of infinite Coxeter groups. The talk, presenting a joint work with Pavel Tumarkin, describes a generalization of this construction leading to a new invariant of bordered marked surfaces, and a geometric interpretation: It occurs that presentations constructed by Barot and Marsh give rise to a construction of geometric manifolds with large symmetry groups, in particular to some hyperbolic manifolds of small volume with proper actions of Coxeter groups.

Ilya Gekhtman (University of Toronto, Toronto)
"Gibbs measures vs. random walks in negative curvature"

The ideal boundary of a negatively curved manifold naturally carries two types of measures. On the one hand, we have conditionals for equilibrium (Gibbs) states associated to Hölder potentials; these include the Patterson-Sullivan measure and the Liouville measure. On the other hand, we have stationary measures coming from random walks on the fundamental group.

The talk, based on a joint work with Gerasimov–Potyagailo–Yang and, partly, on a joint work with Tiozzo, aims to compare and contrast these two classes. First, it is shown that both of these of these measures can be associated to geodesic flow invariant measures on the unit tangent bundle, with respect to which closed geodesics satisfy different equidistribution properties. Second, we show that the absolute continuity between a harmonic measure and a Gibbs measure is equivalent to a relation between entropy, (generalized) drift and critical exponent, generalizing previous formulas of Guivarc'h, Ledrappier, and Blachere–Haissinsky–Mathieu. This shows that if the manifold (or more generally, a $\mathrm{CAT}(-1)$ quotient) is geometrically finite but not convex cocompact, stationary measures are always singular with respect to Gibbs measures.

A major technical tool is a generalization of a deviation inequality due to Ancona saying the so called Green distance associated to the random walk is nearly additive along geodesics in the universal cover.

Dmitry Kleinbock (Brandeis University, Waltham, MA)
"Khintchine-type theorems via L^2 estimates for Siegel transform"

Recently there has been a surge of activity in quantifying the density of values of generic quadratic forms at integer points. The talk, presenting a joint work with Mishel Skenderi, describes some new and quite general results in this direction obtained via the so-called Siegel–Rogers method, which has recently been utilized by Athreya and Margulis, and later by Kelmer and Yu.

Alex Kontorovich (Rutgers University, New Brunswick)
"Sphere Packings and Arithmetic"

The talk describes recent progress in understanding Apollonian-like sphere packings and more general objects, with connections to arithmetic hyperbolic groups, both reflective and non-reflective.

Arie Levit (Yale University, New Haven)
"Quantitative weak uniform discreteness"

This talk, based on a joint work with Gelander and Margulis, describes a quantitative variant of the Kazhdan–Margulis theorem generalized to probability measure preserving actions of semisimple groups over local fields.

Michael Lipnowski (McGill University, Montreal)
"Building grids on $\Gamma\backslash X$ for $\Gamma < \mathrm{SL}_n(\mathbb{Z})$ admitting membership testing"

This talk, presenting a joint work with Aurel Page, describes an algorithm for building grids in metric spaces (M, d_M). The algorithm uses repeated computations of (cutoff) distances $\min\{1, d_M\}$; computations are illustrated in the case of the locally symmetric space of lattices in $\mathbb{R}^n$. A pessimistic outlook of these results for locally symmetric spaces $G(\mathbb{Z})\backslash G(\mathbb{R})/K$, when $G(\mathbb{Z})$ satisfies the congruence subgroup property: The membership testing for finitely generated subgroups of $G(\mathbb{Z})$ is harder than certifying thinness. An optimistic outlook of these results for the same $G(\mathbb{Z})$ is that it gives a prospect for certifying thinness for finitely generated subgroups.

Beibei Liu (Max Plank Institute for Mathematics, Bonn)
"Hausdorff dimension and geometric finiteness in hyperbolic spaces"

Geometric finiteness is a nice property that discrete isometry group of a hyperbolic space can have. One way to define geometric finiteness is to require that the limit set of the group consists of conical limit points and parabolic fixed points. In the talk, it is shown that the limit sets of geometrically infinite Kleinian groups contain continuum of nonconical limit points. One can ask questions relating the measure-theoretic size of the limit set, conical limit set or non-conical limit set, in relation to the geometric finiteness. The talk reviews some recent results and conjectures about Kleinian groups with small Hausdorff dimension, and small critical exponents.

Sara Maloni (University of Virginia, Charlottesville)
"The geometry of quasi-Hitchin symplectic Anosov representations"

Quasi-Hitchin representations in $\mathrm{Sp}(4, \mathbb{C})$ are deformations of Fuchsian (and Hitchin) representations which remain Anosov. These representations acts on the space $\mathrm{Lag}(\mathbb{C}^4)$ of complex lagrangian grassmanian subspaces of $\mathbb{C}^4$. This theory generalizes the classical and important theory of quasi-Fuchsian representations and their action on the Riemann sphere $\mathbb{C}P^1 = \mathrm{Lag}(\mathbb{C}^2)$. The talk (based on a joint work with D.Alessandrini and A.Wienhard) reviews the classical theory as well as the geometry and topology of quasi-Hitchin representations, In particular, it is shows that the quotient of the domain of discontinuity for this action is a fiber bundle over the surface and fibers are described. The fibration map comes from an interesting parametrization of $\mathrm{Lag}(\mathbb{C}^4)$ as the space of regular ideal hyperbolic tetrahedra and their degenerations.

Giuseppe Martone (University of Michigan, Ann Arbor)
"Sequences of Hitchin representations of tree-type"

In this talk some non-trivial sufficient conditions are described for diverging sequences of Hitchin representations, whose limits in the Parreau boundary is given by an action on a tree. These non-trivial conditions are given in terms of Fock-Goncharov coordinates on moduli spaces of positive tuples of flags.

Chen Meiri (Technion, Haifa, Israel)
"First order rigidity of higher-rank arithmetic groups"

In many contexts, there is a dichotomy between lattices in Lie groups of rank one and lattices in Lie groups of higher-rank. In the talk, based on joint works with Nir Avni and Alex Lubotzky, some manifestations of this dichotomy are described in the context of the Model Theory.

Plinio Murillo (KIAS, Seoul, Korea)
"Systole growth on arithmetic locally symmetric spaces"

The systole of a Riemannian manifold is the shortest length of a non-contractible closed geodesic. The purpose of this talk is to survey recent results in systole growth along congruence covers of arithmetic manifolds, and how this information interact with the geometry and the topology of the covers.

Joan Porti (Universitat Autònoma de Barcelona)
"Twisted Alexander polynomials and hyperbolic volume for three-manifolds"

Given a hyperbolic 3-manifold with cusps, one considers the composition of a lift of its holonomy in $\mathrm{SL}(2,\mathbb{C})$ with the irreducible representation in $\mathrm{SL}(n,\mathbb{C})$, that yields a twisted Alexander polynomial $A_n(t)$, for each natural n. In the talk (based on a joint work with L.Bénard, J.Dubois and M.Heusener), it is proven that, for a complex number z with norm one, $\log|A_n(z)|/n^2$ converges to the hyperbolic volume of the manifold divided by 4π, as $n \to \infty$. This generalizes and uses a theorem of W. Mueller for closed manifolds on analytic torsion.

Andrei Rapinchuk (University of Virginia, Charlottesville)
"Eigenvalue rigidity for Zariski-dense subgroups"

This talk is a progress report on the work of Gopal Prasad and Andrei Rapinchuk focused on a new form of rigidity, called the eigenvalue rigidity. The latter is based on the notion of weak commensurability of Zariski-dense subgroups of semi-simple algebraic groups introduced in [38], which provides a convenient way of matching the eigenvalues of semi-simple elements of these subgroups. A detailed analysis of this notion for arithmetic groups allows to resolve some long-standing problems about isospectral compact locally symmetric spaces. Currently, there is growing evidence that some key results can be extended from arithmetic groups to arbitrary finitely generated Zariski-dense subgroups, yielding thereby certain rigidity statements, based on the eigenvalue information, in this generality (including the situations where the subgroups at hand are free groups). This work has led to new directions of research in the theory of algebraic groups, one of which is the analysis of forms of a given absolutely almost simple algebraic group that have good reduction at a given set of discrete valuations of the base field.

Igor Rapinchuk (Michigan State University, East Lansing)
"Abstract homomorphisms of algebraic groups and applications"

This talk presents several results on abstract homomorphisms between the groups of rational points of algebraic groups. The main focus will be on a conjecture of Borel and Tits formulated in their landmark 1973 paper. The presented results settle this conjecture in several cases; the proofs make use of the notion of an algebraic ring. Several applications are given to character varieties of finitely generated groups and representations of some non-arithmetic groups.

Nicolas Tholozan (ENS, Paris)
"Exotic compact quotients of pseudo-Riemannian symmetric spaces"

Let M be a Gromov-Thurston manifold. This talk, presenting a joint work with Daniel Monclair and Jean-Marc Schlenker, describes a construction of proper and cocompact actions of the fundamental group of M on a certain pseudo-Riemannian symmetric space. The talk also explain how the construction relates to the existence of a globally hyperbolic anti-de Sitter manifold with Cauchy hypersurface homeomorphic to M.

Kostas Tsouvalas (University of Michigan, Ann Arbor)
“Characterizing Benoist representations by limit maps”

Anosov representations of word hyperbolic groups form a rich class of discrete subgroups of semisimple Lie groups, generalizing classical convex cocompact groups of real rank one Lie groups. A large class of projective Anosov representations are Benoist representations. This talk, presenting a joint work with Richard Canary, gives a characterization of Benoist representations in terms of the existence of limit maps.

Tengren Zhang (National University of Singapore)
“Regularity of limit curves of Anosov representations”

Anosov representations are representations of a hyperbolic group Γ to a non-compact semisimple Lie group that are “geometrically well-behaved.” In the case when the target Lie group is $\mathrm{PGL}(d, \mathbb{R})$, these representations admit a limit set in the $d-1$ dimensional projective space that is homeomorphic to the boundary of Γ. In this talk, presenting a joint work with A. Zimmer, under some irreducibility conditions, necessary and sufficient conditions are given for when this limit set is a $C^{1,a}$ submanifold.

Andrew Zimmer (Louisiana State University, Baton Rouge)
“Convex co-compact actions of projective linear groups”

This talk, presenting a joint work with Mitul Islam, describes some results concerning convex cocompact subgroups of the projective linear group (as defined by Danciger–Guéritaud–Kassel). These are a special class of discrete subgroups which act convex cocompactly on a properly convex domain in real projective space. In the case when the subgroup is word hyperbolic, these are well studied objects: The inclusion representation is actually an Anosov representation. The non-hyperbolic case is less understood and is the main focus of the talk.

Outcome of the Meeting

Due to late cancellations, the number of participants was 31 instead of the planned 42, but there was a general consensus that the size of the group led to even closer interactions and more focused discussion than is common at such meetings. Some progress was made on problems raised at the meeting, but it is too early to predict the full impact on new research and collaborations from the meeting. Suffice it to say that in conversations at the meeting and since, participants have described the meeting as having been unusually successful.

Participants

Choi, Suhyoung (Korea Advanced Institute of Science and Technology)
Danciger, Jeffrey (University of Texas - Austin)
Detinko, Alla (University of Hull)
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Tholozan, Nicolas (Ecole Normale Supérieure)
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Two-day Workshop Reports

Chapter 30

First Year Mathematics Repository Workshop (19w2256)

February 8 - 10, 2019

Organizer(s): Veselin Jungić (Simon Fraser University), Miroslav Lovrić (McMaster University)

Overview

In the workshop attendance were 24 participants, representing 12 Canadian universities: University of Alberta, University of Calgary, University of Victoria, University of Fraser Valley, Simon Fraser University, University of Regina, Mount Royal University, University of Manitoba, Queen's University, University of Toronto Mississauga, University of Waterloo, and McMaster University.

The workshop was an important event within an ongoing National dialogue on the present and future of teaching first-year mathematics at Canadian universities. The dialogue, initiated by the worksop organizers [2], takes different forms: from informal meetings of colleagues from the same department to discussions and exchanges of ideas over social media; and from conducting surveys and writing academic papers to regional and national workshops and conferences. The workshop was built on, and informed by, the outcomes of the CMS Winter Meeting Education session in Waterloo, Ontario (9 December 2017) and the First Year University Mathematics Across Canada: Facts, Community and Vision conference at the Fields Institute in Toronto, Ontario (27-29 April 2018). The follow-up events are planned at the University of Alberta (3-5 May 2019) and the University of Toronto Mississauga (22-24 May 2020). For the summary of the conference at the Fields Institute please see [1].

The themes that were addressed in the plenary sessions, working groups and other activities related to the so-called "service courses," perhaps best described as (often massive) courses offered by mathematics departments that serve students other than mathematics or statistics majors. 'How do different institutions and different instructors find the balance between introducing a relatively complex math content and meeting the needs of the specific program that the course "services"?'was the guiding question. More specifically, the workshop participants addressed the following questions:

1. What makes a math/stats service course program specific, and what are the challenges?
2. To what extent (if at all) are the service courses outcomes of the collaborations between the department of mathematics and/or statistics and another academic unit?
3. How do we address the diversity of the student populations within service courses?
4. What are the available learning resources for service courses?

The BIRS workshop also served as a crucial step in further promotion and development of The First Year Mathematics and Statistics Courses Repository, a resource supporting an ongoing national dialogue about teaching first-year mathematics and statistics at Canadian universities.[3] This shareable dynamic online database contains extensive data, collected from mathematics instructors across the country, including course content, resource and technology used, learning outcomes, modes of delivery, connections with other courses, as well as informal descriptions of various practices in teaching these courses.

We were able to achieve our main goal to bring together a group of the university mathematics teaching practitioners from across Canada that shared their experiences, views, and approaches to teaching mathematics among themselves, but also with the broader community by critically reviewing data already contained in the repository, providing feedback on the content and functionality of the database, and contributing new content.

Workshop Activities and Discussion

The Banff workshop started on Friday, 8 February, in the afternoon. Although no formal activities were planned, the time was used for introductions and much needed socializing and informal conversations. As is well known (and thus was built into the workshop), many important discussions, exchanges of views and ideas, and building of foundations for future collaborations take place outside of the formal workshop/conference activities. The lounge in Corbett Hall, the fireplace area in particular, proved to be an ideal facilitator for this. Moreover, this informality encouraged openness and the depths of critique that were definitely embraced by the participants, who are weary of daily feeds of statements, documents, and views (mis)guided by university branding proclamations, public relations departments, and political correctness.

The workshop was built on the idea that each participant gets the opportunity to voice their opinion about any of the discussion topics and/or initiate discussion about any relevant new topic. This was achieved by structuring the workshop rather as an *experience* equally owned by each attendee than as a rigid schedule driven sequence of events. For us, as the organizers, it was particularly important to establish the atmosphere of the collegiality, mutual respect, and trust from the very beginning of our meeting. In our view, only in that kind of environment a group of the workshop participants as diverse as our group was could have an honest in depth discussion about the complex issue of teaching first year math courses. For example, the group included some of the leading Canadian post-secondary educators, but also some of the young faculty that are just at the beginning of their teaching careers. We are very proud of the fact that in the attendance we had the same number of the female and male colleagues. We represented Canadian post-secondary institutions *A Mari usque ad Mare*, and occasionally shared unflattering facts about some of our institutions' practices.

The true unifying factor for the group was our shared commitment to support our students in achieving their academic goals and to, by transferring our knowledge of and passion for mathematics to our students, meet our share of responsibility in ensuring that the next generation of scholars holds the torch of mathematics high.

The workshop activities were roughly divided in five categories:

- Plenary talks (3 hours)
- Plenary discussions (4 hours)
- Working groups' discussions (3 hours)
- Math showcase (1.5 hours)
- Social events including meals (10 hours)

The four working groups were as follows:

- Service courses for physical sciences and engineering students;
- Service courses for arts, humanities, social sciences, and business students;
- Service courses for mathematics education students;
- Service math and stats courses for life sciences students.

Each group had one or two *captains* assigned as moderators with the additional duty to provide a report about their working group discussion.

We are happy to report that each workshop participant fully participated in all segments of the workshop.

Instead of commenting on the workshop activities one-by-one, we present some major points that were discussed. Although service courses "service" thousands of students, they are not given the attention, nor resources that they deserve and need, by their home departments or faculties. (Some participants argued that there would be no math and stats departments without the money that the service courses earn.) Junior faculty and sessional instructors, who often teach such courses, are given large teaching loads (5 or up to 7 courses per academic year) with demands on their time that are so severe that they leave very little (or no) time for anything else. However, in spite of this, and with their work penetrating deep into their private and family lives, they innovate, experiment, and put energy into improving the courses they teach. Given extra time, we all could do a lot more – for instance, to have an informed design of a service course, we must communicate with the members of relevant departments across campus. This does not involve a couple of meetings, but rather a continuous effort.

The applications of mathematics and statistics taught in a service course need to be authentic to the students in order for the service course to have value. Needless to say, we are not assuming that a service course for life scientists will educate future researchers in mathematical biology, but can nevertheless bring the applications we study closer to reality. In presenting mathematical and statistical models in our courses, we need to be clear about the assumptions that were made, and about the limitations, both with regards to the situation modeled and the mathematical/ statistical tools used.

Presentation Highlights

Brian Forrest, University of Waterloo:

Things are changing in the math ed community across Canada, it is getting younger. Ph.D. students are becoming more and more serious about the teaching aspects of their education as graduate students.

Young research faculty are under heavy demands and are under pressure to focus on "research first and teaching second".

At Waterloo a significant proportion of service courses are taught by Lecturers, many who are under contract, or post-docs or graduate students (who are not invested in development and innovation).

Gerda de Vries, University of Alberta:

What do/should/can we teach?

- We should have a much wider variety of courses rather than pumping everyone through Calculus.
- Perhaps more specialized courses on abstract mathematical thinking and reasoning.
- There is an expectation for more applied content in specialized calculus courses, yet also the expectation that these courses are interchangeable, leading to courses that are packed with content.

How do/should/can we teach?

- People are starting to experiment with different methods (like blended learning).

How do/should/can we assess?

- We need to get better at articulating what students need to be able to do when they come out of our courses.
- Institutions seem to be moving towards more frequent term assessments, and lower stakes final exams BUT more classes with more frequent assessments can lead to never ending assessments for students.
- There are interesting ways to do mark breakdowns or exam regulations to combat cheating on term work.

Kseniya Garschusk, University of the Fraser Valley, and Andie Burazin, University of Toronto Mississauga:

One definition of a service course is "any course that is included in a program in order to achieve the objectives of the program that is provided by a school other than the school that owns the program".

Learning objectives should be a conversation and collaboration between those who need the course and those who teach the course. Ultimately, however, it is the math departments? responsibility to design and deliver a math course.

Is it important to teach mathematics as a mental activity for critical thinking, or delivering only the mathematical content that is required?

- Both are important, both have value, both are intertwined.
- Too much focus on techniques can lose the focus on the concepts behind those techniques.

Who should teach the services courses?

- It depends on the person, and it depends who you ask.
- Traditional disciplinary boundaries are disappearing, reinforcing the need for communication.

- Some universities have actually hired 'outside' experts (like physicists or biologists) to teach service courses within the mathematics departments.
- We can lose credibility if our 'application' problems are not accurate with respect to their own discipline.
- We can standardize foundational material, and leave the rest flexible to context.
- Blended learning can be used to address the content vs concept dichotomy.

Outcome of the Meeting

Here is a brief summary of the main conclusions of the workshop:

- Math and Stats departments must pay lot more attention to their service courses.
- Service courses provide unique opportunities to teach mathematics that is interesting, exciting, and stimulating, and that addresses authentic life situations. This is where we are forced to re-think the mathematics content, to benefit not only service courses, but all math courses.
- Service courses are mostly taught by younger instructors; often they are on limited-term contracts or hold more permanent, but non-tenure track positions.
- Instructors teaching service courses bring huge amounts of enthusiasm and energy into their courses. They are willing to experiment with a variety of pedagogical approaches and technology (plenty of evidence to this presented at the workshop).
- A successful design of a service course requires continuous communication with faculty in all departments whose students will be taking the course. Course design is an intense, time-consuming process, and those involved in the design should be given time necessary to develop the course.
- Much-needed innovation in math and stats instruction happens in service courses! This is a major reason why math and stats departments across the country should pay more attention to these courses, as well place more resources (human and money) into them.
- For the reasons mentioned above and given the stigma that comes with the attribute "service," it might be a good idea to find a more suitable name; for instance, to rename "service courses" into "mathematics and statistics courses," and refer to their complement as "courses for mathematics and statistics majors."

The next iteration of the national dialogue about teaching the first year math courses in Canada will be hosted by the University of Alberta, Edmonton, AB, between May 3-5, 2019. In 2020, the conference will be hosted by the University of Toronto Mississauga.

Participants

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Chibry, Nancy (University of Calgary)
Coles, Matthew (University of British Columbia)

Davidson, Michelle (University of Manitoba)
de Vries, Gerda (University of Alberta)
DeDieu, Lauren (University of Calgary)
Desaulniers, Shawn (University of Alberta)
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Chapter 31

Precise Computation of Quantum Amplitudes (19w2241)

April 5 - 7, 2019

Organizer(s): Andrzej Czarnecki (Department of Physics, University of Alberta)

Overview of the Field

Quantum amplitudes are needed to predict probabilities and properties of physical processes such as atomic transitions and scattering and decay of elementary particles. Comparisons of such predictions with measurements improve the knowledge of fundamental constants such as particle masses and strengths of interactions, and probe for new phenomena beyond the current theory.

In order to fully exploit the precision of contemporary experiments, amplitudes have to be computed with high-order of quantum effects. For example, in the language of Feynman diagrams, multiple loops must be included. Recently, significant progress has been achieved in the mathematics involved in such calculations. Tools that are being used include large systems of linear difference equations, asymptotic expansions and singular perturbation theory.

Our group at the University of Alberta is among the world leaders in performing such high-precision calculations. We specialize in the computation of processes involving bound particles. Recently, we made a breakthrough in the calculation of magnetic moment of a bound electron [1]. This workshop was intended to build on this success and prepare methods for the next stage of our research.

Recent Developments and Open Problems

The intention of this workshop was to prepare tools for making theoretical predictions to guide and interpret precise experiments. These experiments search for so-called New Physics, that is for phenomena beyond the currently known subatomic models. They are performed primarily in the United States (for example Mu2e at Fermilab) and in Japan (COMET at J-PARC). The subatomic theory group at the University of Alberta specializes in providing such precise predictions for experiments involving bound elementary particles.

One of the objectives was to define observables that should be predicted first. We identified a group of problems related to decays of a muon bound in an atom. We outlined a plan for a series of projects whose aim is to fully characterize the influence of binding on the distributions of decay products.

Binding is interesting from the mathematics point of view because it is a singular perturbation. It introduces a qualitative change in the spectrum of daughter electrons. The reason for this is the presence of the nucleus which is so heavy in comparison with both the muon and the electron that it can absorb momentum almost without taking up any kinetic energy. As a result, the range of energies of the produced electron almost doubles in comparison with decays of a free muon.

Outcome of the Meeting

An important outcome was the start of a collaboration with Professor Jamil Aslam, who arrived from Islamabad, Pakistan. He is an expert in few-body hadronic and electromagnetic systems.

As our first project we decided on a rare decay of a bound muon. When a muon bound in an atom decays, there is a small probability that the daughter electron remains bound. We set out to evaluate that probability. Surprisingly, a significant part of the rate turned out to be contributed by the negative energy component of the wave function, neglected in a previous study. We found a simple integral representation of the rate. In the limit of close muon and electron masses, an analytic formula was derived. We published this result in [2].

In the near future we plan to extend this work. We want to reveal the mechanism that enhances the negative energy contribution. We also plan to derive a closed formula in the limit of very small electron masses. Numerical fits indicate that this limit is singular, that is the dependence on the small ratio of electron-to-muon masses is logarithmic, rather than an integer power. This is another example of a singular perturbation: even though the electron mass is much smaller than the muon mass, it cannot be neglected without a qualitative change of the process. Namely, without the finite mass, the electron would not be bound in the atom: the so called Bohr radius is inversely proportional to the electron mass and tends to infinity when the electron mass tends to zero.

Participants

Aslam, Muhammad Jamil (University of Alberta)
Czarnecki, Andrzej (University of Alberta)

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Chapter 32

Biological Tissue Mathematical Constitutive Models in Human Body Models for Enhanced Human Safety (19w2266)

April 12 - 14, 2019

Organizer(s): D. Cronin (University of Waterloo, Canada), M.B. Panzer (University of Virginia, United States), J. Combest (Global Human Body Models Consortium, Nissan, United States), C. Simms (Trinity College, Dublin, Ireland), D. Gierczycka (University of Waterloo, Canada)

Overview of the Field

Improving safety for human vehicle occupants and vulnerable road users is critical to reduce severe injuries that may lead to fatalities, and low–severity injuries with high societal cost and long–term consequences to quality of life [1]. Computational Human Body Models (HBM) provide a new paradigm for improving human safety through enhanced understanding of injury causation leading to improved safety systems and reduction of injury in impact scenarios [2, 3].

HBMs have evolved significantly over the past decade owing to advanced imaging techniques providing detailed anatomy, high–performance computing enabling large models needed to represent the human body at the tissue level, and the availability of accurate vehicle models and restraint systems to simulate real crash scenarios. However, much of the current research and development for HBM relies on the use of existing biological material data (e.g. stress–strain response for individual tissues) and the implementation of this data in appropriate constitutive models. Biological materials have well–known characteristics of being non–linear, viscoelastic, anisotropic, heterogeneous, and highly variable from person to person. These characteristics, often unquantified in the literature, pose both analytical and numerical challenges when used for simulating impact and injury. Furthermore, owing to the focal nature of impact in crash scenarios, including high deformation rates (up to $\sim$1000 1/s) and large deformations, special requirements exist for numerical stability and accurate representation of material response. Recently, interest in varying occupant postures and positions within the vehicle associated with autonomous vehicles and driver assist systems (e.g. automated braking) have resulted in the need to simulate the human body before impact in loading conditions separate from impact (such as active musculature response, repositioning and unloading in tissues). In addition, there is large variability in the published experimental data and testing methods for tissues which further compounds these challenges. Thus, there is a need to arrive at generally accepted procedures, properties and constitutive models that can be used to model tissues in contemporary HBM.

Workshop Objectives

The overall objective of this workshop was to collaborate with academic and industry experts in the field of computational HBM to discuss the current state of the science on the types of biological tissue models used in current HBMs, the status of material properties in the literature, and the opportunities for improved constitutive models to enhance HBM response and injury prediction. There were four specific aims of the workshop:

1. Review the current state–of–the–art constitutive models and material data for hard and soft tissues, and identify key limitations. This objective was achieved through contributed presentations from the participants, followed by broad and focused group discussions.
2. Investigate current mathematical formulations of constitutive models and discuss the benefits of constitutive model formulations with respect to representation of properties, computational efficiency, and numerical stability at high deformation rates and large deformations.
3. Collaboratively develop a framework for evaluating, verifying and validating proposed constitutive models and implementations.
4. Create a strategy for implementing new constitutive models or material data into HBM and organize follow–on meetings to discuss the outcomes from the workshop.

Presentation Highlights and Scientific Progress Made

The workshop included 24 formal presentations on topics ranging from a broad overview of the state–of–the–art and future directions; to whole body models and validation with experimental data; to constitutive model development and tissue testing; to body region modeling such as the head, neck and spine modeling; to soft tissue modeling such as flesh and adipose tissue; and to numerical challenges and best–practices for HBM. The presenters included academics, industry and students. Two break–out sessions, were held with three groups of 8 participants including three group leaders. The first break–out session identified current challenges in HBM, while the second session led to identification of strength and challenges in this field along with future directions. The breakout session discussions were summarized and shared with the workshop participants.

Outcome of the Meeting

The meeting was a unique opportunity to assemble a diverse group of international experts from academia and industry to discuss the current state of knowledge and to identify challenges. Experts from many countries (Canada, USA, Mexico, United Kingdom, Sweden, Austria, Czech Republic) came together to discuss the development, validation and application of HBMs, and to address a critical need for improved biological tissue mathematical models required for widespread use of these models with particular interest in improving human safety in transportation. This was the inaugural meeting of this group, and the overall consensus was that this type of workshop was needed for the trauma biomechanics research community. Furthermore, the group identified that:

1. the current technical challenges in modeling techniques for soft tissues is a major limiting component in advancing contemporary HBMs,

2. that more experimental tissue data tested in appropriate loading regimes is required for improving the accuracy of the HBMs,

3. that formalized "best practice" protocols are needed for the implementation and use of constitutive models for HBM.

The participants were encouraged by the progress made at this meeting and by the potential for future meetings to continue to working towards common goals. Based on this feedback, a meeting of the group organizers is scheduled for the fall of 2019 to plan for the next steps.

Participants

Adanty, Kevin (University of Alberta)
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Barker, Jeffrey (University of Waterloo)
Combest, John (Nissan, Global Human Body Models Consortium)
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Chapter 33

2019 Ted Lewis SNAP Math Fair Workshop (19w2267)

April 26 - 28, 2019

Organizer(s): Sean Graves (University of Alberta), Tiina Hohn (MacEwan University), Ted Lewis(SNAP Mathematics Foundation & U of Alberta), Trevor Pasanen(University of Alberta)

Introduction

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 presenters mostly consisted of teachers/educators who shared their math fair experiences and success stories. We also had talks about some current research that is taking place in Alberta (University of Alberta and University of Calgary).

This year, two math educators (Maria Omar and Trent Worthington) who hosted their first math fairs in the past two years were able to share their experiences. Maria Omar helps to coordinate a homeschool network called SHiNE (Society for the Homeschool Network of Edmonton). It was great to see how Math Fair could be implemented with this group of very diverse students. Both teachers had marvelous comments about SNAP Math Fairs and are now promoting the idea to other teachers in their respective communities.

2019 Workshop Highlights

We saw a myriad of presentation topics and presentation styles, the only constant was the passion. Two of the main ideas taken from the workshop are the following:

1. Teaching, especially in elementary years, is a very complicated and complex job. Teachers are obliged with the overwhelming task of educating our youth in several curricular subjects, fine and gross motor skills, dealing with emotions, and the list is enormous. In fact the job of a teacher is getting more complex every year and this, as well as increasing classroom sizes and diverse students clearly contributes to the high attrition rate of the profession.

   There is an enormous amount of resource material (in math alone) available for teachers and they do not have enough time to sift through it. It sounds like teachers, especially ones that are early in their careers, would appreciate a primary detailed resource that could guide them through the programs of studies.

2. Play is vital for young learners, this is a big selling point of Math Fair. Another benefit is the cross-curricular opportunities that Math Fair can promote. Thirdly Math Fair promotes opportunities for students to learn and practice communication skills - which seem to be diminishing in our youth.

2019 Workshop Feedback

”I thought the workshop was very good. Some of the presentations covered material that was broader than I expected and did not deal specifically with math fairs. It showed what some people were interested in - namely what ways of presenting or teaching math might help teachers.”

”I appreciated Trent’s presentation and conversations about how incredibly useful he thought math fairs were. They tied math fairs in with the rest of the curriculum, and they came directly from a school teacher.”

Participants

Bowling, Suzanne (Edmonton Public Schools)
Desaulniers, Shawn (University of Alberta)
Farquharson, Keenan (University of Alberta (student))
Francis, Krista (University of Calgary)
Gold Bennett, Ayanna (University of Alberta (undergraduate student))
Graves, Sean (University of Alberta)
Hoffman, Janice (Edmonton Public Schools)
Hohn, Tiina (MacEwan University)
Jones, Carolyn (Edmonton Public Schools - Centre for Education)
Khan, Steven (University of Alberta)
Kinasevich, Robin (Edmonton Public School Board)
Lewis, Ted (SNAP Mathematics Foundation & U of Alberta)
Lorway, Geri (Thinking 101/University of Alberta)
Omar, Maria (SHiNEdmonton)
Pasanen, Trevor (University of Alberta)
Wi, Dami (University of Alberta)
Wong, Catherine (Edmonton Public Schools)
Worthington, Trent (Sir George Simpson School)

Chapter 34

Alberta Number Theory Days XI (ANTD XI) (19w2262)

May 10 - 12, 2019

Organizer(s): Dang-Khoa Nguyen (University of Calgary), Wolfgang Riedler (University of Alberta), Lee Troupe (University of Lethbridge), Peng-Jie Wong (University of Lethbridge)

Introduction

Number theory is a broad and central area of research with many connections and applications to other areas of mathematics and science. It is also an extremely active and diverse area of research. The subject may be divided into several subdisciplines that range from pure mathematics, to more applied areas such as cryptography, computational number theory, and mathematical physics. Some of the pure mathematics subdisciplines are algebraic number theory, arithmetic geometry, analytic number theory, automorphic forms, and representation theory.

Alberta Number Theory Days allows for face-to-face discussion between peers and facilitates collaboration between researchers within the province as well as distinguished out of province participants. As our Albertan universities are far from each other, it is impractical to run a weekly or bi-weekly number theory seminar. Instead this conference allows the community of Alberta number theorists to gather once a year to discuss the latest advances in the field, and in their own research. New connections are made and old associations are renewed, and these personal interactions lead to the conception of new projects. It also allows for the exchange of knowledge, which improves the progress of ongoing projects. Another goal is to provide opportunities for young researchers to present some of their early mathematical work.

This was the eleventh edition of Alberta Number Theory Days. Previous conferences took place in Lethbridge (2008), Calgary (2009), and BIRS (2010, 2011, 2013, 2014, 2015, 2016, 2017, 2018). Moreover, in June 2016, the fourteenth meeting of the Canadian Number Theory Association (CNTA) was hosted by the University of Calgary, with approximately 175 participants.

Outcome of the Meeting

This year, the meeting had a total of eleven talks. One was a plenary lecture given by an out-of-province and well-established researcher. Eight talks were given by faculty members and postdocs from UAlberta, UCalgary, ULethbridge, UBC, and UNBC, and two talks were given by graduate students from UAlberta and UCalgary.

Our success in providing early-career researchers with access to a nourishing research environment is reflected in the participant pool. Indeed, out of the 31 participants, 6 were postdoctoral fellows, and 7 were graduate students. All main Alberta number theory centres were well-represented: 7 participants were from Edmonton, 11 were from Calgary, and 8 were from Lethbridge. Comments made in conversations after the conference suggested that we also achieved the goal of improving connections among number theorists in the region.

Diversity and Inclusion

We strive to improve participation of underrepresented groups in mathematics. We are pleased to report that the plenary lecture was given by a female mathematician and that out of the 11 total talks, 4 were delivered by female mathematicians. Out of the 31 participants, 9 were female and 12 were visible minorities as defined by the Government of Canada.

Highlights of the Meeting

The first highlight was the plenary talk given by Dr. Julia Gordon. Dr. Gordon is an Associate Professor at the University of British Columbia. She earned her doctorate at the University of Michigan in 2003 under the supervision of Thomas Hales. She has been recognised by several appointments and awards including: Fields Institute Postdoctoral Fellow in 2003; University of Toronto Postdoctoral Fellow 2004-2006; NSERC Accelerator Award 2015-2018; and the Michler Prize (AWM and Cornell University) in 2017. In 2019, she has been named the recipient of the Krieger-Nelson Prize by the Canadian Mathematical Society for her contributions to mathematics research.

Dr. Gordon works in representation theory of p-adic groups related to the Langlands Programme, motivic integration, the trace formula, and their applications to arithmetic questions. In particular, with R. Cluckers and I. Halupczok, Dr. Gordon used techniques from the theory of motivic integration to derive uniform estimates for orbital integrals, which have applications to certain L-functions. Furthermore, with J. Achter and S.A. Altug, Dr. Gordon applied the theory of motivic integration to connect different ways of computing the sizes of isogeny classes of abelian varieties. This joint work work was the main topic of her inspiring plenary lecture.

In addition to the plenary lecture, there were 10 excellent talks by Sumin Leem (UCalgary), Jonathan Webster (UCalgary), Jack Klys (UCalgary), Adam Topaz (UAlberta), Karol Koziol (UAlberta), Jamie Juul (UBC), Amir Akbary (ULethbridge), Alia Hamieh (UNBC), Nitin Jumar Chidambaram (UAlberta), and Andrew Fiori (ULethbridge).

The plenary lecture and all of the above talks covered many aspects of modern number theory and presented several interesting directions and open problems for future research. Videos of the plenary lecture and several of the talks are available at www.birs.ca/videos/2019. The following are papers related to some talks given at the meeting. Other talks involve ongoing projects for which published papers or preprints are not yet available.

Participants

Akbary, Amir (University of Lethbridge)
Aygin, Zafer Selcuk (Northwestern Polytechnic)
Chidambaram, Nitin Kumar (Max Planck Institute for Mathematics)
Cunningham, Clifton (University of Calgary)
Das, Sourabh (University of Waterloo)
Fever, Amy (The King’s University)
Fiori, Andrew (University of Lethbridge)
Gordon, Julia (University of British Columbia)
Greenberg, Matthew (University of Calgary)
Gunn, Keira (University of Calgary)
Guy, Richard (The University of Calgary)
Hamieh, Alia (University of Northern British Columbia)
Jacobson, Michael (University of Calgary)
Juul, Jamie (Colorado State University)
Kadiri, Habiba (University of Lethbridge)
Klys, Jack (University of Calgary)
Koziol, Karol (University of Alberta)
Leem, Sumin (University of Calgary)
Ng, Nathan (University of Lethbridge)
Nguyen, Dang Khoa (University of Calgary)
Patnaik, Manish (University of Alberta)
Riedler, Wolfgang (University of Alberta)
Roettger, Eric (Mount Royal University)
Scheidler, Renate (University of Calgary)
Shen, Quanli (University of Lethbridge)
Topaz, Adam (University of Alberta)
Tran, Ha (Concordia University of Edmonton)
Troupe, Lee (University of Lethbridge)
Webster, Jonathan (Butler University)
Wong, Peng-Jie (National Sun Yat-Sen University)
Wong, Tian An (University of British Columbia)

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Chapter 35

Innovations in New Instructor Training (19w2231)

June 21 - 23, 2019

Organizer(s): Carmen Bruni (University of Waterloo), Shawn Desaulniers (University of Alberta), Fok-Shuen Leung (University of British Columbia), Pam Sargent (Yale University)

Introduction

Teaching mathematics is a critical component of any mathematician's career. However, instructor training for mathematicians varies widely across institutions. For example, some universities have a mandatory, credit-bearing orientation course for all instructors prior to teaching, where others allow courses to be taught by graduate students with almost no pedagogical training. This diversity gives rise to a number of interesting questions:

- How much training is appropriate for a novice instructor?
- What are key components of effective instructor training?
- What are key techniques of effective instructor training?
- What is the impact of higher quality teaching on undergraduate education?
- How can one deliver effective instructor training under serious financial/logistical constraints?

There is consensus in the research literature — and indeed in common experience — that a strong mathematical background is insufficient to be a good instructor [3, 5]. However, some research also indicates that good instructor training programs can help novice mathematics instructors make great gains in both pedagogy [1, 2] and pedagogical content knowledge [4]. This research is compelling but emergent: the above questions are still very open, especially in the Canadian context and at the institutional level. The purpose of this workshop was to explore instructor training across institutions, and to allow participants to share their experiences and lessons learned.

Workshop themes

Two underlying themes informed the structure of the workshop and much of the discussion at it.

- The first theme was that resources matter. Despite increasing departmental and institutional interest in mathematics instructor training, acquiring funding and finding willing colleagues for training programs is a perennial challenge.
- The second, related theme was that many local successes have been achieved in instructor training. Faculty members at universities across Canada, many of them junior, have collectively developed many innovative, resourceful training components. Though the components have been unevenly evaluated, their impact appears to be significant. One major issue — which this workshop was aimed at alleviating – is that the components constitute a kind of "patchwork quilt" of training programs. Efforts are likely being unnecessarily duplicated.

Presentation Highlights

Productive discussions were present throughout the workshop. We underline here two types of especially beneficial presentations.

- "Ground-level" presentations provided participants the actual experience of being in a component of instructor training. Two standout presentations were given by Kseniya Garaschuk and Amanda Malloch (University of the Fraser Valley and Camosun College) and Lauren DeDieu (University of Calgary), on using programmed role-play and writing exercises to train instructors for a drop-in tutorial centre and a linear algebra course, respectively. The discussions following these ground-level presentations were especially helpful in allowing participants to translate what they just experienced into the context of their home institution.
- "High-level" presentations provided participants insight into the history, administration and other behind-the-scenes details of instructor training. In one talk, Danny Dyer (Memorial University of Newfoundland), Brian Forrest (University of Waterloo) and Costanza Piccolo (University of British Columbia) discussed developing full-length instructor training courses at their institutions, from the point of view of a developer of a stalled course, an emerging course, and a mature course, respectively. One presentation, singled out as a highlight by many participants in feedback following the workshop, blended the "ground-level" and "high-level" views: Dan Wolczuk (University of Waterloo) and Kari Marken (University of British Columbia) demonstrated and discussed the role of acting and theatre in the classroom.

Outcomes

One of the goals of this workshop was to allow representatives from key institutions across North America, in particular Canada, to gather for an exchange of ideas on instructor training and instructor training programs. This goal was achieved, and a number of follow-up activities are already underway.

- Representatives at the University of British Columbia and Simon Fraser University will collaborate on the development of an instructor-training course at Simon Fraser University. The collaboration between the University of British Columbia and the University of Waterloo on their respective courses is ongoing.
- Representatives at the University of British Columbia and First Nations University will collaborate on the Indigenization of instructor training components.

- Representatives at the University of Toronto will present follow-up sessions at Mathfest and the Canadian Mathematical Society 2019 Winter Meeting.

In addition to these collaborative outcomes, many participants also confirmed that they will be adopting components and techniques from the workshop into their own instructor training programs.

There were also impactful general outcomes. All participants commented at a “speaking circle” at the end of the workshop about their invigorated sense of purpose and camaraderie. One senior faculty member remarked that the workshop was “the best I have ever attended”. We expect that the network initialized at the workshop will persist, and that many of the components of instructor training presented at the workshop will become staples at Mathematics departments throughout Canada.

Participants

Barnes, Julie (Western Carolina University)
Bauer, Mark (University of Calgary)
Blois, Cindy (University of Toronto)
Bruni, Carmen (University of Waterloo)
Coles, Matthew (University of British Columbia)
de Vries, Gerda (University of Alberta)
DeDieu, Lauren (University of Calgary)
Desaulniers, Shawn (University of Alberta)
Doolittle, Edward (First Nations University of Canada)
Dyer, Danny (Memorial University of Newfoundland)
Forrest, Brian (University of Waterloo)
Graves, Sean (University of Alberta)
Haskell, Cymra (University of Southern California)
Khan, Steven (University of Alberta)
Leung, Fok-Shuen (University of British Columbia)
Malloch, Amanda (Camosun College)
Marken, Kari (University of British Columbia)
Mayes-Tang, Sarah (University of Toronto)
Menz, Petra (Simon Fraser University)
Piccolo, Costanza (University of British Columbia)
Sargent, Pam (Yale University)
Smith, Brett (Yale University)
Wolczuk, Dan (University of Waterloo)
Zazkis, Rina (Simon Fraser University)

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Chapter 36

Open Education Resources and Technologies in Mathematics (19w2268)

26 July - 28, 2019

Organizer(s): Sean Fitzpatrick (University of Lethbridge), Jeremy Sylvestre (University of Alberta, Augustana Campus)

Background and Summary

The BIRS Workshop on Open Education Resources and Technologies in Mathematics brought together champions of Open Education Resources (OER) in Alberta, along with leading experts from other institutions in Canada and the United States.

In Alberta and beyond, there is a growing number of mathematics educators involved in creating, modifying, and adopting OER for the academic (and financial) benefit of their students. We convened this workshop to address a significant barrier to development of high quality OER; namely, that many of the people working in this area are doing so independently, unaware of similar efforts elsewhere.

Another issue we hoped to address is awareness of new and exciting software platforms for authoring and publishing OER. As LaTeX is the dominant paradigm for mathematical publishing, including publication of open textbooks, most open textbook authors choose LaTeX as their authoring tool of choice, either out of habit, or due to lack of awareness of other options. While LaTeX allows for beautiful typesetting of mathematics, it is limited to output in PDF format. The use of PDF for textbooks is good for printing, but not for the increasingly large proportion of students who choose to access their course materials electronically. A major problem with PDF is that it typically scores poorly on accessibility tests, since it lacks features available in formats such as HTML for persons with visual impairments, including alt-text descriptions for images, screen reader support for equations, and scalability. Accessibility and student preference are two factors driving the need for high quality mathematical textbooks in HTML. An HTML textbook works well on a larger selection of devices with varying screen sizes. It also allows for the inclusion of interactive content, such as applets, live code, and computer-graded homework problems.

With these two issues in mind, participants in the workshop were given the opportunity to learn about the efforts of their colleagues at other institutions in the OER realm, and they also were able to learn about the most recent developments in some of the most cutting-edge open education technologies.

There were three primary technological themes represented at the workshop:

- The PreTeXt system for open textbook authoring and publishing.
- Online assessment tools, including WeBWorK and STACK.
- The Jupyter notebook system for online coding and scientific computing, and the PIMS Syzygy service.

Taken together, these tools form a robust ecosystem of open, interactive, online content with the potential for transformative enhancement of postsecondary mathematics education.

In keeping with the workshop's goal of introducing participants to each other and to some of the recent technology developments, presentations were kept brief and informal, with most time set aside for working groups. We saw three different types of working groups form:

1. Getting started — the workshop offered an opportunity for participants with no prior experience to learn the basics of working with tools such as PreTeXt and Jupyter.
2. Roundtable discussions — groups of participants got together to form discussion groups dealing with topics ranging from challenges in OER publishing to curriculum issues in elementary linear algebra.
3. Technical — the workshop also provided an opportunity for participants who are active in the development of open education technologies to meet in person to work out software bugs and technical problems.

PreTeXt

The PreTeXt system [1] is an XML vocabulary, together with processing tools, that allows one to author open textbooks with a single set of source files that can be processed into several different outputs, including HTML, LaTeX, and ePub. PreTeXt is undergoing rapid, community-based development, with new features added on a regular basis.

At the BIRS workshop, we heard from Rob Beezer, creator of PreTeXt, about some recent (and exciting) developments, including support for worksheets, lecture slides, and improved accessibility, including output to Braille.

Accessibility is a key feature of PreTeXt, along with interactivity features in HTML, such as embedding of WeBWorK problems and GeoGebra applets. Alex Jordan, another workshop participant, has made major contributions in these areas.

Roughly half of the workshop participants were already familiar with the PreTeXt project. Among the remaining participants, there was definite enthusiasm for PreTeXt as a platform. Following Saturday morning's presentations, one of the working groups formed provided interested participants an opportunity to be guided by Rob through the process of installing and setting up the necessary software to begin using the PreTeXt system, to the point that participants were able to author and produce output for a "minimal working example" document.

Also at the workshop was David Farmer, of the American Institute of Mathematics. David provides a service in support of the PreTeXt project, in which he will automatically convert authors' LaTeX source into PreTeXt. His conversion does about 90% of the job, with some hand-editing required after the fact for the author to complete the process. By the conclusion of the workshop, David managed to perform PreTeXt conversions for three authors:

Joy Morris, Remkes Kooistra, and Robert Petry. Conversions for several more texts by Remkes are planned for the near future.

Assessment

Technological solutions for assessment include both online homework systems and software to support evaluation of written work. WeBWorK [2] is a leading open source online homework system. It is mature, with a large bank of community-contributed problems, and supported by the Mathematical Association of America. As reported by Danny Glin (University of Calgary), a lot of the recent development in WeBWorK is related to making it more portable, so that WeBWorK problems can be embedded in other websites. This technology makes it possible, for example, to have interactive WeBWorK problems included in the HTML version of a PreTeXt book.

There is also a push within the WeBWorK project to improve documentation, with work underway for a new website. One of the working groups spent Saturday morning navigating the website, and giving suggestions for improvement.

While almost everyone at the workshop was familiar with WeBWorK, we also heard about two new developments that generated a lot of interest.

George Peschke and Chris Frei (University of Alberta) told us about their work creating question banks for calculus and linear algebra using the STACK plugin for Moodle [3]. For institutions using Moodle as their LMS, this provides an opportunity to provide online homework with computer-generated formative feedback, without the need for an external system like WeBWorK.

A modern take on traditional assessment was given by Andrew Rechnitzer (UBC). Andrew has created an open source alternative to online grading systems like Crowdmark and Gradescope, written entirely in Python. The PLOM system (PaperLess Online Marking) allows instructors to automatically generate many different versions of a test by mixing different versions of each question. While tests are written in class as usual, his software allows the work to be organized and processed so that markers can work online, and grade only one version of a problem at a time. The use of a rubric with predefined comments increases the quality and consistency of feedback to students, and the software saves time on tedious administrative work.

Jupyter

The Jupyter worksheet [4] has been an important research tool in data science and scientific computation for some time. From Michael Lamoureux (PIMS, University of Calgary), we heard about the PIMS Syzygy project [5], which provides online (browser-based) access to Jupyter using Jupyter hubs powered by Compute Canada. Although Syzygy was originally created as a research service, the fact that anyone with an institutional email address at a participating institution can sign in and access Jupyter's browser-based computing environment has made the service increasingly attractive as a teaching tool.

We heard from several participants who are either already including coding and software in their mathematics teaching, or are hoping to begin doing so.

Michael showed us some of the ways he uses Jupyter in the classroom. After his presentation (and coffee) a working group was formed, led by Patrick Walls (UBC) to get people started on Jupyter/Syzygy. In addition to basic details on accessing and using Jupyter, this group also looked at logistical details, such as distributing notebooks to students, and setting up grading tools that enable instructors to collect and evaluate student work in a Jupyter notebook.

Next steps

A major goal of the workshop was to promote awareness of OER projects, both within Alberta and beyond, and to begin to build a community of OER champions interested in sharing their work and supporting the work of others.

To that end, the workshop was a success. Friday evening provided an informal meeting in which all participants had a chance to share their interests and accomplishments. For those who wanted to share their work in more detail, we set aside time Sunday morning for a series of "lightning presentations" in which participants gave short (5-10 minute) talks about their work in OER.

A collection of resources shared during the lightning presentations can be found at

`https://sites.ualberta.ca/~jsylvest/birs_july_2019/`

To keep the conversation going, we created a Google group, where participants from the workshop, and the broader OER community, can share details on their projects, ask questions, and get support. The group can be found at

`https://groups.google.com/forum/#!forum/oer-math`

The question of how to support and sustain OER in mathematics is a difficult one, and not easily solved in a single weekend. We concluded the workshop with a group discussion on this topic, led by Claude Laflamme (University of Calgary, Lyryx Learning). Questions debated included:

- How do we organize and curate existing OER material?

  The experience of David Farmer with the Curated Courses initiative suggests that this is more difficult than one might expect. We heard from Rob Beezer that work is underway to produce an improved website documenting the many mature PreTeXt projects that currently exist.

  No single website is likely to accomplish the task, which is why community organization and communication is essential, and an outcome of the workshop that will be continuously pursued.

- How do we convince faculty to adopt OER?

  This can be a challenge. Large departments often have textbooks set by committee. Everywhere, faculty have designed their courses around existing commercial textbooks. Champions of OER can have an impact; for example, at the University of Lethbridge, participants Joy Morris and Sean Fitzpatrick have made open textbooks available for at least 10 courses.

  Work underway in the PreTeXt project to integrate ancillary materials such as lecture slides, WeBWorK problems, videos, etc. will also support adoption.

- How do we fund OER development and deployment?

  A common misconception about open textbooks is that they are completely free. This, of course, is false. Aside from the time commitment needed from faculty members to create OER, there is the need to hire support staff (such as summer students), and maintain web servers needed to host content. Interactive content such as WeBWorK problems can be especially costly to maintain.

  We discussed the fact that while there is good support in the USA from the NSF, grant money in support of OER in Canada is limited, and not always available to academic institutions.

  Claude made the suggestion that we work towards establishing a not-for-profit corporate entity to support OER, modelled after the NumFocus Foundation [6], which supports a number of open source projects, including MathJax and Jupyter.

This would certainly be a positive development in support of OER, but not one that we can expect to occur after a single weekend workshop.

Participants

Beezer, Rob (University of Puget Sound)
Davidson, Michelle (University of Manitoba)
Desaulniers, Shawn (University of Alberta)
Doob, Michael (University of Manitoba)
Farmer, David (American Institute of Mathematics)
Fever, Amy (The King's University)
Fitzpatrick, Sean (University of Lethbridge)
Forrest, Brian (University of Waterloo)
Frei, Christoph (University of Alberta)
Glin, Danny (University of Calgary)
Jordan, Alex (Portland Community College)
Kooistra, Remkes (The Kings University)
Laflamme, Claude (University of Calgary and Lyryx Learning)
Lamoureux, Michael (University of Calgary)
Morris, Joy (University of Lethbridge)
Peschke, George (University of Alberta)
Petry, Robert (Campion College at the University of Regina)
Pierce, Virgil (University of Northen Colorado)
Rechnitzer, Andrew (Ubc)
Rosoff, Dave (College of Idaho)
Sylvestre, Jeremy (University of Alberta)
Thangarajah, Pamini (Mount Royal University)
Walls, Patrick (The University of British Columbia)
Wilson, Nicole (University of Lethbridge)

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Chapter 37

Mathematics and Computer Science in Modeling and Understanding of Structure and Dynamics of Biomolecules (19w2257)

August 9 - 11, 2019

Organizer(s): Józef Adam Liwo (University of Gdańsk), Gabriel del Río Guerra (Universidad Nacional Autónoma de México), François Major (Université de Montréal)

Overview of the Field

Mathematical methods are nowadays extensively used in life sciences. On one hand, they are used to construct models of biological structures and processes at all levels of description, from structure and dynamics of biological macromolecules and their assemblies, through the structures and processes occurring in organelles, cells, organisms to modeling populations and whole ecosystems, as well as evolution. On the other hand, numerical mathematics and statistics provide tools to process sophisticated experimental data, extract correlations from databases, as well as simulate the structure and dynamics of the systems studied at different levels of resolution.

The workshop was focused on modeling biological molecules and their dynamics. The scope of this research comprises prediction of protein and RNA structure from sequence alone or in data-assisted mode, modeling the structure of protein assemblies, protein-protein docking, global-optimization methods in relation to these tasks, modeling biomolecule functions, and evolution of biomolecules. This research is of key importance not only because of the continuous quest of mankind to understand the world but also for purely utilitarian reasons such as, e.g., fighting cancer and hereditary diseases or producing better and more resistant crops. Prediction of the structures of biomolecules, mainly proteins, is of utmost importance in this field, because the experimental methods are not sufficient to provide the structures of the newly-discovered proteins. Therefore, the Community Wide Experiments on the Critical Assessment of Techniques for Protein Structure Prediction (CASP) [1] are organized since 1992 to assess the respective methods which, in turn, helps the biological chemists to select the most reliable ones for their research.

Recent Developments and Open Problems

In the last decade, enormous progress was made in the field of molecular modeling. Simulations of protein folding at all-atom level became possible owing to use of distributed computing and construction of dedicated supercomputers [2], and GPU computing [3]. Coarse grained models, in which atoms are grouped into united interaction sites have also been developed, which enable us to extend the simulation time- and size-scales by orders of magnitude [4]. Along with the development of models and simulation techniques, efficient data analysis approaches such as, e.g. principal component analysis, support vector machines, and neural network-based techniques have been developed. Another branch are the modeling methods that use heavy bioinformatics (database) input [5]. These methods integrate database information into modeling by using a variety of approaches; recently the Deep Learning-based methods achieved the top score in CASP13 [6].

Despite these successes, the computational approaches to biomolecular modeling still need improvement, Force fields, both all-atom and coarse-grained, can reproduce the experimental structures of only some proteins and nucleic acids. The availability of low-resolution experimental data (SAXS, CryoEM and ambiguous nuclear magnetic resonance data) pose new challenges to include them in modeling. New methods are also required to analyze the growing amount of experimental data. These topics were addressed during the workshop.

Presentation Highlights

The aim of this workshop was to bring together mathematicians, chemists, biologists, computer scientists, physicists so that they could exchange ideas and share experience. There were 22 participants total (out of initially confirmed 25, because of three last-minute cancellations), including‘ the organizers, all presenting a lecture, a talk, a short talk or a poster. The talks were divided into the following four thematic sessions: (1) *Protein structure and function*, (2) *Topology, disorder, and allostery*, (3) *Structure-function prediction*, (4) *Models and algorithms*, and the opening lecture by Robert Jernigan entitled *The importance of correlations in biology*. The poster presentations concerned coarse-grained modeling of protein structure and dynamics.

In his opening lecture, Robert Jernigan described the new protein-sequence alignment algorithm that he developed. The new algorithm utilizes tertiary structure information on the proximity of the amino acids and cab relate directly protein genome-related data to protein functions, based on accurate protein sequence alignment. Evolutionary relationship between proteins was also covered by Banu Ozkan in her talk on evolutionary aspects of allostery. Allosteric properties of proteins are important for protein function and are the next frontier in structural modeling of macromolecular interactions.

Many talks addressed ab initio and data-assisted modeling of the structures of biological macromolecules. Gregory Chirikjian described a new algorithm that he recently developed to retrieve original structure based on combined cryoelectron microscopy (CryoEM) and small X-ray electron scattering (SAXS) data. He showed that, even with large sections of data missing, the combined approach results in reasonable image restoration, not possible when only data of one kind are used. The method has been tested on model examples by now. Practical protein-structure determination from CryEM data was discussed by Daisuke Kihara who has developed a de novo modeling tool named MAINMAST (MAINchain Model trAcing from Spanning Tree), which enables us to obtain models with a very decent resolution. Marek Cieplak presented a talk on coarse-grained studies of the folding of intrinsically-disordered proteins, demonstrating that knots are formed in the process. Ensemble-based modeling of intrinsically-disordered proteins with the aid of ^{13}C chemical-shift data was presented by Yi He. Nina Pastor presented ta talk on modeling the effect of phosphorylation on the conformation of intrinsically disordered proteins, demonstrating that phosphorylation leads to increasing the content of α-helical structure.

A very interesting talk on accurate ab initio modeling of RNA structure with his simRNA approach that uses coarse-grained statistical potentials was presented by Michał Boniecki. Agnieszka Karczyńska presented protein-structure prediction method with the use of coarse-grained UNRES force field and input from bioinformatics approaches; this method achieved some success in the CASP13 experiment. Ilya Vakser presented a talk on his method of comparative modeling of protein complexes, which performed very well in CASP13. Use of machine learning to protein docking was presented by Marcelino Arciniega.

The topic of protein function was covered by Changbong Hyeon in his talk of cost-precision trade-off and transport efficiency of molecular motors. Using the uncertainty relation, he demonstrated that transport efficiencies of the molecular motors are optimized under experimental conditions. An interesting computational model of kinetochore-microtubule attachments in relation to modeling the process of cell mitosis was presented by Tamara Bidone.

Outcome of the Meeting

As pointed out by many participants, many new scientific contacts were made that are likely develop into collaborations. The participants learned about new methods and could talk in person to their developers. On the other hand, method developers could hear from simulation practitioners in what directions to develop their methodologies.

Participants

Arciniega, Marcelino (Univesidad Autonoma de Mexico)
Bidone, Tamara (University of Utah)
Boniecki, Michał (International Institute of Molecular and Cell Biology in Warsaw)
Brizuela, Carlos (Centro de Investigación Científica y de Educación Superior de Ensenada)
Chirikjian, Gregory (National University of Singapore and Johns Hopkins University)
Cieplak, Marek (Polish Academy of Science)
Del Rio, Gabriel (Universidad Nacional Autónoma de México)
Fontove, Fernando (C3 Idea)
He, Yi (University of New Mexico)
Hernández Rosales, Maribel (CINVESTAV)
Hyeon, Changbong (Korea Institute for Advanced Study)
Jernigan, Robert (Iowa State University)
Karczynska, Agnieszka (University of Gdansk)
Kihara, Daisuke (Purdue University)
Lipska, Agnieszka (University of Gdańsk)
Liwo, Jozef Adam (University of Gdansk)
Lubecka, Emilia (University of Gdańsk)
Ozkan, Banu (Arizona State University)
Pastor, Nina (Universidad Autonoma del Estado de Morelos)
Vakser, Ilya (University of Kansas)
Wu, Zhiyun (Iowa State University)

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Chapter 38

Retreat for Young Researchers in Stochastics (19w2282)

September 27 - 29, 2019

Organizer(s): Chris Hoffman (U. Washington), Ed Perkins (UBC)

Overview

This was the fifth annual meeting of the PIMS Postdoctoral Training Centre in Stochastics (PTCS). The Retreat offers an opportunity for young researchers in pure or applied probability from Western Canada and Washington state to interact, communicate their recent results and ongoing research programs, and initiate new collaborations. Nine postdoctoral fellows affiliated with PTCS, and one Ph.D. student spoke at the meeting. The 27 participants included postdoctoral fellows from U. Washington, U. of Alberta, U. of Calgary, U. Saskatchewan and UBC, Ph.D. students from U. Calgary, U. Alberta, U. Victoria, U. Washington and UBC, and faculty from U. Alberta, U. Calgary, U. Victoria, U. Regina, U. Washington and UBC.

The response from the participants after the retreat was quite positive.

Presentation Highlights

The range of topics from applied statistical hydrology to mathematical finance to the latest developments in random growth models was a striking feature of the workshop.

Chandra Rajulapati (U. Saskatchewan) spoke on modelling precipitation both locally and globally and how global trends provide inputs for urban precipitation estimates. She discussed the considerable challenge of adapting current static models to take account of global trends, notably climate change. She also presented the challenges faced in incorporating the disparate types of data (from ground measurement, satellite input and input from Global Climate Models) into the rainfall predictions. A particular challenge for Canada is the sparseness of on-ground data collection stations as compared to Europe and India, for example. She pointed to some unexpected phenomena which leads to data analysis challenges such as the increased variability of data in urban areas due to the presence of micro climates resulting from buildings and pollution issues.

Two talks on random dynamics from different perspectives were given by Joseph Horan (U. Vic) and Shirou Wang (U. Calgary). Joseph gave an extension of the Peron-Frobenius Theorem for matrices with non-negative entries to a sequence of random operators driven by an ergodic process. In particular he gave a contraction condition under which one has a lower bound on the "spectral gap" in this random setting and hence exponential rates of convergence of the resulting cocycles in Oseledets spaces. His perspective was from that of classical ergodic theory. Shirou Wang's results were from an applied modelling perspective in which the random cocycle structure arises due to extrinsic ergodic noise in the system and is further perturbed by a Markov chain arising from smaller intrinsic noise. She was concerned with convergence of the random invariant laws as the size of the perturbation becomes small to a moving equilibrium under a synchronization assumption on the underlying ergodic sequence of operators. In this setting she did not address the issue of exponentially fast convergence, but found different limiting results on synchronization or desynchronization depending on the strength of the synchronization of the non-perturbed ergodic system or on the regularity of the perturbation. Shirou and Joseph were not aware of each others work prior to the workshop.

There were three interesting presentations on random geometry given by the three postdocs at UBC, Thomas Budzinski, Delphin Senizergues and Yinon Spinka. Senizergues spoke on random growth models for trees based on (possibly random) weights giving the probabilities of attachment. One striking result showed the preferential attachment model (related to a common model for the internet) can be constructed through a particularly simple assignment of the random weights. Several precise results on the asymptotic growth properties of the resulting random trees were obtained. Thomas Budzinski spoke on random gluing models to construct random manifolds from sequences of polygons. This work is closely related to the random maps of Le Gall and Miermont constructed as random metric measure spaces by taking a scaling limit of a random planar map with n vertices as n gets large (one of the most important recent developments in the field [1]), but now the resulting surfaces are no longer conditioned to be spherical and so could be of large genus. A number of detailed properties of the growth dynamics were discussed including the fact that the rescaled vertex degrees in decreasing order converges to a Poisson-Dirichlet process. Spinka spoke on work done recently at UBC with Omer Angel. Their results again considered random geometry, this time given by random metrics on the circle of circumference L obtained by doing $1/2$-percolation between points in countable dense sets which are within distance one. For each L rational the graphs are all isomorphic a.s. and so determine an interesting class of graphs (up to isomorphism) indexed by L. But if L is irrational the resulting random graphs are not isomorphic to each other a.s. Earlier work in this field had focussed on normed linear spaces but this kind of disparate behaviour in the metric space setting was unexpected.

Outcome of the Meeting

The level of talks at this Retreat was extremely high in terms of content and presentation. Four of the ten lectures were given by outstanding young female postdoctoral fellows from U. Alberta, U. Calgary, and U. Saskatchewans A number of the participants wrote after the meeting, all expressing thanks for a stimulating meeting. Yaozhong Hu (CRCI at U. Alberta) pointed to new connections made with faculty and young researchers at U. Calgary.

During the meeting plans were made for an annual conference rotating between sites at UBC, U. Washington, U. Victoria and U. Alberta. A large meeting at UW was planned for 2020 using the final cycle of NSF funding for the PTCS, and a smaller weekend meeting at U. Victoria will be held in April of 2020. This will be followed by a one-week meeting in Victoria in 2021 and a large event at U. Alberta in 2022, with another Summer School in Probability in 2022 at either UA or UBC. It was also agreed that these annual meetings featuring young researchers in Probability from PIMS sites should continue after the end of the funding for the PIMS Postdoctoral Training Centre for Stochastics, It was felt that a 3-day meeting might be better to offer more time for informal discussion. The extra day could be at U. Calgary prior to the weekend meeting at BIRS.

Participants

Barlow, Martin (University of British Columbia)
Budzinski, Thomas (University of British Columbia)
Chen, Yu-Ting (University of Victoria)
Guo, Qi (University of Calgary)
Hoffman, Christopher (University of Washington)
Hong, Jieliang (University of British Columbia)
Horan, Joseph (University of Victoria)
Hu, Yaozhong (University of Alberta)
Kozdron, Michael (University of Regina)
Liu, Shuo (University of Alberta)
Min, Li (University of Alberta)
Perkins, Edwin (University of British Columbia)
Qi, Weiwei (University of Alberta)
Rajulapati, Chandra (University of Manitoba)
Ray, Gourab (University of Victoria)
Richey, Jacob (University of British Columbia)
Rosenberg, Josh (University of Washington)
Sénizergues, Delphin (University of British Columbia)
Sezer, Deniz (University of Calgary)
Shen, Zhongwei (University of Alberta)
Spinka, Yinon (University of British Columbia)
Wang, Shirou (University of Alberta)
Wang, Xiong (University of Alberta)
Wei, Wenning (University of Calgary)
Yi, Yingfei (University of Alberta)
Yi, Yulian (University of Alberta)

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Focused Research Group Reports

Chapter 39

Quantum Field Theory and Factorization Algebras (19frg244)

Feb 17 - 24, 2019

Organizer(s): Dylan Butson (University of Toronto), Kevin Costello (Perimeter Institute), Si Li (Tsinghua University), Philsang Yoo (Yale University)

Overview

Costello and Gwilliam [2] developed a general framework of constructing factorization algebra of quantum observables for any quantum field theory as defined earlier in Costello's book [1].

The Focused Research Group aimed to develop the formalism further toward two goals:

1) capturing bigger generality;
2) allowing concrete computations

The principal focus was to understand various sorts of defects of quantum field theory within the framework. In this report, we record the two main topics that were discussed in the meeting. These in particular include recent developments and open problems, presentation highlights, and scientific progress made.

Semiclassical OPE

OPE of Local Operators

This subsection is a quick summary of Section 10.3 of Costello and Gwilliam [2]. The main result describes the first order in $\hbar$ contribution to the operator product expansion (OPE) of local operators from the foundational construction of the quantum factorization algebra.

Consider classical field theory on $\mathbb{R}^n$ and classical observables $\mathrm{Obs}_0^{\mathrm{cl}}$ supported at $0 \in \mathbb{R}^n$. These are what we call local operators. For $\mathcal{O} \in \mathrm{Obs}_0^{\mathrm{cl}}$, we write $\mathcal{O}(x)$ for its translate to $x \in \mathbb{R}^n$. Then the claim is that the OPE, in the leading order in $\hbar$, gives a Poisson bracket on $\mathrm{Obs}_0^{\mathrm{cl}}$.

Let us understand this from the perspective of factorization algebras. Consider two local operators $\mathcal{O}_1, \mathcal{O}_2 \in \mathrm{Obs}_0^{\mathrm{cl}}$. We look at a factorization product $\widetilde{\mathcal{O}}_1(0) \cdot \widetilde{\mathcal{O}}_2(x) \in \mathrm{Obs}^{\mathrm{q}} q(D(0, 2|x|))$ modulo $\hbar^2$ where $\widetilde{\mathcal{O}}_i$ is a lift to quantum observables defined mod $\hbar^2$. The result modulo $\hbar^2$ is independent of the choice of lifts. As we can, modulo $\hbar$, extend it to $x = 0$, the OPE measures an obstruction to extending this continuously across the origin $x = 0$.

Now we write

$$\widetilde{\mathcal{O}}_1(0) \cdot \widetilde{\mathcal{O}}_2(x) \equiv \hbar \sum_i \mathcal{O}^i(0) F_i(x) + (\text{regular at } x) \qquad \text{modulo } \hbar^2$$

where $\mathcal{O}^i(0)$ is a basis of operators and F_i is an analytic function modulo functions continuous at 0, which we denote by $F_i \in C^\omega(\mathbb{R}^n \setminus 0)/C^0(\mathbb{R}^n)$. Note that this information only depends on $\mathcal{O}, \mathcal{O}'$ and classical field theory; this is a semi-classical computation. Still, this amounts to doing certain simple Feynman diagram computation.

Let us use notation $\{\mathcal{O}_1(0), \mathcal{O}_2(x)\} = \lim_{\hbar \to 0} \hbar^{-1} \mathcal{O}_1(0) \cdot \mathcal{O}_2(x)$ for the OPE. In fact, one obtains a map

$$\{-,-\}\colon \mathrm{Obs}_0^{\mathrm{cl}} \otimes \mathrm{Obs}_0^{\mathrm{cl}} \to \mathrm{Obs}_0^{\mathrm{cl}} \otimes (C^\omega(\mathbb{R}^n \setminus 0)/C^0(\mathbb{R}^n)).$$

The notation is justified because this satisfies the Leibniz rule

$$\{\mathcal{O}_1(0)\mathcal{O}_2(0), \mathcal{O}_3(x)\} = \mathcal{O}_1(0)\{\mathcal{O}_2(0), \mathcal{O}_3(x)\} + \mathcal{O}_2(0)\{\mathcal{O}_1(0), \mathcal{O}_3(x)\}.$$

Formalism for OPE

We want to record the underlying formalism for the above. As a first step, we present the result as a concrete construction. The formalism for extended defects is work in progress. We eventually hope to understand to what extent we can analogously discuss the quantum OPE.

Consider a classical field theory with space of fields $\mathcal{E}$. We have an (IR regulated) propagator $P \in \mathcal{D}(M^2, \mathcal{E}^{\boxtimes 2})$ such that $P|_{M^2 \setminus \Delta} \in C^\infty(M^2 \setminus \Delta, \mathcal{E}^{\boxtimes 2})$. The classical interaction terms are given by $I = \sum_{k \geq 3} I_k$ where $I_k \in \mathrm{Sym}^k_{C^\infty_M}(\mathcal{J}(\mathcal{E})^\vee) \otimes_{D_M} \mathrm{Dens}_M \subset \mathcal{D}(M^k, (\mathcal{E}^!)^{\boxtimes k})_{S_k}$. In this subsection, we work with $M = \mathbb{R}^n$.

As an example, consider scalar theory on M, where $\mathcal{E} = C^\infty(M)$. The propagator is

$$P(x,y) = \int_0^L K_t(x,y)dt \qquad \text{where} \quad K_t(x,y) = \frac{1}{(4\pi t)^{n/2}} e^{-\frac{|x-y|^2}{t}}$$

A generic interaction term may be of the form $I_k(\phi) = \int_M \partial_{i_1}\phi^{j_1} \cdots \partial_{i_l}\phi^{j_l}$ with $\sum_{m=1}^l j_m = k$, where we abuse the notation to write a density as an integral.

To first order in $\hbar$, the only diagrams that will contribute to the OPE of two local operators will be irreducible trees connecting the two. Fix such a diagram, with interaction terms $I_{k_1}, ..., I_{k_p}$ and $p+1$ propogators, $(p-1)$ of them linking the p interaction vertices together in a line, and one on each end which will contract with the local operators of which we are computing the OPE.

Before contracting with the local operators at each end, we have $k = \sum_{i=1}^p k_i - 2p$ external legs of the interaction vertices, and two external legs of propagators, one at each end. Thus, the amplitude of this diagram is given by

$$\widetilde{\mathcal{A}} \quad \in \quad \mathcal{D}(M^2 \times M^k, \mathcal{E}^{\boxtimes 2} \boxtimes (\mathcal{E}^!)^{\boxtimes k}) \cong \mathcal{D}(M^2, \mathcal{E}^{\boxtimes 2}) \hat{\otimes} \mathcal{D}(M^k, (\mathcal{E}^!)^{\boxtimes k})$$

Here is a proposition. The restriction of $\widetilde{\mathcal{A}}$ to the compliment of the diagonal $\Delta = M \hookrightarrow M^2$ satisfies

$$\mathcal{A} := \widetilde{\mathcal{A}}|_{(M^2 \setminus \Delta) \times M^k} \quad \in \quad C^\infty(M^2 \setminus \Delta, \mathcal{E}^{\boxtimes 2}) \hat{\otimes} \mathcal{D}(M^k, (\mathcal{E}^!)^{\boxtimes k}) \quad \subset \quad \mathcal{D}(M^2 \setminus \Delta, \mathcal{E}^{\boxtimes 2}) \hat{\otimes} \mathcal{D}(M^k, (\mathcal{E}^!)^{\boxtimes k})$$

Proof. Follows from the fact that the propogators are smooth away from the diagonal themselves, and that the interactions are strictly supported on the small diagonal, so that contraction with them can not propogate the singularities away from the diagonals. □

Now let us fix two local operators, which for simplicity we assume to be linear in the fields, and thus given by $\mathcal{O}_i \in \mathcal{J}(\mathcal{E})^\vee \otimes \delta_{x_i}$ for $x_i \in M$ and $i = 1, 2$. Let us allow the positions of the local operators to vary, or equivalently view the underlying elements of $\mathcal{J}(\mathcal{E})^\vee$ as flat families of local operators. This is where we used the assumption $M = \mathbb{R}^n$; otherwise one has to be more careful. Then their contraction with $\mathcal{A}$ yields an element $\langle \mathcal{O}_1 \boxtimes \mathcal{O}_2, \mathcal{A}\rangle \in C^\infty(M^2 \setminus \Delta)\hat{\otimes}\mathcal{D}(M^k, (\mathcal{E}^!)^{\boxtimes k})$.

Now, fix a point $w_0 \in M$, choose coordinates x, y on M^2 in a disk $U \times U$ around (w_0, w_0) and let $z = \frac{x-y}{2}$ and $w = \frac{x+y}{2}$ on M^2. We will consider the limit $z \to 0$ with fixed $w = w_0$ which will be the common value $x = y = w_0$ in the limit. Then we have the following proposition.

Fix an expansion

$$\langle \mathcal{O}_1 \boxtimes \mathcal{O}_2, \mathcal{A}\rangle|_{w=w_0} = \sum_j f_j(z) \otimes \mathcal{O}_{(j)} \quad \in C^\infty(U \setminus \{w_0\})\hat{\otimes}\mathcal{D}(M^k, (\mathcal{E}^!)^{\boxtimes k})$$

such that the functions f_j are algebraically linearly independent. Then for each j such that $f_j(z)$ is singular at $z = 0$, the corresponding observable $\mathcal{O}_{(j)}$ is supported at w_0, that is,

$$\mathcal{O}_{(j)} \in \mathrm{Sym}^k(\mathcal{J}(\mathcal{E})^\vee) \otimes \delta_{w_0} \subset \mathcal{D}(M^k, (\mathcal{E}^!)^{\boxtimes k})$$

Instead of providing an abstract proof, let us consider an example illustrating a general feature:

$$F(z) = \int_{x\in\mathbb{R}^n} \left(\int_{t_1=0}^{L} t_1^{-n/2} e^{-|x|^2/t_1}\right)\left(\int_{t_2=0}^{L} t_2^{-n/2} e^{-|x-z|^2/t_2}\right)\varphi(x)$$

Here are some observations one can immediately make:

- For $t_1, t_2 > 0$, the integral over x is clearly convergent from having the exponential.
- Similarly, for x away from 0 and z, the integral over t is convergent near 0 from the exponential.
- (Above proposition) Each of the integrals does yield a singular function, but it yields a well-defined integral kernel for $z \neq 0$, so that the total integral is still convergent if $z \neq 0$.

Now, for z near zero, this integral will typically diverge. We have $\int_{t_1=0}^{L} t_1^{-n/2} e^{-|x|^2/t_1} = |x|^{2-n}\tilde{\Gamma}(n, x)$ where $\tilde{\Gamma}(n, x)$ is regular (and non-vanishing) at $x = 0$.

However, since the rate of blow up of this integrand near 0 is polynomial, for some $d \in \mathbb{N}$ sufficiently large, if we write our field $\varphi(x) = \varphi_{\leq d}(x) + \varphi_{>d}$ where $\varphi_{\leq d}(x)$ is the d^{th} order power series expansion of φ at x and $\varphi_{>d}$ vanishes to order d, then in the corresponding decomposition $F(z) = F_{\leq d}(z) + F_{>d}(z)$ we have that $F_{>d}$ is regular at 0.

Thus, we see that the singular contributions all come from $F_{\leq d}$, but this functional only depends on the power series expansion of φ at 0 to order d, and thus is a local functional.

Koszul Duality for Factorization Algebras

Mathematical Background

The fundamental theorem of deformation theory, for instance, as articulated by Lurie in DAG X, says that over a field k of characteristic 0, there is an equivalence between the ∞-category of differential graded Lie algebras and the one of formal moduli problems. Roughly speaking, the functor $\Psi\colon \mathrm{Lie} \to \mathrm{Moduli}$ is given by

$$\Psi(\mathfrak{g})(R) = \mathrm{MC}(\mathfrak{m}_R \otimes \mathfrak{g})$$

for a commutative differential (non-positively) graded algebra R over k. Here $\mathfrak{m}_R$ is fixed by an augmentation $R \to k$ and MC stands for the space of solutions to the Maurer–Cartan equation. To put it another way, one can find

$$\Psi(\mathfrak{g})(R) = \underline{\mathrm{Map}}_{\mathrm{CAlg}^{\mathrm{aug}}}(C^\bullet_{\mathrm{CE}}(\mathfrak{g}), R) = \underline{\mathrm{Map}}_{\mathrm{Lie}}(\mathfrak{D}(R), \mathfrak{g})$$

where $C^\bullet_{\mathrm{CE}}\colon \mathrm{Lie} \to (\mathrm{CAlg}^{\mathrm{aug}})^{\mathrm{op}}$ is the Chevalley–Eilenberg cochain functor and $\mathfrak{D}\colon (\mathrm{CAlg}^{\mathrm{aug}})^{\mathrm{op}} \to \mathrm{Lie}$ is the Koszul duality functor that is the right adjoint to $C^\bullet_{\mathrm{CE}}$.

In the same paper, Lurie also discusses a formal moduli problem for an associative algebra. Indeed, the statement is that if k is a field (of arbitrary characteristic), there is an equivalence between the ∞-category of augmented $\mathbb{E}_1$-algebras over k and the one of formal $\mathbb{E}_1$-moduli problems. This time, the situation is more symmetric and the functor $\Psi\colon \mathrm{Alg}^{\mathrm{aug}} \to \mathrm{Moduli}^{(1)}$ is given by

$$\Psi(B)(A) = \underline{\mathrm{Map}}_{\mathrm{Alg}^{\mathrm{aug}}}(\mathfrak{D}^{(1)}(B), A) = \underline{\mathrm{Map}}_{\mathrm{Alg}^{\mathrm{aug}}}(\mathfrak{D}^{(1)}(A), B)$$

where $\mathfrak{D}^{(1)}\colon (\mathrm{Alg}^{\mathrm{aug}})^{\mathrm{op}} \to \mathrm{Alg}^{\mathrm{aug}}$ is the Koszul dualty functor. Recall that for an $\mathbb{E}_1$-algebra (or a homotopy associative algebra) A with an augmentation $\varepsilon\colon A \to k$, one can define the Koszul dual algebra $\mathfrak{D}^{(1)}(A)$ as $A^! = \underline{\mathrm{Hom}}_A(k,k)$ where k is understood as a left A-module. We want to read the result as saying that the Koszul dual algebra of an associative algebra A corepresents the "Maurer–Cartan functor", namely,

$$\text{“}\mathrm{MC}(\mathfrak{m}_A \otimes B) \simeq \underline{\mathrm{Map}}_{\mathrm{Alg}^{\mathrm{aug}}}(A^!, B)\text{”}$$

where $\mathfrak{m}_A$ is the augmentation ideal. To put it another way, by applying the Yoneda lemma, we can recover the Koszul dual algebra $A^!$ from the "Maurer–Cartan functor".

QFT Interpretation

We would like to understand the QFT interpretation of this statement.

Here is a general set-up. Suppose we have a field theory on $\mathbb{R} \times X$ and hence a factorization algebra $\mathcal{F}$ on it. Suppose that the theory is topological along $\mathbb{R}$. Then for each point $x \in X$, the factorization algebra $\mathcal{F}_x := \mathcal{F}|_{\mathbb{R}\times x}$ on $\mathbb{R}$ is an $\mathbb{E}_1$-algebra which plays the role of A in the above discussion. For simplicity, we assume that for the projection $\pi\colon \mathbb{R} \times X \to \mathbb{R}$, the pushforward $\pi_*\mathcal{F}$ is trivial, namely, $\pi_*\mathcal{F} \simeq \mathbb{C}$ (or $\mathbb{C}[[\hbar]]$ in the quantum case but this will be omitted below).

Note that there is a map of factorization algebras $\mathcal{F}_x \to \pi_*\mathcal{F}$ on $\mathbb{R}$, because for a small neighborhood U of x we have $\mathbb{R} \times U \hookrightarrow \mathbb{R} \times X$ giving $\mathcal{F}(\mathbb{R} \times U) \to \mathcal{F}(\mathbb{R} \times X)$. Now from the assumption, the map $\mathcal{F}_x \to \pi_*\mathcal{F}$ can be thought of as an augmentation. Physically speaking, this is a choice of a vacuum.

As B is another $\mathbb{E}_1$-algebra, let us think of it as the algebra of observables of a certain topological quantum mechanics. It remains to understand the meaning of $\mathrm{MC}(\mathcal{F}^0_x \otimes B)$, where $\mathcal{F}^0_x \subset \mathcal{F}_x$ is the augmentation ideal. The claim is that

$\mathrm{MC}(\mathcal{F}^0_x \otimes B)$ is the space of ways of coupling the two theories.

Proving this in some generality would involve some nontrivial research work, so we will be content with providing some informal explanation for its few different aspects.

First of all, let us note that it has a classical analogue. That is, if A, B are Poisson algebras, then using a Lie bracket from a Poisson structure, a Maurer–Cartan element corresponds to coupling at the classical level.

Here is an example. Consider 4d Chern–Simons theory on $\mathbb{R}^2_{x,y} \times \mathbb{C}_z$. Consider the system of free fermions on $y = z = 0$. The space of fields is $A \in \Omega^\bullet(\mathbb{R}^2)\widehat{\otimes}\Omega^{0,\bullet}(\mathbb{C}) \otimes \mathfrak{g}$ with $\mathfrak{g} = \mathfrak{gl}_n$ and $\psi = (\psi_i, \psi^j) \in \Omega^\bullet(\mathbb{R}_x, \mathbb{C}^n \oplus (\mathbb{C}^n)^*)$. We know that free fermions lead to the Clifford algebra $B = \mathrm{Cl}(\mathbb{C}^n)$ as the algebra of observables. Hence local observables of the product system are $C^\bullet_{\mathrm{CE},\hbar}(\mathfrak{g}[[z]]) \otimes \mathrm{Cl}(\mathbb{C}^n)$. Here $C^\bullet_{\mathrm{CE},\hbar}(\mathfrak{g}[[z]])$ is an $\mathbb{E}_1$-algebra which is quantization of the Chevalley–Eilenberg complex $(C^\bullet_{\mathrm{CE}}(\mathfrak{g}[[z]], d_{\mathrm{CE}})$.

Let us take its classical limit; the Clifford algebra becomes $\mathrm{Sym}((\mathbb{C}^n \oplus (\mathbb{C}^n)^*))$ with the induced bracket from the pairing $\langle -, - \rangle$; hence we end up with a DG Lie algebra

$$(C^\bullet_{\mathrm{CE}}(\mathfrak{g}[[z]]) \otimes \mathrm{Sym}((\mathbb{C}^n \oplus (\mathbb{C}^n)^*)), d_{\mathrm{CE}}, \langle -, - \rangle).$$

Then its Maurer–Cartan element corresponds to a map of DG Lie algebras $\mathfrak{g}[[z]] \to \mathrm{Sym}((\mathbb{C}^n \oplus (\mathbb{C}^n)^*))$. For instance, $X \mapsto \Phi_X = (\psi \mapsto \langle \psi, X_0 \cdot \psi \rangle)$ is a map of DG Lie algebras, where $X = \sum X_n z^n \in \mathfrak{g}[[z]]$ and we abuse the notation to write $\psi \in \mathbb{C}^n \oplus (\mathbb{C}^n)^*$. Under our correspondence, this defines a coupling $\int_{\mathbb{R}} \psi A \psi$.

Now let us formulate this in a more conceptual way. Let us assume that $(\mathcal{F}_x \otimes B, d_{\mathcal{F}_x \otimes B})$ is quantum observables for topological quantum mechanics. One should imagine $d_{\mathcal{F}_x \otimes B} = Q + \hbar\Delta$, where Δ is the BV differential. In particular, it is an $\mathbb{E}_1$-algebra which can also be regarded as a DG Lie algebra. If it is not topological, one has to keep track of the information of Hamiltonian, but the story will essentially be the same.

From the assumption, we have the local constancy along $\mathbb{R}$, which gives a quasi-isomorphism

$$\mathcal{F}_x \otimes B \simeq \Omega^\bullet(\mathbb{R}) \otimes \mathcal{F}_x \otimes B$$

of DG Lie algebras. Then a Maurer–Cartan element α of $\mathcal{F}_x \otimes B$ corresponds to a Maurer–Cartan element O_α of the right-hand side, which we expand as $O_\alpha = O^{(0)}_\alpha + O^{(1)}_\alpha$ where $O^{(i)}_\alpha$ is of the form degree i. Namely, we have

$$d_{\mathcal{F}_x \otimes B}\alpha + \frac{1}{2}[\alpha, \alpha] = 0 \qquad \longleftrightarrow \qquad \begin{cases} d_{\mathcal{F}_x \otimes B} O^{(0)}_\alpha + \frac{1}{2}[O^{(0)}_\alpha, O^{(0)}_\alpha] = 0 \\ d_{\mathrm{dR}} O^{(0)}_\alpha + d_{\mathcal{F}_x \otimes B} O^{(1)}_\alpha + [O^{(0)}_\alpha, O^{(1)}_\alpha] = 0 \end{cases}$$

The expected claim is that $S_\alpha = \int_{\mathbb{R}} O^{(1)}_\alpha$ is a solution to quantum master equation if and only if α satisfies the Maurer–Cartan equation. Again, proving it in some generality is work in progress.

Moreover, the assumption that $\pi_* \mathcal{F}_x$ is trivial yields $\pi_*(\mathcal{F}_x \otimes B) \simeq B$. From this one can observe that we obtain $\alpha \in \mathcal{F}^0_x \otimes B$ if and only if when we compactify to $\mathbb{R}$ we get the trivial deformation of the topological quantum mechanics.

In sum, $\mathrm{MC}(\mathcal{F}^0_x \otimes B)$ realizes a deformation of the Lagrangian as claimed and $\mathcal{F}^!_x$ is operators of universal QM system we couple at $\mathbb{R} \times x$. This gives all possible ways to couple QM system.

In fact, for 4d Chern–Simons theory, if we want to couple 4d CS with some quantum mechanics with QM operator B, then most general coupling looks like $\sum_n \int (\partial^n_z A)^a \rho_a[n]$, where $\rho_a[n] \in B$. It turns out that for the coupled system to be anomaly-free, $\rho_a[n]$ should satisfy some relations, which one can check to be the relations of the Yangian $Y(\mathfrak{g})$.

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Chapter 40

Towards Spacetime Entanglement Entropy for Interacting Theories (19frg247)

March 31 - April 7, 2019

Organizer(s): Yasaman K. Yazdi (University of Alberta, Canada), Ravi Kunjwal (Perimeter Institute for Theoretical Physics, Canada), Heidar Moradi (University of Cambridge, UK)

Overview

Entanglement entropy was originally conceived in pursuit of an understanding of black hole entropy [1]. The Bekenstein-Hawking thermodynamic entropy of a black hole is proportional to the area of its event horizon. However, the microscopic origin of this entropy has been a mystery. Entanglement entropy, similarly, in many different situations obeys a spatial "area law". This means that in units of the UV cutoff of the theory, it scales proportional to the spatial area of the boundary of the region whose entropy of entanglement is being considered. The area law nature of entanglement entropy, as well as the fact that it has both quantum (entanglement) and gravitational (geometric) features, make it a strong candidate for being the microscopic origin of black hole entropy. Since its conception in 1983, entanglement entropy has also found many important applications in other areas of modern physics such as condensed matter physics [2, 3] and information theory [4]. This has strengthened its role as a foundational concept in fundamental theoretical physics.

Our main motivation in the work we carried out relates back to the original goal of understanding black hole entropy as well as other questions in quantum gravity. Numerous studies have already been made on the connection between entanglement entropy and black hole entropy [5, 6, 7, 8]. While these studies have shed some light on the issue, they have not been conclusive. One of the challenges in studying the entanglement entropy of a black hole is that black holes are truly global and spacetime objects. One would have to know the entire causal history of a spacetime to characterize a black hole. The information in a subregion, much less a moment in time, would not suffice. This is in stark contrast to conventional quantum systems which are typically characterized by states at a "moment in time". There are arguments related to the well-posedness of the initial value problem that in some classical and semiclassical cases justify the characterization of a physical system using data at a moment in time or on a Cauchy surface. In going beyond classical theory and entering the regime of nontrivial semiclassical and full quantum gravity one must insist on finding spacetime tools to probe quantum properties such as entanglement entropy. Freeing quantum characteristics from spatial surfaces would also pave the way for studying dynamical causal structures and spacetimes. These dynamical scenarios are inevitable in full quantum gravity, so it is a worthwhile investment to build a framework that could study them.

Thus we wish to cast entanglement entropy in an explicitly spacetime form. An additional motivation for doing this for entanglement entropy in particular is the crucial role played by the UV cutoff. Entanglement entropy and its properties are quantified with respect to a UV cutoff, without which one would get infinite values. In order for entanglement entropy to serve as an objective measure for a theory in a spacetime without any special frames, we need the UV cutoff to not belong to any special frame. This is only possible if the cutoff is a spacetime rather than spatial cutoff.

Recent Developments and Open Problems

Major strides were made towards an intrinsically spacetime definition of entanglement entropy in work by Sorkin [9]. In this work entanglement entropy was defined in a spacetime framework for a gaussian scalar field in an arbitrary spacetime. This was achieved by expressing the entropy in terms of the spacetime two-point function (or Wightman function) of the theory. Explicitly, in terms of the Wightman function $W(x,y) = \langle 0|\phi(x)\phi(y)|0\rangle$ and the spacetime commutator $\Delta(x,y) = [\phi(x),\phi(y)]$, the entropy is

$$S = \sum_{\lambda} \lambda \ln|\lambda|, \tag{40.0.1}$$

where λ are solutions of the generalized eigenvalue problem

$$Wv = i\lambda\Delta v, \qquad \Delta v \neq 0. \tag{40.0.2}$$

Such a definition was possible because the two-point function contains all the information in a gaussian theory. This definition has been explored in some follow-up work in both continuum spacetimes [10] and discrete causal sets [11]. In both cases the characteristic area law scaling of the entropy was obtained with respect to a covariant UV cutoff set by a smallest eigenvalue of Δ.

To understand the nature of entanglement in general physical theories, which tend to be interacting, it is important to go beyond gaussian theories. The focus of our workshop was to make progress in this direction. An open question is how the entropy can be described by spacetime correlators in such theories. For non-gaussian theories Wick's theorem fails to hold and generally all higher n-point correlation functions are needed to specify the theory. One would therefore expect extensions to Sorkin's formula to depend on these higher order correlators.

Scientific Progress Made

In order to gain deeper intuition about the problem and as a first step towards generalizing the entropy definition (40.0.1)-(40.0.2), we tested the formula under perturbations away from a gaussian theory. The density matrix we considered (expressed in the block-diagonal q-basis of [9]) was

$$\rho_{qq'} = \langle q|\rho|q'\rangle = Ne^{-A/2(q^2+q'^2)-C/2(q-q')^2-\left(\lambda_1\frac{q^4+q'^4}{2}+\lambda_2(q^3q'+qq'^3)+\lambda_3 q^2q'^2\right)}, \tag{40.0.3}$$

where N is a normalization constant, A and C are constant coefficients, and $\lambda_i \ll 1$ set the strength of the perturbations. Equation (40.0.3) is the most general quartic perturbation of a gaussian density matrix that is symmetric in $q \leftrightarrow q'$. Expectation values with respect to such non-gaussian states do not factorize in the sense of Wick's theorem and one would expect higher order correlator contributions to the formulas (40.0.1)-(40.0.2).

For a given density matrix, the entanglement entropy is typically directly computed through

$$S = -\mathrm{tr}\rho \log \rho, \tag{40.0.4}$$

which can be straightforwardly calculated using the replica trick [12, 13],

$$S = -\lim_{n\to 1} \frac{\partial}{\partial n} \mathrm{tr}\left(\rho^n\right) . \tag{40.0.5}$$

Using the replica trick, the entropy can be computed to first order in λ_i using a formalism reminiscent of path integrals. We find

$$\begin{aligned} S = &- \frac{\mu \log \mu + (1-\mu)\log(1-\mu)}{1-\mu} - \frac{3\mu \log \mu}{(\mu+1)(\mu-1)^5\beta^2}\lambda_1 \\ &- \frac{3(\mu+1)\log \mu}{2(\mu-1)^5\beta^2}\lambda_2 - \frac{3(1+\mu+\mu^2)\log\mu}{(\mu+1)(\mu-1)^5\beta^2}\lambda_3 + \mathcal{O}(\lambda^2). \end{aligned} \tag{40.0.6}$$

where

$$\mu = \frac{\sqrt{1+2C/A}-1}{\sqrt{1+2C/A}+1}, \quad \text{and} \quad \beta = \frac{1}{2}\left(A\sqrt{1+2C/A}+A+C\right). \tag{40.0.7}$$

It is useful to express the result in terms of the gaussian form with a perturbed μ which we will call $\mu_{replica}$

$$S = -\frac{\mu_{replica}\log \mu_{replica} + (1-\mu_{replica})\log(1-\mu_{replica})}{1-\mu_{replica}}, \tag{40.0.8}$$

where

$$\mu_{replica} = \mu + \frac{3\mu}{\beta^2(\mu+1)(\mu-1)^3}\lambda_1 + \frac{3(\mu+1)}{2\beta^2(\mu-1)^3}\lambda_2 + \frac{1+\mu+\mu^2}{\beta^2(\mu+1)(\mu-1)^3}\lambda_3 + \mathcal{O}(\lambda^2). \tag{40.0.9}$$

In general we expect that the formulas (40.0.1)-(40.0.2) need to be generalized to include contributions of higher order correlators. However, as a first approximation we tried to compute the formula in the non-gaussian case, by replacing the two-point correlator W with its non-gaussian counterpart. We can express the result as

$$S = -\frac{\mu_{correlation}\log \mu_{correlation} + (1-\mu_{correlation})\log(1-\mu_{correlation})}{1-\mu_{correlation}}. \tag{40.0.10}$$

To our surprise we found that

$$\mu_{replica} = \mu_{correlation}, \tag{40.0.11}$$

despite being computed using very different methods. This implies that Sorkin's proposal still holds for non-gaussian theories (at least to first order in perturbation theory), and nothing besides the (non-gaussian) two-point correlator contributes. This is a nontrivial result and, to our knowledge, the first such example.

Outcome of the Meeting

The main outcome of our meeting was to show that the entropy definition (40.0.1)-(40.0.2) continues to hold to first order in perturbation theory for the quartic perturbations that we considered. More precisely, for our non-gaussian theory, the same gaussian entropy formula holds but with W and Δ replaced by their perturbation-corrected versions. We have written a paper [14] containing the details of our findings. Our results indicate that S may universally depend on W, or at least primarily on W. If this turns out to be true, then it is an example of a physical insight we have gained as a result of working in this spacetime correlation framework for entanglement entropy.

Our work at this stage serves as an important proof of principle that it is possible to formulate entanglement entropy in terms of correlations functions for theories beyond gaussian theories. This opens the door to extending such studies to general interacting theories and conformal field theories.

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Chapter 41

Concentration, Relaxation and Mixing time for Restricted Lattices (19frg225)

May 19 - 26, 2019

Organizer(s): O. Angel (UBC), A. Ben-Hamou (University of Paris, Jusseiux), E. Cohen (CCR-Princeton), C. Roberto (University of Paris, Nanterre), P-M. Samson (University of Paris, Marne La Vallee), A. Stauffer (University of Rome 3), Prasad Tetali (Georgia Institute of Technology)

Overview of the Field

The study of the convergence of Markov chains/processes is a lively and active field in probability theory, with connections with different fields, including statistical mechanics – many models are coming from physics – and combinatorics, related to isoperimetry and functional analysis. Concentration of measure in various non-product spaces is also a fascinating topic with many potential applications, in spite of deep understanding of this phenomenon on product spaces (with product measures). During the Focused Research Group period, as per our submitted proposal, we investigated bounding relaxation and mixing times for two models/problems that have arisen in recent years: The first model was introduced by Jian Ding and Elchanan Mossel as an example of the study of mixing times of Markov chain under monotone censoring. The second model of interest for us is the non-crossing partition lattice which arises as a natural lattice/graph (or Catalan structure) in many topics, including enumerative combinatorics, free probability and statistical physics. Questions of concentration (of measure) and mixing time (of local dynamics) on the non-crossing partition lattice are also compelling and challenging to understand precisely on a host of other combinatorial structures whose enumeration is also given by the sequence of Catalan numbers.

Mixing in a monotone subset of the n-cube. Let $\Omega_n := \{0,1\}^n$ be the n-dimensional hypercube. We consider the standard partial order on $\Omega_n : x \leq y, x, y \in \Omega_n$ if $x_i \leq y_i$ for all $i = 1, \dots, n$. Now a subset $A \subset \Omega_n$ of the hypercube is said to be monotone increasing (or simply increasing) if $x \leq y, \quad x \in A \quad \Longrightarrow \quad y \in A$. There has been recently some effort in understanding the following Poincaré inequality on any monotone increasing set.

Namely, one is interested in estimating the best constant C_P such that, for any $f\colon A \to \mathbb{R}$, it holds

$$\mathrm{Var}_\pi(f) \le C_P \mathcal{E}_\pi(f). \tag{41.0.1}$$

Here $\pi := \frac{1}{|A|}$ is the uniform measure on A (and $|\cdot|$ denotes the cardinal of the set), $\mathrm{Var}_\pi(f) = \pi(f^2) - \pi(f)^2$ is the variance of the function f with respect to the probability measure π (recall that $\pi(g) := \sum_{x\in A} g(x)\pi(x)$ is a short hand notation of the mean of g under π), and

$$\mathcal{E}_\pi(f) := \frac{1}{2}\sum_{x\in A}\sum_{\substack{y\in A:\\ y\sim x}} \pi(x)(f(y)-f(x))^2$$

denotes the Dirichlet form associated to the operator L acting on functions as follows $Lf(x) = \sum_{y\in A, y\sim x} f(y) - f(x)$. Finally $y \sim x$ means that x and y differ only on exactly one coordinate: $x \sim y$ if there exists $j \in \{1,\dots,n\}$ such that $x_i = y_i$ for all $i \ne j$ and $x_j = 1 - y_j$.

Tight estimate on C_P, that possibly depends on A and n, for all monotone set A is still an open question.

Random Catalan Structures. There are many realizations (at least 214, to be precise, according to a recent book by Richard Stanley) as combinatorial structures of the nth Catalan number, for $n \ge 1$. Some well-studied ones include the triangulations of a regular polygon of $n+2$ sides, sets of expressions of balanced parentheses with n left and n right parentheses, non-crossing set partitions of an n-set, pattern 312-avoiding permutations of n distinct integers etc. Each of these realizations comes with its own set of natural local moves which can be used to define a Markov chain on the corresponding combinatorial structures whose equilibrium distribution is uniform over the nth Catalan number many of them. While this study is similar in spirit to understanding the mixing time properties, the cut-off phenomenon etc. of various card shuffles (that generate a permutation of n cards uniformly, or otherwise, at random), progress has been rather limited in analyzing various "Catalan shuffles". A classical example is the Markov chain on triangulations of an n-gon using diagonal flips, whose relaxation time was conjectured by Aldous (more two decades ago) to be of order $n^{3/2}$. The best known lower and upper bounds are of order $n^{3/2}$ (Molloy, Reed and Steiger, 1999), and n^4 (McShine and Tetali, 1999). Tighter bounds on this problem and several other Catalan shuffles are lacking despite much effort.

Recent Developments

Every participant contributed to Monday's session by reminding each other of the principal challenges (as well as related open problems) mentioned in the FRG proposal.

Presentation Highlights

Mixing in a monotone subset of the n-cube. Anna Ben-Hamou and Emma Cohen gave excellent presentations on the status of and recent progress made on the monotone censoring question. Emma described the general status of the problem and known bounds on the quantity C_P defined in the previous section, particularly her work with Piotr Nayar and Prasad Tetali. Anna's presentation is described a bit more in the next section. Paul-Marie Samson described analogous questions (and the convenience of working) in the smooth setting when one considers the real cube, as opposed to the discrete cube.

Random Catalan Structures. Alexandre Stauffer presented a recent result [1], obtained with Alessandra Caraceni, on the mixing time of the edge-flip Markov chain on random quadrangulations of the sphere. In this model, one considers the state space of the Markov chain as the set of all quadrangulations of the sphere with n faces. Such objects are in one-to-one correspondence with labelled plane trees, thus falling into the large class of Catalan structures. Caraceni and Stauffer showed that the relaxation time of this Markov chain is at most $n^{11/2}$ and at least $n^{5/4}$, up to absolute multiplicative constants. It is expected that the lower bound is the correct order for the relaxation. This improves upon a previous result by Budzinski, who showed a lower bound on the (total variation) mixing time of $n^{5/4}$. The best known upper bound on the mixing time is $n^{13/2}$, and is just a corollary of the result of Caraceni and Stauffer.

Scientific Progress Made and Open Problems

Mixing in a monotone subset of the n-cube. Anna Ben-Hamou described progress on the problem in an important case, by proving a Poincaré inequality in the case the monotone subset is covered by a set of minimal elements with disjoint support. During the meeting, we verified that the proof extended to provide the stronger logarithmic Sobolev inequality. The technical details are as follows.

Let $A \subset \{0,1\}^n$ be a monotone subset of the n-dimensional cube, defined by M minimal elements with disjoint support of lengths $L_1, \ldots, L_M$. We denote by π the uniform measure on A, and by μ the uniform measure on $\{0,1\}^n$.

Let $f : A \to \mathbb{R}$ be a given real-valued function on A. For $k \in \{1, \ldots, M\}$, let us define the function f_k on $\{0,1\}^n$ by

$$f_k(x) = \begin{cases} f(x) & \text{if } x \in A, \\ f(x^k) & \text{if } x \notin A, \end{cases}$$

where x^k is the element obtained from x by completing with ones the support of the k^{th} minimal element. The above allows us to use the classical logarithmic Sobolev inequality on the (whole) n-cube, along with much additional work, in obtaining the following theorem.

Theorem 41.0.1. *With $A \subset \{0,1\}^n$ and L_ℓ as above, for any $f : A \to \mathbb{R}$ we have:*

$$\mathrm{Ent}_\pi(f^2) \lesssim \frac{n}{\sum_{\ell=1}^{M} 2^{-L_\ell}} \left(\frac{\max_{1\le \ell \le M} L_\ell}{\min_{1\le k\le M} L_k} \right) \mathcal{E}_\pi(f)\,.$$

Note that this implies that in the case when L_ℓ are all within a constant multiple of each other, we obtain an optimal bound on the log-Sobolev inequality in its depends on n as well as the measure of A.

Random Catalan Structures. The proof of Caraceni and Stauffer goes by the introduction of two new Markov chains on plane trees, called the leaf translation and the leaf replanting chains. In the leaf translation (resp., leaf replanting) chain, one picks an edge of the tree uniformly at random and, if that edge is incident to a leaf of the tree, then the leaf is moved one step clockwise or counterclockwise (resp., is moved to a uniformly random position in the tree). For either chain, the relaxation is shown to be at most $n^{9/2}$, which yields the upper bound of $n^{11/2}$ on the relaxation time of quadrangulations via a standard comparison procedure (which adds a factor of n due to the maximum degree). In terms of lower bounds, the leaf replanting chain has relaxation at least n^2, whereas, as observed by Emma Cohen during the meeting, the leaf translation chain has relaxation at least n^3 as it is a subset of the peak-to-valley (a.k.a. adjacent transposition) chain on Dyck paths.

In an ongoing work, Caraceni and Stauffer are able to adapt the above analysis to derive a polynomial upper bound on the mixing time of p-angulations, for p even. An open problem is to tackle the problem for p odd. In particular, the best known upper bound on the mixing time for the edge-flip Markov chain on triangulations of the sphere (with n faces) is exponential in n.

Open Problems

The Poincaré Inequality on $\{0,\dots,n\}$. It is classical to derive inequalities on $\{0,\dots,n\}$ by projection of the hypercube. In this section, we go through this procedure, starting from (41.0.1). To that purpose, define $S_n(x)=\sum_{i=1}^n x_i$, $x=(x_1,\dots,x_n)\in\{0,1\}^n$. Then, given $f\colon\{0,\dots,n\}\to\mathbb{R}$, apply (41.0.1) to $f\circ S_n$ so that

$$\mathrm{Var}_\pi(f\circ S_n)\le\frac{1}{2}C_P\sum_{x\in A}\sum_{\substack{y\in A:\\ y\sim x}}\pi(x)(f(S_n(y))-f(S_n(x)))^2.$$

Let us introduce some notations. Given $k\in\{0,\dots,n\}$, the k-th section of the hypercube is $C_k:=\{x\in\{0,1\}^n: S_n(x)=k\}$. Then, we set $A_k:=A\cap C_k$ and $\nu(k):=\pi(A_k)=|\{y\in A: S_n(y)=k\}|/|A|$. For any function g on $\{o,\dots,n\}$, we have

$$\mathbb{E}_\pi(g\circ S_n)=\sum_{k=0}^n\sum_{x\in A_k}g(S_n(x))=\sum_{k=0}^n\nu(k)g(k)=\mathbb{E}_\nu(g)$$

so that $\mathrm{Var}_\pi(f\circ S_n)=\mathrm{Var}_\nu(f)$. Similarly the Dirichlet form can be rewritten as

$$\begin{aligned}&\sum_{x\in A}\sum_{\substack{y\in A:\\ y\sim x}}\pi(x)(f(S_n(y))-f(S_n(x)))^2\\&=\sum_{k=1}^n\nu(k)p(k,k-1)(f(k-1)-f(k))^2+\sum_{k=0}^{n-1}\nu(k)p(k,k+1)(f(k+1)-f(k))^2,\end{aligned}$$

where we set $p(k,k-1)=|\{(x,y)\in A_k\times A_{k-1}: y\sim x\}|/|A_k|$ and $p(k,k+1)=|\{(x,y)\in A_k\times A_{k+1}: y\sim x\}|/|A_k|$. By construction, $\nu(k)p(k,k+1)=\nu(k+1)p(k+1,k)$ so that the latter can be interpreted as the Dirichlet form of a Markov process on $\{0,\dots,n\}$ with invariant measure ν and transition probabilities $p(k,k+1)$, $p(k,k-1)$. Using reversibility and additional computations, we infer that for any $f\colon\{0,\dots,n\}\to\mathbb{R}$, it holds

$$\mathrm{Var}_\nu(f)\le C_P\sum_{k=1}^n\nu(k)p(k,k-1)(f(k-1)-f(k))^2$$

which is the Poincaré inequality associated to the Markov process described above on $\{0,\dots,n\}$.

Such an inequality could be analyzed for itself. This amounts to the following question. Given a monotone set A define ν and $p(k,k-1)$ as above: then what is the best constant C such that for all for any $f\colon\{0,\dots,n\}\to\mathbb{R}$, it holds

$$\mathrm{Var}_\nu(f)\le C\sum_{k=1}^n\nu(k)p(k,k-1)(f(k-1)-f(k))^2? \qquad (41.0.2)$$

Mixing times of Catalan Structures. As mentioned above, there are more than 200+ known classes of objects which are enumerated by the Catalan numbers, and each comes with its own "natural" Markov chain:

- Dyck paths support corner flips, ribbon additions, swaps of two (non-adjacent) steps, shifting of a step.
- Non-crossing partitions have merge/split operations and partial rotations.
- Triangulations have edge flips and partial rotations.
- Binary trees have Remy moves and several prune and splice chains.

- Plane trees have in addition leaf translation and leaf replanting.

Understanding the mixing times and spectral gaps of the corresponding Markov chains are open problems for almost all of these, with the ntable exceptions being corner flips on Dyck paths (n^3, Wilson 2004) and Remy moves on binary trees (n^2, Schweinsberg 2001).

These chains are related to each other through bijections between the relevant objects, and through the canonical paths method, so that polynomial bounds can be deduced from other polynomial bounds. However, the arguments here are lossy, and the true exponents are unknown in all other cases.

Outcome of the Meeting

It was an overall productive meeting. Several ideas from combinatorics, functional analysis and probability were exchanged. Partial progress was made on the main problems in the project. Besides the interesting versions mentioned above of the main challenges, additional specific problems such as the one below are identified as the next steps to pursue.

Returning to the various Markov chains on Catalan structures, there is a well-known bijection between triangulations of the n-gon and plane binary trees with n leaves (trees where each internal vertex has degree 3). During the working group meeting, a new Markov chain on plane binary trees was proposed, for which the triangulation of the p-gon corresponds to partial rotations. In this chain, one chooses a leaf and an edge uniformly at random, then breaks the edge into two, and attach the chosen leaf to the unique endpoint of the broken edge that would produce a labelled plane tree. Most of the test functions used to give a lower bound on the relaxation in previous case seem to yield only simple bounds of order n. Is n the correct order of the relaxation time?

Our focused research team agreed to continue collaborating on several of the open problems mentioned above. Relevant technical documents are shared online by the group to help facilitate future research discussions. The team is very grateful for the resources and the conducive atmosphere provided by BIRS and the Banff Center.

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Chapter 42

Analytical Methods for Financial Systemic Risk (19frg270)

May 26 - June 2, 2019

Organizer(s): Tom Hurd (McMaster University), Nils Detering (University of California, Santa Barbara)

Workshop Participants

- Ian Buckley - Canadian Securities Transition Office
- Zachary Feinstein - Washington University in St. Louis
- Mark Flood - University of Maryland
- Grzegorz Halaj - Bank of Canada
- Thilo Meyer-Brandis - Ludwig Maximillians University Munich

Overview of the Field

Systemic risk (SR) is the risk of failure of the financial system, as exemplified by the financial crisis of 2007-2008. Imagining, exploring and analysing potential channels of vulnerability in large-scale financial networks requires a wide range of concepts. Many-body physics, agent-based modelling, random graph theory and mean field games are some of the currently active areas that need to be merged with financial mathematics, computer simulations and probability theory in order to understand such a complex system. The broad goal of this workshop was to capitalize on the opportunity offered by BIRS to bring together an international team of senior researchers in SR to discuss new directions, unsolved problems and the unification of different approaches.

Systemic risk research has developed very extensively over the last 10 years, with major advances in both the scope and depth of questions addressed. As a result, it has become increasingly challenging to maintain a current view of the entire topic, and it is a difficult field to enter as there is no clearly identified main line of research.

However, these characteristics also make it an exciting, innovative topic in financial mathematics, with new people entering from different areas bringing in different mathematical approaches. The book [1] provided an excellent collection of new ideas and results that were coming up soon after the financial crisis when research on systemic risk was expanding rapidly. In a different vein, [2] provided a technical overview of systemic network problems that can be understood with random graph methods. It seems however that now is an excellent time for an up-to-date coherent, textbook style introduction to systemic risk that covers the entire breadth of the field, highlighting a broad range of techniques, delivered at a level accessible to new grad students and people working in the financial regulatory system. This would be an invaluable resource on which to base a comprehensive graduate course or web course targeted at a world wide audience.

Progress made during the workshop

To capitalize on the diverse expertise of the workshop participants, the team decided at the outset to depart from a traditional math workshop setting with specialized talks. Instead, we identified the goal for the team to develop a "hypothetical" Master level course in systemic risk, packaged with a textbook, plus a comprehensive range of subsidiary material. While we began our meeting thinking of this as a good organizational theme, by the end of the very first morning, we realized that this course will be real, not hypothetical, and that the topics to be developed for the course must provide an exact map of the entire subject. Moreover, targeting a hypothetical master level student allowed us to explore the entire subject at an introductory level from different points of view, and also to enter more deeply into specific areas to highlight more advanced research-level techniques. During the BIRS week, we were able to identify some of these specific areas as new open problems that the team may develop into publishable research results.

Based on this "Master Course/Text" theme, we spent much of the workshop scoping out, and teaching each other, the main threads of SR, to identify the overall aims and key results for each thread. By the end of the week, a great deal of progress had been made in identifying the most effective strategies for promoting systemic risk as an area of applied research that has growing strategic and societal importance. In a nutshell, there is a crying need for an unbiased, coherent, and comprehensive summary of the main threads of systemic risk viewed at a global scale.

Since the May 2019 workshop, the BIRS participants are already actively implementing this vision, and have embarked on a 5 year project that can be summarized by the following rough outline of the chapters of our textbook. The team's intention is to engage the broader SR community to add expert co-authors and junior researchers to the many sections under development, while maintaining a firm curatorial control over the content and style. Within one year, we hope to have a preliminary version of the webtext to post in the public domain. Subsequent versions of the webtext will provide the SR community with a continuously evolving review of the entire subject from a global perspective.

1. **Overview of SR** A survey of what systemic risk means, how it can be described, and how it has been treated up to now in the economics literature.

2. **Deterministic Channels of SR** Systemic risk is a multi-faceted phenomenon which intertwines numerous simpler effects or channels. Stress can propagate through default contagion, liquidity contagion or fire-sales to mention just a few examples. To keep the book at an accessible technical level, these channels will be developed using the so-called Eisenberg-Noe framework. The focus here will be on mathematical models that provide a detailed qualitative understanding.

3. **Random Financial Networks** Stochasticity is central to systemic risk. At the simplest level, the deterministic channels just described and modelled act on systems that are not well observed. This uncertainty over the state of the system is best modelled by a random financial network. This chapter will focus on simulation

methods and their relation to mathematical results that can be proven within certain classes of random SR models.

4. **Systemic Risk Data and Calibration** This part of the course/book will give an overview of issues relating to data available for calibrating SR models. The two special characteristics of SR is that the required data is difficult to collect and that it has immense strategic value. Consequently it is never available in the public domain, and data held by government agencies is also incomplete. These facts present an immense challenge to academic researchers. This chapter will review relevant databases in the public domain, survey methods to reconstruct required data missing from the public data, and provide access to archives of benchmark databases, both real and surrogate (simulated).

5. **Application: Macroprudential Stress Testing** The most important practical application of SR theory is at the core of the macroprudential ("macropru") stress testing exercises conducted by the central banks of the major economies. Traditional microprudential ("micropru") stress testing is a well-established procedure run by financial regulators in most developed countries. Large banks are provided with a small number of medium term (several years long) economic scenarios, and the test requires all individual banks to report on the detailed characteristics of their future profit and loss distribution resulting from following their operational strategy. Macropru stress testing extends the micropru test to provide a detailed assessment of the stability of the entire system under the same type of scenario. The central regulator takes the micropru results for the individual banks', and then applies a fully-developed systemic risk model to determine risk measures for the additional damage to the entire system stemming from the knock-on effects of systemic contagion. This final chapter will review the common features of macropru in different countries and delve into the implementation issues that must be addressed.

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Chapter 43

Permutation Polynomials over Finite Fields (19frg263)

June 9 - 16, 2019

Organizer(s): Daniele Bartoli (Università degli Studi di Perugia), Ariane Masuda (New York City College of Technology, CUNY), Qiang Wang (Carleton University)

Overview of the Field

After the seminal works of Hermite [3] and Dickson [2] at the end of the 19^{th} century, many researchers have dedicated themselves to studying permutation polynomials over finite fields, not just because they are interesting in their own right, but also due to their connections with several applications.

Permutation polynomials over a finite field $\mathbb{F}_q$ are polynomials that induce bijections over $\mathbb{F}_q$ as mappings. For example, a monomial x^n permutes $\mathbb{F}_q$ if and only if $\gcd(n, q-1) = 1$. Even though permutation monomials are well understood and simply described, the situation with binomials changes completely as not too many families of permutation binomials are known.

The problems in this area tend to fall into two categories: characterization and enumeration. The first category involves questions regarding criteria and tests for permutation polynomials, relationships between their coefficients, numbers and degrees of their terms, and finding families of permutation polynomials. The second one includes questions about the distribution and number of permutation polynomials of a given degree or special form, bounds and asymptotic formulas for these numbers, and the non-existence of permutation polynomials of certain shapes. In several situations these two kinds of problems are closely related. Applications in Coding Theory, Combinatorial Designs and Cryptography often require permutation polynomials having a particular structure or additional extraordinary properties. Permutation polynomials meeting these conditions are usually difficult to find.

The study of permutation polynomials has greatly benefited from a variety of tools in Algebraic Geometry, Combinatorics and Number Theory that involve algebraic curves, power sums, character sums, among others. Surveys like [6, 7, 4, 5] provide an excellent overview of the area.

Recent Developments and Open Problems

Over the past few decades the majority of papers in this area have been devoted to finding families of permutation polynomials. Many of them have built up on previous works by incorporating new ideas into known techniques. One of the goals of the workshop was to better understand the many existing families of permutation polynomials and see how they are related to each other under a more general framework.

The index of a polynomial was first introduced by Akbary, Ghioca, and Wang in 2009 to study the distribution of permutation polynomials over finite fields [1]. Given a non-constant polynomial g of degree less than $q-1$ over $\mathbb{F}_q$, the index ℓ of g is the unique integer for which g can be written as $a(x^r f(x)^{(q-1)/\ell}) + b$ for some $r \in \mathbb{N}_0$, $a, b \in \mathbb{F}_q$, and $f \in \mathbb{F}_q[x]$. They showed that the density of permutation polynomials in the set of polynomials with prescribed index and exponents is higher when the index is smaller. The index of a polynomial has been also investigated in contexts that do not involve permutation polynomials. For instance, the index of a polynomial is closely related to the concept of the least index of a cyclotomic mapping polynomial. As a consequence, Wan and Wang obtained an index bound for character sums of polynomials over finite fields that is better than the Weil bound in some situations. This has potential applications related to the correlation of sequences, the minimum distance of trace codes, and the number of solutions of Artin-Schreier equations. Very recently Wang wrote a survey [8] on the index approach where a long section is dedicated to classifying permutation polynomials from over 60 papers based on their indices. We note that many results in these papers do not mention the index of the polynomial involved explicitly. So this survey is an important and major step in trying to organize the many existing permutation polynomials. It confirms that the index approach is very promising and provides a rich source of research directions.

In the workshop we aimed to pursue some of these directions. Dickson had already found all permutation polynomials of degree up to 6 back in 1896. More than 100 years passed, and only in 2010 permutation polynomials of degree 7 in finite fields of even characteristic were found. Wang's survey revealed that many known permutation polynomials were identified as having small indices. We thus propose the following.

Problem 1: Classify all permutation polynomials of small indices over $\mathbb{F}_q$ in terms of their coefficients.

Another interesting direction concerns the so-called complete permutation polynomials. A polynomial $f(x) \in \mathbb{F}_q[x]$ is a complete permutation polynomial over $\mathbb{F}_q$ if both $f(x)$ and $f(x) + x$ are permutation polynomials over $\mathbb{F}_q$. Complete permutation polynomials are also related to bent and negabent functions that appear in a number of applications in Coding Theory, Combinatorial Designs and Cryptography. The most studied class of complete permutation polynomials is the monomial one.

Problem 2: Classify families of permutation polynomials or complete permutation polynomials like monomials $a^{-1}x^{\frac{q^n-1}{q-1}+1}$ and sparse permutation polynomials over $\mathbb{F}_{q^n}$ having indices $q-1$, $q+1$, or $c(q^{n-1}+\cdots+q+1)$ for some constant c.

Presentation Highlights

Motivated by the emerging emphasis on permutation rational functions, Bartoli presented a different viewpoint in classifying permutation rational functions of degree 3. He also showed several applications of algebraic curves in combinatorics. In a second talk Bartoli focused on techniques to prove irreducibility and to find irreducible components of curves over finite fields, and on their applications in the study of permutation polynomials, exceptional polynomials, complete mappings, planar polynomials, and APN functions.

Hou talked about a class of permutation trinomials of index $q+1$. He discussed the main ingredients in the proof which involve number theoretic techniques, an application of the Hasse-Weil bound, and symbolic computations of resultants and factorizations.

Wang gave a survey talk on the index approach to study and classify permutation polynomials over finite fields. Permutation polynomials of intermediate indices are a recent focus in this area. They can be related to rational functions and complete mappings, depending on the choice of the index. For instance, Wang presented a construction of permutation polynomials with index $q + 1$ based on rational functions.

Scientific Progress Made

During the meeting, we mainly focused on the classification problem for permutation trinomials. We were able to obtain several non-existence results using the Hermite's criterion and algebraic curves. We expect to have a paper gathering our findings within the next few months.

Throughout the week we spent together, we had many opportunities to talk about the different directions that our area has been taking. The number of papers on permutation polynomials has greatly increased, and many new researchers have joined the area. While we currently have a rich source of results, many of them deal with particular shapes of polynomials. It is a challenge for the community to determine what is known, and whether or not certain results have already been obtained. The discussion led us to consider a long-term project that will involve digging through all papers on permutation polynomials, and classifying them, not just in terms of natural parameters like their degrees, number of terms and finite field orders, but also through their indices. This will be a continuation of the work that Wang initiated in [8]. Our overarching goal is to have a better understanding of what is known, to organize the existing permutation polynomials in a systematic way, and to provide the research community access to the valuable data we will be collecting in the form of an online database and a survey book. The process will likely reveal many interesting interconnections. We greatly believe that this will open doors to further development of new mathematics, and prompt researchers to explore and investigate pertinent questions.

Outcome of the Meeting

The workshop gave a select group the unique opportunity to interact, concentrate efforts, and focus on problems. It was the first forum dedicated to discuss permutation polynomials over finite fields exclusively. Having participants with a diverse range of experience working with permutation polynomials and other related problems was highly important to promote expertise sharing. The group included two Ph.D. students and one postdoctoral fellow. We all greatly benefited from seeing how each one contributed to the discussion by exchanging research experiences. Our week was very productive and inspiring. We expect that our collaboration will give rise to one research article and, as a long-term objective, an online database of permutation polynomials and a book.

Participants

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Chapter 44

Extremal Blaschke products (19frg254)

June 23 - 30, 2019

Organizer(s): Kelly Bickel (Bucknell University), Pamela Gorkin (participant, Bucknell University), Anne Greenbaum (University of Washington), Thomas Ransford (Université Laval), Felix Schwenninger, (University of Hamburg), Elias Wegert (TU Bergakademie Freiberg))

Overview of the Field

One of the most important results in operator theory is due to John von Neumann and states that for a fixed contraction T and polynomial p, the operator norm

$$\|p(T)\| \leq \sup\{|p(z)| : z \in \mathbb{D}\}.$$

Variations of von Neumann's inequality can be extremely useful and are thus frequently the object of study. Matsaev's conjecture, for example, asserts that for every contraction T on L^p (with $1 < p < \infty$) for any polynomial p and S the unilateral shift operator one has

$$\|p(T)\|_{L^p \to L^p} \leq \|p(S)\|_{\ell^p \to \ell^p}.$$

When $p = 2$, this is von Neumann's inequality. However, Drury [10] showed that this conjecture fails in general. Another conjecture in this direction, one for which no known counterexample exists, is the Crouzeix conjecture.

Let A be an $n \times n$ matrix and let $W(A)$ denote the numerical range of A. Recently, Crouzeix and Palencia [6] showed that for every function f holomorphic on an open set containing the closure of $W(A)$, the operator norm of $f(A)$ satisfies

$$\|f(A)\| \leq (1 + \sqrt{2})\ \sup\{|f(z)| : z \in W(A)\}.$$

A simplified version of their proof can be found in [17]. The Crouzeix Conjecture states that $(1 + \sqrt{2})$ may be replaced by 2 and there are several classes of matrices for which this is the case (see, for example, [1, 5, 4, 2, 8, 14]). In particular, the conjecture is true for 2×2 matrices as well as matrices of the form $aI + DP$ or $aI + PD$ where a is a complex number, D is a diagonal matrix, and P is a permutation matrix (see [3] and [15]), 3×3 tridiagonal Toeplitz matrices and matrices in this class with some diagonal entries taken equal to zero, [15].

In 2003, Crouzeix showed that equality is obtained with the sharp constant C for some function $f = B_A \circ \omega$, where ω is a conformal map of the interior of $W(A)$ onto the unit disk and B_A is a Blaschke product of degree less than n. Such a Blaschke product is called an *extremal Blaschke product*. In this workshop, we focused on the study of extremal Blaschke products. That the conjecture holds for A a Jordan block with zeros along the diagonal is not difficult to see; it was later shown in [4] that the conjecture also holds for a perturbed Jordan block

$$J_\nu = \begin{pmatrix} \lambda & 1 & & & \\ & \lambda & 1 & & \\ & & \ddots & \ddots & \\ & & & \ddots & \\ \nu & \cdots & \cdots & & \lambda \end{pmatrix}.$$

These two classes of matrices (Jordan blocks and perturbed Jordan blocks) are special cases of operators known as compressions of the shift operator. Much is known about the numerical range of these operators ([7], [11], [12], [16]), It is natural, then, to consider the conjecture for this special class of operators, as well as the extremal Blaschke products associated with these operators. Beurling's theorem tells us that the invariant subspaces of the shift operator S are of the form $\{\Theta H^2 : \Theta \text{ an inner function}\}$. Therefore, the invariant subspaces for the adjoint of the shift are of the form $K_\Theta := H^2 \ominus \Theta H^2$. The compressed shift operator $S_\Theta : K_\Theta \to K_\Theta$ is defined by

$$S_\Theta(f) = P_\Theta(S(f)),$$

where P_Θ is the projection of the Hardy space H^2 onto K_Θ. Throughout this discussion, Θ denotes a finite Blaschke product.

Presentation highlights and progress made

There are several natural questions that we investigated throughout this workshop. In what follows, let A be an $n \times n$ matrix, let Ω be a simply-connected domain (typically with smooth boundary) containing the spectrum of A, $H_1^\infty(\Omega)$ the unit ball of $H^\infty(\Omega)$, and let f be a holomorphic function continuous on $\overline{\Omega}$ and bounded by 1 on Ω such that

$$\|f(A)\| = \sup\{\|g(A)\| : g \in H_1^\infty(\Omega)\}.$$

As indicated earlier, such an extremal function f can be taken to be a Blaschke product composed with a conformal map and these extremal functions have played an important role in previous investigations of the Crouzeix conjecture. The extremal functions come equipped with extremal vectors, namely unit vectors $x \in \mathbb{C}^n$ so that

$$\|f(A)\| = \|f(A)x\|.$$

These extremal vectors are also quite important and are known to possess special properties. For example, in [2], Caldwell, Greenbaum, and Li showed that if $\|f(A)\| > 1$, then

$$\langle f(A)x, x\rangle = 0. \tag{44.0.1}$$

They used this to provide a new, simple proof of the fact that if Ω is a disk containing $W(A)$, then

$$\|g(A)\| \leq 2 \max_{x\in\Omega} |g(x)|.$$

During this workshop, we primarily investigated these extremal functions and their associated extremal vectors both for $\Omega \supset W(A)$ and for more general Ω.

Topic 1. Extremal Functions. Let $\Omega \supset W(A)$. During this workshop, we both analytically and numerically explored the structure of the associated extremal functions. For example, we observed that if A is normal, then every Blaschke product is extremal for A. After restricting to non-normal matrices, we observed that every degree 1 and degree 2 Blaschke product is extremal for some A. We conjecture that every Blaschke product B with $\deg B \le n-1$ is extremal for some non-normal $n \times n$ matrix A. This seems supported by numerical computations, but analytically showing that some B is extremal for a given A is, in general, very challenging. Additionally, T. Ransford presented a result indicating that there is some open set of $n \times n$ matrices A whose extremal Blaschke products always have maximal degree $n-1$. Thus, in some sense, the number of matrices whose extremal Blaschke product has maximal degree is quite large. We also discussed examples where (up to a conformal map) A has a unique extremal Blaschke product and examples where the Blaschke product associated to A is not unique. The example illustrating non-uniqueness is due to Kenan Li. However, we do not currently have enough such examples to conjecture a pattern.

Besides, if Ω is a disk with center c, then (1) implies that the extremal function satisfies $|f(c)| \le \sqrt{4 - \|f(A)\|^2}$ and the estimate can even be improved by a result due to Drury [9]. As mentioned above, an important class of operators to study are compressions of the shift S_Θ, where Θ is a finite Blaschke product with $\deg \Theta = n$. In this setting, we ran numerous numerical experiments to better understand the associated extremal Blaschke products. Let us denote those functions by B_Θ. The numerical investigations always yielded B_Θ with maximal degree, namely $\deg B_\Theta = n-1$. This generalizes the well-known fact that for the Jordan block J_0 with $\lambda = 0$, the symbol is $\Theta(z) = z^n$ and $\Theta(z)/z$ is an extremal Blaschke product. More generally, if we choose Θ with $\Theta(z) = z\Theta_1(z)$, i.e. so $\Theta(0) = 0$, then the experiments suggest that the appropriately normalized Blaschke products Θ_1 and B_Θ are close to each other. This relationship appears particularly strong if the zeros of Θ_1 are very close to the unit circle $\mathbb{T}$. We expect that these experiments indicate an underlying relation between the symbol Θ and an extremal Blaschke product for S_Θ (see the remarks on future research below).

We also have proved the following:

Theorem. Let $\delta_\Theta = \inf_k \prod_{j \ne k} \rho(z_j, z_k)$, where $z_1, \ldots, z_n$ denote the zeros of the finite Blaschke product Θ and ρ denotes the pseudo-hyperbolic distance. If $\delta_\Theta > 2\sqrt{2}/3$, the operator S_Θ satisfies the Crouzeix conjecture.

Future research. One of our goals is to remove the restriction on δ_Θ in the theorem above.

For the compressed shift S_Θ, we hope to better understand the relationship between the symbol Θ and the extremal Blaschke product. For example, we would like to prove analytically that B_Θ always has maximal degree. The case where the symbol Θ has the form $\Theta(z) = z\Theta_1(z)$ is of special interest, since there seems to be a correlation between Θ_1 and the extremal Blaschke product B_Θ. In particular, if the zeros of Θ_1 approach points on the unit circle, we conjecture that the zeros of B_Θ have the same limit points (provided that the conformal mapping ω is appropriately normalized). Working on a proof of this conjecture will help us to understand the interplay of the symbol and the extremal Blaschke product of S_Θ. It will also yield new insight in the behavior of the functions and operators which play a crucial role in the proof of the main theorem in Crouzeix and Palencia [6]. The theoretical investigation of these problems will be supported by improved and specially designed numerical experiments.

We also plan to study other examples of extremal Blaschke products to formulate stronger conjectures about their degree bounds and uniqueness properties. For example, if A is a 3×3 matrix and its numerical range is a disk, when is the extremal Blaschke product of a particular degree and when is it unique?

Topic 2. Extremal Vectors. We also spent significant time investigating extremal vectors and their interplay with their associated extremal functions. An interesting result (proved beforehand and presented during the workshop by T. Ransford) extends (44.0.1). It says that if an extremal function f factors as $f = f_1 f_2$, then

$$\langle f_1(A)x, \left(\|f(A)\|^2 I - f_2(A)^* f_2(A)\right) x\rangle = 0.$$

During the workshop, we generalized this approach considerably by studying the quantity $\langle h(A)x, x\rangle$, where x is an extremal vector, but h is any function holomorphic on Ω and continuous on $\overline{\Omega}$. In this setting, our main result says that there is a probability measure μ such that

$$\langle h(A)x, x\rangle = \int_{\partial\Omega} h d\mu, \text{ for all } h \in \mathcal{A}(\Omega).$$

Moreover, we are able to say quite a bit about this measure and many of its properties; in fact, we can give an explicit description of it.

In the case of the compression of the shift operator S_Θ and $\Omega = \mathbb{D}$, we can say more. In particular, if B is a Blaschke product of degree strictly less than that of Θ, then results from [18] can be used to show $\|B(S_\Theta)\| = 1$. Von Neumann's inequality says that this is the best possible norm and so, B is an extremal function for S_Θ on $\mathbb{D}$. In this setting, we can compute the dimension of the space of extremal vectors associated to each B and provide explicit formulas for them. Moreover, for each extremal vector x, we have a formula for the associated probability measure μ, which has allowed us to investigate various conjectures about the structure of μ in more general situations.

Future Research. We hope to obtain more information about these μ measures and use them to deduce additional facts about the matrix A and related quantities. For example, given a fixed Ω, this result and some underlying formulas put a number of constraints on the possible extremal vectors of A. Moreover, the quantity $\langle h(A)x, x\rangle$ is always in the numerical range of $h(A)$. It appears that this result could be adapted to provide bounds for both the norm and spectral radius of $h(A)$ (at least for particular types of A and h). The case of S_Θ seems particularly tractable. Specifically, we hope to extend the current work on $\Omega = \mathbb{D}$ to more general domains like the numerical range $W(S_\Theta)$, at least in situations where Θ is simple.

Outcome of the Meeting

As indicated above, we made progress in two directions: a probability measure that appears as an inner product and the numerical range of the compression of a shift operator. We also came across some new extremal problems for Blaschke products that appear to be of interest in their own right. We plan to continue working together on each of these topics to extend the results we have, as well as to look at the relationship between the results.

Participants

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Chapter 45

Novel Mathematical and Statistical Approaches to predicting Species' Movement under Climate Change (19frg248)

July 14 - 21, 2019

Organizer(s): Noelle G. Beckman(Department of Biology and Ecology Center, Utah State University), Michael G. Neubert (Biology Department, Woods Hole Oceanographic Institution)

Overview of the Field

Climate change and habitat loss are two of the primary causes of global biodiversity loss [17, 20]. Areas where a species lives - the geographic range - become gradually unsuitable as the climate changes from that which the species can tolerate to levels of temperature, rainfall, and related variables that no longer support its populations. Under a changing climate, species must ”adapt, move or die” [7]. Here, we consider moving or dying.

Populations need to shift - generally polewards - to track their suitable climate as it shifts. This process is captured by the concept of the velocity of climate change [14, 8]. Based on climate change and the factors that determine its realization in space - location on the globe, local topography, etc - the velocity of climate change represents the rate at which a population must shift to remain in the same climate space over time. Estimated poleward speeds, based on predicted temperature changes by the end of this century, range from 0.08 to 1.26 km yr^{-1} depending on the geographic region [14]. If a species can shift populations at a speed at or above the local velocity of climate change, it has the potential to persist; if it cannot, it is more likely to go extinct.

Habitat loss is the other major cause of biodiversity declines. Globally, 75% of the land surface has been converted by humans [11]. The precise consequences of habitat loss can be considered in terms of the critical patch size. As the area of available habitat declines, the population loses more dispersers beyond the patch edge. At a critical patch size the rate of population growth is not sufficient to counter the loss of dispersers, and the population goes extinct [22, 12]. Thus, species with a lower population growth rate or further dispersal will go extinct sooner as habitat shrinks.

The mathematical literature has explored the invasion and persistence thresholds for species whose habitats shift at a constant speed (e.g., [19, 2, 24, 10, 13, 18]) as extensions of the critical patch size problem for populations diffusing out of a favorable habitat [15]. These studies, based on analyses of models formulated as partial differential equations or integrodifference equations, have helped us to identify some of the species and habitat characteristics that facilitate persistence. In particular, these studies establish a connection between a species' spreading speed (i.e., the rate a population spreads into an empty habitat of infinite extent), its thermal tolerance (which determines the extent of the suitable habitat) and climate velocity (which determines how fast the habitat is shifting).

To apply these models to a particular species, we must estimate the model's parameters from data. Roughly speaking, these data fall in two categories: demographic data and dispersal data. For plants and animals, demographic data, in the form of population projection matrices, have been collected in repositories. For example, matrices for 695 plant species have been assembled in the COMPADRE database [21]. Empirical approaches to measure species' movement, such as the use of molecular markers and GPS tracking, have advanced enormously [6]. These advances are producing an increasing amount of dispersal data, some of which has been gathered together and is available (see, [4]).

Recent Developments and Open Problems

While demographic and dispersal data are increasing, these data remain sparse as they are intensive to collect. For example, there are approximately 391,000 known vascular plant species on Earth [16], and autecological studies to estimate population spread for each are not feasible. Hence, most fundamental research on population dynamics and spread has focused on a few well-parameterized case studies. Projections of population spread in response to climate change have been done for a limited number of species [3, 5]. Nevertheless, the development of risk criteria that can be applied to a wide range of species by conservationists is highly desirable. This will require effectively synthesizing data with mathematical models; challenges to which include simplifying often complex data with minimal loss of information and handling sparsity in data as the size and complexity of data increases. Management decisions for species will require projections of population spread based on realistic demographic and dispersal scenarios that can be generalized to a range of species.

Our objective is to develop mathematical and statistical approaches that take advantage of the increasing amount of biological data to predict invasion and persistence of species in a changing world. In this Focussed Research Group, we aimed to:

1. determine if there is a direct way of going from variability in the input parameters to an estimate of what fraction of species can keep up with climate change.

2. develop a new generation of mechanistic models for growth, survival, fecundity, and dispersal in response to changing temperatures and analyse these models mathematically using methods from traveling wave theory and spreading speeds to examine how changes in temperature will influence invasion/persistence as climate change alters demography and dispersal.

Scientific Progress Made

For **Objective 1**, we developed general mathematical insights on the distribution of spread speeds depending on the distribution of dispersal and demography and their covariation using integrodifference equations (IDEs) and assuming dispersal is normally distributed. In this model there are two random variables, the arithmetic growth rate R and the dispersal coefficient D. We derived the distribution of spreading speeds $\left(C^* = 2\sqrt{RD}\right)$ when each of these parameters was fixed and the other was varying according to an exponential, lognormal, or gamma distribution. We also examined the distribution of spreading speeds when both varied independently assuming both had the same distribution (i.e., exponential, lognormal, and gamma). We then explored the distribution of spreading speeds when R and D are correlated for bivariate lognormal and bivariate gamma distributions. Finally, we considered the distribution of critical patch size $\left(L^* = \pi\sqrt{\frac{D}{R}}\right)$ using the ratio distribution of a bivariate lognormal. Using these mathematical results, we will predict the global distribution of species vulnerabilities to habitat loss and climate change based on global databases. From this, we can estimate the proportion of species that may be at risk to either habitat loss or climate change based on estimates of climate velocity from the literature (e.g. [14]). We will also examine how correlation in dispersal and demography (e.g. dispersal syndromes, [1]) influence critical patch size and spread rates.

For **Objective 2**, we developed specific approaches for incorporating temperature responses of demography and dispersal into mechanistic models. We began with a McKendrick Von Foerster model and then moved to an integrodifference equation with stage-structure. We used ragweed (*Ambrosia artemisiifolia*) as an empirical example. The distribution and shift of populations over space of ragweed is of interest to many people due to its role as an allergen. Much is known about its dispersal and demography, but understanding how increasing temperature will affect dispersal and demography, and therefore the spread and shift in populations is less studied. We decided to examine five different cases of temperature fluctuations within the year: 1) constant, 2) stochastic, 3) periodic, 4) increasing trend, and 5) periodic with increasing trend. We assume that demography (i.e., survival, growth, and reproduction) responds to temperature according to a β distribution. We assumed a Laplace distribution for dispersal and that mean dispersal distance increases with the size of reproductive adults. This model could be expanded to investigate spread across a landscape that varies geographically in temperature as well as including density-dependence in plant performance.

Outcome of the Meeting

We made significant progress on both our objectives and identified several immediate next steps that will result in various products. Results for **Objective 1** will be finalized by participants and a manuscript is in progress that will be submitted within six months. Zhou will lead a project extending the results derived in this meeting to moving habitat models. Participants will gather at the National Institute for Mathematical and Biological Synthesis (NIMBioS) in Spring 2020 to work on this project. Other extensions to the results of **Objective 1** we discussed are 1) examining the distribution of wave speeds when including stage structure and 2) developing similar theory for the furthest forward velocity from a branching process. Initial models that emerged from **Objective 2** will be further developed, analyzed, and parameterized by Bogen and Beckman with data provided by Bullock. We also identified new directions of this work.

Participants

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Research in Teams Reports

Chapter 46

An Optimal Transport Approach to Crop Root Systems and related Multiscale Structures (19rit295)

January 20 - 27, 2019

Organizer(s): Young-Heon Kim (University of British Columbia), Brendan Pass (University of Alberta), David Schneider (University of Saskatchewan)

Overview and background of the project

Given the root systems of several plants with identical genotypes (genome sequence) and grown in the same environment, how does one construct a "typical" representative of the set? What about variation within the set? How might one assess whether root systems of different genotypes are similar or different?

These are all important questions arising in the development of crops with improved traits, for example tolerance to drought or nutrient limitations. Root systems are notoriously difficult to study because, they exhibit biologically important structures with characteristic length scales varying over more than five orders of magnitude — primary roots have lengths on the order of one meter while root hairs (extensions of single cells) have diameters of 10^{-5} meters — but are not self-similar. While sophisticated mathematical techniques such as persistent homology have been applied to roots, most researchers rely an ad hoc collection of phenotypes or traits (e.g., rooting depth, total root length, total root mass, volume of convex hull) [2, 4, 5, 3, 7]. Extensive experience has shown that this ad hoc approach has critical limitations. Figures 46.1 and 46.2 represent two distinct root systems arising from the same species and illustrate the issues of using phenotypes to differentiate between them (their structures are clearly different, but it is not at all clear which traits should be used to quantify the difference).

This research project aims to develop metrics that can be used to quantify the differences between root systems and as a framework for interpolating or averaging over a set of biologically equivalent systems (same genotype and environment). The issue of averaging is ubiquitous in nature. Though most often thought of in the linear context of numbers or vectors, there is also a fairly well developed theory of averaging on metric spaces (collections of objects with a canonical distance, or measure of difference, between any two objects), known as the theory of

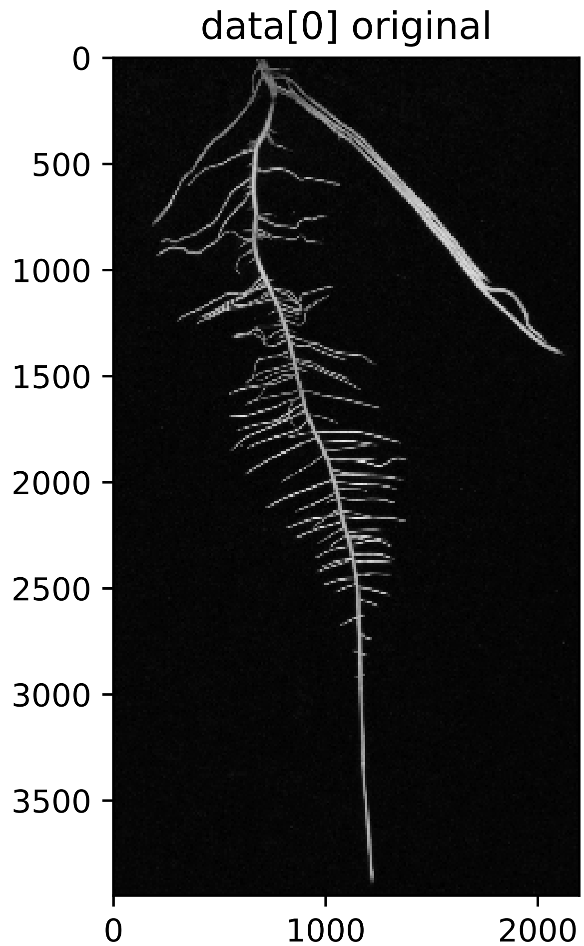

Figure 46.1: Example of root system.

metric barycenters.

Our motivation comes from the relationship of particular phenotypes exhibited by plants to their genotypes and the environmental conditions under which they were grown. Typically, fixed genotypes and environments result in plants with a diverse collection of different root systems, and it is desirable to choose a single system to associate with the genotype/environment pair (how does one "average" in a meaningful way among the various systems with different shapes?) and quantify the variation from that system exhibited by the other samples sharing the same genotype and environment.

The Wasserstein distance, or earth mover's, from optimal transport theory, is commonly used to compare distributions of mass: visualize two mass distribution as piles of dirt with different shapes but the same volume and transform the first pile into the second in a way that minimizes the average distance moved by the dirt. This minimal average distance is then the earth mover's distance, and the theory of its metric barycenters (Wasserstein barycenters) is fairly well developed; see [1] for a seminal paper on Wasserstein barycenters and [6] for an overview

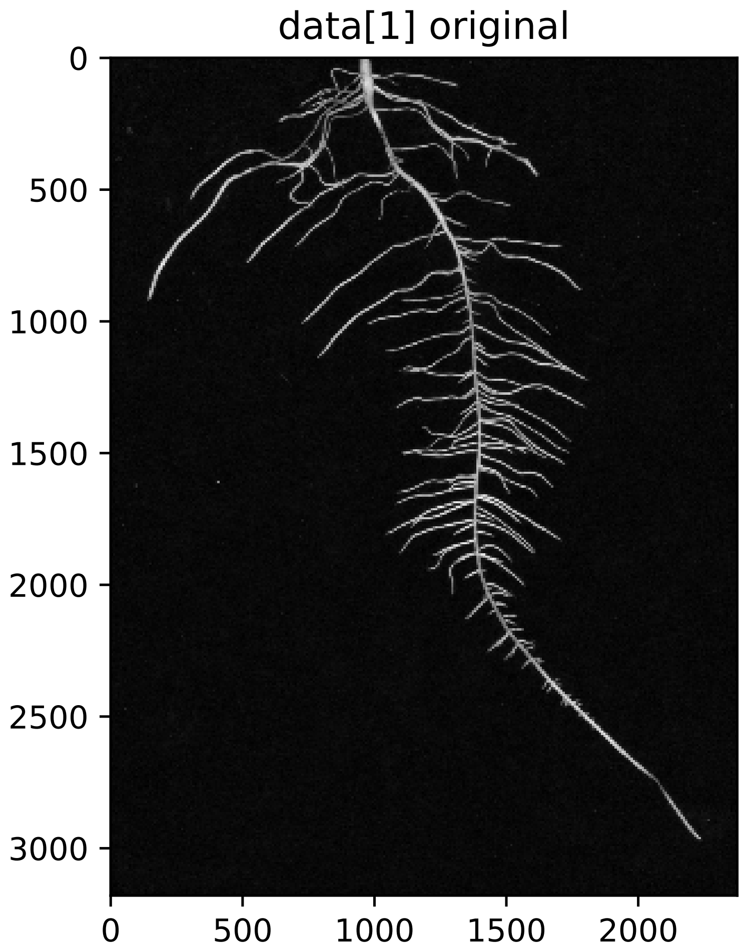

Figure 46.2: Example of a root system.

of numerical methods in optimal transportation. Since one can interpret a root system as a mass distribution, this is in some ways a reasonable candidate for a metric between root systems. However, it fails to account for the topological, dendritic structure exhibited by root systems (for example, a single thick branch will be very close in Wasserstein distance to two thinner branches, emerging from a common node, sitting very close together, but these have very different biological properties). In addition, if we compute the Wasserstein barycenter, or interpolation, of two or more root systems, we generally obtain a distribution of mass, but not necessarily one that resembles a root system (that is, the dendritic structure may be lost). Classical Wasserstein distance is thus not well suited to comparing root systems.

Our proposal is to adapt the earth mover's distance to build a metric better suited for this purpose, a root matcher's metric. When comparing to root systems, one tries to move the mass from one onto the other in way that minimizes as much as possible the overall movement of the mass (as with the earth mover's metric), but also minimizes the distortion of the topology. This will yield a more biologically meaningful way to quantify the difference between two root systems, and the corresponding metric barycenters (defined using the root matcher's metric) will be meaningful representatives of a family of such systems

Objectives of the meeting

The goal of this team meeting is to boost up progress in the very early stage of the proposed research program we have recently initiated; two of us (Kim and Pass) are mathematicians who have been focusing on optimal transport theory, and the third member (Schneider) is a computational biologist who have been working on complex biological systems including analyzing crop root systems. Though we have been having regular research meetings over the internet to discuss issues and exchange ideas, it is desirable for the three of us to meet together in person for a week, free from other distractions, to concentrate on the research problems. This first in-person meeting focused on developing new versions of Wasserstein distance and barycenters which are well suited for analyzing root structures.

Scientific Progress Made

We have developed a new metric on the space of the probability measures that is naturally suited to dentritic structures, including plant roots and trees. Unlike the usual Wasserstein barycenters, interpolants of several root systems (viewed as mass distributions) under this new interpolation seem to largely preserve root like structure (we have already proven the preservation of several desirable properties characteristic of roots systems, while others remain conjectures.) The approach also seems advantageous computationally, and we have almost completed writing code for a preliminary algorithm.

Anticipated Outcome of the Meeting

We are working on three initial papers, one developing the theoretical framework for root matching, targeted towards mathematicians, another focusing on methodological issues (explaining how this framework can be used to distinguish between collections of root systems) and a third targeted towards biologists, in which we apply this methodology to real data and establish distinctions between collections of root systems that previous, phenotype-based approaches were unable to detect.

We are also optimistic that this approach and variations of it will lead to much more fruitful research in the future as well. We plan to hire at least on postdoctoral researcher, working closely with all three us, to investigate future directions.

Our work completed at BIRS represents a first step towards a mathematical foundation of "optimal transport of graphs with spatial embedding and mass," and seems likely to lead to fascinating new questions at the intersection of graph theory and analysis. It is reasonable to expect the same underlying mathematical structure (mass distributions on dendritic structures) to occur in other areas such as vascular structures in leaves, blood vessels and nerves in animals, and trees in decision science. Therefore it is reasonable to expect that this work will be broadly applicable.

Participants

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Chapter 47

Analysis and geometry of several complex variables (19rit242)

April 14 - 20, 2019

Organizer(s): Alexander Nagel (University of Wisconsin-Madison), Malabika Pramanik (University of British Columbia)

Let $\Omega \subseteq \mathbb{C}^d$ be an open connected set, and let $L^2(\Omega)$ denote the Hilbert space of equivalence classes of measurable functions f that are square-integrable with respect to the Lebesgue measure on Ω, i.e., for which

$$||f||^2_{L^2(\Omega)} = \int_\Omega |f(\mathbf{z})|^2 \, d\mathbf{z} < +\infty.$$

The Bergman space $A^2(\Omega)$ given by

$$A^2(\Omega) = \{h \in L^2(\Omega) : h \text{ is holomorphic on } \Omega\}$$

is a closed subspace of $L^2(\Omega)$. The orthogonal projection $\mathcal{P} : L^2(\Omega) \to A^2(\Omega)$ is called the Bergman projection. This operator is given by integration:

$$\mathcal{P}f(\mathbf{z}) = \int_\Omega B(\mathbf{z}, \mathbf{w}) f(\mathbf{w}) \, d\mathbf{w}$$

where $B(\mathbf{z}, \mathbf{w}) : \Omega \times \Omega \to \mathbb{C}$ is the Bergman kernel. Basic properties of the Bergman kernel can be found in [4]. The study of the Bergman kernel and projection has a long and rich history, but many interesting questions remain. Our collaborative research has focused on estimation of the Bergman kernel, see [5], for several different types of domains. We made additional progress during the week-long residence at BIRS. We are currently writing up our results for publication. We briefly summarize them below.

1. Tubes over convex sets and log-convex Reinhardt domains.

A tube over a convex set $\Sigma \subset \mathbb{R}^n$ is the domain

$$T = \{\mathbf{x} + i\mathbf{y} \in \mathbb{C}^n : \mathbf{y} \in \Sigma\}.$$

We say that $\mathcal{R} \subset \mathbb{C}^n$ is a Reinhardt domain if it is invariant under rotations about each coordinate axis[1]. A Reinhardt domain $\mathcal{R}$ is axis-deleted if $\prod_{j=1}^n z_j \neq 0$ for all $(z_1, \ldots, z_n) \in \mathcal{R}$, and is log-convex if

$$\log|\mathcal{R}| = \big\{y_1, \ldots, y_n) \in \mathbb{R}^n : (e^{y_1}, \ldots, e^{y_n}) \in \mathcal{R}\big\}$$

is a convex set. If $\mathcal{R}$ is an axis-deleted log-convex Reinhardt domain then $\Phi(z_1, \ldots, z_n) = (e^{-iz_1}, \ldots, e^{-iz_n})$ is a holomorphic mapping of the tube domain over $\log|\mathcal{R}|$ onto $\mathcal{R}$ and is the universal covering map.

We obtain sharp geometric estimates for the Bergman kernel $B(\mathbf{z}, \mathbf{w})$ and its derivatives on the diagonal $\mathbf{z} = \mathbf{w}$ for tubes T over convex sets Σ and for axis-deleted log-convex Reinhardt domains $\mathcal{R}$. These estimates are given in terms of the volume and other geometric properties of minimal caps of the convex sets Σ or $\log|\mathcal{R}|$. To describe these caps, let $E \subset \mathbb{R}^n$ be a proper[2] open convex set. If $\mathbf{p} \in E$ and $\mathbf{n}$ is a unit vector in $\mathbb{R}^n$, the cap of E through $\mathbf{p}$ in direction $\mathbf{n}$ is the set $C_{\mathbf{p}}(\mathbf{n}) = \big\{\mathbf{y} \in E : \langle \mathbf{y} - \mathbf{p}, \mathbf{n}\rangle \geq 0\big\}$. There is a unit vector $\nu_{\mathbf{p},n} \in \mathbb{R}^n$ so that, if $|E|$ denotes the volume of a set E,

$$|C_{\mathbf{p}}(\nu_{\mathbf{p},n})| = \inf_{\mathbf{n} \in \mathbb{R}^n} |C_{\mathbf{p}}(\mathbf{n})|.$$

Thus $C_{\mathbf{p}}(\nu_{\mathbf{p},n})$ is a cap[3] of E of minimal volume through $\mathbf{p}$. Moreover, $\mathbf{p}$ is the centroid of the convex $(n-1)$-dimensional slice $E_{\mathbf{p}}(\nu_{\mathbf{p}}) = \big\{\mathbf{y} \in E : \langle \mathbf{y} - \mathbf{p}, \nu_{\mathbf{p}}\rangle = 0\big\}$. It follows that there are mutually orthogonal unit vectors $\nu_{\mathbf{p},1}, \ldots, \nu_{\mathbf{p},n-1}$, all orthogonal to $\nu_{\mathbf{p},n}$, and positive constants $\mu_1(\mathbf{p}), \ldots, \mu_{n-1}(\mathbf{p})$ so that

$$E_{\mathbf{p}}(\nu_{\mathbf{p}}) \approx \Big\{\mathbf{y} \in \mathbb{R}^n : \langle \mathbf{y} - \mathbf{p}, \nu_{\mathbf{p},n}\rangle = 0 \text{ and } |\langle \mathbf{y} - \mathbf{p}, \nu_{\mathbf{p},j}\rangle| < \mu_j(\mathbf{p}) \text{ for } 1 \leq j \leq n-1\Big\}.$$

The notation above implies that $E_{\mathbf{p}}(\nu_{\mathbf{p}})$ contains, and is contained in, constant dilates of the parallelepiped appearing on the right hand side, where the implicit constants in the approximation depend only on the dimension n. Let $\Delta(\mathbf{p}) = |C_{\mathbf{p}}(\nu_{\mathbf{p}})|$ be the minimal volume, and let $\mu_n(\mathbf{p}) = \sup_{\mathbf{y} \in E}\langle \mathbf{y} - \mathbf{p}, \nu_{\mathbf{p}}\rangle$.

We now state our diagonal estimates of the Bergman kernel $B_T(\mathbf{z}, \mathbf{w})$ for the tube domain T over a convex set $\Sigma \subset \mathbb{R}^n$. Let $\mathbf{z} = \mathbf{x} + i\mathbf{y}$, $\mathbf{w} = \mathbf{x} + i\mathbf{v} \in T$ and let $\mathbf{p} = \frac{1}{2}(\mathbf{y} + \mathbf{v}) \in \Sigma$. Then $B_T(\mathbf{z}, \mathbf{w}) \approx \Delta(\mathbf{p})^{-2}$ where the implicit constants in the approximation depend only on the dimension n. To estimate derivatives, choose coordinates in $\mathbb{R}^n$ so that the j^{th} coordinate axis is in the direction of $\nu_{\mathbf{p},j}$. Then we show

$$\Big|\partial_{\mathbf{z}}^{\alpha}\partial_{\bar{\mathbf{z}}}^{\beta} B_T(\mathbf{z}, \mathbf{w})\Big| \lesssim \Delta(\mathbf{p})^{-2} \prod_{j=1}^{n} \mu_j(\mathbf{p})^{-\alpha_j - \beta_j}.$$

We also obtain estimates of the Bergman kernel $B_{\mathcal{R}}$ for an axis-deleted log-convex Reinhardt domain $\mathcal{R}$. This time the estimates use the minimal caps of the convex set $\log|\mathcal{R}|$. When the parameters $\mu_1(\mathbf{p}), \ldots, \mu_n(\mathbf{p})$ are all small, the estimates are identical with the tube case. However if some of these parameters are large, the estimates also depend on the number of lattice points in sets of the form

$$\big\{(y_1, \ldots, y_n) \in \mathbb{R}^n : |y_j| < \mu_j(\mathbf{p})^{-1},\ 1 \leq j \leq n\big\}.$$

2. Monomial-type model domains and monomial balls.

For any $\mathbf{m} = (m_1, \ldots, m_n) \in \mathbb{Z}^n$ the function $F_{\mathbf{m}}(\mathbf{z}) = z_1^{m_1} \cdots z_n^{m_n}$ is a monomial which is holomorphic on $\mathbb{C}^n \setminus \big\{\mathbf{z} \in \mathbb{C}^n : \prod_{j=1}^n z_j = 0\big\}$. We obtain diagonal estimates of the Bergman kernel for model domains in $\mathbb{C}^{n+1}$ of the form

$$\Omega = \Big\{(z_1, \ldots, z_n, w) \in \mathbb{C}^{n+1} : \sum_{j=1}^{d} |F_{m_j}(\mathbf{z})|^2 < \operatorname{Im} w\Big\}.$$

[1]This means that if $(z_1, \ldots, z_n) \in \mathcal{R}$ then $(e^{i\theta_1}z_1, \ldots, e^{i\theta_n}z_n) \in \mathcal{R}$ for all $(\theta_1, \ldots, \theta_n) \in \mathbb{R}^n$.
[2]This means that E does not contain any entire straight line.
[3]Note that the minimal cap need not be unique.

To study the Bergman kernel on the diagonal at a point $(0, \ldots, 0, i\delta)$ above the origin, the problem is easily reduced to obtaining diagonal estimates of the Bergman kernel for the domain

$$\Omega_\delta = \Big\{(z_1, \ldots, z_n) \in \mathbb{C}^n : \sum_{j=1}^{d} |F_{m_j}(\mathbf{z})|^2 < \delta\Big\},$$

and this is possible since Ω_δ is a Reinhardt domain. To obtain estimates above some other point $\mathbf{a} = (a_1, \ldots, a_n) \in \mathbb{C}^n$ we observe that Ω is biholomorphic to the domain

$$\Omega(\mathbf{a}) = \Big\{(z_1, \ldots, z_n, w) \in \mathbb{C}^{n+1} : \sum_{j=1}^{d} |F_{m_j}(\mathbf{z}) - F_{\mathbf{m}_j}(\mathbf{a})|^2 < \operatorname{Im} w\Big\}.$$

The domain $\Omega(\mathbf{a})$ is called a monomial ball, and estimating the Bergman kernel on the diagonal then involves the following steps.

1. Obtain a structure theorem for $\Omega(\mathbf{a})$: after a monomial mapping, monomial balls can be written as the Cartesian product of a polydisk and an axis-deleted log-convex Reinhardt domain.

2. Study the behavior of the Bergman kernel under monomial mappings.

3. Compute weighted diagonal estimates for the Bergman kernel on Reinhardt domains.

3. Off-diagonal estimates for tubes over model polynomial domains.

If $\Sigma \subset \mathbb{R}^{n+1}$ is a proper open convex set, the Bergman kernel for the tube T over Σ is given by

$$B_T(\mathbf{z}, \mathbf{w}) = \int_{\mathbb{R}^{n+1}} e^{-2\pi i\langle \mathbf{x}-\mathbf{u},\mathbf{t}\rangle} e^{4\pi\langle \mathbf{p},\mathbf{t}\rangle} \left[\int_\Sigma e^{4\pi\langle \mathbf{s},\mathbf{t}\rangle}\, d\mathbf{s}\right]^{-1} d\mathbf{t},$$

where $\mathbf{z} = \mathbf{x}+i\mathbf{y}$, $\mathbf{w} = \mathbf{u}+i\mathbf{v} \in T$ and $\mathbf{p} = \frac{1}{2}(\mathbf{y}+\mathbf{v}) \in \Sigma$. Here the understanding is that $\big[\int_\Sigma e^{4\pi\langle \mathbf{s},\mathbf{t}\rangle}\, d\mathbf{s}\big]^{-1} = 0$ if $\int_\Sigma e^{4\pi\langle \mathbf{s},\mathbf{t}\rangle}\, d\mathbf{s} = \infty$. To obtain estimates which are better than the estitmates on the diagonal, one must take advantage of the oscillation $e^{-2\pi i\langle \mathbf{x}-\mathbf{u},\mathbf{t}\rangle}$ in the outer integral. We obtain sharp estimates for domains

$$\Sigma = \big\{(y_1, \ldots, y_n, y) = (\mathbf{y}', y) \in \mathbb{R}^{n+1} : y > \Psi(\mathbf{y}')\big\}$$

where $\Psi : \mathbb{R}^n \to \mathbb{R}$ is a convex polynomial of finite line type[4].

For $\mathbf{p}' \in \mathbb{R}^n$ let $\Psi_{\mathbf{p}'}(\mathbf{y}) = \Psi(\mathbf{p}' + \mathbf{y}') - \Psi(\mathbf{p}') - \langle \nabla\Psi(\mathbf{p}'), \mathbf{y}'\rangle$, and note that $\Psi_{\mathbf{p}'}$ is normalized at $\mathbf{p}'$ in the sense that $\Psi_{\mathbf{p}'}(\mathbf{0}') = 0$ and $\nabla\Psi_{\mathbf{p}'}(\mathbf{0}') = \mathbf{0}'$. Our estimates are given in terms of the geometry of the convex set $\big\{\mathbf{s}' \in \mathbb{R}^n : t\Psi_{\mathbf{p}}(\mathbf{s}) \leq 1\big\}$. We show that there is a constant $\kappa \geq 1$ and for each $\mathbf{p} \in \mathbb{R}^n$ and each $t > 0$ there is a choice of coordinates $(s_1, \ldots, s_n)$ in $\mathbb{R}^n$ and positive constants $\mu_1(\mathbf{p}, t), \ldots, \mu_n(\mathbf{p}, t)$ so that

$$\Big\{\mathbf{s} \in \mathbb{R}^n : |s_j| \leq \mu_j(\mathbf{p}, t^{-1})\Big\} \subset \Big\{\mathbf{s} \in \mathbb{R}^n : t\Psi_{\mathbf{p}}(\mathbf{s}) \leq 1\Big\} \subset \Big\{\mathbf{s} \in \mathbb{R}^n : |s_j| \leq \kappa\, \mu_j(\mathbf{p}, t^{-1})\Big\}.$$

Now let $\mathbf{z} = (\mathbf{z}', z) = (\mathbf{x}' + i\mathbf{y}', x + iy)$, $\mathbf{w} = (\mathbf{w}', w) = (\mathbf{u}' + i\mathbf{v}', u + iv) \in \mathbb{C}^{n+1}$, and let

$$\begin{aligned} p &= \frac{1}{2}(y + v) \in \mathbb{R}, & \mathbf{p}' &= \frac{1}{2}(\mathbf{y}' + \mathbf{v}') \in \mathbb{R}^n, \\ \lambda &= (x - u) - \langle \mathbf{x}' - \mathbf{u}', \nabla\Psi(\mathbf{p}')\rangle, & \mu &= 2\big(p - \Psi(\mathbf{p}')\big) \in \mathbb{R}. \end{aligned} \tag{47.0.1}$$

[4]This means that any straight line in $\mathbb{R}^{n+1}$ makes at most finite order of contact with the graph $y_0 = \Psi(y_1, \ldots, y_n)$.

Note that $(\mathbf{p}', p) \in \Sigma$ and that $\mu \geq 0$ with $\mu > 0$ if $(\mathbf{p}', p) \in \text{Int}(\Sigma)$. We show that

$$\Big| B_T\big((\mathbf{z}, z), (\mathbf{w}, w)\big)\Big| \approx |\lambda + i\mu|^{-2} \prod_{j=1}^{n} \Big(|x_j - u_j| + \mu_j\big(\mathbf{p}, |\lambda + i\mu|\big)\Big)^{-2}$$

with corresponding estimates for derivatives of B_T.

4. Additional questions.

We are also working on several related problems.

(a) There has been considerable interest in the formula for Bergman kernels and the L^p boundedness of Bergman projections in tubes over symmetric cones (see for example [3], [2], [1]). We are interested in extending these investigations to tubes over certain classes of non-symmetric cones.

(b) We would like to obtain sharp off-diagonal estimates of the Bergmen kernel for tubes T over bounded convex sets Σ. We can show for example that $|B_T(\mathbf{x} + i\mathbf{y}, \mathbf{u} + i\mathbf{v})| \lesssim e^{-\varepsilon|\mathbf{x}-\mathbf{u}|}$.

Finally we would like to thank BIRS for the opportunity to work together for a week and we greatly appreciate their hospitality.

Participants

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Chapter 48

Stability of multidimensional waves (19rit022)

June 2 - 19, 2019

Organizer(s): Anna Ghazaryan (Miami University, Oxford OH), Stéphane Lafortune (College of Charleston, Charleston SC)

Overview of the subject area of the workshop

Traveling waves are solutions of reaction diffusion equations that preserve their shape while moving in a preferred direction. Traveling waves are basic coherent structures in partial differential equations and they often serve as building blocks for complex patterns. Traveling fronts and pulses are abundant in nature and human activities. They arise in applied problems from different fields: optical communication, combustion theory, biomathematics, chemistry, population dynamics, to name a few. Stability of the wave which describes their resilience under perturbations therefore is important.

In this project we are focused on fronts and pulses which are waves asymptotic to spatially equilibria states of the system. These asymptotic states are called rest states of the wave. Stability theory of the traveling fronts and pulses in reaction-diffusion equations is a vast and current subject [3, 4, 6, 7]. Stability analysis is a multi-step process that involves determining the location of the spectrum of the linearization of the underlying system about the front or pulse. The dynamics near the asymptotic rest states of the wave is responsible for the location of the essential spectrum.

Planar traveling waves in the reaction-diffusion systems has been well studied, but the stability theory theory in the multidimensional cases is not as well developed as for the waves in systems posed on the one-dimensional physical space. In 1997, T. Kapitula in [2] proved one of the most important results for multidimensional, planar waves in equi-diffusive reaction-diffusion systems. The result reduces the problem of investigating the stability of a multidimensional planar front to the stability of the associated one-dimensional front. The result implies that if the one-dimensional front is stable, then small perturbations to the planar front decay algebraically.

In 2016, this result was extended to the cases when the one-dimensional front associated to the planar one is marginally stable. More precisely, its has essential spectrum that extends to the imaginary axes. For these cases, exponential weights technique by Sattinger was combined with Kapitula's approach to prove a result similar to Kapitula's result under assumptions on the nonlinear reaction term in the system and under the same assumption on the diffusion matrix - the diffusion matrix has to be an identity.

The main objective of this collaborative effort is to further generalize these two results. Two main goals is to (1) weaken the assumptions on the nonlinearity in [1] ; (2) to allow for a diagonal diffusion matrix which is not a multiple of an identity. We proposed to work on specific models first and then to work on generalization of the results.

Progress made during the workshop

During the workshop the participants have identified a specific model that exhibits properties relevant to the topic of the workshop. A significant progress was made during the workshop and details of the analysis of the existence of a planar wave and some partial stability results were worked out. In particular, the participants developed an idea that is the key to overcome issues related to the stability analysis described above is to consider waves supported by the system the dynamics of which is governed by a scalar equation. The existence properties and the stability of the wave then will be dictated by the properties of the associated wave in that scalar equation. This potentially will resolve both issues with the non-identity diffusion and the nonlinear stability. The techniques that allow to relate the traveling wave in the full system to the traveling wave in the scalar equation include Geometric Singular Perturbation Theory for the existence, topological methods such as construction of the Stability Index Bundles and the interpretation of the Stability Index Bundle theory to the language of the properties of the projection operators and generated by them semigroups. The group is currently working on a preparation of a manuscript that contains these original technique.

In addition, a number of new research projects were identified and discussed during the workshop. Plans of work for these projects were developed. In particular, one of the projects is related to the possibility of the generalization of the Sattinger's nonlinear stability in exponential weights result. Indeed, the nonlinear stability in an exponentially weighted norm in [5] is inferred for a parabolic system

$$u_t = \mathcal{A}u + f(u, u_x), \;\; u \in R^n,$$

where $\mathcal{A}$ is assumed to be second-order elliptic operator with constant coefficients. There are applications were the waves and the spectrum share the properties with those in [5], but the differential operator $\mathcal{A}$ has variable coefficients. The group discussed issues arising in this case and ways to overcome those.

Participants

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Chapter 49

p-adic dynamics of Hecke operators (19rit245)

June 16 - 23, 2019

Organizer(s): Eyal Z. Goren (McGill University)

The main short-term goal of this research-in-teams project was to extend work done by two separate groups to a wide class of Shimura curves and level structures. The work of the first group, consisting of Herrero-Menares-Rivera-Letelier, studied the dynamics of Hecke operators T_n acting on the j-line, in the p-adic topology, in terms of limit of measures. As a sample result we provide the following: given a j invariant x of a curve with ordinary mod p reduction, denote by $\delta(n)$ the probability measure supported on the orbit $T_n(x)$ of x under the Hecke operator T_n; then

$$\lim_{n\to\infty} \delta(n) = \delta_\zeta,$$

where δ_ζ is the Dirac distribution associated to the Gauss point ζ on the Berkovich projective line. The convergence is in the sense of "weak convergence" of measures. An interesting feature of this result that it requires extending the usual affine line to the Berkovich line to recognize the limit.

The work of the second group, consisting of Goren-Kassaei, in the same setting concerns the dynamics of the iterations $T_\ell^n(x)$ as n goes to infinity, $(\ell, p) = 1$ and ℓ a prime. It contains a weaker statement than the above, but describe the set $T_\ell^n(x)$ nicely using isogeny volcanoes and, more significantly, explains the "error term" in the following sense. There is a minimal n_o such that a point in $T_\ell^{n_o} x$ belongs to the same residue disc as x, due to a cyclic endomorphism f of the mod p reduction of x, and then the dynamics of T_ℓ on this residue disc is given by

$$q \mapsto (1+q)^{\bar{f}/f},$$

where q is the Serre-Tate parameter and $\bar{f}/f$ is a p-adic unit that is explicitly defined.

The papers referred to above are the following. A more precise formulation of these results and, in fact, many more and much harder results can be found there.

- Eyal Z. Goren & Payman L. Kassaei: p-adic dynamics of Hecke operators on modular curves. 38 pp. ArXiv:1711.00269 *Submitted*

- Sebastian Herrero, Ricard Menares & Juan Rivera-Letelier: p-adic distribution of CM points and Hecke orbits I. Convergence towards the Gauss point. *Submitted*

Our goal in this Research-in-Teams project was to take the whole spectrum of results both teams had and to develop them for the case of Shimura curves. Even the case of Shimura curves offers many, perhaps too many, variations. And, the case of modular curves is just a test-ground for a more general study of studying the action of Hecke operators on special subvarieties of Shimura varieties, in the p-adic topology. Such general studies were conducted by Clozel, Ullmo, and others over the complex numbers. The analogous questions for p-adic actions seem to be wide-open, although the mod p action was studied by Chai, Oort, and others.

That said, the setting we considered during this week is that of Shimura curves associated to a quaternion algebra B over $\mathbb{Q}$ and Drinfeld level structure of type $\Gamma_0(n)$. By allowing p to divide the discriminant of B, or not, the level n, or not, we have several situations to consider. During the week we came up with conjectural descriptions of the limit measures
$\lim_{n\to\infty,(n,p)=1} \delta(n)$ when x is ordinary (in most situations), and have made very significant progress towards completing the conjectural description also when x is not ordinary.

The nature of the answer depends very much on whether $p|\mathrm{disc}\, B$, or $p|n$. For $p|\mathrm{disc}\, B$ we were able to use work of Drinfeld and Ribet. For $p|n$ and $B = M_2(\mathbb{Q})$, we were able to use work of Katz-Mazur. The case of $\mathrm{disc}\, B \neq 1$ and $p|n$ is conjecturally understood, but in reality we will have to use Drinfeld level structures for quaternion algebras. This was partially done by K. Buzzard but because he put severe restrictions on n we will have to develop this theory further ourselves. Similar "side projects" – very substantial on their own – came up during the week, but we hope to have solved the conceptual difficulties in carrying them on.

While a lot of work remains, it is safe to say that many of the main obstacles were overcome during this week.

I believe that I describe everyone's experience in saying that this week was one of the best experiences of joint research I have ever participated in. The conditions in BIRS were ideal. For one, the freedom of not needing to worry about meals – three meals provided in the dining hall – freed a lot of time. 2) The room allocated to us had large boards, convenient desks and a laptop projector (and access for wifi). It was excellent for collaboration. 3) The athletic facilities in Banff, and the trekking trails, offered excellent opportunities to break from marathon discussion sessions running from morning till late at night.

Our team members had complementary expertise and that kept discussions lively and interesting. We leave BIRS with a long "to-do" list, among its items are developing further Drinfeld level structures for Shimura curves, using Bruhat-Tits buildings to understand Hecke orbits, studying quadratic forms and equidistribution results for Eichler orders in quaternion algebras, studying metric properties of period maps for moduli of p-divisible groups with a Drinfeld level structure, and much more. We are very tempted to return to Banff to put the finishing touches on the project in the future. In particular, we believe that the atmosphere and working conditions in BIRS will be conducive for the completion of Phase II of our project which is devoted to arithmetic applications.

June 28, 2019

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Chapter 50

Counting V-tangencies and nodal domains (19rit271)

June 30 - July 7, 2019

Organizer(s): Suresh Eswarathasan (Cardiff University, McGill University, Dalhousie University), Igor Wigman (King's College London)

Overview of the Field

Given a "nice" function $f : \mathbb{R}^d \to \mathbb{R}$, $d \geq 2$, or $f : M \to \mathbb{R}$ with M a compact Riemannian d-manifold (equipped with some Riemannian metric), the nodal set of f is its zero set $f^{-1}(0)$; if f is Morse, then its nodal set is a smooth hypersurface. The nodal components of f are the connected components of the nodal set. The most basic question one is interested is in the nodal count of f, i.e. the total number of the nodal components of f, which we denote by $\mathcal{N}(f)$. Classical and celebrated results in $\mathbb{R}^d$ go back to Sturm and Courant.

Understanding the "typical" nature of the nodal structures of Gaussian random fields, rather than individual functions, is an actively pursued subject especially in the last few years. Let us introduce the specific Gaussian random fields of our focus. The space $L^2(M)$ of square-summable functions on M has an orthonormal basis $\{\varphi_j\}_{j=1}^{\infty}$ consisting of Laplace eigenfunctions, i.e.

$$\Delta\phi_j + t_j^2\phi_j = 0, \tag{50.0.1}$$

where Δ is the Laplace-Beltrami operator on M acting on L^2, and $\{t_j\}_{j\geq 0}$ is its purely discrete spectrum

$$0 = t_0 \leq t_2 \leq \ldots,$$

satisfying $t_j \to \infty$. For a "band" $\alpha \in [0, 1)$ and spectral parameter $T > 0$ (with the intention of taking the limit $T \to \infty$), we define the random band-limited functions to be

$$f_T(x) = f_{\alpha;T}(x) = \frac{1}{|\{j : \alpha \cdot T < t_j < T\}|^{1/2}} \sum_{\alpha \cdot T < t_j < T} c_j\varphi_j(x), \tag{50.0.2}$$

where the c_j are independent and identically distributed standard Gaussians. For $\alpha = 1$, we interpret the summation as

$$f_{1;T}(x) = \frac{1}{|\{j : T - \eta(T) < t_j < T\}|^{1/2}} \sum_{T-\eta(T)<t_j<T} c_j \varphi_j(x), \tag{50.0.3}$$

with the convention $\eta(T) = o_{T\to\infty}(T)$ but $\eta(T) \to \infty$; we will drop the subscript α when the context is clear. The breakthrough works of Nazarov-Sodin [NS09, NS15] demonstrate that as $T \to \infty$,

$$\mathbb{E}\left[\left|\frac{\mathcal{N}(f_T)}{Vol(M)\cdot T^2} - c(d,\alpha)\right|\right] \to 0 \tag{50.0.4}$$

with $c(d,\alpha) > 0$ being a universal constant, itself a quantity that has generated tremendous interest.

Focus of the Workshop

For the purposes of the workshop, we first let $\mathtt{V}(M)$ be the class of all C^∞-smooth vector fields on M with finitely many zeros; the class $\mathtt{V}(M)$ is non-empty for every smooth M by the existence of Morse functions (that is, we can simply take the gradient field of a given Morse function). For a nodal component $\gamma \subseteq f_T^{-1}(0)$ and $V \in \mathtt{V}(M)$ fixed, define

$$\mathcal{N}_V(f_T, k) := \#\{\gamma \subseteq f_T^{-1}(0) :\ \gamma \text{ has precisely } k \text{ tangencies w.r.t. } V\}. \tag{50.0.5}$$

Note that we have

$$\mathcal{N}(f_T) = \sum_{k=0}^{\infty} \mathcal{N}_V(f_T, k), \tag{50.0.6}$$

hence turning the nodal count for f_T into a series of counts involving tangencies. Our aim is to understand various asymptotics, in T, surrounding the distribution of the random variable $\mathcal{N}_V(f_T, k)$.

Recent Developments

As inferred in the previous section, one might refine the study of $\mathcal{N}(f_T)$ by separately counting the nodal components of f_T belonging to a given topology class $\mathcal{T}$ or more generally to a class of some prescribed geometric type. For the expected Betti number, or the expected number of components of a certain diffeomorphism type $\mathcal{T}$, Gayet-Welschinger [GW14] were able to obtain upper and lower bounds for the corresponding expected values for the Kostlan ensemble, which is different in many aspects from those considered in (50.0.2) or (50.0.3). A local refinement of their lower bound was very recently obtained by Wigman [Wig19].

The work of Sarnak-Wigman [SW18] provides some finer results surrounding the count for the components of a particular topology $\mathcal{T}$, particularly in the case of ensembles given in (50.0.2) and (50.0.3). To be more specific and for the sake of concreteness, take a 3-dimensional (M, g). The work [SW18] shows the existence of a probability measure $\mu^{H(2)}$, with support on every element n of $\mathbb{Z}_{\geq 0}$, where $\mu^{H(2)}(n)$ gives the expected limiting fraction of nodal components of $f_T^{-1}(0)$ of genus n (in this case, smooth and compact surfaces of genus n). Moreover, this measure is shown to be universal in the sense of its independence of the geometry or topology of M but still dependent on the spectral measure for the corresponding scaling limit $\mathfrak{g}_\alpha$ (attached to the ensemble $\{f_{\alpha,T}\}_{T>0}$) and the dimension d.

Building upon the techniques of Nazarov-Sodin and Sarnak-Wigman, Beliaev-Wigman [BW17] addressed the following question: what is the asymptotic volume distribution of the nodal domains of f_T, the sets where f_T is either positive or negative? A similar deterministic universal law to that established in [SW18] was obtained; some basic qualitative properties of the cumulative probability distribution were also proven.

The interaction between tangent/normal spaces to nodal sets and various other geometric quantities of these submanifolds is another natural topic of study. The work of Dang-Rivière (who themselves were motivated by the work [GW14]) give asymptotics pertaining to the equidistribution (in T^*M) of conormal cycles for f_T on general compact manifolds [DR17]. In the setting of the base space M, the study of the distribution of tangencies to a fixed vector field $V \in \mathtt{V}(M)$ was initiated in the work of Rudnick-Wigman [RW18], who considered a count in the arithmetic setting of the flat torus $M = \mathbb{T}^d$ related to that described in (50.0.5), specifically

$$N_V(f_T) = \#\{x : V(x) \neq 0,\ f_T(x) = V f_T(x) = 0\} \tag{50.0.7}$$

where the f_T is taken to be a Gaussian toral eigenfunction and $V = \zeta \in S^{d-1}$ a fixed direction. The authors obtained asymptotics for $\mathbb{E}\left[N_V(f_T)\right]$, along with some deterministic results, while the subsequent work of Eswarathasan [E18] gave asymptotics for Gaussian spherical harmonics on S^2 for fixed vector fields $V \in \mathtt{V}(M)$.

Scientific Progress Made

Let us encapsulate all the individual counts $\mathcal{N}_V(f_k)$ into a single (random) probability measure, the "direction distribution measure", as follows:

$$\mu_f(V) = \frac{1}{\mathcal{N}(f)} \sum_{k=0}^{\infty} \mathcal{N}_V(f,k) \cdot \delta_k, \tag{50.0.8}$$

on $\mathbb{Z}_{\geq 0}$. Given two probability measures μ_1, μ_2 on $\mathbb{Z}$ we will use the total variation distance function

$$\mathcal{D}(\mu_1, \mu_2) = \sup_{F \subseteq \mathbb{Z}_{\geq 0}} |\mu_1(F) - \mu_2(F)|. \tag{50.0.9}$$

During our week-long workshop, we were able to establish all the necessary details behind the following:

Theorem: Let (M,g) be 2 dimensional. Given $\alpha \in [0,1)$, there exists a (deterministic) probability measure μ_α on $\mathbb{Z}_{\geq 0}$, supported on the positive even integers $2\mathbb{Z}_{>0}$, so that for all $V \in \mathtt{V}(M)$ and every $\varepsilon > 0$,

$$\lim_{T \to \infty} \mathbb{P}\left(\mathcal{D}(\mu_{f_{\alpha;T}}(V), \mu_\alpha) > \varepsilon\right) = 0, \tag{50.0.10}$$

where $\mathcal{D}(\cdot,\cdot)$ is the total variation distance.

This theorem can be seen as the natural next step after those established in [SW18, BW17] with the added property that the support of our limiting direction distribution measure μ_α is "essentially half" that of the connectivity measure introduced by Sarnak-Wigman and is actually independent of V. The remaining case that we would like to include before publication is $\alpha = 1$. The approach we took followed that of [SW18] which itself closely follows that of [NS15]. However, a significant juncture in our methods occurred at the stage of establishing the stability between the nodal counts involving tangencies for f_T and the corresponding counts for the universal scaling limit $\mathfrak{g}_\alpha$. Thanks to some elementary differential geometry in the plane, we were able to reduce the question of counting components whose number of tangencies with respect to V is precisely k to a question of counting components with precisely k points of (quantitative) transversal intersection to another set of curves, namely $\{V f_T = 0\}$.

A critical obstacle that we faced was in showing such components with precisely k transversal intersections, but that also have at least one intersection that is quantitatively near-degenerate, are few; this was a crucial part to establishing our desired stability property. A Kac-Rice calculation allowing us to bound an expected volume however, hinging upon some technical work of Cammarota-Marinnucci-Wigman [CMW16], allowed us to overcome this roadblock.

As mentioned before, the only missing piece before submitting the paper is to show that band-limited ensembles for $\alpha = 1$ give the same measure result as recorded above. The main hurdle en route to this goal is to apply the barrier method of Nazarov-Sodin [NS09, NS15] with added regularity assumptions and allowing our target eigenfunctions to have singular nodal sets. We will work out the details of this approach in the near future.

Outcome of the Meeting

We expect to complete the case of $\alpha = 1$ with relatively few obstructions and hope to subsequently submit our article for publication. We warmly thank BIRS for its hospitality and an environment which is in many ways second to none!

Participants

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section*

Chapter 51

Serre Weight Conjectures for p-adic Unitary Groups (19rit273)

July 7 - 14, 2019

Organizer(s): Karol Kozioł(University of Alberta), Stefano Morra (Université Paris 8)

Context

Our research stay at BIRS was motivated by the **mod-p and p-adic Langlands programs**. These programs constitute a vast web of conjectures which have had tremendous impact on arithmetic algebraic geometry over the past 30 years (e.g., the work of Wiles, Taylor–Wiles, and Breuil–Conrad–Diamond–Taylor on the Taniyama–Shimura–Weil conjecuture, leading to a proof of Fermat's Last Theorem).

More specifically, pursuing the calculations of [BCDT01]and following an early observation of Serre ([Ser87]), Breuil suggested in the early 2000s that certain congruences between modular forms should be explained by a p-adic version of the classical Langlands Correspondence. This "p-adic correspondence" may be stated loosely as follows:

Conjecture 51.0.1. *Let p be a prime number and F be a finite extension of $\mathbf{Q}_p$ (the field of p-adic numbers). Then there is a natural bijection*

$$\left\{\begin{array}{c}\textit{certain continuous representations}\\ \mathrm{Gal}(\overline{F}/F)\to\mathbf{GL}_n(\overline{\mathbf{Q}}_p)\end{array}\right\}\overset{?}{\longleftrightarrow}\left\{\begin{array}{c}\textit{certain continuous representations}\\ \textit{of }\mathbf{GL}_n(F)\textit{ with }\overline{\mathbf{Q}}_p\textit{-coefficients}\end{array}\right\}$$

The connotation of "natural" above means that the bijection should be compatible with the classical local Langlands correspondence with $\mathbf{C}$-coefficients, its geometric realization in the cohomology of arithmetic varieties, and so on.

So far, this conjecture has been made precise and proven **only** for the group $\mathbf{GL}_2(\mathbf{Q}_p)$ (by work of Breuil, Colmez, Emerton, Kisin, Paškūnas and others; see[Ber11] and [Bre12] for a survey). Even in the $\mathbf{GL}_2(\mathbf{Q}_p)$ case its applications are far-reaching, and afford us a better understanding of global objects, such as the absolute Galois group of $\mathbf{Q}$ and cohomology of algebraic varieties.

The starting point in attacking the above conjecture is to consider first an "inertial" version of the above situation with mod-p coefficients, which is the content of Serre's modularity conjecture [Ser87] and its generalization in the form of the Breuil–Mézard conjecture [BM02, Conjecture 1.1]. The latter predicts the complexity of the special fiber of local Galois deformation rings (with p-adic Hodge theoretic conditions) in terms of representation theory of the group $\mathbf{GL}_2(\mathbf{Z}_p)$. Further, the Breuil–Mézard conjecture has now taken on a geometric reformulation, due to Emerton and Gee [EGa], [EGb], which opens up the possibility of importing new tools to handle the problem.

Despite these achievements, we note that $\mathbf{GL}_2$ (or more generally $\mathbf{GL}_n$ for $n \geq 2$) is just an example of reductive groups governing symmetries in nature. One of the most exciting and mysterious aspects in the classical Langlands program is known as **Langlands functoriality**: how can we relate automorphic forms and Galois representations (or, more appropriately, Galois parameters) for various reductive groups (such as unitary groups)? In particular, can we describe such parameters in terms of those pertaining to general linear groups, possibly endowed with additional symmetries?

Background

During our research stay at BIRS we explored the setting above; more precisely, we considered relating Langlands correspondences for $\mathbf{GL}_n$ and those for the unitary group $\mathbf{U}_n$. In this context, we seek a correspondence of the form

$$\left\{ \begin{array}{c} \text{certain continuous representations} \\ \text{Inertia}(\overline{F}/F) \to {}^C\mathbf{U}_n(\overline{\mathbf{F}}_p) \end{array} \right\} \overset{?}{\longleftrightarrow} \left\{ \begin{array}{c} \text{certain continuous representations} \\ \text{of } \mathbf{U}_n(\mathcal{O}_F) \text{ with } \overline{\mathbf{F}}_p\text{-coefficients} \end{array} \right\}$$

(Here, ${}^C\mathbf{U}_n$ is an enhancement of the L-group of $\mathbf{U}_n$ called the **C-group**, and it is the appropriate object to consider in order to make this correspondence compatible with global and cohomological considerations.)

This modification in terms of unitary groups makes the project interesting in several ways: many of the tools used in the $\mathbf{GL}_n$ setting still apply, but we also have base change techniques at our disposal to relate representations of $\mathbf{U}_n$ to those of $\mathbf{GL}_n$. This hints at a **mod-p principle of Langlands functoriality**. Note that we have already proven a version of correspondence above when $n = 2$ in [KM] and the project we started at BIRS explores the extension of our results to higher rank. Moreover, recent advances in the p-adic Langlands correspondence for $\mathbf{GL}_n$ open up the possibility of utilizing novel geometric techniques in the context of unitary groups (namely, moduli stacks of ${}^C\mathbf{U}_n$-valued Galois representations [EGb]and local models of Galois deformation rings [LLHLM]) in order to geometrize the functoriality principle.

In order to properly approach the setup above, we require some input from the Langlands correspondence with $\mathbf{C}$-coefficients. Namely, when dealing with groups other that $\mathbf{GL}_n$, local Galois parameters correspond to "L-packets" on the representation theory side. These are finite sets of smooth $\mathbf{U}_n(F)$-representations characterized by a character identity, and are relevant in the theory of automorphic base change and functoriality over $\mathbf{C}$. In particular, as inertial Galois parameters are the key ingredients used to construct "Breuil–Mézard cycles" on the aforementioned local models, it is now natural to consider packets of Bushnell–Kutzko types, i.e., the smooth, tame $\mathbf{U}_n(\mathcal{O}_F)$-representations appearing in the constituents of an L-packet, and how these inertial packets interact with base change to $\mathbf{GL}_n$. Note that for representations of finite groups of Lie type there is an independent notion of base change, the so called Shintani lift, which is given in purely representation theoretic terms. In particular, Shintani lifting is naturally well-suited for combinatorics à la Breuil–Mézard. (It is indeed a conjecture, verified in low-rank cases [AL05], that the Shintani lift is compatible with automorphic base change.)

Note that the interaction of packets of Bushnell–Kutzko types and automorphic base change gives us the intriguing opportunity to formulate a geometric version of the functoriality principle in terms of the Breuil–Mézard conjecture and Emerton–Gee stacks: we expect the natural morphism between C-dual groups ${}^C\mathbf{U}_n \to {}^C\mathbf{GL}_n$ to induce morphisms $M(\lambda)^{\nabla_\tau}_{\mathbf{U}_n} \to M(BC(\lambda))^{\nabla_{BC(\tau)}}_{\mathbf{GL}_n}$ between local models of [LLHLM] and the stacks $\overline{\mathcal{X}}_{\mathbf{U}_n} \to \overline{\mathcal{X}}_{\mathbf{GL}_n}$ of [EGb]. In particular, part of our project would consist in understanding how the notions of Breuil–Mézard cycles interact with the map of cycles induced by the morphisms above.

Results

The main focus of our research activity at BIRS consisted in understanding the combinatorics of L-packets and how the Bushnell–Kutzko types interact with base change. Our starting point was the paper of DeBacker–Reeder [DR09] which contains an exhaustive study of L-packets associated to tame regular semisimple elliptic Galois parameters ϕ, for a wide class of p-adic Lie groups (including our $\mathbf{U}_n$). These L-packets are constructed by inducing certain Deligne–Lusztig representations $\sigma(\phi)$ (of certain varying compact subgroups), and the ellipticity condition on ϕ ensures that $\sigma(\phi)$ is cuspidal. Consequently, the DeBacker–Reeder construction produces, starting from $\sigma(\phi)$, a "supercuspidal" representation π in the L-packet Π_ϕ associated to ϕ. (It is conjectured -and likely- that the DeBacker–Reeder construction does indeed give the local Langlands correspondence for $\mathbf{U}_n$ with $\mathbf{C}$-coefficients.)

Given this construction, we examined the tame $\mathbf{U}_n(\mathcal{O}_F)$-representations contained in the L-packet Π_ϕ. Making a detailed study of the construction of [DR09], we sketched a strategy (and verified it in several low-rank cases) for the proof of the following fact: if ϕ is as above, then the packet Π_ϕ contains a unique tame $\mathbf{U}_n(\mathcal{O}_F)$-representation σ. Moreover, if we let $\mathrm{BC}(\Pi_\phi)$ denote the automorphic base change of Π_ϕ to $\mathbf{GL}_n(E)$ (where E denotes the quadratic unramified extension of F), then $\mathrm{BC}(\Pi_\phi)$ contains a unique tame $\mathbf{GL}_n(\mathcal{O}_E)$-representation, which is precisely the Shintani lift of σ. We hope to flesh out the ideas of this argument soon.

Aside from the above result, we moreover outlined a strategy to remove the assumption on ellipticity for the inertial Galois parameter, which goes as follows. We checked that a tame regular semisimple Galois parameter ϕ actually factors through (the dual group of) a Levi subgroup M of $\mathbf{U}_n(F)$, and decomposes as a direct sum of elliptic tame regular semisimple Galois parameter for the Levi blocks. In particular we can construct, via [DR09], an L-packet of smooth M-representations, which we then parabolically induce to $\mathbf{U}_n(F)$.

The relation between these parabolically induced representations and the L-packet of ϕ is not immediate. Indeed, the parabolic induction of supercuspidal representation of M need not be irreducible, and the classification of tame regular semisimple Galois parameters given by [SZ18] requires the knowledge of Langlands quotients. Because of this, more work will be required in order to precisely formulate and prove the necessary results.

The "local automorphic" results obtained above are an excellent starting point towards the proofs of Serre conjectures and geometric Breuil–Mézard conjectures for unitary groups. The other ingredients required (such as the relevant calculations in p-adic Hodge theory and additional results from the global theory of automorphic forms on unitary groups) constitute some of the other (substantial) pieces, and we plan to pursue these directions further in the future.

Participants

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Chapter 52

Dispersion Interactions via Optimal Transport (19rit280)

29th September - 10th October, 2019

Organizer(s): Augusto Gerolin (Theoretical Chemistry, VU Amsterdam), Mircea Petrache (Mathematics, PUC Chile)

Overview of the Field

Accurately predicting electronic structure from first principles is crucial for many research areas such as chemistry, solid-state physics, biophysics and material sciences. In principle, the electronic structure is determined by the Schrödinger equation, which can only be solved in practice for few electrons. Kohn-Sham (KS) Density functional theory (DFT) has been a real breakthrough for electronic structure calculations. KS DFT uses the one-electron density and a non-interacting wave function as basic variables, much simpler quantities than many-electron wave-functions, allowing to treat realistic large systems [2, 6, 7, 8, 9, 10, 13].

In the Hohenberg and Kohn formulation of DFT[6, 10, 13] the electronic-ground state properties are calculated by minimizing a functional $E[\rho]$ with respect to $\rho(x_i)$, the one-body particle density[1],

$$E[\rho] = F^{HK}_{\hbar}[\rho] + \int_{\mathbb{R}^3} V(x)\rho(x)dx, \qquad \rho(x_i) = N\int_{\mathbb{R}^{3(N-1)}} |\psi(x_1, x_2, \dots, x_N)|^2 dx_1 \dots \hat{dx_i} \dots x_N,$$

where N denote the number of electrons, ψ is the wave-function, V an external potential, which is due to the nuclei, and $F^{HK}_{\hbar}[\rho]$ is an universal functional, the so-called Hohenberg-Kohn functional (or Levy-Lieb functional) [2, 10, 13].

For every density $\rho \geq 0$ in $\mathbb{R}^3$ the functional $F^{HK}_{\hbar}[\rho]$ is defined as a minimization problem on a space of wave functions subject to a highly non-linear constraint $\psi \mapsto \rho$

$$F^{HK}_{\hbar}[\rho] = \inf_{\psi\mapsto\rho} \int_{(\mathbb{R}^d)^N} \hbar^2|\nabla\psi|^2 + V_{ee}|\psi|^2 dx, \quad V_{ee}(x_1, \dots, x_N) = \sum_{i=1}^{N}\sum_{j=i+1}^{N} \frac{1}{|x_j - x_i|}, \qquad (52.0.1)$$

[1]The idea of formulate the ground state problem in terms of the electronic density alone comes from Thomas–Fermi (TF) model [4, 15]. L. H. Thomas and E. Fermi are viewed as precursors of the modern Density Functional Theroy.

$$\textit{and} \quad \psi \mapsto \rho \quad \textit{stands for} \quad \int_{\mathbb{R}^{3(N-1)}} |\psi(x_1,\ldots,\hat{x}_j,\ldots,X_N)|^2 dx_1 \ldots d\hat{x}_j \ldots dx_N = \rho(x_j), \, \forall j = 1,\ldots,N.$$

Although the Hohenberg-Kohn theory guarantees the existence of such functional $F_{\hbar}^{HK}[\rho]$, in practical, approximations are needed. In classical Kohn-Sham DFT, the minimization of $E[\rho]$ is done under the assumption that the kinetic energy dominates over the electron-electron interaction by introducing the functional $T_s[\rho]$, corresponding to the minimum of the expectation value of the kinetic energy alone over all fermionic wave functions yielding the given ρ. The remaining part of the exact energy functional, $E_{Hxc}[\rho] = F_{\hbar}^{HK}[\rho] - T_s[\rho]$, is usually approximated by splitting it into the sum of the classical Hartree functional and the exchange-correlation (xc) energy E_{xc}, that is the crucial quantity to be approximated.

In addition, Kohn-Sham DFT obviously encounters difficulties when particle-particle interactions play a more prominent role. In such cases, the physics of $F_{\hbar}^{HK}[\rho]$ is completely different than the one of the Kohn-Sham non-interacting system.

An alternative approach, more suitable to study strongly-correlated electrons (SCE), were introduced by M. Seidl, P. Gori-Giorgi and co-authors (e.g. [1, 5, 14]). The so-called SCE limit is defined as the semi-classical limit $\hbar \to 0$ of $F_{\hbar}^{HK}[\rho]$ keeping the one-body density fixed. In [2, 3, 11] this limit was shown to be equal to an optimal transport problem with finitely many probability measures (marginals) $\mu_1,\ldots,\mu_N$ and Coulomb cost:

$$V_{ee}[\rho] = \inf\left\{ \int_{(\mathbb{R}^d)^N} V_{ee}(x_1,x_2,\ldots,x_N)d\gamma(x_1,\ldots,x_N) \; : \; \begin{array}{l} e_i : (\mathbb{R}^d)^N \to \mathbb{R}^d \\ (e_i)_\sharp \gamma = \mu_i \end{array} \text{ and } 1 \leq i \leq N \right\}, \quad (52.0.2)$$

where $e_1,\ldots,e_N : (\mathbb{R}^d)^N \to \mathbb{R}^d$ denotes the canonical projections. The probability measure γ are called couplings or transport plans, and give the joint probability distribution of the marginals $\mu_1,\ldots,\mu_N$. In the DFT context, the multi-marginal optimal transportation problem with Coulomb cost is a lower bound for the internal part of the *ground state energy* (Hohenberg-Kohn functional) of a time-independent Electronic Schrödinger equation describing the evolution of a molecular system of N-electrons under Coulomb electron-electron interaction [2].

Objectives of the meeting

The goal of this team meeting is to boost up progress in the very early stage of the proposed research program we have recently initiated. Augusto Gerolin is a mathematician working at the Theoretical Chemistry Department at Vrije Universiteit Amsterdam (VU Amsterdam), which has been developing Optimal Transport methods in Density Functional Theory; Mircea Petrache is a mathematician working at the Pontificia Universidad Católica de Chile, which among other interests have been studying ground state energies and assymptotic behavoir of clusters of molecules in different contexts.

Augusto Gerolin together with Quantum Matter research group at the VU Amsterdam has been developing physical models on dispersion interaction via the SCE-formalism in DFT. The main goal of this team meeting is to start a rigorous mathematical framework, based on Optimal Transport Theory, to describe quantum interactions between molecules (e.g. Hydrogen bond, van der Waal's, dipole-dipole force) in the so-called strong-interaction limit. Although we have been done several online meetings, it was fundamental for both of us to meet personally and to focus on full week in the problem.

Scientific Progress Made

In the physical-chemistry literature, dispersion interactions, have been always considered out of the realm of the strong-interaction limit, and, more generally, have been usually treated in a conceptually separate framework from

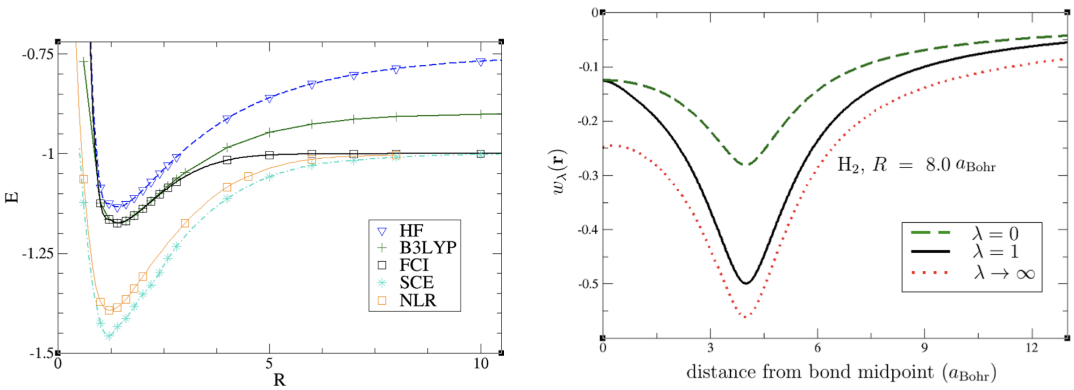

Figure 52.1: From [16][Left] H_2 dissociation curves obtained by different methods, including Hartree-Fock, B3LYP, FCI, LDA and SCE. [Right] Energy densities in the xc hole of eq 30 for H_2 at R = 8.0 at different strenght $\hbar$ values: 0, 1, and ∞. (for all details see [16])

the problem of strong correlation. During the meeting, we make the first step in understanding the mathematical framework allowing to study Dispersion interaction in the strongly-correlated limit.

The relevance of the strong-interaction limit for dispersion is already hinted in the fundamental work of E. Lieb and W. Thirring [12]. The conceptual difference with respect to other physical and theoretical investigations available in the literature is that during the meeting the analysis were done with the density constraint ρ, using the a highly non-local functional $V_{ee}[\rho]$ and to study the asymptotic behaviour of the ground state energy of the coupled system $\alpha\beta$ in function of the distance of the molecules α and β.

Outcome of the Meeting

The work developed at BIRS allowed us to be one step forward in understanding dispersion interactions via Optimal Transportation techniques. We will continue developing the theory and we plan to write a paper containing the results obtained at Banff.

Participants

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