ACTIVITY REPORT 2018/2019
Doctoral Program in Mathematics

The report covers the period from 1 September 2018 – 31 August 2019
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New PhD students enrolled
# Faculty Members

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<th><strong>Director</strong></th>
<th>Fabio Nobile (from 1.1.2019)</th>
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| **Commission** | Annalisa Buffa  
Friedrich Eisenbrand  
Kathryn Hess Bellwald  
Clément Hongler (new member since 1.7.2019)  
Joachim Krieger (until 30.6.2019)  
Thomas Mountford  
Sophia C. Olhede (new member since 1.7.2019)  
János Pach (until 30 June 2019)  
Marc Troyanov  
Maryna Viazovska (new member since 1.7.2019) |
| **Student Representative** | Ondine Chanon |
| **Administration** | Anna Dietler |
| **Thesis Directors** |  
Prof. Assyrr Abdulle  
Prof. Buffa Annalisa  
Dr. Boris Buffoni  
Prof. Maria Colombo  
Prof. Robert Dalang  
Prof. Bernard Dacorogna  
Prof. Anthony C. Davison  
Prof. Simone Deparis  
Prof. Friedrich Eisenbrand  
Prof. Damir Filipovic  
Prof. Kathryn Hess Bellwald  
Prof. Jan S. Hesthaven  
Prof. Clément Hongler  
Prof. Dimitar Jetchev  
Prof. Juhan Aru  
Prof. Daniel Kressner  
Prof. Joachim Krieger  
Prof. John H. Maddocks  
Prof. Philippe Michel  
Prof. Nicolas Monod  
Prof. Stephan Morgenthaler  
Prof. Thomas Mountford  
Prof. Hoài-Minh Nguyên  
Prof. Fabio Nobile  
Prof. Sophia C. Olhede  
Prof. János Pach  
Prof. Victor Panaretos  
Prof. Zsolt Pataki  
Prof. Marco Piccaso  
Prof. Amin Shokrollahi  
Prof. Joachim Stubbe  
Prof. Donna Testerman  
Prof. Marc Troyanov  
Prof. Maryna Viazovska |
## EDMA Courses

### Fall 2018

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<tr>
<td>Arithmetic of elliptic curves - MATH-695</td>
<td>P. Michel, M. Viazovska</td>
</tr>
<tr>
<td>Positive characteristic algebraic geometry - MATH-697</td>
<td>Z. Patakfalvi</td>
</tr>
<tr>
<td>The Fourier transform in algorithms and optimization - MATH-696</td>
<td>F. Eisenbrand</td>
</tr>
<tr>
<td>Topics in Mathematical Physics - MATH-669</td>
<td>C. Hongler</td>
</tr>
<tr>
<td>Working Group in Algebraic Groups I - MATH-625(1)</td>
<td>D. Testerman</td>
</tr>
<tr>
<td>Working Group in Topology I - MATH-726</td>
<td>K. Hess Bellwald</td>
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<th>Dates</th>
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<tr>
<td>Summer School on Generalized Curvature - MATH-668</td>
<td>M. Troyanov</td>
<td>2.-7.9.2018</td>
</tr>
<tr>
<td>Elastic rods and Birods I - MATH-610(I)</td>
<td>J. Maddocks</td>
<td>11.-15.2.2019</td>
</tr>
<tr>
<td>Elastic rods and Birods II - MATH-610(II)</td>
<td>J. Maddocks</td>
<td>9.4.-22.5.2019</td>
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<tr>
<td>Isogeometric Analysis for the approximation of PDEs - MATH-652</td>
<td>H. Vazquez</td>
<td>9.4.-22.5.2019</td>
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<tr>
<td>Quantum groups and crystal bases - MATH-617</td>
<td>T. Gerber</td>
<td>8.4.-31.5.2019</td>
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<tr>
<td>Topics in the theory of Markov processes - MATH-618</td>
<td>G. Pavliotis</td>
<td>6.3.-4.4.2019</td>
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<td>Course</td>
<td>Instructor(s)</td>
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<tr>
<td>Convex geometry: Probabilistic methods and metric embeddings - MATH-698</td>
<td>A. Davison, D. Goldstein, S. Morgenthaler, V. Panaretos</td>
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<td>Positive characteristic algebraic geometry II - MATH-651</td>
<td>Z. Patakfalvi</td>
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<td>Topics in 2D continuum random geometry - MATH-654</td>
<td>J. Aru</td>
<td></td>
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<tr>
<td>Topics in Geometric Analysis II - 731(2)</td>
<td>M. Troyanov</td>
<td></td>
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<tr>
<td>Working Group in Algebraic Groups II - MATH-625(2)</td>
<td>D. Testerman</td>
<td></td>
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<tr>
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<td>K. Hess Bellwald</td>
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Candidacy Exams

Luigi De Rosa
Regularity of Incompressible Fluids
Partial Differential Equations

Date: September 9, 2018 Transfer from Uni Zürich
Thesis director: Maria Colombo
Co-director: Camillo De Lellis

Ondine Chanon
Model simplification in isogeometric analysis with hierarchical B-splines

Date: September 7, 2018
Thesis director: Annalisa Buffa
President of the Jury: Joachim Krieger
Jury member: Marco Picasso

Stefania Ebli
Signal Processing on Simplicial Complexes

Date: September 18, 2018
Thesis director: Kathryn Hess Bellwald
President of the Jury: Victor Panaretos
Jury member: Pierre Vandergheynst

Jonathan Koh Boon Han
Quantifying Hail Risk: Contributions to Spatial Extremes

Date: October 9, 2018
Thesis director: Anthony C. Davison
President of the Jury: Kathryn Hess Bellwald
Jury member: Stephan Morgenthaler

Eva Vidlicková
Dynamical low rank approximation for random time dependent PDEs

Date: September 14, 2018
Thesis director: Fabio Nobile
President of the Jury: Annalisa Buffa
Jury member: Jan S. Hesthaven
Emelie K. Arvidsson
Vanishing Theorems for Fano-type varieties in positive characteristic
Date: October 8, 2018
Thesis director: Zsolt Patakfalvi
President of the Jury: Kathryn Hess Bellwald
Jury member: Philippe Michel

Davide Pradovera
Model order reduction based on functional rational approximants for parametric PDEs with meromorphic structure.
Date: October 15, 2018
Thesis director: Fabio Nobile
President of the Jury: Annalisa Buffa
Jury member: Daniel Kressner

Guillaume Buro
Espaces métriques et structures Finslériennes de basse régularité
Date: January 25, 2019
Thesis director: Marc Troyanov
President of the Jury: Thomas Mountford
Jury member: Maria Colombo

Tomas Masák
Nonparametric covariance estimation for space-time processes: separability and beyond
Date: January 29, 2019
Thesis director: Victor Panaretos
President of the Jury: Fabio Nobile
Jury member: Anthony Davison

Quentin Posva
On the application of K-stability to families of Fano varieties
Date: March 1, 2019
Thesis director: Zsolt Patakfalvi
President of the Jury: Kathryn Hess Bellwald
Jury member: Philippe Michel

Soumaya Elkantassi
Likelihood Inference on the Boundary
Date: February 14, 2019
Thesis director: Anthony C. Davison
President of the Jury: Fabio Nobile
Jury member: Stephan Morgentaler
Nicolò Ripamonti  Data-driven POD-Galerkin closure based on Mori-Zwanzig formalism
Date: February 20, 2019
Thesis director: Jan S. Hesthaven
President of the Jury: Joachim Krieger
Jury member: Fabio Nobile

Ana-Maria Retegan  Behavior of semisimple elements in irreducible representations of simple algebraic groups
Date: June 24, 2019
Thesis director: Donna Testerman
President of the Jury: Kathryn Hess Bellwald
Jury member: Jérôme Scherer

Laya Ghodrati  Smoothing in the Wasserstein Space
Date: June 27, 2019
Thesis director: Victor Panaretos
President of the Jury: Kathryn Hess Bellwald
Jury member: Stephan Morgenthaler

Silja Haffter  On stability and regularity problems in fluid dynamics and related problems
Date: August 28, 2019
Thesis director: Maria Colombo
President of the Jury: Fabio Nobile
Jury member: Joachim Krieger

Arthur Jacot-Guillarmod  Theory of Deep Neural Networks: Neural Tangent Kernel
Date: August 29, 2019
Thesis director: Clément Hongler
President of the Jury: Thomas Mountford
Jury member: Matthieu Wyart

Kartik Waghmare  Completions of Partially Specified Covariance Functions
Date: August 30, 2019
Thesis director: Victor Panaretos
President of the Jury: Thomas Mountford
Jury member: Sofia Olhede
Prizes and Awards

Mathematics Doctoral Thesis Award December 2018
given to

DIMITRI WYSS
PhD student of Tamás Hausel

for important contributions to arithmetic algebraic geometry, in particular for developing naive motivic Fourier transform for Nakajima quiver varieties, and for advancing $p$-adic integration techniques to successfully attack cohomological conjectures arising at the juncture of mathematical physics and the number theoretic Langlands program.

Doctoral Program Thesis Distinction 2018

DIMITRI S. WYSS
Phd student of Tamás Hausel
Motivic and $p$-adic Localization Phenomena

THIMOTHÉE N. POUCHON
Phd student of Assyr Abdulle
Effective models and numerical homogenization methods for long time wave propagation in heterogeneous media

Other Awards

GIACOMO ROSILHO DE SOUZA
Phd student of Assyr Abdulle

Giacomo Rosilho de Souza was awarded the Butcher prize 2019 for the best paper by a PhD student at the International Conference on Scientific Computation and Differential Equations.
In this thesis, we solve two different problems.

The first part solves the system of linear partial differential equations

\[ dw + a \wedge w = f, \]

in an open set \( \Omega \), as well as the linear system of equations

\[ da \wedge u = \beta, \]

where \( a: \Omega \to \Lambda^1, \ f: \Omega \to \Lambda^{k+1} \) and \( \beta: \Omega \to \Lambda^{k+2} \) are given and \( w, u: \Omega \to \Lambda^k \) are the unknowns. We show that if \( \text{rank}[da] \equiv 2m \geq 2(k + 1) \), those equations have at most one solution, if \( \text{rank}[da] \equiv 2m \geq 2(k + 2) \) and \( \beta = df + a \wedge f \), they are equivalent and if \( \text{rank}[da] \equiv 2m \geq 2(n - k) \) the first equation always admits a solution. Moreover, we build an operator \( N^k \) defined on \((k - 1)\)-forms such that if \( \text{rank}[da] \equiv 2m \geq 2(n - k + 1) \) and \( w \) is such that \( dw + a \wedge w = 0 \), then there exists \( \varphi \) such that \( N^k(\varphi) = w \).

The first equation is a generalization of the Poincaré lemma since if \( a \) is exact, the solution of this equation are a consequence of this classical result. However, as soon as \( a \) is non exact, the study of the problem changes significantly.

The second part solves the system of linear partial differential equations

\[ A\nabla u + (\nabla u)^t A = F, \]

in \( \Omega \), where \( A \in \mathbb{R}^{n \times n} \) and \( F: \Omega \to \mathbb{R}^{n \times n} \) are given and \( u: \Omega \to \mathbb{R}^n \) is the unknown. We give necessary conditions and sufficient conditions for existence of solutions of the equation above and the equation together with a boundary Dirichlet condition, that is, \( u = u_0 \) on the boundary. We give criteria when \( A \) is symmetric in which case the equation is a generalization of the symmetric gradient equation \( \nabla u + (\nabla u)^t = F \), when \( A \) is skew-symmetric in which case the equation is a generalization of the curl equation \( \nabla u - (\nabla u)^t = F \). Finally, we give criteria when \( A \) doesn’t verify any symmetry hypothesis.
During the past decade, model order reduction (MOR) has been successfully applied to reduce the computational complexity of elliptic and parabolic systems of partial differential equations (PDEs). However, MOR of hyperbolic equations remains a challenge. Symmetries and conservation laws, which are a distinctive feature of such systems, are often destroyed by conventional MOR techniques, resulting in a perturbed and often unstable reduced system. The goal of this thesis is to study and develop model order reduction techniques that can preserve nonlinear invariants, symmetries, and conservation laws and to understand the stability properties of these methods compared to conventional techniques. Hamiltonian systems, as systems that are driven by symmetries, are studied intensively from the point of view of MOR. Furthermore, a conservative model reduction of fluid flow is presented. It is illustrated that conserving invariants, conservation laws, and symmetries not only result in a physically meaningful reduced system but also result in an accurate and robust reduced system with enhanced stability.
Scaling and Resilience in Numerical Algorithms for Exascale Computing

The first Petascale supercomputer, the IBM Roadrunner, went online in 2008. Ten years later, the community is now looking ahead to a new generation of Exascale machines. During the decade that has passed, several hundred Petascale capable machines have been installed worldwide, yet despite the abundance of machines, applications that scale to their full size remain rare. Large clusters now routinely have 50,000+ cores, some have several million. This extreme level of parallelism, that has allowed a theoretical compute capacity in excess of a million billion operations per second, turns out to be difficult to use in many applications of practical interest. Processors often end up spending more time waiting for synchronization, communication, and other coordinating operations to complete, rather than actually computing. Component reliability is another challenge facing HPC developers. If even a single processor fail, among many thousands, the user is forced to restart traditional applications, wasting valuable compute time. These issues collectively manifest themselves as low parallel efficiency, resulting in waste of energy and computational resources. Future performance improvements are expected to continue to come in large part due to increased parallelism. One may therefore speculate that the difficulties currently faced, when scaling applications to Petascale machines, will progressively worsen, making it difficult for scientists to harness the full potential of Exascale computing.

The thesis comprises two parts. Each part consists of several chapters discussing modifications of numerical algorithms to make them better suited for future Exascale machines. In the first part, the use of Parareal for Parallel-in-Time integration techniques for scalable numerical solution of partial differential equations is considered. We propose a new adaptive scheduler that optimize the parallel efficiency by minimizing the time-subdomain length without making communication of time-subdomains too costly. In conjunction with an appropriate preconditioner, we demonstrate that it is possible to obtain time-parallel speedup on the nonlinear shallow water equation, beyond what is possible using conventional spatial domain-decomposition techniques alone. The part is concluded with the proposal of a new method for constructing Parallel-in-Time integration schemes better suited for convection dominated problems.

In the second part, new ways of mitigating the impact of hardware failures are developed and presented. The topic is introduced with the creation of a new fault-tolerant variant of Parareal. In the chapter that follows, a C++ Library for multi-level checkpointing is presented. The library uses lightweight in-memory checkpoints, protected through the use of erasure codes, to mitigate the impact of failures by decreasing the overhead of checkpointing and minimizing the compute work lost. Erasure codes have the unfortunate property that
if more data blocks are lost than parity codes created, the data is effectively considered unrecoverable. The final chapter contains a preliminary study on partial information recovery for incomplete checksums. Under the assumption that some meta knowledge exists on the structure of the data encoded, we show that the data lost may be recovered, at least partially. This result is of interest not only in HPC but also in data centers where erasure codes are widely used to protect data efficiently.
Kazhdan’s Property (T) and Property (FH) for measured groupoids

Introduced 50 years ago by David Kazhdan, Kazhdan’s Property (T) has quickly become an active research area in mathematics, with a lot of important results. A few years later, this property has been generalized to discrete group actions by Robert J. Zimmer. Then, more recently, Claire Anantharaman-Delaroche has generalized it to measured groupoids.

In this work, we will continue to study this property for measured groupoids. We will introduce the Property (\(T_c\)) for locally compact group actions, a generalization via compact sets of the Property (T) for discrete group actions of R. J. Zimmer. We will develop Kazhdan’s Property (T) for measured groupoids, and, for transformation group groupoids, a close link between these two properties will be proved. Then we will define and study a generalization of Property (FH) for measured groupoids. Finally, we will prove a generalization to measured groupoids of the Delorme-Guichardet theorem, which states an equivalence between Property (FH) and Property (T). This has also been proved by C. Anantharaman-Delaroche, but in a different context.
On some problems related to 2-level polytopes

In this thesis we investigate a number of problems related to 2-level polytopes, in particular from the point of view of the combinatorial structure and the extension complexity. 2-level polytopes were introduced as a generalization of stable set polytopes of perfect graphs, and despite their apparently simple structure, are at the center of many open problems ranging from information theory to semidefinite programming. The extension complexity of a polytope $P$ is a measure of the complexity of representing $P$: it is the smallest size of an extended formulation of $P$, which in turn is a linear description of a polyhedron that projects down to $P$. In the first chapter, we examine several classes of 2-level polytopes arising in combinatorial settings and we prove a relation between the number of vertices and facets of such polytopes, which is conjectured to hold for all 2-level polytopes. The proofs are obtained through an improved understanding of the combinatorial structure of such polytopes, which in some cases leads to results of independent interest. In the second chapter, we study the extension complexity of a restricted class of 2-level polytopes, the stable set polytopes of bipartite graphs, for which we obtain non-trivial lower and upper bounds. In the third chapter we study slack matrices of 2-level polytopes, important combinatorial objects related to extension complexity, defining operations on them and giving algorithms for the following recognition problem: given a matrix, determine whether it is a slack matrix of some special class of 2-level polytopes. In the fourth chapter we address the problem of explicitly obtaining small size extended formulations whose existence is guaranteed by communication protocols. In particular we give an algorithm to write down extended formulations for the stable set polytope of perfect graphs, making a well known result by Yannakakis constructive, and we extend this to all deterministic protocols.
Functional Peaks-Over-Threshold Analysis for Complex Extreme Events

Most current risk assessment for complex extreme events relies on catalogues of similar events, either historical or generated artificially. In the latter, no existing methods produce completely new events with mathematically justified extrapolation above observed level of severity. This thesis contributes to the development of stochastic generators of events based on extreme value theory, with a special focus on natural hazards.

The sources of historical meteorological records are multiple but climate model output is attractive for its spatial completeness and homogeneity. From a statistical perspective, these are massive gridded data sets, which can be exploited for accurate estimation of extreme events. The first contribution of this thesis describes methods of statistical inference for extremal processes that are computationally tractable for large data sets. We also relate the extremal behaviour of aggregated data to point observations, a result that we use to downscale gridded data to local tail distributions. These contributions are illustrated by applications to rainfall and heatwaves.

Building stochastic generators of extreme events requires the extension of classical peaks-over-threshold analysis to continuous stochastic processes. We develop a framework in which characterization of complex extremes can be motivated by field-specific expertise. The contribution includes the description of the theoretical limiting distribution of functional exceedances, called the generalized r-Pareto process, the functional equivalent of the generalized Pareto distribution, for which we describe statistical inference procedures, simulation algorithms and goodness-of-fit diagnostics. We apply these results to build a stochastic weather generator of extreme wind storms over Europe.
The detection of two-component mixture alternatives. Theory and methods

In this thesis, we deal with one of the facets of the statistical detection problem. We study a particular type of alternative, the mixture model. We consider testing where the null hypothesis corresponds to the absence of a signal, represented by some known distribution, e.g., Gaussian white noise, while in the alternative one assumes that among observations there might be a cluster of points carrying a signal, which is characterized by some distribution \( G \). The main research objective is to determine a detectable set of alternatives in the parameter space combining the parameters of \( G \) and the mixture proportion \( p \). We focus is on the finite sample sizes and wish to study the possibility of detecting alternatives for fixed \( n \), given pre-specified error levels. The first part of the thesis covers theoretical results. Specifically, we introduce a parametrization which relates the parameter space of an alternative to the sample size, and present the regions of detectability and non-detectability. The regions of detectability are the subsets of the new parameter space (induced by the parametrization) where for a prespecified type I error rate, the type II error rate of the likelihood ratio test (LRT) is bounded from above by some constant. To move towards the real data applications, we also check the performance of some non-parametric testing procedures proposed for this problem and some widely used distributions. In the second part of the thesis, we use this argument to develop a framework for clinical trial designs aimed at detecting a sensitive-to-therapy subpopulation. The idea of modeling treatment response as a mixture of subpopulations originates from treatment effect heterogeneity. Methods studying the effects of heterogeneity in the clinical data are referred to as subgroup analyses. However, designs accounting for possible response heterogeneity are rarely discussed, though in some cases they might help to avoid trial failure due to the lack of efficacy. In our work, we consider two possible subgroups of patients, drug responders and drug non-responders. Given no preliminary information about patients’ memberships, we propose a framework for designing randomized clinical trials that are able to detect a responders’ subgroup of desired characteristics. We also propose strategies to minimize the number of enrolled patients whilst preserving the testing errors below given levels and suggest how the design along with all testing metrics can be generalized to the case of multiple centers. The last part of the thesis is not directly related to the preceding parts. We present two supervised classification algorithms for real-data applications.
Approximate Cloaking via Transformation Optics for Electromagnetic Waves

Cloaking via transformation optics was introduced by Pendry, Schurig, and Smith for the Maxwell system and Leonhardt in the geometric optics setting. They used a singular change of variables which blows up a point into a cloaked region. The same transformation had been used by Greenleaf, Lassas, and Uhlmann in an inverse context. This singular structure implies difficulties not only in practice but also in analysis. To avoid using the singular structure, regularized schemes have been proposed. One of them was suggested by Kohn, Shen, Vogelius, and Weinstein for which they used a transformation which blows up a small ball instead of a point into the cloaked region. In this thesis, we study the approximate cloaking via transformation optics for electromagnetic waves in both the time harmonic regime and time regime. In the time-harmonic regime, the cloaking device only consists of a layer constructed by the mapping technique, no (damping) lossy-layer is required. Due to the fact that no lossy layer is required, resonance might appear. The analysis is therefore delicate and the phenomena are complex. In particular, we show that the energy can blow up inside the cloaked region in the resonant case and whereas cloaking is achieved in both non-resonant and resonant cases. Moreover, the degree of visibility depends on the compatibility of the source inside the cloaked region and the system. These facts are new and distinct from known mathematical results in the literature. In the time regime, the cloaking device also consists of a fixed lossy layer. Our approach is based on estimates on the degree of visibility in the frequency domain for all frequency in which the frequency dependence is explicit. The difficulty and the novelty in the analysis are in the low and high frequency regimes. To this end, we implement the variational technique in low frequency and the multiplier and duality techniques in high frequency domain. The first part of the thesis is inspired by the work of Nguyen and the second part by the work of Nguyen and Vogelius on the wave equation.
A Gauss-Bonnet Theorem for Asymptotically Conical Manifolds and Manifolds with Conical Singularities

The purpose of this thesis is to provide an intrinsic proof of a Gauss-Bonnet-Chern formula for complete Riemannian manifolds with finitely many conical singularities and asymptotically conical ends. A geometric invariant is associated to the link of both the conical singularities and the asymptotically conical ends and is used to quantify the Gauss-Bonnet defect of such manifolds. This invariant is constructed by contracting powers of a tensor involving the curvature tensor of the link. Moreover this invariant can be written in terms of the total Lipschitz-Killing curvatures of the link. A detailed study of the Lipschitz-Killing curvatures of Riemannian manifolds is presented as well as a complete modern version of Chern’s intrinsic proof of the Gauss-Bonnet-Chern Theorem for compact manifolds with boundary.
Knapsack problems give a simple framework for decision making. A classical example is the min-knapsack problem (MinKnap): choose a subset of items with minimum total cost, whose total profit is above a given threshold. While this model successfully generalizes to problems in scheduling, network design and capacitated location, its dynamic programming approaches do not. One often relies on strong polyhedral relaxations for corresponding integer programs instead. Among other results, we construct such a relaxation for the time-invariant incremental knapsack problem (IIK), and study classes of valid inequalities for MinKnap.

IIK is covered in the first part of this thesis. It is a generalization of the max-knapsack problem to a discrete multi-period setting. At each time, capacity increases and items can be added, but not removed from the knapsack. The goal is to maximize the sum of profits over all times. IIK models scenarios in specific financial markets and governmental decision processes. It is known to be strongly NP-hard and there has been work on approximation algorithms for special cases. We settle the complexity of IIK by designing a PTAS, and provide several extensions of the technique.

The second part is on MinKnap and divided into two chapters. One is motivated by a recent work on disjunctive relaxations for MinKnap with fixed objective function, where we reduce the size of the construction. The other focuses on a class of bounded pitch inequalities, that generalize the unweighted cover inequalities for MinKnap. While separating over pitch-1 inequalities is NP-hard, we show that approximate separation over the set of pitch-1 and pitch-2 inequalities can be done in polynomial time. We also investigate integrality gaps of linear relaxations for MinKnap when these inequalities are added. Consequently we show that, for any fixed $t$, the $t$-th CG closure of the natural relaxation has unbounded gap. The last chapter deals with questions in clustered planarity testing. The Hanani-Tutte theorem is a classical result that characterizes planar graphs as graphs that admit a drawing in the plane in which every pair of edges not sharing a vertex cross an even number of times. We generalize this result to clustered graphs with two disjoint clusters, and show that a straightforward extension to flat clustered graphs with three or more disjoint clusters is not possible. For general clustered graphs we show a variant of the Hanani-Tutte theorem in the case when each cluster induces a connected subgraph. We conclude by a short proof, using matroid intersection, for a result by Di Battista and Frati on embedded clustered graphs.
Stochastic approximation methods for PDE constrained optimal control problems with uncertain parameters

We consider the numerical approximation of a risk-averse optimal control problems constrained by an elliptic Partial Differential Equation (PDE) with random coefficients. Specifically, the control function is a deterministic distributed forcing term that minimizes the expected mean squared distance between the state (i.e. solution to the PDE) and a target function, subject to a regularization for well posedness. For the computation of the approximated optimal control, we combine different approximation steps, namely: a Finite Element discretization of the underlying PDEs; a quadrature formula to approximate the expectation in the objective functional; and gradient type iterations to compute the approximated optimal control. We start by considering a Monte Carlo quadrature formula, based on random points, and compare the complexity of a full gradient method, in which the finite element discretization and the Monte Carlo sample are chosen initially and kept fixed over the gradient iterations, with a Stochastic Gradient (SG) method in which the expectation in the computation of the steepest descent direction is approximated by an independent Monte Carlo estimator, with small sample size, at each iteration, and the finite element discretization is possibly refined along the iterations. We then extend the SG method, by replacing the single evaluation of the gradient on a single mesh, by a multilevel Monte Carlo (MLMC) estimator of the gradient, that exploits a hierarchy of finite element discretizations. We propose, in particular, strategies to increase the numbers of discretization levels and Monte Carlo samples per level along the iterations, to achieve an optimal complexity. As a last approach, we consider a tensorized Gaussian quadrature formula, in the case where the randomness in the PDE can be parametrized by a small number of random variables, and propose to use a generalized version of the Stochastic Average Gradient method (SAGA) to compute the approximated optimal control. SAGA is a type of SG algorithm with a fixed-length memory term, which computes at each iteration the gradient of the loss functional in only one quadrature point, randomly chosen from a possibly non-uniform distribution. For all the methods developed in this work, we present a full theoretical error and complexity analysis. Specifically, we show that the SG strategy, when combined with a Monte Carlo approximation, results in an improved computational complexity with respect to a full gradient approach, and, incorporating a MLMC estimator, improves further the complexity. On the other hand, SAGA is well adapted when a quadrature formula with spectral convergence properties is considered, and the resulting algorithm has a similar asymptotic complexity as the full gradient method, although with possibly better pre-asymptotic behavior. All theoretical error estimates and complexity results are confirmed by some numerical experiments.
Penalization and Bayesian numerical methods for multiscale inverse problems

In this thesis we consider inverse problems involving multiscale elliptic partial differential equations. The name multiscale indicates that these models are characterized by the presence of parameters which vary on different spatial scales (macroscopic, microscopic, mesoscopic, etc.). The variations at the smallest scales make these equations very difficult to approximate also when considering forward problems, since classical numerical methods require a mesh resolution at the finest scales, hence a computational cost that is often prohibitive. For this reason one prefers to apply homogenization or effective methods which, neglecting what happens at the smallest scales, are able to provide accurate macroscopic solutions to the problem. For what concerns the solution of inverse problems, we propose then a new numerical algorithm based on homogenization techniques, model order reduction and regularization methods.

First, we consider elliptic operators whose tensor varies on a microscopic scale. Under the assumption that the nature of its micro structure is known, we aim at recovering a macroscopic parameterization of the tensor from measurements originating from the full multiscale model, using homogenization. Practical examples include multi-phase media whose constituents are known, but their respective volume fraction is unknown. We consider the Calderón’s formulation of the inverse problem. We prove that, under some regularity assumptions on the fine scale tensor, the effective inverse problem, with observed data consisting of the homogenized Dirichlet to Neumann (DtN) map, is also well-posed. We then solve the problem by considering finite measurements of the multiscale DtN map and using Tikhonov regularization, and we establish a convergence result of the solution by means of G-convergence.

In a second stage, we consider a Bayesian approach which allows for uncertainty quantification of the results. We prove existence and well-posedness of the effective posterior probability measure, obtained by homogenization of the observation operator. By means of G-convergence we characterize the discrepancy between the fine scale and the homogenized model, and we prove convergence of the effective posterior towards the fine scale posterior in terms of the Hellinger distance. We also propose a numerical procedure to estimate the homogenization error statistics, which, if included in the inversion process, allow to account for approximation errors.

Finally, we deal with multiscale inverse problems for the linear elasticity equation. In this context we assume that the heterogeneity of the material is determined by its geometry rather than by the coefficients of the equation. In particular, we consider porous media with random perforations and, following the Bayesian approach, we solve the inverse problem of determining the elastic properties of an hypothetical isotropic material. We prove the existence and well-
posedness of the effective posterior measure, as well as its convergence in the fine scale limit by means of G-convergence. We conclude by describing a new probabilistic numerical method which computes a new posterior measure that accounts for approximation errors and reveals the uncertainty intrinsic in the numerical method.
Large-scale variational inference for Bayesian joint regression modelling of high-dimensional genetic data

Genetic association studies have become increasingly important in understanding the molecular bases of complex human traits. The specific analysis of intermediate molecular traits, via quantitative trait locus (QTL) studies, has recently received much attention, prompted by the advance of high-throughput technologies for quantifying gene, protein and metabolite levels. Of great interest is the detection of weak trans-regulatory effects between a genetic variant and a distal gene product. In particular, hotspot genetic variants, which remotely control the levels of many molecular outcomes, may initiate decisive functional mechanisms underlying disease endpoints.

This thesis proposes a Bayesian hierarchical approach for joint analysis of QTL data on a genome-wide scale. We consider a series of parallel sparse regressions combined in a hierarchical manner to flexibly accommodate high-dimensional responses (molecular levels) and predictors (genetic variants), and we present new methods for large-scale inference.

Existing approaches have limitations. Conventional marginal screening does not account for local dependencies and association patterns common to multiple outcomes and genetic variants, whereas joint modelling approaches are restricted to relatively small datasets by computational constraints. Our novel framework allows information-sharing across outcomes and variants, thereby enhancing the detection of weak trans and hotspot effects, and implements tailored variational inference procedures that allow simultaneous analysis of data for an entire QTL study, comprising hundreds of thousands of predictors, and thousands of responses and samples.

The present work also describes extensions to leverage spatial and functional information on the genetic variants, for example, using predictor-level covariates such as epigenomic marks. Moreover, we augment variational inference with simulated annealing and parallel expectation-maximisation schemes in order to enhance exploration of highly multimodal spaces and allow efficient empirical Bayes estimation.

Our methods, publicly available as packages implemented in R and C++, are extensively assessed in realistic simulations. Their advantages are illustrated in several QTL applications, including a large-scale proteomic QTL study on two clinical cohorts that highlights novel candidate biomarkers for metabolic disorders.
Metallic aluminium plays a key role in our modern economy. Primary metallic aluminium is produced by the transformation of aluminium oxide using the Hall-Héroult industrial process. This process, which requires enormous quantities of energy, consists in performing the electrolysis of an aluminium oxide solute in large pots and with hundreds of thousands of amperes of electrical current.

The topic of this thesis is the study of some selected aspects of the modelisation of the electrolysis process from the point of view of numerical simulation. This thesis is divided in two parts.

The first part is focused on the numerical modelisation of the alumina powder dissolution and transport in the electrolytic bath as a function of the bath temperature. We provide a mathematical model for the transport and dissolution of the alumina powder, followed by its time and space discretisation by means of a finite element method. Finally, we study the behavior of this numerical model in the case of an industrial electrolysis pot.

The second part is devoted to the development of a numerical scheme for the approximation of the fluid flows in an electrolysis pot. The scheme relies on a Fourier basis decomposition of the unknowns. The amplitude of each Fourier component satisfies a partial differential equation which is expliciete derived. The solution of this equation is approximated by means of a finite element method. Finally, the approximate fluid flow obtained with this new method is compared with the solution provided by the reference model in an industrial electrolysis pot.
Automatic L2 Regularization for Multiple Generalized Additive Models

Multiple generalized additive models are a class of statistical regression models wherein parameters of probability distributions incorporate information through additive smooth functions of predictors. The functions are represented by basis function expansions, whose coefficients are the regression parameters. The smoothness is induced by a quadratic roughness penalty on the functions’ curvature, which is equivalent to a weighted $L_2$ regularization controlled by smoothing parameters. Regression fitting relies on maximum penalized likelihood estimation for the regression coefficients, and smoothness selection relies on maximum marginal likelihood estimation for the smoothing parameters.

Owing to their nonlinearity, flexibility and interpretability, generalized additive models are widely used in statistical modeling, but despite recent advances, reliable and fast methods for automatic smoothing in massive datasets are unavailable. Existing approaches are either reliable, complex and slow, or unreliable, simpler and fast, so a compromise must be made. A bridge between these categories is needed to extend use of multiple generalized additive models to settings beyond those possible in existing software. This thesis is one step in this direction. We adopt the marginal likelihood approach to develop approximate expectation-maximization methods for automatic smoothing, which avoid evaluation of expensive and unstable terms. This results in simpler algorithms that do not sacrifice reliability and achieve state-of-the-art accuracy and computational efficiency.

We extend the proposed approach to big-data settings and produce the first reliable, high-performance and distributed-memory algorithm for fitting massive multiple generalized additive models. Furthermore, we develop the underlying generic software libraries and make them accessible to the open-source community.


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Procrustes Metrics and Optimal Transport for Covariance Operators

Covariance operators play a fundamental role in functional data analysis, providing the canonical means to analyse functional variation via the celebrated Karhunen-Loéve expansion. These operators may themselves be subject to variation, for instance in contexts where multiple functional populations are to be compared. Statistical techniques to analyse such variation are intimately linked with the choice of metric on the space of such operators, as well as with their intrinsic infinite-dimensionality.

We will show that we can identify the space of infinite-dimensional covariance operators equipped with the Procrustes size-and-shape metric from shape theory, with that of centred Gaussian processes, equipped with the Wasserstein metric of optimal transportation. We then describe key geometrical and topological aspects of the space of covariance operators endowed with the Procrustes metric. Through the notion of multicoupling of Gaussian measures, we establish existence, uniqueness and stability for the Fréchet mean of covariance operators with respect to the Procrustes metric. Furthermore, we provide generative models that are canonical for such metrics.

We then turn to the problem of comparing several samples of stochastic processes with respect to their second-order structure, and we subsequently describe the main modes of variation in this second order structure. These two tasks are carried out via an Analysis of Variance (ANOVA) and a Principal Component Analysis (PCA) of covariance operators respectively. In order to perform ANOVA, we introduce a novel approach based on optimal (multi)transport and identify each covariance with an optimal transport map. These maps are then contrasted with the identity with respect to a norm-induced distance. The resulting test statistic, calibrated by permutation, outperforms the state-of-the-art in the functional case. If the null hypothesis postulating equality of the operators is rejected, thanks to a geometric interpretation of the transport maps we can construct a PCA on the tangent space with the aim of understanding sample variability. Finally, we provide a further example of use of the optimal transport framework, by applying it to the problem of clustering of operators. Two different clustering algorithms are presented, one of which is innovative. The transportation ANOVA, PCA and clustering are validated both on simulated scenarios and real dataset.
Extensive amenability and a Tits alternative for topological full groups

This dissertation investigates the amenability of topological full groups using a property of group actions called extensive amenability. Extensive amenability is a core concept of several amenability results for groups of dynamical origin. We study its properties and present some applications. The main result of the thesis is such an application, a Tits alternative for topological full groups of minimal actions of finitely generated groups. On the one hand, we show that topological full groups of minimal actions of virtually cyclic groups are amenable. On the other hand, if $G$ is a finitely generated not virtually cyclic group, we construct a minimal free action of $G$ on a Cantor space such that the topological full group contains a non-abelian free group.
Maximal subgroups acting with two composition factors on irreducible representations of exceptional algebraic groups

Let $Y$ be a simply connected simple algebraic group over an algebraically closed field $k$ of characteristic $p$ and let $X$ be a maximal closed connected simple subgroup of $Y$. Excluding some small primes in specific cases, we classify the $p$-restricted irreducible representations of $Y$ on which $X$ acts with exactly two composition factors. This work follows on naturally from the classification of irreducible subgroups of exceptional algebraic groups given by Testerman.
Contributions to Likelihood-Based Modelling of Extreme Values

Extreme value analysis is concerned with the modelling of extreme events such as floods and heatwaves, which can have large impacts. Statistical modelling can be useful to better assess risks even if, due to scarcity of measurements, there is inherently very large residual uncertainty in any analysis. Driven by the increase in environmental databases, spatial modelling of extremes has expanded rapidly in the last decade. This thesis presents contributions to such analysis.

The first chapter is about likelihood-based inference in the univariate setting and investigates the use of bias-correction and higher-order asymptotic methods for extremes, highlighting through examples and illustrations the unique challenge posed by data scarcity. We focus on parametric modelling of extreme values, which relies on limiting distributional results and for which, as a result, uncertainty quantification is complicated. We find that, in certain cases, small-sample asymptotic methods can give improved inference by reducing the error rate of confidence intervals. Two data illustrations, linked to assessment of the frequency of extreme rainfall episodes in Venezuela and the analysis of survival of supercentenarians, illustrate the methods developed.

In the second chapter, we review the major methods for the analysis of spatial extremes models. We highlight the similarities and provide a thorough literature review along with novel simulation algorithms. The methods described therein are made available through a statistical software package.

The last chapter focuses on estimation for a Bayesian hierarchical model derived from a multivariate generalized Pareto process. We review approaches for the estimation of censored components in models derived from (log)-elliptical distributions, paying particular attention to the estimation of a high-dimensional Gaussian distribution function via Monte Carlo methods. The impacts of model misspecification and of censoring are explored through extensive simulations and we conclude with a case study of rainfall extremes in Eastern Switzerland.
Generalized Norm-compatible Systems on Unitary Shimura Varieties

We define and study in terms of integral Iwahori-Hecke algebras a new class of geometric operators acting on the Bruhat-Tits building of connected reductive groups over $p$-adic fields. These operators, which we call $U$-operators, generalize the geometric notion of "successors" for trees with a marked end. The first main contributions of the thesis are:

(i) the integrality of the $U$-operator over the spherical Hecke algebra using the compatibility between Bernstein and Satake homomorphisms,

(ii) in the unramified case, the $U$-operator attached to a minuscule cocharacter is a right root of the corresponding Hecke polynomial.

In the second part of the thesis, we study some arithmetic aspects of special cycles on (products of) unitary Shimura varieties, these cycles are expected to yield new results towards the Bloch-Beilinson conjectures. As a global application of (ii), we obtain:

(iii) the horizontal norm relations for these GGP cycles for arbitrary $n$, at primes where the unitary group splits.

The general local theory developed in the first part of the thesis, has the potential to result in a number of global applications along the lines of (iii) (involving other Shimura varieties and also vertical norm relations) and offers new insights into topics such as the Blasius-Rogawski conjecture as well.
A sequence-dependent coarse-grain model of B-DNA with explicit description of bases and phosphate groups parametrised from large scale Molecular Dynamics simulations

We introduce a sequence–dependent coarse–grain model of double–stranded DNA with an explicit description of both the bases and the phosphate groups as interacting rigid–bodies. The model parameters are trained on extensive, state–of–the–art large scale molecular dynamics (MD) simulations. The model paradigm relies on three main approximations: 1) nucleic acid bases and phosphate groups are rigid, 2) interactions are nearest–neighbour and can be modelled with a quadratic energy, 3) model parameters have dimer sequence dependence. For an arbitrary sequence, the model predicts a sequence–dependent Gaussian equilibrium probability distribution. The parameter set comprises dimer–based elements, which are used to reconstruct mean configurations, called ground–states, which can have strong non–local sequence dependence, and precision matrices, or stiffness matrices, for any sequence of any length. This prediction step is sufficiently efficient that it is straightforward to construct probability density functions for millions of fragments each of length a few hundred base–pairs. The estimation of a parameter set consists in minimising the sum of Kullback–Leibler divergences between Gaussians predicted by the model and analogous Gaussians estimated directly from MD simulations of a training library of sequences. The training library comprises a short list of short palindromic DNA sequences. We designed the palindromic library using an ad hoc algorithm to include multiple instances of all independent tetramer sub–sequences. We exploit palindromic symmetry properties to study the convergence of the statistics extracted from MD simulations of palindromes and to define palindromically symmetrised estimators of first and second centred moments. The computation of the parameter set is delicate and needs the use of sophisticated numerics. We present an efficient and reliable procedure for estimating a complete parameter set which involves a generalisation of the classic Fisher information matrix and its relationship to the relative entropy, or Kullback–Leibler divergence. The model is a computationally efficient tool that allows the study of the mechanical properties of double–stranded DNA of arbitrary length and sequence. We use the model to study the sequence–dependent rigidity of DNA and we compute sequence–dependent apparent and dynamic persistence lengths. The explicit treatment of the phosphate group also allows computation of sequence–dependent grooves widths. Moreover, with fine–grained representation of predicted ground–states, we can also study sequence–dependence of sugar puckering modes and BI–BII backbone conformations.
On the Dynamics of Magnetic Swimmers in Stokes Flow

In the past decade, the engineering community has conceived, manufactured and tested micro-swimmers, i.e. microscopic devices which can be steered in their intended environment. Foreseen applications range from microsurgery and targeted drug delivery to environmental decontamination. This thesis presents a mathematical analysis of the dynamics of rigid magnetic swimmers in a Stokes flow driven by a steadily rotating external uniform magnetic field. The swimmer is assumed to be made of a permanent magnetic material and to be placed in a fluid that fills an infinite enveloping space. A specific swimmer is prescribed by its magnetic moment and mobility matrix. For a given swimmer, its dynamics depend on two parameters that can be changed during an experiment: the Mason number, related to the magnitude and angular speed of the magnetic field, and the conical angle between the magnetic field and its axis of rotation. As these two parameters vary, strikingly different regimes of response occur. The swimmer’s trajectory is entirely governed by its rotational dynamics: once its orientation dynamics are known, its position trajectory can be recovered. For neutrally buoyant swimmers, this work provides a complete classification of the steady states of the rotational dynamics, along with a study of non-steady solutions in the asymptotic limits of small and large Mason number, and small conical angle. Predicted out-of-equilibrium solutions are in good agreement with numerical simulations. Full swimmer trajectories corresponding to steady states and periodic solutions of the rotational dynamics are then recovered. Finally, the effect of buoyancy is taken into account, and the relative equilibria of swimmers with a different density than that of the fluid are determined when the axis of rotation of the magnetic field is aligned with gravity.