Spectral Geometry:
Theory, Numerical Analysis and Applications

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1 Overview of the Field

Spectral geometry is an area of mathematics at the intersection of analysis, partial differential equations and differential geometry. It investigates the properties of eigenvalues and eigenfunctions of the Laplacian and other operators, including their dependence on the geometric, topological and dynamical features of the underlying space (e.g. a Riemannian manifold or a Euclidean domain).

Originally, spectral geometry was motivated by the study of mathematical models of physical processes, such as vibration, heat propagation, oscillations of fluids and quantum-mechanical effects. The quest to better understand these phenomena lead to the development of powerful analytic and numerical methods in geometric spectral theory and also had a profound impact on engineering applications. In recent years, new and somewhat unexpected applications of these techniques to computer science have emerged, notably to shape recognition and machine learning. These applications, in turn, inspire new exciting theoretical and computational challenges.

Spurred by recent fast-paced progress on theoretical and applied aspects of spectral geometry, our workshop brought together experts on theoretical, numerical and applied aspects of this discipline, with the objective to foster interactions and promote new collaborations. To our knowledge, no interdisciplinary meetings of this kind have been held previously, and by all accounts the meeting led to a variety of new research collaborations and open problems.

2 Recent Developments

There is a long history of fruitful interactions between geometric spectral theory, numerical analysis and computer science. In recent years, the interplay between these fields has reached new heights due to the emergence of increasingly powerful computers, new motivating applications and more efficient numerical algorithms.

Numerical calculations serve as an indispensable source of intuition and are behind many important advances in spectral geometry. In particular, numerical experiments played a stimulating role in recent breakthrough research on nodal portraits of random linear combinations of eigenfunctions (see, for instance, [SSS16, SW15, CS14]). Numerical methods are actively used in the rapidly developing theory of spectral minimal partitions (see [BNH11, BNH17]). For low eigenvalues, numerical experiments are a major source of conjectures in shape optimization problems (see [JLN*05, AF12, ABN15, BBG94]). An exciting new trend is to use numerical analysis not only to formulate conjectures, but to actually prove theorems in spectral geometry [BF16, pol] using rigorous computer-assisted methods.

Some of the most important recent applications of spectral geometry lie in the areas of shape analysis and machine learning (see [ZGL03, BN03, RWP06, BNS06, CL06, CL06, DBG*06, JMS08, OSG08, SOG09, OMMG10, OBCS*12, OMPG13, ROA*13, CSBC*17]). These applications are based on the properties of spectral quantities such as heat kernels and eigenfunctions associated with the Laplacian (see, for instance, [BBG94, JMS08]). As it is now well-understood, the Laplacian on a Riemannian manifold carries a lot of information about intrinsic geometry. To capture the extrinsic geometry of shapes using spectral quantities, however, one needs to use other operators. A natural choice is the Dirichlet-to-Neumann operator, which, incidentally, has been in the focus of intensive research in theoretical spectral geometry in recent years (see [PS15, GPPS14, FS11, FS16, GP17, AKO17, BBG94]). The collection of eigenvalues of the Dirichlet-to-Neumann operator is also called the Steklov spectrum, as it is precisely the spectrum of the Steklov boundary value problem. Recent advances in the study of the Steklov spectrum, particularly, of the corresponding geometric invariants, open up a number of promising new applications to shape analysis (see [WBCPS17]).

Accompanying these developments, the design and analysis of high-accuracy discretization methods for spectral problems and optimal design has been the focus of intense research activity in numerical analysis. A plethora of discretization techniques—including methods based on particular solutions [BHT15], spectral methods, finite element methods [Bof10, CGS15] and integral equation methods [ABN15]—have been developed. Each of these methods presents both advantages and challenges in the numerical analysis, and this analysis in turn leads us to improved understanding of the properties of the eigenvalues and eigenfunctions of the operators under investigation, and can spark entirely novel areas of development. For example, as described in [Bof10], the use of very common Lagrange finite elements for the Maxwell eigenvalue problem was shown to yield the wrong spectrum even on simple geometries, motivating the large-scale adoption of the edge finite elements. The design of numerical methods for inverse problems has lead to the investigation of (nonlinear and non self-adjoint) transmission eigenvalue problems, and this in turn lead to the design of novel methods. The computations were used extensively to enhance our understanding of the situations under which the existence of such eigenvalues could be proven. The design of a boundary integral method for mixed Dirichlet-Neumann eigenvalues of the Laplacian is necessarily intertwined with a careful study of the asymptotic behaviour of the eigenfunctions [ABN15].

Upon discretization, the resulting large discrete systems have been coupled to state-of-the-art eigenvalue solvers and optimization methods. Naïve approaches do not suffice, and the design of good algorithms in this area has yielded many interesting and challenging research directions, due to the potentially nonlinear/non-convex nature of the objective function to be optimized. If the eigenvalues are clustered, or if the original spectrum is not discrete, these problems are much harder, see e.g. [GGO13].

Another fascinating and important area of investigation seeks to provide computable error bounds and eigenvalue enclosures, e.g. [Liu15]. These bounds are crucial if numerical methods are to be used for formulating conjectures.

Finally, practitioners in geometry processing, computer graphics, medical imaging, machine learning, and other computational disciplines have employed spectral geometry to great effect, improving the quality and flexibility of algorithms for a broad range of geometric tasks. The most exciting research in this field requires synthesis of theoretical, numerical, and applied ideas to motivate practical research problems, extract detailed understanding of underlying models, and formulate discrete approximations that provide a stable, faithful link between theory and practice.

3 Presentation Highlights

In view of the interdisciplinary nature of the workshop, the talks were equally divided into three main themes: theory, numerics and applications. In each theme, one talk was reserved for an overview of the subject. All speakers were advised to give colloquium-style presentations accessible to non-experts.

3.1 Theoretical aspects of spectral geometry

A broad historical overview of theoretical advances in spectral geometry from Lord Rayleigh and Hermann Weyl to our time was presented by Michael Levitin. He described some major results on eigenvalue estimates, spectral asymptotics and spectral geometry of the Dirichlet-to-Neumann map. These were recurrent themes during the workshop, and Michael's talk served as an excellent introduction to the subject.

The talks by Dorin Bucur and Mikhail Karpukhin were concerned with shape optimization for Laplace eigenvalues on Riemannian manifolds and Euclidean domains. Dorin Bucur presented his recent work with Antoine Henrot [BH18] on the maximization of the second nonzero Neumann eigenvalue on Euclidean domains. They have shown that among all domains (not necessarily connected) of given volume, the second nonzero Neumann eigenvalue is maximized by a disjoint union of two identical balls. This result extends the 2009 theorem of Girouard, Nadirashvili and Polterovich [GNP09] who proved a similar statement for simply connected planar domains. Mikhail Karpukhin reported on his recent joint work with Nadirashvili, Penskoi and Polterovich on a sharp isoperimetric inequality for all Laplace eigenvalues on a sphere [KNPP17]. It was shown that for any positive integer k, the k-th nonzero eigenvalue on the two-dimensional sphere endowed with a Riemannian metric of fixed area, is maximized in the limit by a sequence of metrics converging to a union of k touching identical round spheres. This proved a conjecture posed by Nadirashvili in 2002.

David Sher and Asma Hassannezhad spoke about recent progress in understanding spectral asymptotics for Steklov-type problems on Euclidean domains. David Sher presented his recent joint work with Levitin, Parnovski and Polterovich on the proof of the two-term asymptotic formula for sloshing (mixed Steklov–Neumann) eigenvalues on planar domains [LPPS17]. In particular, this result confirmed the 1983 conjecture of Fox–Kuttler [FK83] and could be considered a first step towards obtaining sharp spectral asymptotics for the Steklov eigenvalues (or, equivalently, eigenvalues of the Dirichlet-to-Neumann map) on polygons. Asma Hassannezhad's talk was based on her joint work with Ari Laptev [HL17] on estimates on the Riesz means for the eigenvalues of mixed Steklov problems on Euclidean domains of arbitrary dimension.

Virginie Bonnaillie-Noël presented a collection of analytic and numerical results on spectral minimal partitions. Earlier developments on this topic were mostly concerned with either sums or maxima of the first eigenvalues of a partition. The talk focused on recent advances in the general case of the p-norm of the vector composed by the first eigenvalues of each subdomain of the partition. Some of these results were obtained jointly with Beniamin Bogosel [BNB16, BBN17].

Yaiza Canzani presented her recent joint works with John Toth and Jeffrey Galkowski [CGT18, CT16] on estimates of the averages of Laplace eigenfunctions over Riemannian submanifolds. Particularly strong results were obtained for surfaces with an Anosov geodesic flow, such as surfaces of negative curvature.

3.2 Numerical methods

Jeff Ovall presented an overview of discretization strategies and methods for locating the eigenvalues of discrete systems. Naïve implementations of discretizations can lead to problematic results, and this point was highlighted by simple examples. Next, he presented a filtered subspace iteration strategy for (possibly) unbounded self-adjoint operators. The method is analyzed in a fairly general framework. The bulk of the computational effort in the algorithm involves approximating the action of the resolvent at a few points along a contour enclosing the eigenvalues of interest.

David Colton provided a survey of transmission eigenvalue problems. These arise in inverse scattering theory, and are non-self-adjoint in nature. Transmission problems exhibit fascinating spectral properties and many open questions remain: indeed, the existence of the spectrum is only guaranteed under fairly restrictive assumptions on the contrast parameter. Whether these can be relaxed is an interesting open question. A remarkable connection (due to Fioralba Cakoni and Sagun Chanillo) between the location of transmission eigenvalues for automorphic solutions of the wave equation in the hyperbolic plane and the Riemann hypothesis was also briefly discussed.

The spectral indicator method described by Jiguang Sun is an efficient method for determining the location and multiplicity of eigenvalues in the complex plane. The indicators are inexpensive to compute, and the method is memory-efficient even for large spectral problems.

There is an intimate connection between the numerical analysis of wave scattering problems and the calculation of spectra; the family of time-domain spectral methods have typically relied on the availability of eigenfunctions of the Laplacian on a given domain to serve as an efficicent basis. These can, however, be prohibitively expensive to compute on complex geometries. Oscar Bruno described the need for spectrally accurate algorithms for both scattering and spectral problems, and discussed some of the key ideas behind integral-equation based approaches.

Xuefeng Liu presented the recent progress in providing guaranteed eigenvalue bounds in computation. For all but the simplest geometries the eigenvalues of elliptic operators are computed via approximation; it is important to be able to state computable intervals around the approximate eigenvalue within which the true eigenvalue is guaranteed to lie. Such a method is now available using finite element methods, and guaranteed eigenvalue bounding strategies for the Laplace, the Biharmonic, the Stokes, the Steklov operators were presented. A related talk was given by Joscha Gedicke on his joint worith with Carsten Carstensen. He discussed recent results on guaranteed lower bounds for eigenvalues of the Laplace operator on arbitrary coarse meshes using the nonconforming Crouzeix-Raviart finite element method. This approach was shown to yield guaranteed eigenvalue bounds of surprisingly high accuracy.

Francesca Gardini's talk was concerned with the adaptive finite elmeent method for eigenvalue problems. In particular, she explained how this method could be used to approximate multiple eigenvalues and clusters of eigenvalues. Optimal convergence of the method for the Laplace eigenvalue problem in mixed form was also discussed.

Sebastien Dominguez presented his joint work with Nilima Nigam and Jiguang Sun on Jones modes in Lipschitz domains. The Jones eigenvalue problem is an overdetermined problem, where the Neumann eigenvalue problem for linear elasticity is coupled with a constraint on the normal trace of the displacement along the boundary. It is relatively unexplored and has many interesting features, notably its sensitive dependence on boundary geometry. In the talk, existence of eigenpairs for this eigenvalue problem was proved in two and three dimensions, and some numerical results were presented on simple geometries.

The meeting concluded by the talk of Braxton Osting on his joint work with Dong Wang and Ryan Viertel on diffusion generated methods for target valued maps. Diffusion generated methods were discused for minimizing the Dirichlet energy of a function taking values in a wide class of target sets. Applications to finding Dirichlet partitions, generating quadrilateral meshes and solving certain inverse problems were presented.

3.3 Applications

Justin Solomon gave a survey of applications of spectral geometry to different disciplines in computer science, including computer graphics, machine learning, and medical imaging. The key theme in his talk was to show how the numerical methods and theoretical results covered in the previous survey talks are incorporated into algorithms that leverage the geometry of scanned shapes and abstract clouds of data points.

Ron Kimmel reported on applications of spectral geometry to surface classification. The classification problem is to find an algebraic representation for each surface that would be similar for objects within the same class and preserve dissimilarities between classes. He discussed how to transform the geometric problem of surface classification into an algebraic form of classifying matrices. The eigenfunctions of the Laplacian with two distinct metrics on a surface are used extensively [AKR13]. Another key topic is the connection with deep learning techniques, and a new approach for encoding geometric intuition into modeling, training, and testing. The key idea is to design learning algorithms to use geometric representations and invariants, for applications from shape matching, facial surface reconstruction from a single image, to reading facial expressions [RSK16, RSOEK17, SRK17].

Etienne Vouga described preliminary results on inverse spectral problems, namely how to embed a piece of geometry given its Laplace–Beltrami spectrum. His talk covered a promising new algorithm leveraging spherical conformal parameterization techniques to pose the problem in terms of optimization over spherical harmonic coefficients. Preliminary experiments show some promise for practical tools that solve the inverse spectral problem numerically.

Mirela Ben-Chen and Amir Vaxman demonstrated the value of spectral geometry algorithms for problems involving vectors and frames on discrete surfaces. Prof. Ben-Chen's talk focused on an operator-based approach to vector field processing, representing fields not as collections of direction vectors but rather as derivative operators discretized as matrices; her work reveals new discretization techniques with structure-preserving properties, as well as applications to field design [ABCCO13, AOCBC15] and simulation [AWO*14, AVW*15]. Prof. Vaxman presented efforts to unify directional field processing with subdivision operators for discrete surfaces, providing a representation of vector fields compatible with subdivision-based superresolution.

Hervé Lombaert demonstrated the value of spectral techniques for medical image processing [LGPC11], in particular correspondence between 3D brain models gathered using MRI. In this domain, spectral algorithms allow for efficient and accurate intrinsic matching of neuroimaging data, enabling tools that transfer labels and other information across multiple scans and subjects [LAA15].

Finally, Yu Wang showed that intrinsic surface-based algorithms for geometry processing can be extended to incorporate volumetric information by replacing the Laplacian with the Dirichlet-to-Neumann operator [WBCPS17]. His application of the boundary element method (BEM) enables volumetric shape analysis without tetrahedral remeshing to fill the volume bounded by a surface. Intriguing theoretical questions arise from his work involving the behavior of integral operators involved discretizing the Dirichet-to-Neumann operator in the case of open surfaces.

4 Outcomes of the Meeting

The intents of this meeting were to (a) capture the state-of-the-art in the theory, numerical analysis and applications of spectral geometry, (b) provide a forum for experts in these typically disparate communities to interact and (c) identify common challenges or problems of mutual interest. As is typical in many mathematical disciplines, several subcommunities of researchers make significant progress with little "cross-pollination", sharing their results with others who may benefit or have ideas for extension.

The current workshop was demonstrably successful in achieving these goals. Longer tutorial and survey-style talks from theory, numerics and applications set a common technical base and vocabulary among the participants. For instance, we saw that the 'stiffness matrix' in finite elements is the 'cotangent Laplacian' in discrete differential geometry. Shorter talks presented the state-of-the-art from the viewpoint of the subcommunities, and the tutorials prepared all the participants to understand some of the recent developments in the field more broadly, as well as to launch meaningful interactions and collaborations. The breaks and open problem sessions generated several interactions and inspired research projects of mutual interest. Here is a sampling of open problems:

4.1 Inferring interior structure of Mars from spectral data

The first seismometer is about to land on Mars in November 2018. Amongst other data, it will be able to measure the spectrum of free elastic oscillations of the planet. What can be inferred about the internal structure of Mars from this data? Do discontinuities in the media have a "spectral fingerprint" in terms of heat invariants, Weyl asymptotics, or some other spectral quantity? As a simple first model, one may consider the Neumann spectrum of the Laplace-Beltrami operator on a Riemannian manifold with boundary when the metric has a conormal jump or other singularities across a hypersurface.

This problem was presented by Joonas Illmavirta.

4.2 A numerical analysis for the Jones eigenvalue problem in elasticity in curvilinear domains

An unusual eigenvalue problem in elasticity was introduced by D.S. Jones [Jon83], in the larger context of fluid-structure and elastodynamic transmission problems. Stated abstractly, the eigenvalue problem is as follows. Let Ω be an open and bounded domain in $\mathbb{R}^d$ with reasonable boundary, and $\lambda, \mu \in \mathbb{R}$ are given constants so that $\mu > 0, \lambda + \frac{2}{d}\mu > 0$. We seek nontrivial $\mathbf{u}$, vector fields in Ω, and $\omega^2 \in \mathbb{C}$ such that

$$\mathcal{L}\mathbf{u} := \mu\Delta\mathbf{u} + (\lambda + \frac{2}{d}\mu)\mathrm{grad}\,\mathrm{div}\mathbf{u} = \omega^2\mathbf{u} \tag{1}$$

in Ω. On the boundary we enforce the natural boundary condition for the *Lamé* operator $\mathcal{L}$. In addition, we enforce $\mathbf{u} \cdot \mathbf{n} = 0$ on the boundary of Ω, where $\mathbf{n}$ is the unit outer normal to the boundary (defined a.e.). It was only recently established that this constrained eigenvalue problem has a discrete countable spectrum in non-axisymmetric domains with Lipschitz boundaries; it was shown by Hargé in 1990 that the set of C^∞ domains which do not support such a spectrum is dense amongst all possible C^∞ domains. It is clear that any rigid rotation is a Jones mode in a disk, and so zero is an eigenvalue of $\mathcal{L}$ in some instances.

We would like to understand the approximation problem of computing these eigenmodes in curvilinear domains. A standard mesh of triangles will not approximate the boundary exactly, and a consistency error is committed. Certain coercivity constants degenerate in the passage from polygonal domains with many sides to a curvilinear domain, and therefore one question is: In what situations does the Jones spectrum on approximating domains approach the true Jones spectrum, and at what rate? Another question is: Can one develop a stable approximation scheme for the eigenmodes in curvilinear domains?

This problem was presented by Nilima Nigam.

4.3 Discrete isoperimetric inequalities

Fine-grained results characterize isoperimetry in terms of the eigenvalues of the Laplacian operator for shapes embedded in the plane; for instance, the shape extremizing the first eigenvalue is a circle. No analogous results, however, are known about discrete Laplacian operators, e.g. the cotangent Laplacian from first-order finite elements on a triangle mesh. Suppose the topology of a triangle mesh with n vertices is fixed. Then, we could consider the first nonzero Laplacian eigenvalue of the mesh to be a function $\lambda(X) : \mathbb{R}^{n\times 2} \to \mathbb{R}_+$, where $X \in \mathbb{R}^{n\times 2}$ gives the positions of the vertices in the plane. Then, we could ask the usual isoperimetric question: What configuration of vertices in X extremizes $\lambda(X)$ subject to a constraint on the area covered by X in the plane?

Similarly, if we fix the boundary of a polygonal region $\Omega \subseteq \mathbb{R}^2$, we have many choices of triangulations in the interior of Ω. A distinguishing feature of the discrete problem is that different triangulations of the same region in the plane may have different spectra. Hence, we can ask: What conditions on a mesh of Ω make for larger or smaller principal eigenvalues?

This problem was presented by Justin Solomon.

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