Laplace-Beltrami operator – the Swiss Army knife of shape analysis problems

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ABSTRACT

The Laplace-Beltrame operator (LBO) is the extension of the Laplacian to non-Euclidean domains. Its spectral decomposition has many physical interpretations and can be numerically computed on various discrete domains ranging from point clouds to volumetric images. In this talk I will review several computational shape analysis problems in which the LBO spectral decomposition has established itself as particularly useful.

The differential geometry of spaces of polygons and polymers

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ABSTRACT

We are interested in understanding the geometry of the Riemannian manifold of space polygons. Applications include the study of random walks and polymers, linkages, and protein shapes. In this talk, we focus on the space of equilateral polygons (these model polymers and arc-length parametrized curves). We will first discuss the space of closed equilateral polygons as a symplectic reduction of the space of open polygons (this structure was introduced by Millson and Kapovich [1]). This structure provides a natural way to understand the probability measure on random equilateral polygons [2] and leads to a natural sampling algorithm for random polygons [3], which is now being extended to a deeper combinatorial understanding of polygon spaces [4]. The symplectic structure on polygon space provides the correct probability measure, but distorts the metric. This makes shape clustering and classification harder to do. To end the talk, we'll discuss some work in progress on making the metric structure more easily visible by writing the closed polygons as a quotient space (instead of a subspace) of the open polygons using the Möbius group.

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Topological approach to modeling spatial cognition

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ABSTRACT

Understanding the neural mechanisms learning and memory is impossible without a theoretical apparatus explaining how the inputs provided by individual neurons combine at the ensemble scale. We developed a theoretical approach that helps understanding how individual cells in mammalian hippocampus interact with one another to enable (or prevent) accurate spatial information from being encoded. Our key hypothesis is that the hippocampal representation of space is a topological framework —a topological memory map —which geometric details can be situated as necessary. Our computational model can be used to assess the contributions made by various physiological parameters into spatial learning, given a sufficiently detailed input about neuronal spiking.

Biologically relevant distances between morphological surfaces representing teeth and bones

Ingrid Daubechies

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ABSTRACT

The talk describes new distances between pairs of two-dimensional surfaces (embedded in three-dimensional space) that use both local structures and global information in the surfaces. These are motivated by the need of biological morphologists to compare different phenotypical structures, to study relationships of living or extinct animals with their surroundings and each other. This is typically done from carefully defined anatomical correspondence points (landmarks) on the teeth and bones. We are working on building algorithms for automatic morphological correspondence maps, without any preliminary marking of special features or landmarks by the user. This is an ongoing project by a collaboration of mathematicians, computer scientists, biologists and statisticians.

Mathematicians helping Art Historians and Art Conservators

Ingrid Daubechies

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ABSTRACT

In recent years, mathematical algorithms have helped art historians and art conservators putting together the thousands of fragments into which an unfortunate WWII bombing destroyed world famous frescos by Mantegna, decide that certain paintings by masters were "roll mates" (their canvases were cut from the same bolt), virtually remove artifacts in preparation for a restoration campaign, get more insight into paintings hidden underneath a visible one,...

The presentation will review these applications, and give a glimpse into the mathematical aspects that make this possible.

Normal Modes and Structural Transitions in Biological Macromolecules

Marc Delarue

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ABSTRACT

I will review our recent work towards making Normal Modes well adapted for studying Conformational transitions in very large systems. To tackle large systems, coarse-graining becomes necessary and I will describe a new method to perform rigourous Decimation of the system while preserving low-frequency normal modes. In addition, robust normal modes obtained by a combination of elastic networks and Delaunay tessalation will be presented. These robust Normal Modes have been used successfully to refine models against either x-ray data or cryo-EM maps. Finally, in the case where axial symmetry exists in the model, I will show that symmetricity of the modes is an excellent criterion to choose the most effective modes to describe the transition, using as examples structures solved in the lab.

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On the applicability of convex relaxations for matching symmetric shapes

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ABSTRACT

The problem of finding a near-isometry between two (discretized) shapes is often modeled as a quadratic assignment problem, and solved using convex relaxations. in the talk we will analyze the successfulness of the doubly stochastic (DS) relaxation for isometric matching problems. We will review results showing that DS is successful for almost all asymmetric shapes, and present our results which show that DS is successful for almost all shapes with reflective symmetry. We also provide example of simple symmetry groups for which the DS relaxation is never successful.

If time permits we will discuss similar results we obtained for an SDP relaxation of the Procrustes matching problem.

Shapes, radius functions, and persistent homology

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ABSTRACT

Given a protein in terms of spheres, the family of alpha shapes gives a multi-scale representation of the shape. We study the radius function on the Delaunay mosaic that governs this family and work out the related construction of the family of wrap complexes. In combination with persistent homology, this gives a powerful tool to construct a multi-scale shape representation with high topology fidelity.

A Metric on the space of Genus Zero shapes

Joel Hass

University of California at Davis, USA

ABSTRACT

I will discuss a method of comparing shapes based on finding an optimal conformal diffeomorphism between two surfaces. This method gives a metric on the space of Riemannian surfaces of genus zero. I will also describe some alternative approaches to comparing genus zero shapes with cone points, based on comparing conformally equivalent hyperbolic orbifolds. This allows specifying landmarks when comparing surfaces and has been used to compare brain cortices.

Applications of Conformal Geometry in Brain Mapping and Computational Anatomy

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ABSTRACT

Brain mapping research combines many different fields of study to investigate and understand the anatomy, growth, development, function, and changes of a healthy brain as we age, or the progression of disease. Magnetic resonance imaging (MRI) data enables researchers from fields outside medicine to develop and offer new tools to the study of the human brain. Mathematics, computation, and modeling play important roles in contributing new ideas to understanding the brain.

In this presentation, I will discuss some of the conformal geometric methods that my research group is using to study the human brain. The cortical folding patterns of each human brain are unique. This uniqueness, along with the highly folded nature of the human brain makes it difficult to compare function, anatomy, and changes due to disease or aging across individuals. I will discuss how we are using MRI data, image segmentation, and topology methods to construct a triangulated mesh representing a cortical surface and then create a conformal "flat" map of the surface. Conformal maps preserve angles and their orientation. The Uniformization Theorem, which is a generalization of the Riemann Mapping Theorem [1], says there is a unique conformal transformation to the complex plane, hyperbolic disc, or (Riemann) sphere. I will discuss a method known as circle packing which we are using to create our quasi-conformal "flat" maps of the brain [2]. I will also discuss how we are using these conformal maps, along with conformal invariants, such as extremal length, and harmonic measure to explore and compare specific regions of the human brain. If time permits, I will also present some other geometric methods we are using to investigate the development of the folding patterns of the human brain.

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Minimum action principles and shape dynamics

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ABSTRACT

The functions of all life forms depend on organization in space and time. Spatial organization involves the interactions of shapes with their surroundings, while organization in time concerns changes in shape. Geometric methods therefore play an essential role in the analyses and simulations of biological systems. Geometry and topology are now used regularly for representing, searching, simulating, analyzing, and comparing biological systems. In this talk, I will focus on the latter. I will present a new method for computing a distance between two shapes embedded in three dimensional space. Instead of comparing directly the geometric properties of the two shapes, we measure the cost of deforming one of the two shapes into the other. The deformation is computed as the geodesic between the two shapes in the space of shapes. The geodesic is found as a minimizer of the Onsager Machlup action, based on an elastic energy for shapes. I will illustrate applications of this method to geometric morphometrics using data sets representing bones and teeth of primates. Experiments on these data sets show that the method performs remarkably well both in shape recognition and in identifying evolutionary patterns, with success rates similar to, and in some cases better than, those obtained by expert observers.

Geometric Optimization for Surface Parameterization

Shahar Kovalsky

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ABSTRACT

Surface parameterization is often a key component in the analysis and comparison of shapes. Consequently, efficient computation of parameterizations becomes essential, for example, in the analysis of high-resolution shapes or for the joint parameterization of multiple shapes.

I will begin with a brief introduction to surface parameterization and its computation, motivated by the problem of learning correspondences over a collection of biological shapes. Then, I will discuss an ongoing project that requires highly efficient computation of parameterizations and present our recent work on geometric optimization that enables it.

Orbifold-Tutte Embedding and Deep Learning on Surfaces

Yaron Lipman

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ABSTRACT

Tutte's graph drawing algorithm is a popular technique for embedding planar graphs in the plane as it guarantees validity, simple to compute, and minimizes a natural distortion energy. In this talk we show how Tutte's algorithm can be generalized to handle a rich set of target domains called Orbifolds. Orbifolds are intriguing simple surfaces generated by symmetry groups acting on two-dimensional Euclidean, hyperbolic and spherical domains. We demonstrate how the Orbifold-Tutte embedding can be used for defining Convolution Neural Networks on genus-zero surfaces and explore some applications such as semantic surface segmentation and biological landmark detection.

This is a joint work with Noam Aigerman, Haggai Maron and others I'll mention in the talk.

Phage capsid structure: Theory, phage lifestyle constraints, and environmental diagnostic

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ABSTRACT

Phages are viruses that infect bacteria and are the most abundant entity on the planet. About eighty percent of these viruses are made of a protein shell—the capsid—that stores the phage genome, adopts an icosahedral shape, and has a tail that inoculates the genome into the bacterial host. These phages have tuned this architecture to succeed in all sorts of environments from the cold waters of the arctic and the hot springs of Yellowstone to the mucosal surfaces of the human gut. We hypothesize that the malleable and rapidly evolving structure of tailed phages can be used as an early predictor of ecosystem changes due to environmental factors. To address this, we developed a mathematical model that predicts the structure of phages based on accessible environmental data such as phage genome size or capsid size. We validated the theory for 30 phages that are well-characterized structurally, and we applied the model to predict the structure associated to 500 phage genomes that have been annotated with the bioinformatic platform PhAnToMe. The structural analysis of these phages show that the lysogenic lifestyle—which allows phages to integrate in the bacterial host—imposes a strong constraint on the structure of the phage capsid. The lytic lifestyle—associated to the predatory life cycle of phage—promotes instead structural variability of the capsid. Despite the biological reason for this result remains unclear, our methodology provides a new approach to study the emergence of lysogeny, which has been linked to diseases and ecosystem degradation. To this end, we have analyzed phage samples from the Curonian Lagoon (near the Baltic sea), and we predict the emergence of lysogeny on the nearshore of Klaipeda. This methodology has a broad range of potential applications, for example, in the diagnosis of lysogenic variation within the human digestive tract and respiratory tract.

A discrete uniformization theorem and its applications

Feng Luo

Rutgers University, USA

ABSTRACT

We will discuss our work on discrete conformal geometry of polyhedral surfaces. A notion of discrete conformal equivalence of polyhedral surfaces is introduced and a discrete version of the uniformization theorem for compact polyhedral surfaces is established. We show that the discrete conformality is algorithmic and converges to the smooth conformal geometry. Applications to computer graphics will be addressed. This is a joint work with David Gu, Jian Sun, and Tianqi Wu.

Persistent Homology of Asymmetric Networks

Facundo Memoli

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ABSTRACT

I'll discuss recent work on trying to adapt persistent homology methods to datasets that exhibit asymmetry. Natural candidates are the Rips and Cech filtrations. Whereas the Rips filtration can unambiguously be generalized directly, generalizing the Cech filtration gives rise to two different versions: the sink and the source filtrations. It turns out that the Rips filtration imposes a symmetrization on the data whereas the Cech filtrations do not, thus making them more suitable for the analysis of intrinsically asymmetric data. By generalizing a theorem of Dowker we can prove that the persistent homologies of these two Cech filtrations are isomorphic. We establish the stability of these constructions under a metric between networks that generalizes the Gromov-Hausdorff distance. I'll also describe some results ve that characterize the persistence diagrams of some likely "motifs" in real (e.g. biological) networks: cycle-networks, which are directed analogues of the standard (discrete) circle. Finally, as an application, I'll show some computational results about classifying simulated networks arising from hippocampal cells.

The search for Transition Paths: some applications to biological systems

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The French Alternative Energies and Atomic Energy Commission (CEA), France

ABSTRACT

Transition paths are the stochastic paths that take a system from one state to another. In presence of high barriers, transitions are exponentially rare events, that require very long simulation times. In this talk, we show how transition paths can be formulated as conditioned stochastic paths, that can be generated exactly by a modified Langevin equation. Their generation requires much shorter simulation times than unconstrained paths. We illustrate the method on some analytical models, and show how it can be applied to the knotting-unknotting of circular DNA (in presence of topoisomerase), and to some allosteric transitions in proteins.

Spectral Approaches to Partial Shape Matching

Emanuele Rodolà[a,b] and Michael M. Bronstein[a,c,d]

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ABSTRACT

Shape correspondence is a fundamental problem in computer graphics and vision, with applications ranging from robotic vision to medical imaging and biological sciences. A particularly challenging setting of this problem arises when the shapes are allowed to undergo *non-rigid* deformations and only *partial data* are available. In this talk we will consider a hybrid approach operating in the spectral as well as the spatial domain to deal with this challenging setting. After introducing some basic notions of spectral shape analysis and functional correspondence, we will present a non-rigid multi-part shape matching algorithm [1,2]. In the most general setting, we assume to be given a reference shape and its multiple parts undergoing a non-rigid deformation. Each of these parts of interest can be additionally contaminated by clutter [3], may overlap with other parts, and there might be missing parts or redundant ones. Our method simultaneously solves for the segmentation of the reference model, and for a dense correspondence to (subsets of) the parts. Experimental results on synthetic as well as real data demonstrate the effectiveness of the proposed approach in dealing with this challenging matching scenario.

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Description and Comparison of Protein 3d-Structures with Emphasis on (Bio)-Topology

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ABSTRACT

The talk shortly introduces protein structure and present arguments why methods for comparing protein structures are need and are needed to be further developed. Structure comparison is fundamental for our understanding of proteins, specifically for studying their sequence and structural evolution and for guiding our efforts to predict their structures from their sequences of amino acids.

All methods for structural alignment of protein structures are based on a notion of geometric difference between two aligned substructures. Coordinate based structural alignment methods optimize a score based on the distances between aligned residue pairs after superposition. In a morph given by the linear interpolation between two superimposed structures the aligned residues, traverse these distances. Current alignment scores do not take into account if this implied morph is easy to perform, will cause steric clashes, or more severally, if it will cause (bio)-topological changes of the compared structures. I present novel algorithms designed to distinguish such cases introducing an analogy of Reidemeister moves for protein structures.

Another strategy to separate protein fold-classes is to use sufficiently power full geometric invariants to describe protein chains or sub-sets of these. Usually the number of protein structures dominates the calculation time of a descriptor-based method. Therefor such methods are usually significantly faster than pair alignment methods. I will present some descriptor families and results from applying them to search for both global (folds), intermediate (linking and poking) and local geometry in proteins. If time permits, I will point out new directions of our research.

Animal Behavior and Conformal Geometry

Ajay Mathuru[a,b] and Matt Stamps[a]

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ABSTRACT

A fundamental objective of neuroscience is to establish meaningful correlations between the observed behaviors of an organism and the neural activity in its brain. While there are well-developed measures for neural activity, it is difficult to objectively quantify animal behavior. This talk will present some preliminary findings on the application of computational conformal geometry to quantify differences in movement, specifically alarm behavior, of medaka and zebrafish in response to Schreckstoff (a fear-inducing pheromone). This is joint work with Haroun Chahed and Goh Rui Zhe.

Topology with Biological Applications

John M. Sullivan

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ABSTRACT

Given a topological object, one can search for an optimal shape by minimizing some geometric energy. After briefly reviewing the use of surface bending energy to model membrane shapes, we turn our attention to tight knots and links. While such ropelength minimizers have also been used in the study of knotted polymers like DNA, we discuss a more direct application: tight configurations of periodic woven or tangled structures provide a good model, for instance, of keratin filaments in skin cells.

Viruses and Geometry: New Insights into Virus structure, Assembly and Evolution

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ABSTRACT

Viruses are remarkable examples of order at the nanoscale. The capsids of many viruses, enclosing and protecting their genomes, are organised in lattice-like arrangements with overall icosahedral symmetry. Mathematical techniques from group, graph and tiling theory can therefore be used to characterise their architectures. In this talk, I will introduce our mathematical approach to the modelling of viral capsids (e.g. [1, 2]), and demonstrate its applications in vaccine design ([3, 4]). I will then present our Hamiltonian path approach to the modelling of genome packing in RNA viruses that underpins the discovery of an RNA-encoded assembly instruction manual in a wide range of viruses [4], including Picornavirusus [5], Hepatitis C [6] and Hepatitis B virus [7]. Finally, I will introduce our models of virus assembly [8] and demonstrate how they can be used to develop implicit fitness functions that shed new light on viral evolution and anti-viral drug therapy [9].

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Translating changing shapes into therapies

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ABSTRACT

The applications of physics in the biological sciences has opened up new paths to develop hypotheses underpinning mechanism in biology. Developing models to understand the role of dynamics of biomolecules in their interactions with other molecules has opened up a new window of opportunity to develop agents that can modulate these interactions and engineer new therapies.