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Abstracts

Applied Topology in Frontier Sciences

(11–22 July 2022)

1 Henry Adams

Colorado State University, USA
The persistent topology of optimal transport based thickenings

Abstract

The input to persistent homology is a filtration - an increasing sequence of spaces. We recast filtrations arising in applied topology, including Cech and Vietoris-Rips filtrations, in terms of optimal transport. This perspective faithfully preserves the (undecorated) persistence diagram. Furthermore, these optimal transport filtrations have nicer metric properties enabling simpler proofs of results such as Hausmann's theorem or homotopy types of Vietoris-Rips thickenings of spheres. Joint work with Michał Adamaszek, Florian Frick, Michael Moy, Facundo Mémoli, and Qingsong Wang.

2 Javier Arsuaga

University of California Davis, USA
DNA knotting in liquid crystalline phases

Abstract

The genome of some viruses, such as bacteriophages or human herpes, is a double stranded DNA (dsDNA) molecule that is stored inside a viral protein capsid at concentrations ranging from 200 mg/ml to 800mg/ml and osmotic pressures of 70 atmospheres. The organization of the viral genome under

these extreme physical conditions is believed to be in a liquid crystalline state and topologically knotted.
Cryoelectron microscopy (cryoEM) analysis of viral genomes reveal characteristics of the genome inside the capsid. Near the surface of the viral capsid the DNA is organized in a series of concentric layers followed by an isotropic arrangement of DNA fibers near the center of the capsid. In this talk, I will discuss cryoEM observations of the structure of the genome, how the arrangement of the genome changes with the ionic conditions of the environment and the length of the genome being packed. We propose a continuum liquid crystalline model for the organization of the genome that shows bifurcation solutions determined by the relation between the bending rigidity and twisting of the liquid crystal. We also discuss how these conformations are related to DNA knotting.

Work in collaboration with C Calderer and P. Liu (U. Minnesota)

3 Kathryn Hess Bellwald

EPFL, Switzerland
Of mice and men

Abstract

Motivated by the desire to automate classification of neuron morphologies, we designed a topological signature, the Topological Morphology Descriptor (TMD), that assigns a "barcode" to any any finite binary tree embedded in R^3. Using the TMD we performed an objective, stable classification of pyramidal cells in the rat neocortex, based only on the shape of their dendrites. In this talk, I will introduce the TMD, then focus on a very recent application to comparing mouse and human cortical neurons and characterizing the differences between them. This talk is based on collaborations led by Lida Kanari of the Blue Brain Project.

4 Igor Berezovsky

*A*STAR, Singapore*
Protein allostery: from molecular bases to practical implications

Abstract

We present a computational model, Structure-Based Statistical Mechanical Model of Allostery (SBSMMA), that makes it possible to tackle the problem of modulating the energetics of protein allosteric communication. In the context of the energy landscape paradigm, allosteric signalling is always a result of perturbations, such as ligand binding, mutations, and intermolecular interactions. The calculation of local partition functions in the protein harmonic model with perturbations allows us to evaluate the energetics of allosteric communication. Using SBSMMA, The Allosteric Signalling Map (ASM) providing a comprehensive residue-by-residue allosteric control over the protein activity can be obtained for any structure of interest. The Allosteric Probing Map (APM), in turn, allows one to perform the fragment-based-like computational design experiment aimed at finding leads for potential allosteric effectors.We will discuss the model itself, its usability for the analysis and prediction of allosteric regulation, and potential for using in biomedical applications, such as diagnostics and drug design.

5 Ginestra Bianconi

Queen Mary University of London, UK

The dynamics of higher-order networks: the effect of topology and triadic interactions

Abstract

Higher-order networks capture the interactions among two or more nodes and they are ubiquitous in complex systems. Here we show that higher-order interactions are responsible for new dynamical processes that cannot be observed in pairwise networks. We will cover how topology is key to define synchronization of topological signals, i.e. dynamical signal defined not only on nodes but also on links, triangles and higher-dimensional simplicies in simplicial complexes. Moreover we will reveal how triadic interactions can turn percolation into a fully-fledged dynamical process in which nodes can turn on and off intermittently in a periodic fashion or even chaotically leading to period doubling and a route to chaos of the percolation order parameter.

6 Jason Cantarella

University of Georgia, USA
Topological polymers and random embeddings of graphs

Abstract

Most biopolymers studied are either linear (such as DNA, RNA, or proteins) or circular (DNA minicircles, mitochondrial DNA). However, in the past decade, chemists have made enormous progress in synthesizing "topological" polymers whose graph types are more complicated, creating theta-curve polymers, "tadpole" or "lasso" polymers, and even $K_{3,3}$ and K_4 polymers. To understand the behavior of these more complicated polymers in solution, we require a mathematical theory which describes random embeddings of these graphs. Such a theory was created by James, Guth, and Flory in the 20th century to study elasticity, but it was restricted to simple Gaussian interactions between monomers. In this talk, we discuss a generalization of their theory which describes arbitrary interaction potentials. This new theory allows us to describe (for instance) freely-jointed networks or networks with steric interactions between monomers.

Authors: Jason Cantarella, Tetsuo Deguchi, Clayton Shonkwiler, Erica Uehara.

7 Wojtek Chacholski

KTH Royal Institute of Technology, Sweden
Homological algebra and persistence

Abstract

There is a growing interest in TDA community regarding homological invariants of persistent modules. In my talk I will describe a set up for relative homological algebra with computationally effective methods based on Koszul complexes for calculating associated Betti diagrams. This is a joint work with A. Guidolin, I. Ren, M. Scolamiero, F. Tombari.

8 Chao Chen

Stony Brook University, USA
Topology-driven learning for biomedical image analysis

Abstract

Extraction and analysis of complex biomedical structures such as vessels, tissue and neurons are crucial for understanding the underlying biological functionality and disease progression. Topological loss, based on the theory of persistent homology, plays an important role in these problems. In this talk, we will discuss several recent results of topology-driven learning. We will propose a probabilistic model for topology-aware segmentation. The model will learn a parametric probabilistic model in the space of topological structures. This will be very powerful in segmentation tasks especially when we have limited annotations. We will also discuss the convergence behavior of topological loss and topological constraints in multi-label segmentation.

9 Jiahui Chen

Michigan State University, USA
Evolutionary de Rham-Hodge method

Abstract

The de Rham-Hodge theory is a landmark of the 20^{th} Century's mathematics and has had a great impact on mathematics, physics, computer science, and engineering. This work introduces an evolutionary de Rham-Hodge method to provide a unified paradigm for the multiscale geometric and topological analysis of evolving manifolds constructed from filtration, which induces a family of evolutionary de Rham complexes. While the present method can be easily applied to close manifolds, the emphasis is given to more challenging compact manifolds with 2-manifold boundaries, which require appropriate analysis and treatment of boundary conditions on differential forms to maintain proper topological properties. Three sets of unique evolutionary Hodge Laplacians are proposed to generate three sets of topology-preserving singular spectra, for which the multiplicities of zero eigenvalues correspond to exactly the persistent Betti numbers of dimensions 0, 1, and 2. Additionally, three sets of non-zero eigenvalues further reveal both topological persistence and

geometric progression during the manifold evolution. Extensive numerical experiments are carried out via the discrete exterior calculus to demonstrate the potential of the proposed paradigm for data representation and shape analysis. To demonstrate the utility of the proposed method, the application is considered for the protein B-factor predictions of a few challenging cases for which other existing models do not work well.

10 Carina Curto

The Pennsylvania State University, USA
Graph rules and topological insights for inhibitory network dynamics

Abstract

Many networks in the nervous system possess an abundance of inhibition, which serves to shape and stabilize neural dynamics. The neurons in such networks exhibit intricate patterns of connectivity, whose structure controls the allowed patterns of neural activity. In this talk, we will focus on inhibitory threshold-linear networks whose dynamics are dictated by an underlying directed graph. We'll introduce a set of parameter-independent graph rules that enable us to predict features of the dynamics from properties of the graph. Graph rules also lead us to consider some natural topological structures, such as nerves and sheaves, stemming from various graph covers. Our results provide a direct link between the structure and function of inhibitory networks, and yield new insights into how connectivity may shape dynamics in real neural circuits. We will illustrate this with some applications to central pattern generator circuits and related examples of neural computation.

11 Yuri Dabaghian

The University of Texas Health Science Center at Houston (UTHealth), USA
Spatial representability of neuronal activity

Abstract

A dominating approach to interpreting spiking activity in various parts of the brain is based on identifying "firing fields"—regions in physical or configuration spaces that elicit neuronal responses. Common examples include

hippocampal place cells that fire at preferred locations in the navigated environment, head direction cells that fire at preferred orientations of the animal's head, view cells that respond to preferred spots in the visual field, etc. Historically, firing fields in all these cases were discovered empirically, by trial and error. However, the existence and a number of properties of the firing fields can be established theoretically, through topological analyses of the simplicial complexes that represent neuronal spiking activity. We also discuss topological and geometric conditions required for establishing "inherent spatiality" of neuronal activity produced by generic types of spiking neuronal networks.

12 Isabel Darcy

University of Iowa, USA
Modeling knotted proteins with tangles

Abstract

A protein is a linear chain of amino acids. In rare cases the protein can fold into a 3-dimensional structure that contains a local knot. Local knots with up to 6 crossings have been observed in some proteins. In all cases, these knots come from the family of twist knots. We use 2-string and 3-string tangles to explain why twists knots are more likely to be observed. This is joint work with Garrett Jones and Puttipong Pongtanapaisan.

13 Tamal K. Dey

Purdue University, USA
New results in computing zigzag and multiparameter persistence

Abstract

In this talk we present the following two results: (i) Zigzag persistence, a powerful extension of the standard persistence, is known to be more costly to compute than the non-zigzag persistence. We show how to narrow this efficiency gap. Our main result is that an input zigzag filtration can be converted to a non-zigzag filtration of same length with a very little cost. Furthermore, the barcode of the original filtration can be easily read from

the barcode of the converted filtration. Our experiment shows that this indeed allows substantial performance gain over the existing state-of-the-art softwares. We can take advantage of this result for computing generalized rank invariants involving 2-parameter persistence due to our next finding; (ii) We show that the generalized rank over a finite interval I of a 2-parameter persistence module M is equal to the full rank of the zigzag module that is induced on a certain path in I tracing mostly its boundary. Among others, we apply this result to obtain an improved algorithm for determining if a given 2-parameter module is interval decomposable and, if so, to compute all intervals supporting its summands. This is joint work (i) with Tao Hou and (ii) with Woojin Kim and Facundo Memoli.

14 Massimo Ferri

Università di Bologna, Italy
Digraph persistence

Abstract

First, the basic notions of non-simplicial persistence will be recalled: persistence functions, steady and ranging sets; a few examples in graphs will be shown. Then, the extendability to directed graphs will be made explicit by the persistence functions relative to: strong components, hubs, kernels.

15 Patrizio Frosini

Università di Bologna, Italy
On the use of group equivariant non-expansive operators for topological data analysis and geometric deep learning

Abstract

Group equivariant non-expansive operators (GENEOs) have been recently introduced as mathematical tools for approximating data observers, when data are represented by real-valued or vector-valued functions. The use of these operators is based on the assumption that the interpretation of data depends on the geometric properties of the observers. In this talk we will illustrate some recent results in the theory of GENEOs, showing how these

operators could be used for topological data analysis and geometric deep learning.

16 Tomas Gedeon

Montana State University, USA
Extremal event graphs: a stable tool for analyzing noisy time series data

Abstract

Local maxima and minima, or extremal events, in experimental time series can be used as a coarse summary to characterize data. However, the discrete sampling in recording experimental measurements suggests un- certainty on the true timing of extrema during the experiment. This in turn gives uncertainty in the timing order of extrema within the time series. Motivated by applications in genomic time series and biological network analysis, we construct a weighted directed acyclic graph (DAG) called an extremal event DAG using techniques from persistent homology that is robust to measurement noise. Furthermore, we define a distance between extremal event DAGs based on the edit distance between strings. We prove several properties including local stability for the extremal event DAG distance with respect to pairwise L_∞ distances between functions in the time series data. We apply the new method to quantify similarity in replicate experiments of microarray yeast cell cycle data and to provide quantitative evidence that an intrinsic oscillator drives the blood stage cycle of the malaria parasite Plasmodium falciparum.

17 Xinqi Gong

Renmin University of China, China
Multibody protein interaction complex structure prediction

Abstract

Improved from our dimer protein-protein docking methods, in the last several years we have designed new deep learning algorithms to predict the interface residue pair in trimer, tetramer and even bigger multibody protein complex structures. Furtherly, we assembled a holistic procedure for multibody protein interaction complex structure prediction, which can give out results from monomer sequences. Trained and tested on an experimental dataset, our procedure show promise advances and advantages.

18 Yasuaki Hiraoka

Kyoto University, Japan
Girth, magnitude homology, and phase transition of diagonality

Abstract

We study the magnitude homology of graphs focusing mainly on the relationship between its diagonality and the girth. Magnitude and magnitude homology are formulations of the Euler characteristic and the corresponding homology, respectively, for finite metric spaces, first introduced by Leinster and Hepworth-Willerton. Several authors study them restricting to graphs with path metric, and some properties which are similar to the ordinary homology theory have come to light. However, the whole picture of their behavior is still unrevealed, and it is expected that they catch some geometric properties of graphs. In this talk, we show that the girth of graphs partially determines magnitude homology, that is, the larger girth a graph has, the more homologies near the diagonal part vanish. Furthermore, applying this result to a typical random graph, we investigate how the diagonality of graphs varies statistically as the edge density increases. In particular, we show that there exists a phase transition phenomenon for the diagonality. This talk is based on the joint work with Asao and Kanazawa (https://arxiv.org/abs/2101.09044).

19 Nataša Jonoska

University of South Florida, USA
Topological and algebraic models for studying DNA self-assembly

Abstract

There is an increased necessity for mathematical study of self-assembly of various phenomena ranging from nano-scale structures, material design, crystals and nano devices. We present a range of topological questions associated with DNA self-assembly and three dimensional structures. The questions vary from topological graph theory related to DNA strand routing a three-dimensional mesh, to questions in knot theory related to structural embeddings in 3D, to algebraic descriptions related to Jones monoids associated with DNA origami.

20 Jürgen Jost

Max Planck Institute for Mathematics in the Sciences, Germany
Graphs, hypergraphs and network analysis

Abstract

I shall discuss two approaches for the empirical analysis of network data, spectra of Laplace operators and discrete curvature, and develop the underlying mathematical theory.

21 Vitaliy Kurlin

University of Liverpool, UK
Geometric Data Science challenges and solutions

Abstract

We discuss the recent advances [1-4] in Geometric Data Science studying computable and continuous metrics on finite and periodic sets of points considered up to rigid motion or more general isometry in any Euclidean or metric space. The classical distance matrix is a complete isometry invariant of any ordered finite set but becomes computationally infeasible for comparing unordered sets. The bottleneck distance takes infinite value and is also discontinuous even on lattices. The persistent homology is an isometry invariant of finite point sets and turned out to be much weaker than previously anticipated [2]. Some of these challenges were recently resolved by the Data Science Theory and Applications group in the Liverpool Materials Innovation Factory. The space of all 2D lattices up to rigid motion and uniform scaling was described as a 2D sphere without one point [3]. All 660K+ periodic crystals in the CSD were distinguished by 200B+ pairwise comparisons of new isometry invariants over two days on a modest desktop computer, establishing the Crystal Isometry Principle [4]: any real crystal is uniquely determined by its geometry of atomic centers. Hence all periodic crystals live in a common Crystal Isometry Space (CRISP) extending Mendeleev's table of elements.

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22 Claudia Landi

Università degli Studi di Modena e Reggio Emilia, Italy
Computing the matching distance of 2-parameter persistence modules from critical values

Abstract

Persistence modules are defined by applying homology to filtered cell complexes. Multi-parameter persistence modules are a promising tool in the topological data analysis of multivariate data. Unfortunately, they come with heavy computational and theoretical intricacies. In this talk, I'll show that in the case with two parameters, entrance values of critical cells in the bifiltration determine exactly the matching distance of 2-parameter persistence modules, yielding an algorithm for its computation. This is joint work with Asilata Bapat, Robyn Brooks, Celia Hacker, Barbara Mahler, and Elizabeth Stephenson.

23 Ran Levi

University of Aberdeen, UK
Persistence module calculus

Abstract

The concept of a persistence module was introduced in the context of topological data analysis. In its original incarnation a persistence module is defined to be a functor from the poset of nonnegative real numbers with theory natural order to the category of vector spaces and homomorphisms. These are referred to as single parameter persistence modules and are a fundamental and useful concept in topological data analysis when the source data depends on a single parameter. The concept naturally lends itself to generalisation, and one may consider persistence modules as functors from an arbitrary poset (or more generally an arbitrary small category) to some abelian target category. In other words, a persistence module is simply a representation of the source category in the target abelian category. As such much research was dedicated to studying persistence modules in this context. Unsurprisingly, it turns out that when the source category is more general than a linear order, then its representation type is generally wild. In particular, keeping in mind

that persistence module theory is supposed to be applicable, computability of general persistence modules is very limited. In this talk I will describe the background and motivation for persistence module theory and introduce a new set of ideas for local analysis of persistence module by methods borrowed from spectral graph theory and multivariable calculus.

24 Jie Liang

University of Illinois at Chicago, USA

Non-diffusive topological structure of reactions dynamics of complex molecules and stochastic landscapes of molecular networks

Abstract

We describe recent developments in understanding the topological structures of complex biological systems of 1) molecular reactions of activated processes and 2) probability landscape of reaction networks. For molecular reactions of activated processes, we describe an exact approach based on persistent homology to quantify the topology of dynamic probability surface of barrier-crossing. For the simplest complex activated process of alanine-dipeptide isomerization, we find that instead of a saddle-point in the free energy surface, the transition state ensemble (TSE) at the barrier top form the most prominent probability H_0 peak in the high-dimensional configuration-time space after reactants/products. Furthermore, this reactive region is vorticle and has strong rotational fluxes, which cannot be described by Kramers' diffusion-based theory. For stochastic reaction networks, we show the persistent homology of the high-dimensional probability landscapes obtained using the finite-buffer ACME methods can be computed. Furthermore, defining topological properties of the landscapes can be quantified, including the degree of multistability by H_0, the oscillatory cycles by H_1, and higher-order oscillatory membranes by H_2. We also give examples of phase diagrams over the parameter space of multistability of a class of stochastic reaction network. These results show that topological data analysis and persistent homology can provide powerful means towards understanding naturally occurring physical dynamic processes and stochastic interaction networks. (Join work with Farid Manuchehrfar, Wei Tian, Huiyu Li, Ao Ma, Hubert Wagner, and Herbert Edelsbrunner).

25 Haiyan Liu

University of Science & Technology of China, China
Data-driven methods for de novo protein design

Abstract

Computational protein design brings the capability of inventing de novo proteins to fulfill various structural and functional needs from therapeutics to bio-catalysis. The two problems at the bottom of de novo protein design are, first, how to effectively generate function-fulfilling backbones that are designable (meaning there are indeed amino acid sequences that fold into the backbone structures), and second, sequence design or inverse protein folding (meaning to select amino acid sequences that fold into given designable backbones). We have shown that an effective neural network energy function named SCUBA (for SideChain Unknown Backbone Arrangement) for backbone design and our previous data-driven sequence selection method ABACUS2 together can design proteins of novel structures from scratch. More recently, we developed ABACUS-R, a deep learning-based model for sequence design that outperforms the statistical energy function method ABACUS in success rate and precision in wet experiments. Propelled by the unprecedented accumulation of sequence and structural data and increasingly powerful artificial intelligence tools, data-driven methods are progressing rapidly and extending the range of biomolecular structures and functions amenable to de novo design.

26 Benzhuo Lu

LSEC, Institute of Computational Mathematics, CAS, China
Molecular sparse representation by a 3D ellipsoid radial basis function neural network via L1 regularization

Abstract

The three-dimensional structures and shapes of biomolecules provide essential information about their interactions and functions. Unfortunately, the computational cost of biomolecular shape representation is an active challenge which increases rapidly as the number of atoms increase. Recent developments in sparse representation and deep learning have shown significant

improvements in terms of time and space. A sparse representation of molecular shape is also useful in various other applications, such as molecular structure alignment, docking, and coarse-grained molecular modeling. We have developed an ellipsoid radial basis function neural network (ERBFNN) and an algorithm for sparsely representing molecular shape. To evaluate a sparse representation model of molecular shape, the Gaussian density map of the molecule is approximated using ERBFNN with a relatively small number of neurons. The deep learning models were trained by optimizing a nonlinear loss function with L1 regularization. Experimental results reveal that our algorithm can represent the original molecular shape with a relatively higher accuracy and fewer scale of ERBFNN. Our network in principle is applicable to the multiresolution sparse representation of molecular shape and coarse-grained molecular modeling.

27 Kelly Maggs

EPFL, Switzerland

Morse theoretic signal compression and reconstruction on chain complexes

Abstract

In this work, we provide an approach to signal compression and reconstruction on chain complexes that leverages the tools of algebraic discrete Morse theory. The main goal is to reduce and reconstruct a based chain complex together with a set of signals on its cells via deformation retracts, with the aim of preserving parts of the global topological structure of both the complex and the signals. We first prove that any deformation retract of real degree-wise finite-dimensional based chain complexes is equivalent to a Morse matching. We then study how the signal changes under particular types of Morse matching, showing its reconstruction error is trivial on specific components of the Hodge decomposition. Furthermore, we provide an algorithm to compute Morse matchings which locally minimizes reconstruction error.

28 Konstantin Mischaikow

Rutgers, The State University of New Jersey, USA
Identifying nonlinear dynamics with high confidence from sparse data

Abstract

There are a variety of statistical techniques that given sufficient time series identify explicit models, e.g. differential equations or maps, that are then evaluated to predict dynamics. However, chaotic dynamics and bifurcation theory implies sensitivity with respect to small errors in data and parameters, respectively. This suggests a potential inherent instability in going directly from data to models. We propose a novel method, combining Conley theory and Gaussian Process surrogate modeling with uncertainty quantification, through which it is possible to characterize local and global dynamics, e.g., existence of fixed points, periodic orbits, connecting orbits, bistability, and chaotic dynamics, with lower bounds on the confidence that this characterization of the dynamics is correct.

29 Julie Mitchell

Oak Ridge National Laboratory, USA
Machine learning models for biophysics

Abstract

Protein interactions govern most physiological processes. Predicting the structure of protein interactions is an important open question, as is understanding the impacts of mutations on the strength of association. I will discuss the use of machine learning to develop predictive models for these questions. In addition, recent work on generative adversarial networks for protein structure design will be presented.

30 Marian Mrozek

Jagiellonian University, Poland
Some recent advances in combinatorial topological dynamics

Abstract

Forman's work on discrete Morse theory set foundations for the field of combinatorial topological dynamics. The theory has found applications in the study of the topological shape of data. To make this approach successful in describing the dynamics encoded in data, Forman's work has recently been extended towards the Conley theory. I will present some new results in this direction.

31 Bradley J. Nelson

The University of Chicago, USA
Induced maps and dimension reduction

Abstract

The homology functor in algebraic topology is a key construction motivating persistent homology and its variants. This talk will focus on how induced maps on the homology of spaces can be used to understand dimension reduction. We will discuss how interleavings can be used to characterize the topological fidelity of an embedding. We will also present an extension of the acyclic carrier theorem that allows for the general construction of maps in the context of filtrations to gain a more detailed understanding of maps between filtrations.

32 Duc Nguyen

University of Kentucky, USA
Persistent spectral graph and differential geometry-assisted AI for drug design

Abstract

Nowadays, machine learning, especially deep learning, is the main workhorse in many applications from speech recognition to molecular design. However, identifying the most promising drug candidates for combating the deadly and newly emerging diseases such as COVID-19 still poses a big challenge for any AI-based models due to the high dimensionality of the biological datasets and the lack of properly encoded chemical and physical information. To address these issues, my lab has developed several powerful mathematical representations for the diverse biological datasets in the low-dimensional spaces, namely

persistent graph theory, persistent homology, and differential geometry. By carefully designing cutting-edge convolutional neural networks, graph neural networks, and recurrent neural networks integrating with attention and transformer gate mechanisms to tailor these mathematical features, we arrived at novel models not only perform well on virtual screening targeting important drug properties but also have the ability to design new drugs at an unprecedented speed. In recent years, our team has emerged as a top winner in D3R Grand Challenges, a worldwide annual competition series in computer-aided drug design.

33 Andreas Ott

Karlsruhe Institute for Technology, Germany

Vietoris-Rips transformations in multipersistent homology and an application to viral evolution

Abstract

Multi-parameter persistent homology naturally arises in applications of persistent topology to data that come with extra information depending on additional parameters, like for example time series data. In this talk, I will introduce the concept of a Vietoris-Rips transformation, a method that reduces the computation of the one-parameter persistent homology of pathwise subcomplexes in multi-filtered flag complexes to the computation of the Vietoris-Rips persistent homology of certain semimetric spaces. As an application, I will present the CoVtRec pipeline and explain how Vietoris-Rips transformations greatly improve the topology-based surveillance of the convergent evolution of the coronavirus SARS-CoV-2. This is joint work with Maximilian Neumann, Michael Bleher, Lukas Hahn, Samuel Braun, Holger Obermaier, Mehmet Soysal and René Caspart.

34 Keith Promislow

Michigan State University, USA

Singular-Enthalpic limit for charged diblock polymer blends

Abstract

Polymers are fundamental to modern materials, playing crucial roles in biology and in advanced materials for industrial and energy conversion applications. Functional polymers contain charged or polarizable groups that induce strong interactions with solvent and with other polymers. System behaviors become increasingly complex when combining several types of polymers or multiple solvents. We present a derivation of a phase field model from a self-consistent mean field approach in the singular-enthalpic limit. This broad scaling combines entropy, enthalpy, and pressure: pressure is large and enforced through incompressibility, enthalpy is smooth, entropy is singular in key regions. The singular enthalpy limit renders these fundamental systems amenable to analysis, resolving the connection problem for optimal packings of diblock polymers by patching linear enthalpic flows to the stable and unstable manifolds of fixed points from a vicinity of the singular entropy domain to find points of intersection. This has applications to the self-assembly of charged polymers and the stacking behavior of the associated bilayer vesicles that have broad application to photosynthesis, through Thylakoid membranes, and the behavior of organelles such as the Golgi apparatus. We address terms that are likely to be excluded by this approach, and outline a framework in which machine learning could assist in model improvement.

35 Hans Riess

University of Pennsylvania, USA
Lattice-valued network sheaves

Abstract

In this talk, we develop a discrete Hodge theory for network sheaves and cosheaves in the data category of complete lattices and Galois connections. The key development is the Tarski Laplacian, an endomorphism on the cochain complex whose fixed points agree with global sections in degree zero. After laying the foundation for the basic theory, we, then, introduce some motivating examples of lattice-valued network (co)sheaves and the heat flow dynamics the Tarski Laplacian induces.

36 Vanessa Robins

Australian National University, Australia
Stability of persistence diagrams derived from digital images

Abstract

The physical properties of porous and granular materials critically depend on the topological and geometric details of the material micro-structure. For example, the way water flows through sandstone depends on the connectivity and diameters of its pores. Persistent homology of a signed Euclidean distance function provides a comprehensive description of both pore and grain structure and highlights properties such as the percolating length scales in porous materials, the degree of consolidation in sandpacks/ sandstones, and the distribution of fluid trapping in two-phase fluid experiments imaged using x-ray micro-CT. My Women in Computational Topology group recently established rigorous results describing how persistence diagrams of signed Euclidean distance functions change with lowered image resolution. This talk will summarise those results and discuss their consequences for applied image analysis.

37 Primoz Skraba

Queen Mary University of London, UK
Understanding random persistence diagrams

Abstract

This talk will cover recent advances in understanding persistence diagrams arising from distance function to a "random sample." This setting is commonly arises in topological data analysis and over the last few years there has been steady progress in the area of stochastic topology. I will cover theoretical results such as new limit theorems as well as experimental evidence for the phenomena of universality – a common arising from diagrams of this type. Several conjectures will be presented as well as other possible directions and open questions.

38 Iskander Taimanov

Novosibirsk State University, Russia
Topological and geometrical characterization of three-dimensional porous media

Abstract

We discuss approcahes to numerical topological and geometrical characterization of porous media based on persistent homology and Minkowski functionals.

39 Julien Tierny

CNRS - Sorbonne Université, France
Wasserstein distances, geodesics and barycenters of merge trees

Abstract

In this talk, I will present a unified computational framework for the estimation of distances, geodesics and barycenters of merge trees. We extend recent work on the edit distance and introduce a new metric, called the Wasserstein distance between merge trees, which is purposely designed to enable efficient computations of geodesics and barycenters. Specifically, our new distance is strictly equivalent to the L2-Wasserstein distance between extremum persistence diagrams, but it is restricted to a smaller solution space, namely, the space of rooted partial isomorphisms between branch decomposition trees. This enables a simple extension of existing optimization frameworks for geodesics and barycenters from persistence diagrams to merge trees. We introduce a task-based algorithm which can be generically applied to distance, geodesic, barycenter or cluster computation. The task-based nature of our approach enables further accelerations with shared-memory parallelism. Extensive experiments on public ensembles and SciVis contest benchmarks demonstrate the efficiency of our approach – with barycenter computations in the orders of minutes for the largest examples – as well as its qualitative ability to generate representative barycenter merge trees, visually summarizing the features of interest found in the ensemble. We show the utility of our contributions with dedicated visualization applications: feature tracking, temporal reduction and ensemble clustering. We also provide a lightweight C++ implementation that can be used to reproduce our results.

40 Reidun Twarock

University of York, USA

Virus structure and function through the lens of viral tiling theory: novel opportunities for antiviral therapy and virus nanotechnology

Abstract

Viral capsids are molecular Trojan horses built from protein, that enable viral genomes to invade host cells and replicate. These protein containers are repurposed as virus-like particles for a wide range of applications, including vaccine design, cargo storage and diagnostics, that require control over their assembly and disassembly. In this talk, I will demonstrate how insights into the mathematical principles governing virus architecture not only answer fundamental biological questions regarding the evolution of viral capsid architectures, but also provide a key to unlocking their nanotechnological potential. By combining tiling theory with stochastic simulations, I will explain the particle polymorphism seen in virus-like particle assembly, and introduce a percolation theory of virus capsid disassembly. I will also use Viral Tiling Theory as a mathematical microscope to elucidate the mechanisms by which larger and more complex capsid architectures efficiently assemble from their molecular components.

41 Chandra Verma

*A*STAR, Singapore*

Some shape based explorations and manipulations of biomolecules

Abstract

Conservation in biology offers a great opportunity for the exploration of similarities in shapes and hence functions of biomolecules, at different levels of resolution. In addition they also offer the potential to develop novel probes that can be exploited towards the development of highly specific therapeutics.

42 Andrei Yu. Vesnin

Novosibirsk State University, Russia

Topological indices of fullerenes

Abstract

In molecular topology and mathematical chemistry, the notion of topological indices is used for molecular descriptors based on molecular graphs of chemical compounds. One of the most known topological indices is the Wiener index introduced by H. Wiener in 1947. Topological indices are widely used in the study of Quantitative Structure-Activity Relationships in which properties of molecules are correlated with their chemical structure. We will discuss Wiener index of fullerene graphs. Its properties, generalizations, and relations with hyperbolic volume of fullerenes obtained in [1-4] will be presented.

43 Bei Wang

University of Utah, USA

Hypergraph Visualization: Topological Simplification and Comparisons

Abstract

Hypergraphs capture multi-way relationships in data, and they have consequently seen a number of applications in higher-order network analysis, computer vision, geometry processing, and machine learning. First, we study hypergraph visualization via its topological simplification. We put vertex simplification and hyperedge simplification in a unifying framework using tools from topological data analysis. In simplifying a hypergraph, we allow vertices to be combined if they belong to almost the same set of hyperedges, and hyperedges to be merged if they share almost the same set of vertices. Second, we develop the theoretical foundations for studying the space of hypergraphs using ingredients from optimal transport. By enriching a hypergraph with probability measures on its nodes and hyperedges, as well as relational information capturing local and global structure, we obtain a general and robust framework for studying the collection of all hypergraphs. This talk is based on joint works with Youjia Zhou, Archit Rathore, Emilie Purvine, Samir Chowdhury, Tom Needham, and Ethan Semrad.

44 Rui Wang

Michigan State University, USA

Persistent Laplacian and its applications in SARS-CoV-2

Abstract

Persistent homology (PH) is one of the most popular tools in topological data analysis (TDA). However, it is not sensitive to homotopic shape evolution, which is essential for protein-protein interactions (PPIs). Therefore, persistent spectral graph (PSG) theory is introduced to create a unified low-dimensional multiscale paradigm for revealing topological persistence and extracting geometric shapes from high-dimensional datasets. In PSG theory, families of persistent Laplacian matrices (PLMs) corresponding to various topological dimensions are constructed via filtration to sample a given dataset at multiple scales. The harmonic spectra from the null spaces of PLMs offer the same topological invariants, namely persistent Betti numbers, at various dimensions as those provided by PH, while the non-harmonic spectra of PLMs give rise to additional geometric analysis of the shape of the data. This work developed Persistent Laplacian-based deep learning models to systematically evaluate the SARS-CoV-2 variants' infectivity. Our comparative analysis of Alpha, Beta, Gamma, Delta, Lambda, Mu, and Omicron BA.1, BA.1.1, BA.2, BA.2.11, BA.2.12.1, BA.3, BA.4, and BA.5 unveils that Omicron BA.2.11, BA.2.12.1, BA.4, and BA.5 are more contagious than BA.2 and have high potential to become new dominating variants in the world.

45 Junjie Wee

Nanyang Technological University, Singapore
Mathematical AI for molecular sciences

Abstract

With great accumulations in experimental data, computing power and learning models, artificial intelligence (AI) is making great advancements in molecular sciences. Recently, the breakthrough of AlphaFold 2 in protein folding herald a new era for AI-based molecular data analysis for materials, chemistry, and biology. A major challenge remains in AI-based molecular sciences which is to design and achieve effective molecular descriptors or fingerprints. In this talk, we propose several advanced mathematical based representations and featurizations. Molecular structures and their interactions can be represented by graphs, simplicial complexes (Rips complex, Neighborhood complex, Dowker complex, and Hom-complex) and hypergraphs. Molecular representations can be systematically featurized using various persistent

invariants, including persistent homology, persistent Ricci curvature, persistent spectral, and persistent Tor-algebra. These features are combined with machine learning and deep learning models to form quantitative prediction models. Our models have demonstrated great advantage over traditional models in drug design, material informatics and chemical informatics.

46 Zenghui Zhang, John

NYU Shanghai, China
Computational study of protein-ligand and protein-protein interactions

Abstract

Protein-ligand and protein-protein interactions are fundamental processes in biology and their accurate prediction remains a grand challenge in computational biology. In this talk, we present some recent work in protein-ligand and protein-protein interactions. The reported work involved development of machine learning methods to accurately predict complex structures in protein-ligand systems as well as methods to predict binding energies and mutational effects in protein-protein interaction.

47 Yingkai Zhang

New York University, USA
Integrating machine learning and molecular modeling for drug design

Abstract

The overall goal of our lab is to develop and apply state-of-the-art computational tools for rational drug design. In this talk, I will present our recent advances in targeting protein-protein interactions, developing machine-learning based protein-ligand scoring functions, and advancing deep learning models in chemistry.

48 Huan-Xiang Zhou

University of Illinois Chicago, USA
Thermodynamic and dynamic properties of phase-separated biomolecular condensates

Abstract

Biomolecular condensates, formed through phase separation, mediate crucial cellular functions and are linked with neurodegeneration and cancer. Yet we are only starting to gain a glimpse of physical understanding of their properties and complex behaviors [1]. In this talk I will present our recent theoretical and experimental studies into the physical determinants for the thermodynamic and dynamic properties of biomolecular condensates. We found that the equilibrium of condensate formation can be regulated by adding macromolecular components, and macromolecular regulators fall into three architypes, depending on whether their interactions with condensate drivers are dominated by steric repulsion, or are weakly or strongly attractive [2, 3]. Matching effects of macromolecular regulators on phase equilibrium and on interfacial tension are predicted from computational studies [4] and confirmed experimentally [5]. The disparity in interaction strength and in structural compactness among macromolecular components leads to multiphase organization [6,7], and to widely varying fusion speeds among different condensates [8]. Probe by optical tweezers has revealed that condensates are viscoelastic rather than purely viscous [9]. Shear relaxation spans timescales from milliseconds to seconds, and is a governing measure for dynamic processes ranging from fusion to condensate aging. These insights serve to bridge the gap in understanding between the biology and physics of biomolecular condensates.