Workshop Schedule

August 28, 13:50-18:25 (CET)	13:50-14:00 **Opening remarks** **Chair: Jurgen Jost** 14:00-14:50 **Herbert Edelsbrunner** *"The intrinsic volumes of a space filling diagram and their derivatives"* 14:50-15:40 **Ginestra Bianconi** *"The topological Dirac operator and the dynamics of topological signals"* 15:40-16:30 **Vidit Nanda** *"Principal components along quiver representations"* **15 Minutes Time Break** 16:45-17:35 **Konstantin Mischaikow** *"Solving systems of ordinary differential equations via combinatorial homological algebra"* 17:35-18:25 **Guowei Wei** *"How Math and AI are revolutionizing biosciences"*
August 29, 9:00-12:35 (CET)	**Chair: Herbert Edelsbrunner** 09:00-09:50 **Stefania Ebli** *"Simplicial Neural Networks"* 09:50-10:40 **Claudia Landi** *"Discrete Morse Theory meets Multi-Parameter Persistence"* **15 Minutes Time Break** 10:55-11:45 **Francesco Vaccarino** *"Parallel decomposition of persistence modules through interval bases"* 11:45-12:35 **Mattia G. Bergomi** *"Comparing Neural Networks via Generalized Persistence"*
August 29, 14:00-18:25 (CET)	**Chair: Konstantin Mischaikow** 14:00-14:50 **Jurgen Jost** *"Geometry and topology of data"* 14:50-15:40 **Kelin Xia** *"Persistent function based machine learning for drug design"* 15:40-16:30 **Robert Ghrist** *"Laplacians and Network Sheaves"* **15 Minutes Time Break** 16:45-17:35 **Sayan Mukherjee** *"Modeling shapes and fields: a sheaf theoretic perspective"* 17:35-18:25 **Vasileios Maroulas** *"Random Persistence Diagram Generator"*
August 30, 9:00-12:35 (CET)	**Chair: Marian Mrozek** 09:00-09:50 **Hiraoka Yasuaki** *"On characterizing rare events in persistent homology"* 09:50-10:40 **Andreas Ott** *"A persistent topology approach for the surveillance of coronavirus mutations"* **15 Minutes Time Break** 10:55-11:45 **Wojciech Chacholski** *"Enabling a machine to sense geometry"* 11:45-12:35 **Patrizio Frosini** *"On the role of group equivariant non-expansive operators in Topological Data Analysis"*
August 30, 14:00-18:25 (CET)	**Chair: Vidit Nanda** 14:00-14:50 **Marian Mrozek** *"Combinatorial vs. Classical Dynamics: Recurrence"* 14:50-15:40 **Massimo Ferri** *"Selection of points in persistence diagrams"* 15:40-16:30 **Ran Levi** *"An application of neighbourhoods in directed graphs in the classification of binary dynamics"* **15 Minutes Time Break** 16:45-17:35 **Facundo Mémoli** *"Other Persistence Invariants: homotopy and the cohomology ring"* 17:35-18:25 **Henry Adams** *"Vietoris-Rips complexes of hypercube graphs"*

Titles and abstracts

August 28, 14:00-18:25 (CET)

The intrinsic volumes of a space filling diagram and their derivatives

Herbert Edelsbrunner

Abstract. The morphological approach to modeling the free energy in molecular dynamics by Roth and Mecke suggests to write it as a linear combination of weighted versions of the four intrinsic volumes of a space filling diagram: the volume, the area, the total mean curvature, and the total Gaussian curvature. Based on the Alpha shape representation of a union of solid spheres, we derive formulas for the weighted intrinsic volumes as well as for their derivatives.

Acknowledgements. The formulas for the weighted volume and the area derivatives go back to joint work with Robert Bryant, Patrice Koehl, and Michael Levitt more that a decade ago, while the formulas for the weighted mean and Gaussian curvature derivatives have been obtained recently in collaboration with Arseniy Akopyan.

The topological Dirac operator and the dynamics of topological signals

Ginestra Bianconi

Abstract: Topological signals associated not only to nodes but also to links and to the higher dimensional simplices of simplicial complexes are attracting increasing interest in signal processing, machine learning and network science. Typically, topological signals of a given dimension are investigated and filtered using the corresponding higher-order Laplacian. In this talk, I will cover notable spectral properties of higher-order Laplacians and I will reveal how these properties affect higher-order diffusion and higher-order synchronization dynamics. Moreover, I will introduce the topological Dirac operator that can be used to process simultaneously topological signals of different dimensions. I will discuss the main spectral properties of the Dirac operator defined on networks, simplicial complexes and multiplex networks, and their relation to higher-order Laplacians. Finally, I will show how the Dirac operator allows to define topological synchronization of locally coupled topological signals defined on nodes and links of a network.

Principal components along quiver representations

Vidit Nanda

Abstract: Many interesting objects across pure and applied mathematics (including single and multiparameter persistence modules, cellular sheaves and connection matrices) are most naturally viewed as vector-space valued representations of a quiver. In this talk, I will describe a practical framework for dimensionality reduction, comparison and optimization over a wide class of such objects. This is joint work with Anna Seigal and Heather Harrington.

Solving systems of ordinary differential equations via combinatorial homological algebra

Konstantin Mischaikow

Abstract: Using the simplest possible nontrivial model system (2-dimensional with continuous piecewise linear nonlinearities, but a high dimensional parameter space) and as many pictures as possible I will outline how one can efficiently compute a homological representation of dynamics and then demonstrate that these computations are valid for the differential equation of interest. Furthermore, I will argue that a predetermined finite set of these computations captures dynamics over “all” (this will be explicitly defined) of parameter space. This is joint work with W. Duncan, D. Gameiro, M. Gameiro, T. Gedeon, H. Kokubu, H. Oka, B. Rivas, and E. Vieira.

How Math and AI are revolutionizing biosciences
Guo-Wei Wei

Abstract: Mathematics underpins fundamental theories in physics such as quantum mechanics, general relativity, and quantum field theory. Nonetheless, its success in modern biology, namely cellular biology, molecular biology, biochemistry, and genetics, has been quite limited. Artificial intelligence (AI) has fundamentally changed the landscape of science, technology, industry, and social media in the past few years and holds a great future for discovering the rules of life. However, AI-based biological discovery encounters challenges arising from the structural complexity of macromolecules, the high dimensionality of biological variability, the multiscale entanglement of molecules, cells, tissues, organs, and organisms, the nonlinearity of genotype, phenotype, and environment coupling, and the excessiveness of genomic, transcriptomic, proteomic, and metabolomic data. We tackle these challenges mathematically. Our work focuses on reducing the complexity, dimensionality, entanglement, and nonlinearity of biological data in AI. We have introduced evolutionary de Rham-Hodge, persistent cohomology, and persistent spectral graph theories to achieve high-level abstractions of biological systems and thus significantly enhance AI's ability to handle excessively large biological datasets. Using our mathematical AI approaches, my team has been the top winner in D3R Grand Challenges, a worldwide annual competition series in computer-aided drug design and discovery for years. Using one million genome isolates from patients, we prove for the first time that the emergency of SARS-CoV-2 variants is determined by natural selection. We also accurately predicted vaccine-escape, fast-growing, and antibody-disruptive viral mutations.

August 29, 9:00-12:35 (CET)

Simplicial Neural Networks
Stefania Ebli

Abstract: In this talk I will present simplicial neural networks (SNNs), a generalization of graph neural networks to data that live on a class of topological spaces called simplicial complexes. These are natural multi-dimensional extensions of graphs that encode not only pairwise relationships but also higher-order interactions between vertices - allowing us to consider richer data, including vector fields and n-fold collaboration networks. We define an appropriate notion of convolution that we leverage to construct the desired convolutional neural networks. We test the SNNs on the task of imputing missing data on coauthorship complexes. Finally, I will highlight some future directions of learning on simplicial complexes.

Discrete Morse Theory meets Multi-Parameter Persistence
Claudia LANDI

Abstract: Discrete Morse theory permits reducing a cell complex to the critical cells of a gradient vector field. Critical cells carry all the relevant homological information about the input data. Multiparameter persistence is a promising tool in topological data analysis of multivariate data that still needs to maintain its promises due to its heavy computational burden and its theoretical intricacies. In the last years, in a joint effort with a number of collaborators I've been investigating the connections between these two theories. Firstly, with Bapat, Brooks, Hacker, and Mahler, we prove that the entrance values of critical cells are sufficient to determine the fibered rank invariant. Secondly, with Scaramuccia, Iuricich, and De Floriani, we show that reduction to the Morse complex allows to speed up algorithms for multiparameter persistence computation; Thirdly, with Scaramuccia and Guidolin, we derive Morse inequalities for the Betti numbers of multi-parameter persistence modules. In this talk, I will report on such a thread of findings.

Parallel decomposition of persistence modules through interval bases
Francesco Vaccarino

Abstract: We introduce an algorithm to decompose any finite-type persistence module with coefficients in a field into what we call an "interval basis". This construction yields both the standard persistence pairs of Topological Data Analysis (TDA), as well as a special set of generators inducing the interval decomposition of the Structure theorem. The computation of this basis can be distributed over the steps in the persistence module. This construction works for general persistence modules on a field, not necessarily deriving from persistent homology. We subsequently provide a parallel algorithm to build a persistent homology module over by leveraging the Hodge decomposition, thus providing new motivation to explore the interplay between TDA and the Hodge Laplacian.

Comparing Neural Networks via Generalized Persistence

Mattia G. Bergomi (speaker), Pietro Vertechi

Abstract: Artificial neural networks are often used as black boxes to solve supervised tasks. At each layer, the network updates its representation of the dataset to minimize a given error function, depending on the correct assignment of predetermined labels to each observed data point. On the other end of the spectrum, topological persistence is commonly used to compare hand-crafted low-dimensional data representations. Here, we provide an application of rank-based persistence, a generalized persistence framework that allows us to characterize the data representation generated at each layer of an artificial neural network and compare different neural architectures.

August 29, 14:00-18:25 (CET)

Geometry and Topology of Data

Jürgen Jost

Abstract: Data sets are often equipped with distances between data points, and thereby constitute a discrete metric space. We develop general notions of curvature that capture local and global properties of such spaces and relate them to topological concepts such as hyperconvexity. This also leads to a new interpretation of TDA.

Persistent function based machine learning for drug design

Kelin Xia

Abstract: Effective molecular representation is key to the success of machine learning models for drug design. In this talk, we will discuss a series of new persistent functions, including persistent spectral, persistent Ricci curvature, and hypergraph-based persistent homology. Based on these persistent representations, molecular descriptors or fingerprints can be generated and further combined with machine learning models, such as random forest, gradient boosting tree, and convolutional neural network. Dramatically different from traditional graph/network or geometric models, these molecular features can characterize the intrinsic multiscale topological information within molecules, thus have a better transferability for machine learning models. Our persistent function-based learning models are tested on three most commonly-used databases including PDBbind-2007, PDBbind-2013, and PDBbind-2016. It is found that our models outperform all the machine learning models with traditional molecular descriptors.

Laplacians and Network Sheaves

Robert Ghrist

This talk will begin with a simple introduction to cellular sheaves as a generalized notion of a network of algebraic objects. With a little bit of geometry, one can often define a Laplacian for such sheaves. The resulting Hodge theory relates the geometry of the Laplacian to the algebraic topology of the sheaf. By using this sheaf Laplacian as a diffusion operator, one can do dynamics on sheaves, which leads to decentralized methods for computing sheaf cohomology. The talk represents joint works with Jakob Hansen and Hans Riess.

Modeling shapes and fields: a sheaf theoretic perspective

Sayan Mukherjee

Abstract: We will consider modeling shapes and fields via topological and lifted-topological transforms. Specifically, we show how the Euler Characteristic Transform and the Lifted Euler Characteristic Transform can be used in practice for statistical analysis of shape and field data. The Lifted Euler Characteristic is an alternative to the. Euler calculus developed by Ghrist and Baryshnikov for real valued functions. We also state a moduli space of shapes for which we can provide a complexity metric for the shapes. We also provide a sheaf theoretic construction of shape space that does not require diffeomorphisms or correspondence. A direct result of this sheaf theoretic construction is that in three dimensions for meshes, 0-dimensional homology is enough to characterize the shape.

Random Persistence Diagram Generator
Vasileios Maroulas

Abstract: We will discuss in this talk a method of generating random persistence diagrams (RPDG). RPDG is underpinned (i) by a parametric model based on pairwise interacting point processes for inference of persistence diagrams (PDs) and (ii) by a reversible jump Markov chain Monte Carlo (RJ-MCMC) algorithm for generating samples of PDs. The parametric model combines a Dirichlet partition to capture spatial homogeneity of the location of points in a PD and a step function to capture the pairwise interaction between them. The RJ-MCMC algorithm incorporates trans-dimensional addition and removal of points and same-dimensional relocation of points across samples of PDs.

August 30, 9:00-12:35 (CET)

On characterizing rare events in persistent homology
Hiraoka Yasuaki

Abstract: Indecomposables obtained through decompositions of persistent homology are regarded as topological summary of real data. However, as is well known, there exist pathologically complicated indecomposables in multi-parameter persistent homology in purely algebraic setting, and this fact makes it difficult to build mathematical theory on that setting. Our fundamental question is, how much should we care about such complicated indecomposables in the real data, and what is a suitable framework to study this question? In this talk, after explaining motivations from materials science, we will show several ongoing mathematical results, especially, (1) large deviation principle on 1 parameter persistent homology, and (2) law of large numbers on multi-parameter persistent homology. Then we will discuss how these two results (partially) answer to the original question.

A persistent topology approach for the surveillance of coronavirus mutations
Andreas Ott

Abstract: The COVID-19 pandemic has initiated an unprecedented worldwide effort to characterize its evolution through the mapping of mutations in the genome of the coronavirus SARS-CoV-2. Ideally, one would like to quickly identify new mutations that could confer adaptive advantages, such as higher infectivity or immune evasion, by leveraging the large number of genomes. One way of identifying adaptive mutations is by looking at convergent mutations, mutations in the same genomic position that occur independently. However, the large number of currently available genomes precludes the efficient use of standard phylogeny-based methods. In this talk, I will present a fast and scalable approach for the early warning and surveillance of emerging adaptive mutations based on persistent homology. It identifies convergent mutations merely by their topological footprint and thus overcomes limitations of current phylogenetic inference techniques. This allows for an unbiased and rapid analysis of large viral datasets. Joint work with Ulrich Bauer, Michael Bleher, Mathieu Carriere, Lukas Hahn, Juan Angel Patino-Galindo, and Raul Rabadan.

Enabling a machine to sense geometry
Wojciech Chachólski

Abstract: I will explain how to construct a reach space of kernels on persistent modules called stable ranks, enabling a machine intelligence to sense some geometry. I will illustrate how to use this sense in some synthetic and real applications.

On the role of group equivariant non-expansive operators in Topological Data Analysis
Patrizio Frosini

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 results in the theory of GENEOs, showing how these operators can be used in Topological Data Analysis.

August 30, 14:00-18:25 (CET)

Combinatorial vs. Classical Dynamics: Recurrence
Marian Mrozek

Abstract: The study of combinatorial dynamical systems goes back to the seminal 1998 papers by Robin Forman. The main motivation to study combinatorial dynamics comes from data science. Combinatorial dynamics also provides very concise models of dynamical phenomena. Moreover, some topological invariants in combinatorial dynamics like the Conley index or Morse decomposition may be relatively easily analyzed via persistence. Recently, some formal ties between combinatorial and classical dynamics in gradient-like setting have been established. In the talk, I will present some extensions of these results for recurrent behavior. These results, in particular, may be useful in some computer assisted proofs in dynamics. Based on joint work with R. Srzednicki, J. Thorpe and Th. Wanner.

Selection of points in persistence diagrams
Massimo Ferri

Abstract: The need for point selection in a persistence diagram is shown. We recall V. Kurlin's selection criterion, intended for producing a hierarchy of segmentations out of a point cloud: diagonal gaps. We also show some applications of it on generalised persistence functions. Then we introduce the Ziqqurat, a 3D construction built on a persistence diagram D, and define a filtering function on it. Out of the filtration of the Ziqqurat we obtain a ranking of the points of D. We show its effect in noise reduction.

An application of neighbourhoods in directed graphs in the classification of binary dynamics
Ran Levi

Abstract: A binary state on a graph means an assignment of binary values to its vertices. For example, if one encodes a network of spiking neurons as a directed graph, then the spikes produced by the neurons at an instant of time is a binary state on the encoding graph. Allowing time to vary and recording the spiking patterns of the neurons in the network produces an example of a binary dynamics on the encoding graph, namely a one-parameter family of binary states on it. The central object of study in this talk is the neighbourhood of a vertex v in a graph $\mathcal{G}$, namely the subgraph of $\mathcal{G}$ that is generated by v and all its direct neighbours in $\mathcal{G}$. We present a topological/graph theoretic method for extracting information out of binary dynamics on a graph, based on a selection of a relatively small number of vertices and their neighbourhoods. As a test case we demonstrate an application of the method to binary dynamics that arises from sample activity on the Blue Brain Project reconstruction of cortical tissue of a rat.

Other Persistence Invariants: homotopy and the cohomology ring
Facundo Mémoli, Ling Zhou

Abstract: In this work, we study both the notions of persistent homotopy groups and persistent cohomology rings. In the case of persistent homotopy, we pay particular attention to persistent fundamental groups for which we obtain a precise description via dendrograms, as a generalization of a similar structure existing for persistent PI-0, i.e. for hierarchical clustering. We also study the notion of persistent rational homotopy groups and exhibit pairs of filtrations which are confounded by persistent homology but are distinguished by persistent homotopy groups. In the case of persistent cohomology, we consider a certain persistent graded ring structure induced by the cup product. We then identify a notion of persistence cup-length diagram which can be computed efficiently and, in analogy with the case of persistent homotopy, also complements the information captured by persistent homology.

Vietoris-Rips complexes of hypercube graphs
Henry Adams

Abstract: Questions about Vietoris-Rips complexes of hypercube graphs arise naturally from problems in genetic recombination, and also from Kunneth formulas for persistent homology with the sum metric. We describe the homotopy types of Vietoris-Rips complexes of hypercube graphs at small scale parameters. In more detail, let Q_n be the vertex set of the hypercube graph with 2^n vertices, equipped with the shortest path metric. Equivalently, Q_n is the set of all binary strings of length n, equipped with the Hamming distance. The Vietoris-

Rips complex of Q_n at scale zero is 2^n points, and the Vietoris-Rips complex of Q_n at scale one is the hypercube graph, which is homotopy equivalent to a wedge sum of circles. We show that the Vietoris-Rips complex of Q_n at scale two is homotopy equivalent to a wedge sum of 3-spheres, and furthermore we provide a formula for the number of 3-spheres as a function of n. Many questions about the Vietoris-Rips complexes of hypercube graphs at larger scale parameters remain open. We describe these questions, and pose some conjectures motivated by homology computations in Ripser++. Joint work with Michal Adamaszek.