# The 2nd Young Topologist Seminar

**(July 4-8, 2022, Beijing Time)**

## Schedule: (Zoom: 638 227 8222 Password: BIMSA)

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|---|---|---|---|---|
| **July 4 (Monday)** | *Chair: Jie Wu* | | | |
| | 8:30-8:40 | Opening ceremony | | |
| | *Chair: Masud Rana* | | | |
| | 8:40-9:30 | Michael Moy | | |
| | 9:30-10:20 | Masud Rana | | |
| | | | | |
| **July 5 (Tuesday)** | *Chair: Yuan Wang* | | *Chair: Chuan-Shen Hu* | |
| | 8:40-9:30 | Depeng Gao | 15:00-15:50 | Yasharth Yadav |
| | 9:30-10:20 | Yuan Wang | 15:50-16:40 | Chuan-Shen Hu |
| | | | 16:40-17:30 | Shiquan Ren |
| | | | | |
| **July 6 (Wednesday)** | *Chair: Tomoki Uda* | | *Chair: Xiang Liu* | |
| | 8:40-9:30 | Zehua Lai | 15:00-15:50 | Ben Zhang |
| | 9:30-10:20 | Tomoki Uda | 15:50-16:40 | Xiang Liu |
| | | | 16:40-17:40 | Wojciech Reise |
| | | | | |
| **July 7 (Thursday)** | *Chair: Luis Scoccola* | | *Chair: Isaac Ren* | |
| | 8:40-9:30 | Jian Liu | 15:00-15:50 | Chenguang Xu |
| | 9:30-10:20 | Luis Scoccola | 15:50-16:40 | Isaac Ren |
| | | | 16:40-17:30 | Enhao Liu |
| | | | | |
| **July 8 (Friday)** | *Chair: Shizuo Kaji* | | *Chair: Jasna Urbančič* | |
| | 8:40-9:30 | Mengmeng Zhang | 15:00-15:50 | Milton |
| | 9:30-10:20 | Shizuo Kaji | 15:50-16:40 | Jasna Urbančič |
| | | | 16:40-17:30 | Dong Chen |

## Program：

| **July 4, 2022** | | |
|---|---|---|
| Time | Speaker | Title |
| 8:30-8:40 | Jie Wu | *Opening ceremony* |
| 8:40-9:30 | Michael Moy | *Vietoris Rips metric thickenings: persistent homology and homotopy types* |
| 9:30-10:20 | Masud Rana | *Multiscale Molecular Surface-Based Machine Learning Models for Protein-Ligand Binding Affinity Prediction* |

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| **July 5, 2022** | | |
| Time | Speaker | Title |
| 8:40-9:30 | Depeng Gao | *Porous Synthesis in Free Form Model by Persistent Homology* |
| 9:30-10:20 | Yuan Wang | *Topological Inference of Brain Signals and Networks* |
| Break | | |
| 15:00-15:50 | Yasharth Yadav | *Graph Ricci curvatures reveal atypical functional connectivity in autism spectrum disorder* |
| 15:50-16:40 | Chuan-Shen Hu | *Multi-parameter Persistent Homology Arising from Image Processing* |
| 16:40-17:30 | Shiquan Ren | *Categorifying The Constrained Embedded Homology of Hypergraphs* |
| | | |
| **July 6, 2022** | | |
| Time | Speaker | Title |
| 8:40-9:30 | Zehua Lai | *Embedding models for Grassmannians and flag manifolds* |
| 9:30-10:20 | Tomoki Uda | *Stability of Reeb Posets by Interleaving Distance* |
| Break | | |
| 15:00-15:50 | Ben Zhang | *Explaining Deep Neural Networks Using Functional Networks and Persistent Homology* |
| 15:50-16:40 | Xiang Liu | *Persistent functions based machine learning for drug design* |
| 16:40-17:40 | Wojciech Reise | *A tutorial on persistent homology with GUDHI and giotto-tda* |
| | | |
| **July 7, 2022** | | |
| Time | Speaker | Title |
| 8:40-9:30 | Jian Liu | *On the Cayley-persistence algebra* |
| 9:30-10:20 | Luis Scoccola | *Bottleneck stability for invariants of multi-parameter persistence modules* |
| Break | | |
| 15:00-15:50 | Chenguang Xu | *Interval approximations for fully commutative quivers* |
| 15:50-16:40 | Isaac Ren | *Relative homological algebra and Koszul complexes for multi-parameter persistence modules* |
| 16:40-17:30 | Enhao Liu | *Curse of Dimensionality in Persistence Diagrams* |
| | | |
| **July 8, 2022** | | |
| Time | Speaker | Title |
| 8:40-9:30 | Mengmeng Zhang | *The Delta-twisted Homology and Fiber Bundle Structure of The Twisted Simplicial Sets* |
| 9:30-10:20 | Shizuo Kaji | *Configuration space of Moebius Kaleidocycle* |
| Break | | |
| 15:00-15:50 | Milton,Chi-Chong Wong | *Topological and Geometric Learning Methods for Fine-Grained 3D Shape Segmentation* |
| 15:50-16:40 | Jasna Urbančič | *Optimizing Embeddings using Persistence* |
| 16:40-17:30 | Dong Chen | *Persistent path homology in molecular and materials sciences* |

## Titles and Abstracts

*Speaker:* **Michael Moy** ( Colorado State University, USA )

*Title:* **Vietoris Rips metric thickenings: persistent homology and homotopy types**

*Abstract:* Vietoris-Rips metric thickenings are constructions similar to traditional Vietoris-Rips simplicial complexes. In this talk, I will describe important properties that make them helpful for studying persistent homology and improving the understanding of Vietoris-Rips complexes. This includes recent results showing the persistence homology of Vietoris-Rips metric thickenings agrees with that of the simplicial complexes, which additionally implies the stability of persistent homology for Vietoris-Rips metric thickenings. I will also present recent work that finds the homotopy types of the Vietoris-Rips metric thickenings of the circle at all scale parameters and describe how the techniques used may eventually lead to a Morse-like theory for metric thickenings.

*Speaker:* **Masud Rana** ( University of Kentucky, USA )

*Title:* **Multiscale Molecular Surface-Based Machine Learning Models for Protein-Ligand Binding Affinity Prediction**

*Abstract:* The molecular surfaces have been a great tool to study the biological properties of molecules and biomolecules. However, they need to be integrated into the reign of physical base models to reveal the information of interest that hinders the applications of the molecular surface for diverse and complex biomolecular structures. In this talk, we will present novel molecular surface representations embedded in different scales of the element interactive manifolds featuring the dramatically dimensional reduction and accurately physical and biological properties encoders. Those low-dimensional surface-based descriptors are ready to be paired with any advanced machine and deep learning algorithms to explore the essential structure-activity relationships that give rise to the element interactive surface area-based scoring functions (EISA-score). The newly developed EISA-score has outperformed many state-of-the-art models, including various well-established surface-related representations, in standard PDBbind benchmarks.

*Speaker:* **Depeng Gao** ( Zhejiang University, China )

*Title:* **Porous Synthesis in Free Form Model by Persistent Homology**

*Abstract:* Porous structure, a three-dimensional structure with a complex topology, has been widely applied in aerospace, paramedical, transportation, and other fields. In the porous structure design, porous structures derived from nature usually have better properties than artificial porous structures. In this talk, a reverse design method for synthesizing a porous model from a porous sample will be presented. A large-scale porous structure can be synthesized from a small-scale porous sample. Then the connectivity of the porous structure and its pores are optimized through persistent homology. The aim of this talk is to show the effectiveness of persistent homology when optimizing topologically complex structures, such as porous structures. Furthermore, a new representation of porous structure through an implicit B-spline will be presented, and the experiments show high controllability and extensive application potential of this representation.

*Speaker:* **Ben Zhang** ( Zhejiang University, China )

*Title:* **Explaining Deep Neural Networks Using Functional Networks and Persistent Homology**

*Abstract:* The layered structure of deep neural networks hinders the use of numerous analysis tools and thus the development of its interpretability. Inspired by the success of functional brain networks, we propose a novel framework for interpretability of deep neural networks, that is, the functional network. We construct the functional network of fully connected networks and explore its small-worldness. In our experiments, the mechanisms of regularization methods, namely, batch normalization and dropout, are revealed using graph theoretical analysis and topological data analysis. Our empirical analysis shows the following: (1) Batch normalization enhances model performance by increasing the global efficiency and the number of loops but reduces adversarial robustness by lowering the fault tolerance. (2) Dropout improves generalization and robustness of models by improving the functional specialization and fault tolerance. (3) The models with different regularizations can be clustered correctly according to their functional topological differences, reflecting the great potential of the functional network and topological data analysis in interpretability.

*Speaker:* **Yuan Wang** ( University of South Carolina, USA )

*Title:* **Topological Inference of Brain Signals and Networks**

*Abstract:* Neuroimaging data from diverse clinical groups often requires considerable technicality and computational power to adequately quantify the heterogeneity of the underlying data structure. Motivated by topological data analysis, we now take a new angle on neuroimaging data by characterizing the shape of brain signals and networks with persistent homology and incorporating the shape information in inference procedures to delineate topological group differences in the signals and networks. We ensure scalability to maintain computational efficiency for large-scale datasets. With findings from recent studies, we showcase how clinical questions in brain disorders are addressed using these novel topological methods.

*Speaker:* **Yasharth Yadav** ( The Institute of Mathematical Sciences, India )

*Title:* **Graph Ricci curvatures reveal atypical functional connectivity in autism spectrum disorder**

*Abstract:* Functional connectivity refers to the temporal correlations between activation patterns of distinct regions in the brain, which is measured by the means of functional magnetic resonance imaging (fMRI). Over the past few years, there has been an increasing interest in the geometric and topological characterization of human brain functional connectivity networks. In this talk, I will present the results of our recent data-driven study, where we applied geometry-inspired measures of Forman-Ricci and Ollivier-Ricci curvature to compare functional connectivity networks of individuals with autism spectrum disorder (ASD) and typically developing controls from the Autism Brain Imaging Data Exchange I (ABIDE-I) dataset. We found brain-wide ASDrelated changes in functional connectivity for both Forman-Ricci and Ollivier-Ricci curvatures. Further, we found that Forman-Ricci curvature can also identify potential ASD-related regions in the brain, and explored the functional role of these regions in ASD. Finally, we provided an external validation of our results by collecting experimental evidence from non-invasive brain stimulation studies. We showed that brain regions with curvature differences overlap with those brain regions whose non-invasive stimulation improves ASDrelated symptoms. These results suggest the utility of graph Ricci curvatures in characterizing atypical connectivity of clinically relevant regions in ASD and other neuro developmental disorders.

*Speaker:* **Chuan-Shen Hu** ( Nanyang Technological University, Singapore )

*Title:* **Multi-parameter Persistent Homology Arising from Image Processing**

*Abstract:* Topological Data Analysis (TDA) is one of the fast-growing research topics in applied mathematics, using algebraic topology techniques to capture features from data. In the last decade, a generalization of PH called the multiparameter persistent homology (or multiparameter persistence) had become a well-known research target in TDA. So far, methods in extracting features from multiparameter persistence are limited and examples of multiparameter filtration are still rare. This talk will introduce how we propose a framework to construct multiparameter filtrations from digital images through image processing techniques, such as mathematical morphology and distance transform. Multiparameter persistence derived from these techniques is more efficient for computing and contains intuitive geometric attributes of objects, such as the sizes or robustness of local objects in digital images. We also involve these features to remove the salt and pepper noise in digital images as an application. Finally, I will discuss possible future approaches, such as using sheaf theory to extract features from this generalized algebraic model.

*Speaker:* **Shiquan Ren** ( Henan Normal University, China )

*Title:* **Categorifying The Constrained Embedded Homology of Hypergraphs**

*Abstract:* Hypergraphs are high-dimensional generalizations of graphs. A hypergraph can be obtained by deleting some non-maximal simplices from a simplicial complex. Given a finite set V, the complete hypergraph Δ[V] on V is 2^V, where 2^V is the powerset of V. If a hypergraph is the complement of a simplicial sub-complex of Δ[V], then we call

this hypergraph an independence hypergraph. Let HI be the category whose objects are hypergraphs and whose morphisms are injective morphisms of hypergraphs. Let SI be the category whose objects are simplicial complexes and whose morphisms are injective simplicial maps. Let IHI be the category whose objects are independence hypergraphs and whose morphisms are injective morphisms of hypergraphs. In this talk, we construct some modules (which will be called the constrained embedded (co)homology) on HI. As particular cases, we construct some modules (which will be called the constrained homology) on SI as well as some modules (which will be called the constrained cohomology) on IHI. We prove some Künneth-type formulae and some Mayer-Vietoris sequences. As applications, we construct the persistence constrained embedded (co)homology and discuss the topological data analysis (TDA) of hyper-networks. This is a joint work with Prof. Jingyan Li.

*Speaker:* **Zehua Lai** ( The University of Chicago, USA )

*Title:* **Embedding models for Grassmannians and flag manifolds**

*Abstract:* There are two widely used models for the Grassmannian, as the set of equivalence classes of orthogonal matrices, and as the set of trace-k projection matrices. We present an alternative by representing k-dimensional subspaces as symmetric orthogonal matrices of trace 2k-n. We show that differential geometric objects and operations have closed-form analytic expressions that are computable with standard numerical linear algebra. In the proposed model, these expressions are considerably simpler and exhibit clear signs of numerical stability. Using this embedding, we also derive an embedding for flag manifolds that has similar advantages.

*Speaker:* **Tomoki Uda** ( Tohoku University, Japan )

*Title:* **Stability of Reeb Posets by Interleaving Distance**

*Abstract:* A Reeb graph summarizes topology of a real-valued function. Silva et al. proposed the interleaving distance between two Reeb graphs and proved the stability theorem. As a result of their framework dealing with a graph as a topological space, the estimation of this metric is rough in terms of data resolution. To remedy this issue, we will introduce another interleaving distance between trees as posets. In the talk we will explain this metric comparing two Reeb trees from viewpoint of data analysis and sketch out stability theorem of Reeb posets.

*Speaker:* **Xiang Liu** ( Nankai University and BIMSA, China )

*Title:* **Persistent functions based machine learning for drug design**

*Abstract:* Artificial intelligence (AI) based drug design has demonstrated great potential to fundamentally change the pharmaceutical industries. However, a key issue in all AI-based drug design models is efficient molecular representation and featurization. Recently, topological data analysis (TDA) has been used for molecular representations and its combination with machine learning models have achieved great successes in drug design. In this talk, we will introduce our recently proposed persistent models for molecular representation and featurization. In our persistent models, molecular interactions and structures are characterized by various topological objects, including hypergraph, Dowker complex, Neighborhood complex, Hom-complex. Then mathematical invariants can be calculated to give quantitative featurization of the molecules. By considering a filtration process of the representations, various persistent functions can be constructed from the mathematical invariants of the representations through the filtration process, like the persistent homology and persistent spectral. These persistent functions are used as molecular descriptors for the machine learning models. The state-of-the-art results can be obtained by these persistent functions based machine learning models.

*Speaker:* **Dong Chen** ( Peking University, Shenzhen Graduate school & BIMSA, China )

*Title:* **Persistent path homology in molecular and materials sciences**

*Abstract:* Path homology introduced by Yau and coworkers is mathematically rich and opens new directions in both pure and applied mathematics. As a generalization, persistent path homology (PPH) enables a multiscale analysis of directed graphs (digraphs) and networks. In this work, we introduce PPH to analyze and characterize directed structures in molecular and material sciences. PPH unveils the Jahn-Teller effect and distinguishes different catalysts with the same conformation in materials science. We also propose angle-based persistent path homology to discriminate spatial isomers in molecular science, including Cis-Trans structures and chiral molecules. Additionally, angle-based PPH uncovers unique structural units with mirror symmetry that may be present in high-entropy alloys. Finally, PPH is applied to systems biology to describe the blood coagulation formation, revealing its pivoting stages

*Speaker:* **Wojciech Reise** ( Paris-Saclay University, France)

*Title:* **A tutorial on persistent homology with GUDHI and giotto-tda**

*Abstract:* Persistent homology, a tool from Topological Data Analysis, has witnessed an increasing number of applications. Numerous implementations of complex constructions, reduction algorithms and vectorization methods for persistent homology are now widely available, making topological descriptors accessible and computable in different contexts. In the first part of the talk, we will study a topological inference example, highlighting the features and flexibility of Gudhi: a library with efficient and flexible algorithms to construct simplicial complexes and compute geometric approximations of shapes. In the second part of the talk, we will focus on a time-series classification example, where we will illustrate the functionalities of giotto-tda: a Python library that integrates high-performance C++ implementations with machine learning via a scikit-learn–compatible API.

*Speaker:* **Jian Liu** ( Hebei Normal University and BIMSA, China )

*Title:* **On the Cayley-persistence algebra**

*Abstract:* In this topic, we introduce a persistent (co)homology theory for Cayley digraph grading. We give the algebraic structures of Cayley-persistence object. Specifically, we consider the module structure of persistent (co)homology and prove that the persistent cohomology is an algebra with respect to the persistence-cup product. As an application on manifolds, we show that the persistent (co)homology is closely related to the persistent map of fundamental classes.

*Speaker:* **Luis Scoccola** ( Northeastern University, USA )

*Title:* **Bottleneck stability for invariants of multiparameter persistence modules**

*Abstract:* Unlike one-parameter persistence modules, for which we have the barcode, persistence modules with two or more parameters do not admit a complete discrete invariant, and thus incomplete invariants must be used to study the structure of such modules in practice. The Hilbert function and the multigraded Betti numbers are among the simplest such incomplete invariants, and, although these invariants are already being used in applications, it is a priori unclear whether they satisfy a stability result analogous to the stability of the one-parameter barcode. I will present joint work with Steve Oudot in which we prove bottleneck stability results for multigraded Betti numbers, the Hilbert function, and finer invariants.

*Speaker:* **Chenguang Xu** ( Kyoto University, Japan )

*Title:* **Interval approximations for fully commutative quivers**

*Abstract:* A central topic in recent research regarding topological data analysis has been the study of multi-parameter persistent homology. The existence of infinitely many non-intervals makes discrete complete invariants impossible, as opposed to the one-parameter case. To address that challenge, here we present a framework for estimating the information contained in a fully commutative quiver through the use of interval representations. We apply the method to both finite and infinite types of commutative ladders. For finite type cases, this technique reveals several types of information extraction methods from an interval using zigzag representations, enabling us to compute the indecomposable decomposition of finite type commutative ladders without using a representation explicitly. For infinite type cases, we propose a new invariant called connected persistence diagram using a selected type of interval approximation. This invariant is then used to study the topology of crystal structures.

*Speaker:* **Isaac Ren** ( Kungliga Tekniska högskolan, Sweden )

*Title:* **Relative homological algebra and Koszul complexes for multiparameter**

**persistence modules**

*Abstract:* In single-parameter persistence, persistence modules can be decomposed exactly into so-called bars. In multiparameter persistence, the theory becomes much more complex. One approach is to approximate multiparameter persistence modules by their resolution of free modules, whose Betti diagrams can be computed effectively using Koszul complexes. In this talk, I will generalize this approach to projective resolutions relative to well-chosen families of simpler modules, including generalizations of the one-dimensional bars. I will also show how, under certain conditions, we can also compute the Betti diagrams of these resolutions using Koszul complexes.

*Speaker:* **Enhao Liu** ( Kyoto University, Japan )

*Title:* **Curse of Dimensionality in Persistence Diagrams**

*Abstract:* Topological data analysis brings topological perspective to data analysis and becomes an important tool in exploring the shape of data. In recent decades, high dimension low sample size (HDLSS) data are encountered frequently in many fields. Particularly when HDLSS data comes to statistical analysis, it gives rise to several difficult problems. For example, applying classical PCA onto the HDLSS data performs very poorly due to inconsistencies. These inconsistencies in statistical analysis of HDLSS data is called the curse of dimensionality. On the other hand, persistent homology has been proved to be robust even in the presence of noise. So we are inspired to investigate the applicability of persistence diagrams in the HDLSS setting. In this talk, we will first show the asymptotic behavior of persistence diagrams of high dimensional random data. This can be achieved by using a geometric representation of high dimensional random vectors and taking into account the stability property of persistence diagram. As a result of the asymptotic behavior, we show the unreliability of using observed persistence diagrams in reality due to the presence of high dimensional noise, this suggests that there also exists the curse of dimensionality in persistence diagrams. Finally, we claim that simple application of PCA is not sufficient to completely eliminate the curse of dimensionality in persistence diagrams due to strong domination of high dimensional noise.

*Speaker:* **Mengmeng Zhang** ( Hebei Normal University and BIMSA, China )

*Title:* **The Delta-twisted Homology and Fiber Bundle Structure of The Twisted Simplicial Sets**

*Abstract:* Different from the classical homology theory, the $\delta$-(co)homology（weighted alternative homology）was introduced by Alexander Grigor'yan, Yuri Muranov and Shing-Tung Yau. For understanding the ideas of $delta$-homology, Li, Vershinin and Wu introduced $delta$-twisted homology and homotopy in 2017. On the other hand, the twisted Cartesian product of simplicial sets was introduced by Barratt, Gugenheim and Moore, playing a key role for establishing the simplicial theory of fibre bundles and fibrations. In this talk, i will report our recent progress for unifying $delta$-homology and twisted Cartesian product. We introduce $\Delta$-twisted Carlsson construction, whose

abelianization gives a twisted chain complex generalizeing the $delta$-homology and show its Mayer-Vietoris Sequence. Moreover, we introduce the concept of $\Delta$-twisted Cartesian product as a generalization of the twisted Cartesian product, and explore the fiber bundle structure.

*Speaker:* **Shizuo Kaji** ( Kyushu University, Japan)

*Title:* **Configuration space of Moebius Kaleidocycle**

*Abstract:* The configuration of points in the Euclidean space satisfying certain geometric constraints has long been a research topic in geometry and topology, sometimes concerning the analysis of mechanical linkages. In this talk, we consider the configuration of lines in the Euclidean space, which provides a model for a certain type of mechanical linkage. The linkage is also popular as an origami toy and is called Kaleidocycle. We see how geometry and topology help to analyse Kaleidocycles:

- We construct a flow on the configuration space by a semi-discretisation of the classical sine-Gordon equation, which generates the characteristic "everting motion" of a Kaleidocycle.
- We show the motion preserves a discretised version of the elastic energy.
- We construct a special family of Kaleidocycles, which we have named the Mobius Kaleidocycle, by a variational calculus.

We will also discuss a wide range of conjectures and open problems:

- There are discrete Mobius strips with a three pi twist, but there does not seem to exist a pi twist one.
- The Mobius Kaleidocycle may be a rare example of a single-degree-of-freedom underconstrained linkage; its configuration space is identified as a singular manifold of a function, and it is conjectured to be homeomorphic to a circle.
- Two variational problems, one on the twist rate and the other on the discrete elastic energy, seem to coincide to provide a characterisation of the Mobius Kaleido cycles.

*Speaker:* **Milton, Chi-Chong Wong** ( University of Macau, China )

*Title:* **Topological and Geometric Learning Methods for Fine-Grained 3D Shape Segmentation**

*Abstract:* Fine-grained 3D segmentation is an important task in 3D object understanding, especially in applications such as intelligent manufacturing or parts analysis for 3D objects. However, many challenges involved in such a problem are yet to be solved, such as i) interpreting the complex structures located in different regions for 3D objects; ii) capturing fine-grained structures with sufficient topology correctness. Current deep learning and graph machine learning methods fail to tackle such challenges and thus provide inferior performance in fine-grained 3D analysis. In this talk, I'll present how methods in topological data analysis can be incorporated with geometric deep learning model for the task of fine-grained segmentation for 3D objects. Topological Data Analysis (TDA) is an emerging field which infers relevant topological and geometric features from complex data, where persistence diagram (PD) is used as the most common topological representation. However, the irregular cardinality and permutation of persistence diagram elements bring difficulties in deployment to downstream machine learning tasks. The second part of this talk will focus on the workable solutions for this problem.

*Speaker:* **Jasna Urbančič** ( Queen Mary University of London, UK )

*Title:* **Optimizing Embeddings using Persistence**

*Abstract:* We look to optimize Takens-type embeddings of a time series using persistent (co)homology. Such an embedding carries information about the topology and geometry of the dynamics of the time series. Assuming that the input time series exhibits some prescribed qualitative behaviour: periodic, quasi-periodic, or recurrent behavior, we can use continuous optimization over persistence diagrams to find good embeddings with respect to these properties. In this talk I will describe this approach which provides a practical approach to finding good embeddings. I will also discuss what we know about the space of these embeddings and gradients on the persistent homology as well as open questions. This is joint work with Primož Škraba.