Xiang Liu, Doctor

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Department of Mathematics, Michigan State University, 619 Red Cedar Road, East Lansing, MI 48824

Education

2021/09 – 2024/06 **Ph.D. in Applied Topology**
Chern Institute of Mathematics, Nankai University
supervised by **Prof. Kelin Xia** and **Prof. Huitao Feng**

2017/09 – 2020/12 **M.S in Algebraic Topology**
School of Mathematical Sciences, Nankai University
supervised by **Prof. Xiangjun Wang**

2013/09 – 2017/06 **B.E in Software Engineering**
College of Software, Jilin University

Research Experience

2024/08 – Present **Postdoctoral Scholar** Department of Mathematics, Michigan State University. In Prof. **Guowei Wei**'s group.

2023/11 – 2024/05 **Joint Phd Student** School of Physical and Mathematical Sciences, Nanyang Technological University. In Prof. **Kelin Xia**'s group.

2022/06 – 2023/09 **Visiting Scholar** Yanqi Lake Beijing Institute of mathematical sciences and applications (BIMSA). In Prof. **Jie Wu**'s group.

2020/09 – 2021/09 **Visiting Research Fellow** Center for Topology and Geometry based Technologies, Hebei Normal University. In Prof. **Jie Wu**'s group.

2019/12 – 2020/07 **Visiting Student** School of Physical and Mathematical Sciences, Nanyang Technological University. In Prof. **Kelin Xia**'s group.

Research Interests

Topological Data Analysis

Topological Deep Learning

Mathematical AI

Machine/Deep Learning

Preprints

1. Chuan-Shen Hu, **Xiang Liu**, Kelin Xia. A Physics-informed Sheaf Model. *arXiv preprint arXiv:2501.06197*, (2024)
2. **Xiang Liu**, Ran Liu, Jingyan Li, Rongling Wu, Jie Wu. IntComplex for high-order interactions. *arXiv preprint arXiv:2412.02806*, (2024)

Research Publications

1. Xinyu You, **Xiang Liu**, Chuan-Shen Hu, Kelin Xia, Tze Chien Sum. Quotient Complex Transformer (QCformer) for Perovskite Data Analysis. *Cell Reports Physical Science*, (2026)

2. **Xiang Liu**, Zhe Su, Yongyi Shi, Yiying Tong, Ge Wang, Guo-Wei Wei. Manifold Topological Deep Learning for Biomedical Data. *Nature Communications*, (2026).

3. Zhe Su, **Xiang Liu**, Layal Bou Hamdan, Vasileios Maroulas, Jie Wu, Gunnar Carlsson, Guo-Wei Wei. Topological data analysis and topological deep learning beyond persistent homology-a review. *Artificial Intelligence Review*, (2025)

4. **Xiang Liu**, Junjie Wee, Guo-Wei Wei. Topological Machine Learning for Protein-Nucleic Acid Binding Affinity Changes Upon Mutation. *Machine Learning: Science and Technology*, (2025)

5. **Xiang Liu**, Xuefei Huang, Guo-Wei Wei. Topological Learning Prediction of Virus-like Particle Stoichiometry and Stability. *Biophysical Journal*, (2025)

6. Yaxing Wang, **Xiang Liu**, Yipeng Zhang, Xiangjun Wang, Kelin Xia. Join Persistent Homology (JPH)-Based Machine Learning for Metalloprotein–Ligand Binding Affinity Prediction. *Journal of Chemical Information and Modeling*, (2025)

7. Cong Shen, **Xiang Liu**, Jiawei Luo, Kelin Xia. Torsion Graph Neural Networks. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, (2025)

8. Li Feng, Dengcheng Yang, Sinan Wu, Chengwen Xue, Mengmeng Sang, **Xiang Liu**, Jincan Che, Jie Wu, Claudia Gragnoli, Christopher Griffin, Chen Wang, Shing-Tung Yau, Rongling Wu. Network modeling and topology of aging. *Physics Reports*, 1101, (2025)

9. Li Feng, Huiying Gong, Shen Zhang, **Xiang Liu**, Yu Wang, Jincan Che, Ang Dong, Christopher H. Griffin, Claudia Gragnoli, Jie Wu, Shing-Tung Yau, Rongling Wu. Hypernetwork modeling and topology of high-order interactions for complex systems. *The Proceedings of the National Academy of Sciences (PNAS)*, 121(40), e2412220121 (2024)

10. Huiying Gong, Hongxing Wang, Yu Wang, Shen Zhang, **Xiang Liu**, Jincan Che, Shuang Wu, Jie Wu, Xiaomei Sun, Shougong Zhang, Shing-Tung Yau, Rongling Wu. Topological change of soil microbiota networks for forest resilience under global warming. *Physics of Life Reviews*, (2024)

11. Longlong Li, **Xiang Liu**, Guanghui Wang, Yu Guang Wang, Kelin Xia. Path Complex Neural Network for Molecular Property Prediction. *ICML 2024 Workshop on Geometry-grounded Representation Learning and Generative Modeling*, (2024)

12. **Xiang Liu**, Huitao Feng, Jie Wu, Kelin Xia. Computing hypergraph homology. *Foundations of Data Science*, 6(2), 172-194 (2024)

13. Shuang Wu, **Xiang Liu**, Ang Dong, Claudia Gragnoli, Christopher Griffin, Jie Wu, Shing-Tung Yau, Rongling Wu. The metabolomic physics of complex diseases. *The Proceedings of the National Academy of Sciences (PNAS)*, 120(42), e2308496120 (2023)

14. Jialin Bi, JunJie Wee, **Xiang Liu**, Cunquan Qu, Guanghui Wang, Kelin Xia. Multiscale Topological Indices for the Quantitative Prediction of SARS CoV-2 Binding Affinity Change upon Mutations. *Journal of Chemical Information and Modeling*, 63(13), 4216-4227 (2023)

15. Kelin Xia, **Xiang Liu**, Junjie Wee. Persistent Homology for RNA Data Analysis. *Homology Modeling: Methods in Molecular Biology*, 2627:211-229 (2023)

16. **Xiang Liu**, Huitao Feng, Zhi Lü, Kelin Xia, Persistent Tor-algebra for protein–protein interaction analysis, *Briefings in Bioinformatics*, 24(2) 2023;, bbad046, https://doi.org/10.1093/bib/bbad046. (2023)

17. Ran Liu, **Xiang Liu**, Jie Wu. Persistent Path-Spectral (PPS) Based Machine Learning for Protein–Ligand Binding Affinity Prediction. *Journal of Chemical Information and Modeling* 63(3), 1066-1075. (2023)

18. **Xiang Liu**, Huitao Feng, Jie Wu, Kelin Xia. Hom-Complex-Based Machine Learning (HCML) for the Prediction of Protein–Protein Binding Affinity Changes upon Mutation. *Journal of Chemical Information and Modeling* 62(17), 3961-3969. (2022)

19. Li Xiao-Shuang, **Xiang Liu**, Le Lu, Xian-Sheng Hua, Ying Chi, and Kelin Xia. Multiphysical graph neural network (MP-GNN) for COVID-19 drug design. *Briefings in Bioinformatics*, *23*(4); bbac231, (2022).

20. **Xiang Liu**, Huitao Feng, Jie Wu, Kelin Xia, Dowker complex based machine learning (DCML) models for protein-ligand binding affinity prediction, *Plos Computational Biology*, 18(4), e1009943, (2022)

21. **Xiang Liu**, Kelin Xia, Persistent Tor-algebra based stacking ensemble learning (PTA-SEL) for protein-protein binding affinity prediction, *ICLR 2022 Workshop on Geometrical and Topological Representation Learning*, GTRL 2022 Poster, (2022)

22. Peiran Jiang, Ying Chi, Xiao-Shuang Li, Zhenyu Meng, **Xiang Liu**, Xian-Sheng Hua, Kelin Xia, Molecular persistent spectral image (Mol-PSI) representation for machine learning models in drug design, *Briefings in Bioinformatics*, *23*(1); bbab527, (2022)

23. **Xiang Liu**, Kelin Xia. Neighborhood Complex Based Machine Learning (NCML) Models for Drug Design. *Interpretability of Machine Intelligence in Medical Image Computing, and Topological Data Analysis and Its Applications for Medical Data. Springer, Cham*, 87-97. **(Spot Light)** (2021)

24. **Xiang Liu**, Huitao Feng, Jie Wu, Kelin Xia, Persistent spectral hypergraph based machine learning (PSH-ML) for protein-ligand binding affinity prediction, *Briefings in Bioinformatics*, *22*(5); bbab127, (2021)

25. **Xiang Liu**, Xiangjun Wang, Jie Wu, Kelin Xia, Hypergraph based persistent cohomology (HPC) for molecular representations in drug design, *Briefings In Bioinformatics*, *22*(5); bbaa411, (2021)

Reviewed Journals

Communications Chemistry

Journal of Chemical Information and Modeling

ACS Omega

Computers in Biology and Medicine

Briefings in Bioinformatics

BMC Bioinformatics

Scientific Reports

Molecular Diversity

Computational Biology and Chemistry

The Journal of Supercomputing

Journal of Computational Biophysics and Chemistry