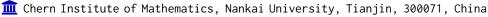
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Education

2021/09 − ····· Ph.D. Chern Institute of Mathematics, Nankai University supervised by Prof. Kelin Xia and Prof. Huitao Feng

2017/09 − 2020/12 M.S School of Mathematical Sciences, Nankai University supervised by Prof. Xiangjun Wang

Research Experience

Joint Phd Student School of Physical and Mathematical Sciences, Nanyang Technological University. In Prof. Kelin Xia's group.

visiting scholar Yanqi Lake Beijing Institute of mathematical sciences and applications (BIMSA). In Prof. Jie Wu's group.

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Visiting student School of Physical and Mathematical Sciences, Nanyang Technological University. In Prof. Kelin Xia's group.

Research Interests

Topological/Geometric data analysis Mathematical AI Machine/Deep learning

Research Publications

- 1. 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)
- 2. 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)
- 3. Kelin Xia, **Xiang Liu**, Junjie Wee. Persistent Homology for RNA Data Analysis. *Homology Modeling: Methods in Molecular Biology*, 2627:211-229 (2023)
- 4. **Xiang Liu**, Huitao Feng, Zhi Lü, Kelin Xia, Persistent Tor-algebra for protein–protein interaction analysis, *Briefings in Bioinformatics*, 24(2) 2023;, bbado46, https://doi.org/10.1093/bib/bbado46. (2023)

- 5. 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)
- 6. **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)
- 7. 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).
- 8. **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)
- 9. **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)
- 10. 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)
- 11. **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)*
- 12. **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)
- 13. **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)

Academic Activities

- Invited speaker, BIMSA workshop on digraph topology and GLMY theory, BIMSA, November 24-26, 2023
- Invited speaker, TDA Seminar at Mathematical Science Research Center, Chongqing University of Technology, November 16, 2023
- Poster, The first International Congress of Basic Science, BIMSA, July 16-28, 2023
- Invited speaker, Advances in Homotopy Theory IV, BIMSA, June 19-23, 2023
- Invited speaker, Topology and application seminar, Shihezi University, May 20-22, 2023
- Invited speaker, Nankai 2023 Topology and its application Seminar, Nankai University, May 13-15, 2023
- Invited speaker, BIMSA Topology Seminar, BIMSA, December 26, 2022
- Invited speaker, Applied topology seminar, Liaoning Normal University, December 9-11, 2022
- Poster, ICMMA 2022 International Conference on "Topology and its Applications to Engineering and Life Science", November 29, 2022
- Invited speaker, Seminar at Southern University of Science and Technology, Department of Mathematics, September 19, 2022
- Invited speaker, The 2nd Young Topologist Seminar, BIMSA, June 4-8, 2022

- Poster, ICLR 2022 Workshop on Geometrical and Topological Representation Learning, April 29, 2022
- Invited speaker, Topological Data Analysis and its Applications for Medical Data (MICCAI 2021), September 27, 2021 (Spot Light)
- Invited speaker, International Conference and Summer School on Applied Topology, Shijiazhuang, August 1-15, 2021
- Invited speaker, Applied topology seminars, Dalin University of Technology, June 6-11, 2021
- Invited speaker, Applied topology winter school and seminars, Liaoning Normal University (Online meeting), December 13-16, 2020
- Invited speaker, The first Joint workshop on Topology and Data Science, Chongqing University of Science and Technology, August 25-29, 2020.
- Participation, Workshop on Computational Topology at Dalian, Dalian University of Technology, July 21-31, 2019

Seminar Organized

 Organizer (with Jie Wu, Jingyan Li), BIMSA Math and Biology Seminar, BIMSA, September 23— December 30, 2022