

SHUANGLI LI

Room 1003, Building 2, USTC ◇ Hefei, Anhui, China, 230026
+86 187-5693-2998 ◇ lsl1997@mail.ustc.edu.cn

EDUCATION

University of Science and Technology of China (USTC) *September 2019 - 2025 (Expected)*
A three-year Ph.D. in Computer Science, School of Computer Science and Technology (Master to Ph.D)
Advisor: Prof. Hui Xiong, AAAS/IEEE Fellow

University of Science and Technology of China (USTC) *September 2015 - June 2019*
B.S. in Computer Science and Technology

INTERN EXPERIENCE

Business Intelligence Lab, Baidu Inc *July 2020 - Present*
Research Intern on geometric graph neural networks and spatial-temporal data mining
Advisor: Dr. Jingbo Zhou

Core R&D platform, iFLYTEK *September 2018 - December 2018*
Algorithm Engineer Intern on educational natural language processing

RESEARCH EXPERIENCE

Spatial Graph Model for Business Relationship Mining *February 2019 - May 2023*
Research on Intelligent Business *Business Intelligence Lab, Baidu Research*

- Applied graph mining methods from a geospatial perspective and studied multiple relationships (e.g., competitive or complementary) in the scenario of business development.
- Designed an inference model tailored for a spatial heterogeneous graph to predict the competitive relationships between locations. The related paper has been published on KDD'20.
- Developed a spatially evolving self-supervised model to discover the multi-temporal relationships between business entities. The related paper has been accepted for the coming KDD'23.

Geometric Deep Learning for Drug Discovery *July 2020 - March 2023*
Research on Intelligent Healthcare *Business Intelligence Lab, Baidu Research*

- Proposed several graph representation learning frameworks to study how spatial relationships and geometric structures can be leveraged to enhance the process of drug discovery.
- Designed 3D geometric-aware graph neural networks to learn the protein-ligand structure for accurate binding affinity prediction to rank drugs. Two papers have been published on KDD'21 and TKDE'23.
- Combined the 2D and 3D molecular structures with a geometry-aware contrastive learning framework to predict the molecular property. The related paper has been published on AAAI'22.

Large Language Models for Information Extraction *December 2023 - Now*
Research on LLM-driven Applications *Business Intelligence Lab, Baidu Research*

- Proposed a multi-agent framework to perform language rule mining for large-scale corpus. Each LLM agent can generate the relation patterns to benefit efficient relation extraction.
- Trained the large language models with supervised fine-tuning and multi-phase reinforcement learning to strengthen the capability of LLMs for pattern mining and adapt to the multi-agent extraction tasks.

PUBLICATIONS

1. **Shuangli Li**, Jingbo Zhou, Tong Xu, Liang Huang, Fan Wang, Haoyi Xiong, Weili Huang, Dejing Dou, and Hui Xiong. GIANT: Protein-Ligand Binding Affinity Prediction via Geometry-aware Interactive Graph Neural Network, IEEE Transactions on Knowledge and Data Engineering (TKDE), Accepted, 2023.

2. **Shuangli Li**, Jingbo Zhou, Ji Liu, Tong Xu, Enhong Chen, and Hui Xiong. Multi-Temporal Relationship Inference in Urban Areas, In Proceedings of the 29th ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD'23), Long Beach, pp. 1316-1327, 2023.
3. **Shuangli Li**, Jingbo Zhou, Tong Xu, Dejing Dou, Hui Xiong. GeomGCL: Geometric Graph Contrastive Learning for Molecular Property Prediction, In Proceedings of the 36th AAAI Conference on Artificial Intelligence (AAAI'22), Online, pp. 4541-4549, 2022.
4. **Shuangli Li**, Jingbo Zhou, Tong Xu, Liang Huang, Fan Wang, Haoyi Xiong, Weili Huang, Dejing Dou, Hui Xiong. Structure-aware Interactive Graph Neural Networks for the Prediction of Protein-Ligand Binding Affinity, In Proceedings of the 27th ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD'21), Online, pp. 975-985. 2021.
Ranked 12nd of Paper Digest Most Influential Papers in KDD 2021
5. **Shuangli Li**, Jingbo Zhou, Tong Xu, Hao Liu, Xinjiang Lu, Hui Xiong. Competitive Analysis for Points of Interest. In Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD'20), Online, pp. 1265-1274. 2020.
6. Rui Zha, Le Zhang, **Shuangli Li**, Jingbo Zhou, Tong Xu, Hui Xiong, Enhong Chen. Scaling up Multivariate Time Series Pre-Training with Decoupled Spatial-Temporal Representations. In Proceedings of IEEE International Conference on Data Engineering (ICDE'24), 2024. Accepted.
7. Shengzhe Zhang, Liyi Chen, Chao Wang, **Shuangli Li**, Hui Xiong. Temporal Graph Contrastive Learning for Sequential Recommendation. In Proceedings of the AAAI Conference on Artificial Intelligence (AAAI'24), 2024. Accepted.
8. Jingbo Zhou, Tao Huang, **Shuangli Li**, Renjun Hu, Yanchi Liu, Yanjie Fu, and Hui Xiong. Competitive Relationship Prediction for Points of Interest: A Neural Graphlet Based Approach. IEEE Transactions on Knowledge and Data Engineering (IEEE TKDE), 2021. Accepted.
9. Hui Luo, Jingbo Zhou, Zhifeng Bao, **Shuangli Li**, J. Shane Culpepper, Haochao Ying, Hao Liu, and Hui Xiong. Spatial object recommendation with hints: When spatial granularity matters. In Proceedings of the 43rd International ACM SIGIR Conference on Research and Development in Information Retrieval (SIGIR'20), pp. 781-790. 2020.
10. Yuhan Ye, Jingbo Zhou, **Shuangli Li**, Congxi Xiao, Haochao Ying, and Hui Xiong. Hierarchical Cross-level Graph Contrastive Learning for Drug-Drug Interaction Prediction. In Proceedings of 29th International Conference on Database Systems for Advanced Applications (DASFAA'24), 2024. Accepted.
11. Yuhan Ye, Jingbo Zhou, **Shuangli Li**, Congxi Xiao, Haochao Ying, and Hui Xiong. Hierarchical Structure-aware Graph Prompting for Drug-Drug Interaction Prediction. In The European Conference on Machine Learning and Principles and Practice of Knowledge Discovery in Databases (PKDD'24), 2024. Accepted.

AWARDS

Baidu Scholarship Top 20 Candidates	2023
SIGKDD Student Travel Award	2023
Outstanding Intern at Business Intelligence Lab, Baidu	2023
PaddlePaddle Developers Experts (PPDE)	2022
Global Digital Technology Scholarship	2022
Yuan-Qing Scholarship	2021
Outstanding Intern at Baidu Research	2021
National Scholarship	2020
The Champion of CCF Big Data Computing Intelligence Contest (BDCI)	2020
Academic Scholarship (USTC), Grad 1	five times from 2019 to 2023
Outstanding Undergraduate Graduate in USTC	2019
Outstanding Student Scholarship (USTC), Silver Medal	2018

Program Committee Member

- The 30th ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD-2024)
- The 38th AAAI Conference on Artificial Intelligence (AAAI-2024)
- SIAM International Conference on Data Mining (SDM-2024)
- The 29th ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD-2023)
- The 35th AAAI Conference on Artificial Intelligence (AAAI-2021)

Journal Reviewer

- IEEE Transactions on Knowledge and Data Engineering (TKDE)
- IEEE Transactions on Neural Networks and Learning Systems (TNNLS)
- IEEE/ACM Transactions on Computational Biology and Bioinformatics (TCBB)
- Neural Networks