JUNJIE XU

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SUMMARY

- **Ph.D.** candidate in Machine Learning with **5+** years of R&D experience in the field.
- **Research Interests**: AI for Science, LLM, Graph Learning, Geometric Deep Learning.
- **18 papers** published (NeurIPS, ICLR, ICML, KDD, etc) or under submission, with **800+ citations** as of 09/2025.
- Extensive industry experiences conducting research and developing ML algorithms for real-world applications.

EDUCATION

The Pennsylvania State University, University Park, USA 08/2021 - Present
Ph.D. candidate in Informatics
Advisor: Dr. Suhang Wang & Dr. Xiang Zhang

Huazhong University of Science and Technology, Wuhan, China 09/2017 - 06/2021
B.E. in Software Engineering
GPA: 3.91/4.00

University of California, Berkeley, Berkeley, USA 01/2020 - 06/2020
Exchange student in Computer Science

PEER-REVIEWED & PREPRINT PAPERS

[1] DualEquiNet: A Dual-Space Hierarchical Equivariant Network for Large Biomolecules
Junjie Xu, Jiahao Zhang, Mangal Prakash, Xiang Zhang, Suhang Wang
NeurIPS 2025

[2] A Comprehensive Survey of Small Language Models in the Era of Large Language Models: Techniques, Enhancements, Applications, Collaboration with LLMs, and Trustworthiness
Fali Wang, Zhiwei Zhang, Xianren Zhang, Zongyu Wu, Tzuhao Mo, Qiuhao Lu, Wanjing Wang, Rui Li, **Junjie Xu**, Xianfeng Tang, Qi He, Yao Ma, Ming Huang, Suhang Wang
TIST, Transactions on Intelligent Systems and Technology

[3] Beyond Sequence: Impact of Geometric Context for RNA Property Prediction
Junjie Xu, Artem Moskalev, Tommaso Mansi, Mangal Prakash, Rui Liao
ICLR 2025, also appears in AIDrugX @ NeurIPS 2024, AI for New Drug Modalities @ NeurIPS 2024

[4] Robustness-Inspired Defense Against Backdoor Attacks on Graph Neural Networks
Zhiwei Zhang, Minhua Lin, **Junjie Xu**, Zongyu Wu, Enyan Dai, Suhang Wang
ICLR 2025 (Oral)

[5] Geometric Hyena Networks for Large-scale Equivariant Learning
Artem Moskalev, Mangal Prakash, **Junjie Xu**, Tianyu Cui, Rui Liao, Tommaso Mansi
ICML 2025 (Spotlight)

[6] HARMONY: A Multi-Representation Framework for RNA Property Prediction
Junjie Xu, Artem Moskalev, Tommaso Mansi, Mangal Prakash, Rui Liao
AI4NA @ ICLR 2025 (Oral)

[7] Stealing Training Graphs from Graph Neural Networks
Minhua Lin, Enyan Dai, **Junjie Xu**, Jinyuan Jia, Xiang Zhang, Suhang Wang
KDD 2025

[8] LanP: Rethinking the Impact of Language Priors in Large Vision-Language Models
Zongyu Wu, Yuwei Niu, Hongcheng Gao, Minhua Lin, Zhiwei Zhang, Zhifang Zhang, Qi Shi, Yilong Wang, Sike Fu, **Junjie Xu**, Junjie Ao, Enyan Dai, Lei Feng, Xiang Zhang, Suhang Wang
ArXiv 2025

[9] Let's Grow an Unbiased Community: Guiding the Fairness of Graphs via New Links
Jiahua Lu, Huaxiao Liu, Shuotong Bai, **Junjie Xu**, Renqiang Luo, Enyan Dai
ArXiv 2025

[10] Shape-aware Graph Spectral Learning
Junjie Xu, Enyan Dai, Dongsheng Luo, Xiang Zhang, Suhang Wang
CIKM 2024

[11] LLM and GNN are Complementary: Distilling LLM for Multimodal Graph Learning
Junjie Xu, Zongyu Wu, Minhua Lin, Xiang Zhang, Suhang Wang
ArXiv 2024

[12] A Comprehensive Survey on Trustworthy Graph Neural Networks: Privacy, Robustness, Fairness, and Explainability
Enyan Dai, Tianxiang Zhao, Huaisheng Zhu, **Junjie Xu**, Zhimeng Guo, Hui Liu, Jiliang Tang, Suhang Wang
Machine Intelligence Research

[13] HC-GST: Heterophily-aware Distribution Consistency based Graph Self-training
Fali Wang, Tianxiang Zhao, **Junjie Xu**, Suhang Wang
CIKM 2024

[14] Enhancing GNNs with Limited Labeled Data by Actively Distilling Knowledge from LLMs
Quan Li, Tianxiang Zhao, Lingwei Chen, **Junjie Xu**, and Suhang Wang
BigData 2024

[15] Self-Explainable Graph Neural Networks for Link Prediction
Huaisheng Zhu, Dongsheng Luo, Xianfeng Tang, **Junjie Xu**, Hui Liu, Suhang Wang
ArXiv 2023

[16] HP-GMN: Graph Memory Networks for Heterophilous Graphs
Junjie Xu, Enyan Dai, Xiang Zhang, Suhang Wang
ICDM 2022

[17] Revisiting Time Series Outlier Detection: Definitions and Benchmarks
Kwei-Herng Lai, Daochen Zha, **Junjie Xu**, Yue Zhao, Guanchu Wang, Xia Hu
NeurIPS 2021, Datasets and Benchmarks Track

[18] TODS: An Automated Time Series Outlier Detection System
Kwei-Herng Lai, Daochen Zha, Guanchu Wang, **Junjie Xu**, Yue Zhao, Devesh Kumar, Yile Chen, Purav Zumkhawaka, Mingyang Wan, Diego Martinez, Xia Hu
AAAI 2021, Demo track

WORK EXPERIENCE

Pinterest 05/2025 - 08/2025
Machine Learning Intern; *Advisor: Liangzhe Chen & Siyuan Gao* Palo Alto, CA, US

Cross-domain Ads Sequence Recommendation

- Integrated sequences from ads and organic domains using novel transformer-based models, enabling unified representation learning and stronger **cross-domain recommendations**.
- Explored **generative recommendation** with LLMs, prototyping recommendation generation and preference alignment to improve relevance and user engagement.

Johnson & Johnson 05/2024 - 11/2024
Research Intern; *Advisor: Mangal Prakash* New Brunswick, NJ, US

Geometric Deep Learning for RNA Prediction

- Generated and refined RNA datasets encompassing **1D, 2D, and 3D** structures; constructed graphs and geometric graphs based on 2D and 3D structures.
- Conducted extensive benchmarking of state-of-the-art models across 1D, 2D, and 3D methods, evaluating model **scalability, robustness to noise, and generalization** under real-world challenges.
- Developed **3D geometric RNA modeling** methods with hierarchical multidimensional GNNs, integrating multi-scale structures to achieve SOTA performance.

Rice University 05/2020 - 06/2021
Research Assistant; *Advisor: Xia "Ben" Hu* TX, US

Automated Time-series Outlier Detection System

- Developed a **full stack and automated** machine learning system with preprocessing, feature extraction, detection algorithms, and human-in-the-loop interfaces.
- Integrated a wide range of algorithms including PyOD. Revisited the definition of the time-series anomalies and proposed a taxonomy for point-wise, piece-wise, and pattern-wise anomalies.
- Implemented AutoML for knowledge-free pipeline construction and automatic optimization of module combinations. Developed GUI to improve usability. [Code] (Github 1.6k+ stars, 200 forks); [Website]; [Video].

SERVICE

Reviewer & Program Committee
NeurIPS (2025, 2024, 2023, 2022); ICLR (2026, 2025, 2024); ICML (2025, 2024); AAAI (2026, 2025); ICDM (2024, 2023, 2022); LoG (2024, 2023); KDD (2023, 2022); WSDM (2023); CIKM (2023); WWW (2022); TKDD; PAKDD; ICWSM

TEACHING EXPERIENCE

Teaching Assistant, PSU

ETI 461: Database Management and Administration	Fall 2025
DS 310: Machine Learning for Data Analytics	Spring 2025
IST 597: Machine Learning on Graphs	Spring 2024
HCDD 364W: Methods for Studying Users	Spring 2024
DS 305: Algorithmic Methods & Tools	Fall 2023

HONORS & AWARDS

NeurIPS Scholar Award	NeurIPS, 2025
ICLR Student Travel Award	ICLR, 2025
IST Travel Award	IST PSU, 2022, 2025
ICDM Student Travel Award	ICDM, 2022
Graham Endowed Fellowship	PSU, 2021
Mitacs Globalink Research Scholarship	China Scholarship Council, 2020
Scholarship for Academic Excellence	HUST, 2017, 2018, 2019

SKILLS

Languages	English (Fluent), Mandarin (Native)
Programming	Python, Java, Matlab, C
Deep Learning	PyTorch, PyTorch Geometric, VERL, DGL, Tensorflow, PyTorch Lightning, e3nn