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**: LLM, AI for Science, Graph Learning, Geometric Deep Learning.
- **18 papers** published (NeurIPS, ICLR, ICML, KDD, etc) or under submission, with **900+ citations** as of 11/2025.
- Extensive industry experiences conducting research and developing ML algorithms for real-world applications.

EDUCATION

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

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

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

SELECTED PAPERS

For the full publication list, please refer to Google Scholar.

[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] LLM and GNN are Complementary: Distilling LLM for Multimodal Graph Learning
Junjie Xu, Zongyu Wu, Minhua Lin, Xiang Zhang, Suhang Wang
BigData 2025

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

[7] 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

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

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

[10] 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

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

EXPERIENCE

Penn State University 08/2021 - Present
Research Assistant University Park, PA, US

Memory-Augmented LLM Agent with Reinforcement Learning

- Developed a **memory-editing LLM agent** capable of structured CRUD operations over **long multi-turn** dialogues using **reinforcement learning** (PPO, GRPO, etc.) with per-edit **counterfactual QA rewards** and **evidence-aware retrieval**.
- Built a **VERL-based RL pipeline** with custom environments, trajectory data, multi-GPU rollout, and a unified memory/answering policy, enabling **long-range reasoning** and **persistent memory construction** in LLMs.

Multi-modal Knowledge Distillation with LLM for Molecule Property Prediction

- Investigated the impact of **multi-modal inputs**—including text, molecular diagrams, node features, and graph structures—on molecule property prediction, and **fine-tuned** LLMs to strengthen their ability to encode and integrate these modalities.
- Implemented **knowledge distillation** from Large Language Models to smaller models (e.g., GNNs, MLPs), improving **efficiency** and reducing **inference cost** while preserving strong representation learning performance.

Pinterest 05/2025 - 08/2025
Machine Learning Intern Palo Alto, CA, US

Cross-domain Ads Sequence Recommendation

- Integrated ad and organic user sequences into a unified transformer-based model, learning shared latent representations that strengthen **cross-domain modeling** and improve **multi-source recommendations**.
- Prototyped **LLM-driven generative recommendation**, leveraging preference modeling and alignment techniques to produce personalized item suggestions and strengthen user engagement signals.

Johnson & Johnson 05/2024 - 11/2024
Research Intern 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 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 (2025-2022); ICLR (2026-2024); ICML (2025-2024); AAAI (2026-2025); ICDM (2024-2022); 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 - 2019

SKILLS

Languages	English (Fluent), Mandarin (Native)
Deep Learning	PyTorch, PyTorch Geometric, DGL, e3nn, TensorFlow, PyTorch Lightning
LLM & Agents	vLLM, HuggingFace, LoRA, RLHF (PPO/GRPO/VERL), RAG
Tools & Infra	CUDA, Weights & Biases, Ray, Docker, Linux, Git