Xu Shen

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Education

Jilin University   Changchun, China
M.ENG. in Computer Science and Technology, expected in June 2026.   Sept 2023 – Present

- Advisor: Prof. *Xin Wang.*
- Honors: Academic Performance Scholarship (2023 & 2024), Outstanding Graduate Student Award (2024)

Ningbo University   Ningbo, China
B.ENG. in Computer Science and Technology   Sept 2019 – June 2023

- GPA: 3.55/4.0
- Honors: Zhejiang Provincial Government Scholarship (2020 & 2022)

Research Interests

- Trustworthy Deep Learning (OOD generalization and representation power of GNNs)
- Theory and Applications of Generative Models (diffusion model, LLMs)

Publications (* indicates equal contribution)

- **Xu Shen**, Pietro Lio, Lintao Yang, Ru Yuan, Yuyang Zhang, Chengbin Peng. *Graph rewiring and preprocessing for graph neural networks based on effective resistance.* IEEE Transactions on Knowledge and Data Engineering (**TKDE**), 2024. [Paper] [Code]

- **Xu Shen**, Yili Wang, Kaixiong Zhou, Shirui Pan, Xin Wang. *Optimizing ood detection in molecular graphs: A novel approach with diffusion models.* Proceedings of the 30th ACM SIGKDD Conference on Knowledge Discovery and Data Mining (**KDD**), 2024. [Paper] [Code]

- Yili Wang*, Yixin Liu*, **Xu Shen***, Chenyu Li*, Kaize Ding, Rui Miao, Ying Wang, Shirui Pan, Xin Wang *Unifying Unsupervised Graph-Level Anomaly Detection and Out-of-Distribution Detection: A Benchmark.* The Thriteen International Conference on Learning Representations (**ICLR**), 2025. [Paper] [Code]

- **Xu Shen**, Yixin Liu, Yili Wang, Rui Miao, Yiwei Dai, Shirui Pan, Xin Wang. *Raising the Bar in Graph OOD Generalization: Invariant Learning Beyond Explicit Environment Modeling.* arXiv preprint (**submit to KDD**), 2025. [Paper] [Code]

Selected Research Experiences

- **Graph rewiring for alleviating over-smoothing and over-squashing**

  - **Objective:** Rewiring the graph structure using effective resistance to adjust imbalanced regions aims to mitigate both over-smoothing and over-squashing.
  - **Methods:**
    - Theoretical analysis establishes the relationship between effective resistance, over-smoothing, and over-squashing.
    - A rewiring method is proposed to simultaneously mitigate over-smoothing and over-squashing by balancing effective resistance values in the graph.
  - **Outcome:** A research paper published in **TKDE 2024** (Publication #1)

- **Leveraging diffusion models for OOD detection in molecular graphs**

  - **Objective:** Utilizing diffusion models to generate prototype graphs for distinguishing whether input molecular graphs in the testing phase are OOD samples.
  - **Methods:**

- Proposing a naive validation model, GR-MOOD, which reconstructs inputs and uses reconstruction quality as the OOD judgment score.
- Generating prototype graphs to avoid reconstructing each input graph with a diffusion model, leading to an efficient OOD detection model: PGR-MOOD.

- **Outcome:** A research paper published in **KDD 2024** (Publication #2)

Service

- Conference Reviewer: NeurIPS (2024-2025), ICLR'25, ICML'25, KDD'25.

Skills

Programming Language: C++, C, Python

Tool and Software: LaTeX, Matplotlib, Git

Language: Chinese (native), English (CET6 511)