LINGXIAO ZHAO

CONTACT

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EDUCATION

Carnegie Mellon University

Pittsburgh, PA, USA Ph.D. in Machine Learning (joint Public Policy) Aug. 2018 to Now

Advisors: Prof. Leman Akoglu, Prof. Aarti Singh

Ph.D. Committee: Prof. Leman Akoglu, Prof. Aarti Singh, Prof. Andrej Risteski, Dr. Neil Shah

Carnegie Mellon University Pittsburgh, PA, USA M.S. in Electrical and Computer Engineering, GPA: 3.90/4.00 Aug. 2016 to Dec. 2017

Xi'an Jiaotong University Xi'an, Shaanxi, China B.S. in Electrical Engineering, Rank: 7/370 Aug. 2012 to July 2016

EXPERIENCE

Apple Inc., Research Intern. with Navdeep Jaitly. May 2023 to Aug. 2023

- Working on improving *pre-training* convergence and generalization of large language model.

with Haggai Maron. Nvidia, Reserach Intern. May 2022 to Aug. 2022

- Working on graph generative model.

with Neil Shah. Snap Inc., Reserach Intern. May 2021 to Aug. 2021

- Working on improving expressivity of graph neural network.

IBM Research, Research Intern. with *Charu Aggarwal*. May 2020 to Aug. 2020

- Working on graph-level anomaly detection, with GNN based approach.

RESEARCH INTEREST

Graph is a powerful representation that captures interactions between identities. My work focuses on solving some fundamental problems of Graph Neural Networks, such as breaking depth-limitation, relaxing homophily requirement, learning better structure, and improving expressiveness. My recent work is focusing on discrete-state diffusion, graph generation, and graph pretraining, with a final goal of building a generative foundation model on graph. In future, I'm interested in 1) combining graph models and LLMs to boost LLMs' reasoning and emergent abilities in different stages, and towards a multimodal foundation model; 2) understanding LLM's reasoning limitation within single step, and improving LLM planner with graph; 3) leveraging graph and relational structure to improve RAG. I am also interested in scientific discovery and AI for Science with LLM and graph.

AWARDS

• Daniel and Rise Nagin Dissertation Fellowship	Aug. 2023
• NeurIPS 2022 Travel Grant	Oct. 2022
• SIGIR Student Travel Grant	Sep. 2018
• Outstanding Student Pacesetter (Only 10 students in 3800 undergraduates)	Oct. 2015

• National Scholarship (Rank 4/370 and 5/370, respectively)

• Outstanding Winner (highest) In MCM/ICM¹ (0.19% worldwide)

Oct. 2015, Oct. 2014

April. 2014

PUBLICATIONS

st denotes equal contribution.

Preprints

- 1. Improving Training Stability and Generalization of Transformer Intern project at Apple, under preparation
- Improving and Unifying Discrete- & Continuous-time Discrete Denoising Diffusion <u>Under Review, ICML 2024</u> <u>Lingxiao Zhao*, Xueying Ding*</u>, Lijun Yu, Leman Akoglu
- Pard: Permutation-Invariant Autoregressive Diffusion for Graph Generation <u>Under Review, ICML 2024</u> <u>Lingxiao Zhao, Xueying Ding, Leman Akoglu</u>
- 4. On the Expressive Power of Spectral Invariant Graph Neural Networks

 <u>Under Review, ICML 2024</u>

 Bohang Zhang, **Lingxiao Zhao**, Haggai Maron
- End-to-End Augmentation Hyperparameter Tuning for Self-Supervised Anomaly Detection <u>Under Review, ICML 2024</u> Jaemin Yoo, Lingxiao Zhao, and Leman Akoglu

Refereed Conference Publications

- Descriptive Kernel Convolution Network with Improved Random Walk Kernel [WWW 2024]
 Jeremy Lee*, Lingxiao Zhao*, Leman Akoglu
- 2. Anomaly Detection of Attributed Multi-graphs with Metadata [BigData 2023] Konstantinos Sotiropoulos*, Lingxiao Zhao*, Pierre Jinghong Liang, Leman Akoglu
- 3. DSV: An Alignment Validation Loss for Self-supervised Outlier Model Selection [PKDD 2023] Jaemin Yoo, Yue Zhao, Lingxiao Zhao, and Leman Akoglu
- 4. Sign and Basis Invariant Networks for Spectral Graph Representation Learning [ICLR 2023] Derek Lim*, Joshua Robinson*, Lingxiao Zhao, Tess Smidit, Suvrit Sra, Haggai Maron, Stefanie Jegelka.
- 5. A Practical, Progressively-Expressive GNN [NeurIPS 2022] Lingxiao Zhao, Louis Härtel, Neil Shah, Leman Akoglu
- 6. Hyperparameter Sensitivity in Deep Outlier Detection [NeurIPS 2022]
 Xueying Ding, Lingxiao Zhao, Leman Akoglu
- 7. Graph-level Anomaly Detection with Unsupervised GNNs [ICDM Short, 2022] Lingxiao Zhao, Saurabh Sawlani, Arvind Srinivasan, Leman Akoglu
- 8. From Stars to Subgraphs: Uplifting Any GNN with Local Structure Awareness [ICLR 2022] Lingxiao Zhao, Wei Jin, Leman Akoglu, Neil Shah

¹The Mathematical Contest in Modeling/The Interdisciplinary Contest in Modeling: comap.com

9. Graph Condensation for Graph Neural Networks [ICLR 2022] Wei Jin, Lingxiao Zhao, Shichang Zhang, Yozen Liu, Jiliang Tang, Neil Shah

10. Fast Attributed Graph Embedding via Density of States Saurabh Sawlani, **Lingxiao Zhao**, Leman Akoglu [ICDM 2021]

- 11. Graph unrolling networks: Interpretable neural networks for graph signal denoising 2021 IEEE Transactions on Signal Processing Siheng Chen, Yonina C. Eldar, Lingxiao Zhao
- 12. Beyond Homophily in GNNs: Limitations and Effective Designs [NeurIPS 2020] Jiong Zhu, Yujun Yan, Lingxiao Zhao, Mark Heimann, Leman Akoglu, Danai Koutra
- 13. Connecting Graph Convolutional Net and Graph-Regularized PCA [ICML Workshop 2020] Lingxiao Zhao, Leman Akoglu
- 14. PairNorm: Tackling Oversmoothing in GNNs Lingxiao Zhao, Leman Akoglu

[ICLR 2020]

15. A Quest for Structure: Jointly Learning Graph and Semi-Supervised Classification [CIKM 2018] Xuan Wu*, Lingxiao Zhao*, Leman Akoglu. (* equal contribution)

Refereed Journal Publications

- Heterophily and Graph Neural Networks: Past, Present and Future 2023 IEEE Data Engineering Bulletin, June 2023 Jiong Zhu, Yujun Yan, Mark Heimann, Lingxiao Zhao, Leman Akoglu, Danai Koutra
- Density of States for Fast Embedding Node-Attributed Graphs 2022 Knowledge and Information System Joural Lingxiao Zhao, Saurabh Sawlani, Leman Akoglu
- On Using Classification Datasets to Evaluate Graph Outlier Detection: Peculiar Observations 2021 Big Data Journal Lingxiao Zhao, Leman Akoglu

ACADEMIC SERVICE

Program Committee Member, Conference Reviewer

• International Conference on Machine Learning (ICML)

2022

• Conference on Neural Information Processing Systems (NeurIPS)

2021-2023

• International Conference on Learning Representations (ICLR)

2022 - 2024

• Learning on Graphs Conference (LoG)

2022

TEACHING

- Teaching assistant for CMU 95-869 Big Data and Large Scale Computing (2020, 2021, 2022)
- Teaching assistant for CMU 95-828 Machine Learning for Problem Solving (2021, 2022)
- Teaching assistant for CMU 90-812 Introduction to Programming with Python (2019)
- Teaching assistant for CMU 10-725 Convex Optimization (2019)

SKILLS

Languages: Python, MATLAB, Java, C, C++, LATEX, Bash

Frameworks: Pytorch, Tensorflow

Large-Scale Computing: MapReduce, Hadoop, Spark, Pig

Web: HTML, CSS, Bootstrap, Jekyll

SELECTED PROJECTS

Generative Pretraining on Graphs

Jan. 2023 to Now

Proposed an autoregressive based diffusion model, it builds the foundation of graph pretraining.

- Unified continuous- & discrete-time discrete-state diffusion which supports diverse noises.
- Proposed an local diffusion model that generates graph block-by-block, autoregressively.
- Working on using the designed blockwise diffusion model to perform generative pretraining.

From Stars to Subgraphs: Uplifting Any GNN

Mar. 2021 to Oct. 2021

Proposed the first general framework to boost expressiveness of any GNN

- Designed a general framework to uplift any GNN, by generalizing MPNN's aggregation field from stars to subgraphs and encoding subgraphs with the (base) GNN.
- Proved the expressiveness is strictly better than 1-WL, while being not less powerful than 3-WL.
- Designed effective and efficient realizations: different encodings and distance-to-centroid feature.
- Designed SubgraphDrop that greatly reduces memory cost and still keeps same performance.

Tackling oversmoothing problem in GNNs

March 2019 to Sept. 2019

Proposed the first normalization layer in GNNs, for solving oversmoothing

- Studied oversmoothing thoroughly with SGC, which decouples the effect of oversmoothing on performance drop of increasing layers from overfitting and vanishing gradient problems.
- Proposed an efficient and effective normalization layer, PairNorm, that "pushes" oversmoothed node representations away from each other. PairNorm greatly improves robustness of depth.
- Studied a new setting: Semi-Supervised Learning with large percentage missing feature problem, where PairNorm greatly boost performance for all three types of GNN (SGC,GCN,GAT).

COURSEWORK

Carnegie Mellon University

- 10-716: Advanced Machine Learning
- 10-725: Convex Optimization
- 10-708: Probabilistic Graphical Model
- 10-705: Intermediate Statistics
- 10-605: Machine Learning in Large Datasets
- 11-785: Introduction to Deep Learning
- 15-213: Introduction to Computer System
- 15-214: Pinciples of Software Construction
- 15-780: Artificial Intelligence
- 15-659: Probability and Computing
- 15-650: Algorithm and Data Structure
- 36-731 & 36-732: Causal Inference
- 36-707: Regression Analysis
- 15-859: Spectral Graph Theory
- 10-703: Deep Reinforcement Learning