

Mufei Li

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Education

- **Georgia Institute of Technology** Georgia, United States
Ph.D., Machine Learning Aug 2023 -
- **New York University Shanghai** Shanghai, China
B.S., Honors Mathematics Sep 2014 - May 2018

Professional Experience

- **Software Development Engineer II** Shanghai, China
Amazon Web Services Shanghai AI Lab Jul 2020 - Jun 2023
- **Software Development Engineer I** Shanghai, China
Amazon Web Services Shanghai AI Lab Feb 2019 - Jul 2020
- **Research Assistant** Shanghai, China
New York University Shanghai Jun 2018 - Feb 2019

Selected Publications

- Mufei Li*, Siqi Miao*, Pan Li, **Simple is Effective: The Roles of Graphs and Large Language Models in Knowledge-Graph-Based Retrieval-Augmented Generation**, International Conference on Learning Representations (ICLR), 2025 (*Equal contribution).
- Mufei Li, Viraj Shitole, Eli Chien, Changhai Man, Zhaodong Wang, Srinivas Sridharan, Ying Zhang, Tushar Krishna, Pan Li, **LayerDAG: A Layerwise Autoregressive Diffusion Model for Directed Acyclic Graph Generation**, International Conference on Learning Representations (ICLR), 2025.
- Tengfei Ma, Xiang Song, Wen Tao, Mufei Li, Jiani Zhang, Xiaoqin Pan, Yijun Wang, Bosheng Song, Xiangxiang Zeng, **Towards Synergistic Path-based Explanations for Knowledge Graph Completion: Exploration and Evaluation**, International Conference on Learning Representations (ICLR), 2025.
- Eli Chien, Mufei Li, Anthony Aportela, Kerr Ding, Shuyi Jia, Supriyo Maji, Zhongyuan Zhao, Javier Duarte, Victor Fung, Cong Hao, Yunan Luo, Olgica Milenkovic, David Pan, Santiago Segarra, Pan Li, **Opportunities and challenges of graph neural networks in electrical engineering**, Nature Reviews Electrical Engineering, 2024.
- Mufei Li, Eleonora Kreačić, Vamsi K. Potluru, Pan Li, **GraphMaker: Can Diffusion Models Generate Large Attributed Graphs?**, Transactions on Machine Learning Research (TMLR), 2024.
- Fabio Broccatelli, Richard Trager, Michael Reutlinger, George Karypis, Mufei Li, **Benchmarking Accuracy and Generalizability of Four Graph Neural Networks Using Large In Vitro ADME Datasets from Different Chemical Spaces**, Molecular Informatics, 2022.
- Ziqi Chen, Bo Peng, Vassilis N. Ioannidis, Mufei Li, George Karypis, Xia Ning, **CTKG: A Knowledge Graph for Clinical Trials**, Scientific Reports, 2022.

- Fengqing Lu, [Mufei Li](#), Xiaoping Min, Chunyan Li, Xiangxiang Zeng, **De novo generation of dual-target ligands using adversarial training and reinforcement learning**, Briefings in Bioinformatics, 2021.
- [Mufei Li](#), Jinjing Zhou, Jiajing Hu, Wenxuan Fan, Yangkang Zhang, Yaxin Gu, George Karypis, **DGL-LifeSci: An Open-Source Toolkit for Deep Learning on Graphs in Life Science**, ACS Omega, 2021.
- Vassilis N. Ioannidis, Xiang Song, Saurav Manchanda, [Mufei Li](#), Xiaoqin Pan, Da Zheng, Xia Ning, Xiangxiang Zeng, George Karypis, **DRKG - Drug Repurposing Knowledge Graph for Covid-19**, preprint, 2020.
- Minjie Wang, Da Zheng, Zihao Ye, Quan Gan, [Mufei Li](#), Xiang Song, Jinjing Zhou, Chao Ma, Lingfan Yu, Yu Gai, Tianjun Xiao, Tong He, George Karypis, Jinyang Li, Zheng Zhang, **Deep graph library: A graph-centric, highly-performant package for graph neural networks**, arXiv, 2019.

Honors and Awards

- Georgia Tech ECE Fellowship
- Top Reviewer for NeurIPS 2024

Peer Review Service

- Conference on Neural Information Processing Systems (NeurIPS), 2024
- International Conference on Learning Representations (ICLR), 2025
- International Conference on Machine Learning (ICML), 2025
- IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI), 2024
- Transactions on Machine Learning Research (TMLR), 2025
- ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD), 2024
- Learning on Graphs Conference (LoG), 2024
- Asian Conference on Machine Learning (ACML), 2024

Talks & Tutorials

- [Mufei Li](#), Fabio Broccatelli, **Accelerating Drug Discovery with Multitask Graph Neural Networks**, Nvidia GTC, 2021.
- Zichen Wang, Vassilis N. Ioannidis, Huzefa Rangwala, Tatsuya Arai, Ryan Brand, [Mufei Li](#), Yohei Nakayama, **Graph Neural Networks in Life Sciences: Opportunities and Solutions**, KDD tutorial, 2022.

Teaching Assistant

- ECE 6254 Statistical Machine Learning