

# Mufei Li

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Homepage: <https://mufeili.github.io>

## 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

## Publications

- [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**, arXiv, 2024.
- [Mufei Li\\*](#), Siqi Miao\*, Pan Li, **Simple is Effective: The Roles of Graphs and Large Language Models in Knowledge-Graph-Based Retrieval-Augmented Generation**, arXiv, 2024 (\*Equal contribution).
- 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.
- Mufei Li, Hao Zhang, Xingjian Shi, Minjie Wang, Zheng Zhang, **A Statistical Characterization of Attentions in Graph Neural Networks**, ICLR Workshop on Representation Learning on Graphs and Manifolds, 2019.
- 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

- IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI)
- Conference on Neural Information Processing Systems (NeurIPS), 2024
- International Conference on Learning Representations (ICLR), 2024
- 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