Mufei Li

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Homepage: https://mufeili.github.io

Education

Georgia Institute of Technology
Ph.D., Machine Learning
Georgia, United States
Aug 2023 -

New York University Shanghai
B.S., Honors Mathematics
Shanghai, China
Sep 2014 - May 2018

Professional Experience

Software Development Engineer II
Amazon Web Services Shanghai AI Lab
Shanghai, China
Jul 2020 - Jun 2023

Software Development Engineer I
Amazon Web Services Shanghai AI Lab
Shanghai, China
Feb 2019 - Jul 2020

Research Assistant
New York University Shanghai
Shanghai, China
Jun 2018 - Feb 2019

Publications

- 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.

Selected Projects

- Deep Graph Library (DGL)

    - A popular library for graph neural networks (GNNs), with more than 10K stars on GitHub
    - Core member of the development team since its early stage
    - My work involves designing and implementing Application Programming Interfaces (APIs) and operators, adding unit tests, writing documentation and blogs, conducting code reviews, reading latest research papers, adding model examples, mentoring interns, and supporting customers

- DGL-LifeSci

    - A DGL-based library for applying GNNs to life science, with applications of molecular property prediction, chemical reaction prediction, molecular generative models, and binding affinity prediction
    - Lead of the development team, with members having a background in CS or Life Science
    - Designed and implemented a command-line interface driven by the feedback of domain experts

- GNNLens2

    - An interactive visualization tool for GNNs, in collaboration with a team from HKUST and SMU that work on information visualization
    - In addition to graph visualization for GNNs, it allows comparing various subgraphs. This can benefit the study of instance-based GNN explainability methods.
    - Lead of the development team

Talks & Tutorials

- <u>Mufei Li</u>, Fabio Broccatelli, **Accelerating Drug Discovery with Multitask Graph Neural Networks**, Nvidia GTC, 2021.

- Zichen Wang, Vassilis N. Ioannidis, Huzefa Rangwala, Tatsuya Arai, Ryan Brand, <u>Mufei Li</u>, Yohei Nakayama, **Graph Neural Networks in Life Sciences: Opportunities and Solutions**, KDD tutorial, 2022.

Skills

- Writing: **LaTeX**, **Markdown**

- Programming Languages: **Python**, Bash, C++, R, MATLAB, Java, Mathematica

- Machine Learning: **PyTorch**, TensorFlow, Transformers, Scikit-learn, XGBoost, TensorBoard, Captum

- Data Science: Conda, NumPy, SciPy, Pandas, Jupyter Notebook, Matplotlib, Seaborn

- Graph Representation Learning and Graph Analytics: **DGL**, PyTorch Geometric, NetworkX, cuGraph

- Software Development: Sphinx, Jenkins, Pytest, Docker

- Amazon Web Services: S3, **EC2**, SageMaker, Comprehend Medical

- Web Development: TypeScript, HTML, CSS

- Natural Language Processing: NLTK, spaCy

- Reinforcement Learning: Gym, MuJoCo