Mufei Li

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github: https://github.com/mufeili

Education

- **New York University Shanghai** — Shanghai, China
  B.Sc. Honors Mathematics — *Sep 2014 - Jun 2018*
  - Graduated with distinction "cum laude", GPA 3.74/4.0
- **New York University** — New York City, U.S.
  Study Away Program, Math & Science — *Sep 2016 - Jun 2017*
  - GPA 4.0/4.0

Professional Experience

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

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

Selected 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.
- 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.

Full list: https://scholar.google.com/citations?user=lwbnLDYAAAAJhl=en

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.

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