Shengchao Liu

CONTACT INFORMATION

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EDUCATION

MILA, Montreal, QC, Canada Jan 2020 - June 2024 (expected)

Doctor of Philosophy, Computer Science

- Advisor: Prof. Jian Tang
- Directions: Molecular Representation Learning with Limited Data

University of Wisconsin-Madison, Madison, WI, USA Aug 2015 - Aug 2018

Master of Science, Computer Science

- Main Advisor: Prof. Anthony Gitter
- Collaborated Advisors: Prof. Dimitris Papailiopoulos, Prof. Yingyu Liang
- Thesis: Exploration on Deep Drug Discovery: Representation and Learning

Shandong University, Jinan, Shandong, China Sep 2011 - June 2015

Bachelor of Engineering, Software Engineering

- GPA: 90.49/100, Rank: 4/320

PROFESSIONAL EXPERIENCE

ServiceNow (ElementAI), Montreal, QC, Canada

Machine Learning Research Intern June 2021 - Jan 2022

- Advisors: Dr. Pierre-André Noël, Dr. David Vázquez

HEC Montréal, Montreal, QC, Canada

Teaching Assistant Jan 2021 - May 2021

- MATH 80600A: Machine Learning II, Deep Learning and Applications

IQVIA, Cambridge, MA, USA

Machine Learning Research Intern June 2019 - Aug 2019

- Advisor: Dr. Cao (Danica) Xiao

University of Wisconsin-Madison, Madison, WI, USA

Associate Researcher Dec 2018 - May 2019

- Advisor: Prof. Anthony Gitter

Research Assistant Aug 2016 - Aug 2018

- Advisor: Prof. Anthony Gitter

Teaching Assistant Jan 2016 - May 2016

- CS 564: Database Management Systems: Design and Implementation

Facebook Software Developer, Menlo Park, CA, USA

Internship on Machine Learning (Full-Time Return Offer) May 2016 - Aug 2016

Selected Publications

Unsupervised Discovery of Steerable Factors in Structure Data. *S. Liu*, Y. Du*, H. Wang, J. Lasenby, B. Zhou, J. Tang.* [In Submission to ICML 2022]

Evaluating Self-Supervised Learned Graph Representations. *H. Wang*, S. Liu*, J. Kaddour*, Q. Liu*, J. Tang, J. Lasenby, M. Kusner.* [In Submission to ICML 2022]

Pre-training Molecular Graph Representation with 3D Geometry. *S. Liu, H. Wang, W. Liu, J. Lasenby, H. Guo, J. Tang.* [ArXiv; Self-Supervised Learning Workshop NeurIPS 2021; ICLR 2022]

Multi-task Learning with Domain Knowledge for Molecular Property Prediction. *S. Liu, M. Qu, Z. Zhang, H. Cai, J. Tang.* [AI for Science Workshop NeurIPS 2021; AISTATS 2022]

Bad Global Minima Exist and SGD Can Reach Them. *S. Liu, D. Papailiopoulos, D. Achlioptas.* [Identifying and Understanding Deep Learning Phenomena Workshop ICML 2019 (oral); NeurIPS 2020]

N-Gram Graph: Simple Unsupervised Representation for Graphs, with Applications to Molecules. *S. Liu, M. F. Demirel, Y. Liang.* [MLMM Workshop NeurIPS 2018; NeurIPS 2019 (Spotlight)]

Loss-Balanced Task Weighting to Reduce Negative Transfer in Multi-Task Learning. *S. Liu, Y. Liang, A. Gitter.* [AAAI-SA 2019]

Atomo: Communication-efficient Learning via Atomic Sparsification. *H. Wang, S. Sievert, Z. Charles, S. Liu, D. Papailiopoulos, S. Wright.* [NeurIPS 2018]

Selected Manuscripts, Preprints, and Symposiums

An Analysis of Attentive Walk-Aggregating Graph Neural Networks. *M. F. Demirel, S. Liu, S. Garg, Y. Liang.* [ArXiv, In Submission to ICLR 2022]

Evaluating scalable supervised learning for synthesize-on-demand chemical libraries. *M. Alnammi, S. Liu, S. S. Ericksen, G. E. Ananiev, A. F. Voter, S. Guo, J. L. Keck, F. M. Hoffmann, S. A. Wildman, A. Gitter.* [ChemRxiv]

A Survey on Graph Representation Learning for Drug Development. *S. Liu, A. Deac, V. Verma, C. Chen, J. Tang.* [Manuscript]

Research Interests

Self-Supervised Learning, Multi-task Learning, Graph Representation Learning, Deep Generative Model, Deep Learning Interpretability, Drug Discovery.

Languages

Python, Java, C++, Matlab, Julia, PHP, C#, CSS, JavaScript.
Specifically in Python: Pytorch, Pytorch Geometric, DGL, OGB, TensorFlow.

Activities & Awards

Main organizer for AI for Science Workshop, NeurIPS 2021
Main contributor to three public GNN git repositories (similar to PyG): TorchDrug
Reviewer for NeurIPS (2019,2021), ICML (2020, 2021), ICLR (2021,2022), AISTATS (2022), AAAI (2021)
Travel Award, Conference on Neural Information Processing Systems 2018
Travel Award, Midwest Biopharamceutical Statistics Workshop 2018
Third Prize, ACM-ICPC North Central Regional 2015
First Prize, Microsoft College Code Competition(MSFT3C) in the year 2015, 2016
TGIF Czars Organizer, SACM at UW-Madison 2015, 2016
Vice-captain of Shandong University ACM-ICPC Laboratory 2013, 2014
The First Class National Scholarship in the year 2013, 2014