

SULIN LIU

 sulinliu@mit.edu

 [liusulin.github.io](https://github.com/liusulin)

 [GitHub](#)

 [LinkedIn](#)

Research Interests

Currently, I focus on diffusion/flow based generative models, particularly in discrete state spaces, such as diffusion language models. I develop core machine learning methods to improve model scalability or capability in both training and inference. I also collaborate closely with domain scientists to apply generative models to scientific discovery and simulation. More broadly, I am passionate about using AI to model and solve complex real-world problems.

Work Experiences

2023 - present	Postdoctoral Associate, MIT - Design and innovate diffusion/flow based generative models, with applications to language modeling, image generation and scientific simulation	Mentors : Rafael Gómez-Bombarelli , Tommi Jaakkola
2021 May-Aug.	Research Engineer Intern, Facebook (Meta) Research - Formulated and pioneered sparse Bayes optimization for interpretable/simple policy search. Published to a methodology paper, successfully deployed the method in products	Mentors : Ben Letham , Eytan Bakshy
2015-17	Research Engineer, Nanyang Technological University, Singapore - Led research in distributed multi-task learning and optimization	Advisor : Sinno Pan

Education

2017-2023	Ph.D. in Electrical and Computer Engineering, Princeton University - Thesis : Scalable and Interpretable Learning with Probabilistic Models for Knowledge Discovery, advised by Ryan Adams (CS) and Peter Ramadge (ECE)
2011-2015	B.Eng. in Electrical Engineering, National University of Singapore - Minor in Mathematics. Thesis advisor : Cheong Loong Fah - Thesis : 3D Scene Reconstruction for Indoor Environment Based on Multiview Homographies
2014	Exchange student, Georgia Institute of Technology - 9 students selected university wide

Honors and Awards

2024	Material sciences track highlight (best paper) prize, ICML Workshop on Machine Learning for Life and Material Science : From Theory to Industry Applications
2024	NERSC Generative AI for Science Award : Generative AI for Rigorous Thermodynamics of Material, 18500 A100 GPU node hours, - <i>awarded by National Energy Research Scientific Computing Center (NERSC)</i>
2023	Schmidt Science Fellows - MIT Nomination (Withdrawn due to conflict)
2022	Princeton ECE Travel Grant Award
2022	NeurIPS Top Reviewer Award, 8%
2020	Azure Cloud Computing Proposal Award, \$10,000

2019	NeurIPS Top Reviewer Award, 50%
2018	Anthony Ephremides Fellowship - <i>awarded to the top first year Ph.D. student in the information science track</i>
2017	Princeton University Fellowship in Natural Sciences and Engineering - <i>tuition, fees, stipends</i>
2017	KDD Conference Travel Award
2014	IEEE Eta Kappa Nu Honor Society
2014	Faculty of Engineering Annual Book Prize - <i>awarded to student with the best performance in wireless communications</i>
2013	ST Electronics Book Prize - <i>awarded to the top sophomore in Electrical Engineering</i>
2011-15	Singapore Ministry of Education Undergraduate Scholarship - <i>tuition, fees, stipends</i>

Selected Publications (Full publications at [8](#))

2024	Sulin Liu , Juno Nam, Andrew Campbell, Hannes Stärk, Yilun Xu, Tommi Jaakkola, Rafael Gómez-Bombarelli Think While You Generate : Discrete Diffusion with Planned Denoising, Under submission Paper . Code .
2024	Juno Nam, Sulin Liu , Gavin Winter, KyuJung Jun, Soojung Yang, Rafael Gómez-Bombarelli Flow Matching for Accelerated Simulation of Atomic Transport in Materials, Under submission . <i>Material Sciences Best Paper Prize at ICML'24 Workshop on Machine Learning for Life and Material Science</i> Paper .
2023	Sulin Liu , Peter J. Ramadge, Ryan P. Adams Generative Marginalization Models, in ICML 2024 . <i>Contributed talk at ICML'23 SPIGM Workshop</i> . Paper . Code . Video .
2023	Sulin Liu *(equal contr.), Qing Feng*, David Eriksson*, Benjamin Letham, Eytan Bakshy Sparse Bayesian Optimization, in AISTATS 2023 . <i>Contributed talk at NeurIPS'22 Workshop on Gaussian Processes, Spatiotemporal Modeling, and Decision-making Systems</i> Paper . Code . Video .
2020	Sulin Liu , Xingyuan Sun, Peter J. Ramadge, Ryan P. Adams Task-Agnostic Amortized Inference of Gaussian Process Hyperparameters, in NeurIPS 2020 . <i>Spotlight Talk at ICML'20 AutoML workshop</i> Paper . Code . Slides . Video .

Invited talks

2024	Think While You Generate : Discrete Diffusion with Planned Denoising <i>Invited talk at Google Deepmind Generative Modeling, Sampling and Transport Seminar Series, 2024.</i>
2023	Deep-Learning-Enabled Probabilistic Models for Knowledge Discovery <i>Invited talk at Hong Kong University Institute of Data Science, 2023.</i>
2023	Deep-Learning-Enabled Probabilistic Models for Knowledge Discovery <i>Invited talk at Westlake University, 2023.</i>
2023	Deep-Learning-Enabled Probabilistic Models for Knowledge Discovery <i>Invited talk at Caltech, Cornell, Columbia, MIT for Postdoc Fellowship Application 2023.</i>

Professional Services

Conference Reviewing

NeurIPS (2018-), ICML (2019-), ICLR (2019-), AMCL (2020-21), KDD (2021), SDM (2021), AAAI (2020-21)

Journal Reviewing

TPAMI (2021-), JMLR (2020-), Science Advances (2023), JACS (2024)

Workshop Reviewing

NeurIPS 22' AI for Accelerated Materials Design Workshop, AI for Science Workshop

Graduate Coursework

- **ML** : Machine Learning and Pattern Recognition, Theoretical Machine Learning, Theoretical Deep Learning, Theory of Deep Weakly Supervised Learning
- **Stats and Optimization** : Statistical Theory and Methods, High-Dimensional Probability, Statistical Optimization and Reinforcement Learning, Linear and Nonlinear Optimization, Optimization for Machine Learning, Large-Scale Optimization
- **Control & Robotics** : Safety-Critical Robotic Systems

Teaching Experiences

Princeton University

Co-Instructor : SML 310 Research Projects in Data Science (Fall'21, Spring'22).

Teaching Assistant : COS 424 Fundamentals of Machine Learning (Fall '20), COS 302 Mathematics for Machine Learning (Spring'20), ELE 535 Machine Learning and Pattern Recognition (Fall'18, '19), SML 201 Introduction to Data Science (Spring'19)

National University of Singapore

Lab tutor : CS1010E Programming Methodology (Fall'14, Spring'15).

Open Source Projects

Creator and Co-creator :

- DDPD <https://github.com/liusulin/DDPD>
- MAM : <https://github.com/PrincetonLIPS/MaM>
- AHGP : <https://github.com/PrincetonLIPS/AHGP>
- ProBF : <https://github.com/athindran/ProBF>

Developer and Contributor :

- BoTorch : <https://github.com/pytorch/botorch>
- Ax : <https://github.com/facebook/Ax>

Programming Skills and Interests

- **Proficient** : Python (PyTorch, Numpy, Transformers), MATLAB, \LaTeX , Git, Slurm, Bash/Zsh
- **Familiar** : JAX, TensorFlow, C/C++, Java, Parameter Server, HTML/CSS, VHDL
- **Interests** : Coffee, Snowboarding, Basketball, Table Tennis, Longboarding, GeoGuessr