

Yining (Sam) Huang

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EDUCATION

- University of Pennsylvania** Aug. 2025 - Present
PhD in **Computer Science** GPA: 3.9/4.0
Advisor: Jacob Gardner
Research Areas: Agentic AI, AI for Scientific Research, AI for RNA Design
- Harvard University** Aug. 2023 – May. 2025
Master's in **Biomedical Informatics** GPA: 4.0/4.0
Advisor: Debora Marks
Research Areas: Protein Language Models, Geometric Deep Learning, Generative Models
- Northwestern University** Sep. 2019 – Jun. 2023
Bachelor of Science in **Computer Science & Statistics**, Minor in **Mathematics & Finance** GPA: 4.0/4.0
Advisor: Bradly Stadie, Liu Han
Research Areas: Reinforcement Learning, Network Analysis

PUBLICATIONS

- [1] Natalie Maus, Yimeng Zeng, Haydn Thomas Jones, **Yining Huang**, Gaurav Ng Goel, Alden Rose, Kyurae Kim, Hyun-Su Lee, Marcelo Der Torossian Torres, Fangping Wan, Cesar de la Fuente-Nunez, Mark Yatskar, Osbert Bastani, Jacob R. Gardner. **Purely Agentic Black-Box Optimization for Biological Design**. ICML 2026 (Under Review). [paper]
- [2] Felix Teufel, Aaron W Kollasch, **Yining Huang**, Ole Winther, Kevin K Yang, Pascal Notin, Debora Marks. **Few-shot Protein Fitness Prediction via In-context Learning and Test-time Training**. NeurIPS 2025: AI for Science Workshop. [paper]
- [3] Zuobai Zhang*, Pascal Notin*, **Yining Huang**, Aurelie Lozano, Vijil Chenthamarakshan, Debora Marks, Payel Das, Jian Tang. **Multi-Scale Representation Learning for Protein Fitness Prediction**. NeurIPS 2024: Conference on Neural Information Processing Systems. [paper]
- [4] Guanghao Wei*, **Yining Huang***, Chenru Duan, Yue Song, Yuanqi Du. **Navigating Chemical Space with Latent Flows**. NeurIPS 2024: Conference on Neural Information Processing Systems. [paper]
- [5] **Yining Huang***, Zuobai Zhang*, Jian Tang, Debora Marks, Pascal Notin. **Augmenting Evolutionary Models with Structure-Based Retrieval**. ICML 2024: ML4MLS Workshop. [paper]
- [6] Dina Sharon*, **Yining Huang***, Motolani Oyewole, Sammy Mustafa. **How to Go with The Flow: An Analysis of Flow Matching Molecular Docking Performance with Priors of Varying Information Content**. ICLR 2024: GEM Workshop. [paper]
- [7] **Yining Huang***, Steffanie Paul*, Debora Marks. **An Energy Based Model for Incorporating Sequence Priors for Target-Specific Antibody Design**. NeurIPS 2023: GenBio Workshop. [paper]
- [8] Zaixi Zhang*, Jiaxian Yan*, **Yining Huang***, Qi Liu, Enhong Chen, Mengdi Wang, Marinka Zitnik. **Geometric Deep Learning for Structure-Based Drug Design: A Survey**. ACM Computing Survey. [paper]
- [9] Yuanqi Du*, Yingheng Wang*, **Yining Huang**, Jianan Canal Li, Yanqiao Zhu, Tian Xie, Chenru Duan, John Gregoire, Carla P Gomes. **M²Hub: Unlocking the Potential of Machine Learning for Materials Discovery**. NeurIPS 2023: Conference on

Neural Information Processing Systems (Datasets and Benchmarks Track). [paper]

[10] Qiwen Zhang, Xueke Tian, Guang Chen, Ze Yu, Xiaojian Zhang, Jingli Lu, Jinyuan Zhang, Peile Wang, Xin Hao, **Yining Huang**, Zeyuan Wang, Fei Gao, Jing Yang. **A Prediction Model for Tacrolimus Daily Dose in Kidney Transplant Recipients With Machine Learning and Deep Learning Techniques**. Frontiers in Medicine. [paper]

(* Equal Contribution)

TEACHING EXPERIENCES

CIS 6200: Advanced Machine Learning (Graduate-level) Jan. 2026 – May. 2026

Teaching Assistant - Instructor: Prof. Jacob Gardner

- Assisted in teaching a PhD-level machine learning seminar.

STAT415 Introduction to Machine Learning (Graduate-level) Mar. 2023 – Jun. 2023

Teaching Assistant - Instructor: Prof. Bradly Stadie

- Assisted in designing and teaching a core PhD-level course on machine learning.

CS336 Design & Analysis of Algorithms Mar. 2022 – Jun. 2022

Teaching Assistant - Instructor: Prof. Donald Stull

- Led weekly office hours and graded weekly proof-based assignments with detailed feedback.

HONORS

Summa Cum Laude 2023

McCormick School of Engineering High Honor 2019 - 2023

Tau Beta Pi - The Engineering Honor Society 2021

RELEVANT COURSEWORK

Computation: Agentic AI, Natural Language Processing, Reinforcement Learning, Graph Neural Networks, CUDA Programming, MLOps, Quantum Computing, Optimization, Time Series Modeling, Probability, Statistics, Stochastic Processes, Bayesian Statistics

Biology: Computational Biology, Clinical Informatics, Cell Biology, Physiology, Genetics, Single-Cell Analysis, Rare Diseases

TECHNICAL SKILLS

Programming Languages: Python, C, C++, Java, SQL, R, Rust, HTML/CSS, JavaScript, Racket

Languages: Chinese, English