Jiaqi Luo

Georgia Institute of Technology, Atlanta, GA
+1 404 784 1391 ⋄ jiaqi@gatech.edu

EDUCATION

Georgia Institute of Technology, School of Computational Science and Engineering August 2023 - August 2028 (estimate)
Ph.D. student in computational science and engineering, advised by Prof. Yunan Luo

Tsinghua University, Institute for Interdisciplinary Information Sciences (Yao Class) August 2019 - June 2023
Bachelor of computer science and technology
College entrance examination grade: 695/750; Rank: No.1 in Shanxi Province, China

RESEARCH INTERESTS

I have a wide range of research interests, including machine learning, deep learning and their application to computational biology. I aim to utilize statistical and machine learning techniques to build tools that can solve real-world problems.

SKILLS

Programming: Python, C/C++

Quantitative research: statistical modeling, data analysis

Machine learning: deep learning, language models, graph neural networks, representation learning.

Computational biology: protein sequence design, protein function prediction

PROJECTS

Learning maximally spanning representations improves protein function annotation
Research project advised by Prof. Yunan Luo

- Designed a novel deep learning framework inspired by neural collapse to refine the representations of pretrained protein language models for protein function annotation. The learned function-aware protein sequence representations can improve the performance on multiple function annotation tasks for both high and low-frequency classes, mitigating the *long-tail* data imbalance problem.
- Accepted by RECOMB 2025.

Pareto-optimal sampling for multi-objective protein sequence design
Research project advised by Prof. Yunan Luo

- Designed a novel multi-objective protein design framework, which combined a gradient-guided Markov Chain Monte Carlo (MCMC) sampling algorithm with Pareto-optimal gradient composition scheme. The framework can design novel protein sequences with enhanced properties with up to 15 mutations away from the wild-type sequences.
- Paper under journal revision.

Classifier-guided diffusion for molecular design with enhanced synthesizability
Bachelor thesis project advised by Prof. Jianzhu Ma

- Used classifier-guided diffusion model to generate novel molecules with better synthesizability that binds to the given protein pocket.

Contrastive learning of protein representations with graph neural networks for structural and functional annotations
Summer research project advised by Prof. Yunan Luo

- Used contrastive learning together with graph neural networks to learn protein representations from structure and sequence, which can be used for structural and functional annotation transfer.

HONORS AND AWARDS

First Prize in 18-th Challenge Cup National College Student Curricular Academic Science and Technology Works Competition — September 2023
Social Work Excellence Award of IIIS — September 2020
The Scholarship for freshmen of Tsinghua University — September 2019
Provincial 1st Prize in Chinese High School Mathematics League (1%) — September 2018
Provincial 1st Prize in Chinese High School Mathematics League (3%) — September 2017

INTERNSHIPS

Quantitative research intern at X-square Investment — June 2022 - September 2022

· During the internship, I worked on developing machine learning models to predict per-day and per-minute stock price changes for 4,000 stocks in Chinese market.

PUBLICATIONS

Learning maximally spanning representations improves protein function annotation — December 2024
Jiaqi Luo, *Yunan Luo*

· Accepted by *RECOMB 2025* (Preparing camera-ready abstract).

Leveraging conformal prediction to annotate enzyme function space with limited false positives — May 2024
Kerr Ding, ***Jiaqi Luo***, *Yunan Luo*

· Accepted by *PLOS Computational Biology.*

Contrastive learning of protein representations with graph neural networks for structural and functional annotations — October 2022
Jiaqi Luo, *Yunan Luo*

· Accepted by *Pacific Symposium on Biocomputing 2023 (PSB).*

HOBBIES

I have a wide range of hobbies, including but not limited to Rubik's Cube, Texas Hold'em, Snooker, Table Tennis and Badminton.