Fengyu Yang

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About me

I am currently a Ph.D. candidate at the University of North Carolina at Chapel Hill, advised by Prof. Shahar Kovalsky. My research focuses on *Differentiable Optimization*, *Machine Learning*, and *Statistical Modeling*. I am currently a Research Scientist intern at ByteDance Seed-AI for Science team, working on AI-driven protein structure reconstruction. I will graduate in May 2026 and am seeking full-time AI/ML research scientist positions starting Summer 2026.

Education

University of North Carolina, Chapel Hill
Ph.D. in Applied Mathematics, Minor in Statistics & Operations Research — Aug. 2021 – May 2026

University of Chicago
M.S. in Computational and Applied Mathematics, GPA: 3.8/4.0 — Sept. 2019 – Mar. 2021

Shandong University
B.S. in Statistics of Mathematics School, GPA: 90/100 — Sept. 2015 – June 2019

Research Experience

Differentiation Through Black-box Convex Optimization Solvers
Advisor: Shahar Kovalsky

- Developed modular convex optimization layer that enables differentiation for **any forward solver** with seamless integration into neural networks and bi-level optimization tasks, addressing limitation in existing methods that rely on specific forward solvers. Achieved **3 orders** of magnitude performance improvements on large-scale problems.
- Extended methodology to broader convex optimization problems including Second-Order Cone Programming and Semidefinite Programming.

Coupling Structural and Functional Brain Connectome
Advisor: Shahar Kovalsky

- Developed model for jointly analyzing brain structure connectome (DT-MRI) and the temporal dynamics of individual brain regions (fMRI) using **graph spectral analysis** and **signal processing**, uncovering cognitive and motor mechanisms while providing insights into degenerative processes associated with aging and diseases.

Methods of Moments for 3D Particle Ab Initio Modeling
Advisor: Yuehaw Khoo

- Developed method of moments approach for ab initio 3D molecular reconstruction from 2D projected cryogenic electron microscopy (cryo-EM) images.
- Formulated mathematical framework using representation theory, harmonic analysis and numerical analysis, generalizing viewing angle distribution representation to **arbitrary basis functions**, enabling enhanced representation power for diverse real data distributions.
- Implemented algorithms in MATLAB and validated reconstruction accuracy on synthetic data.

Professional Experience

ByteDance — May 2025 – Present
Seed-AI for Science, Research Scientist Intern — San Jose, CA

- Leading development of the **first** systematic PyTorch-based open-source cryo-EM reconstruction software **from scratch**, addressing limitations of traditional tools with poor extensibility and limited GPU acceleration, delivering superior performance and enhanced extensibility for AI-based method development.
- Executed complete software development lifecycle independently, from design to deployment.
- Developing **AI foundation generative model** using flow matching and discrete posterior sampling, integrating the software for downstream biology tasks, enabling enhanced protein structure prediction.
- Delivered core reconstruction module that achieves high-resolution 3D protein density reconstruction. Implemented **Distributed Data Parallel (DDP)** scaling across multiple GPUs and nodes, achieving 10x computational speedup.

Argonne National Laboratory May 2023 - Aug. 2023

Givens Associate, Advisor: Prof. Mihai Anitescu Chicago, IL

- Developed statistical parametric model for analyzing positional and substitutional disorder in crystallography.
- Proved theoretical convergence of algorithms with Julia implementation presented at DOE conference.

Deloitte Consulting (Shanghai) Aug. 2018 - Feb. 2019

Data Visualization & Analyst Intern Beijing, China

- Developed business intelligence dashboards for world-renowned companies; facilitated 4 bidding projects with 2 completed orders and 1 consulting project successfully delivered.

Publications

C. W. Magoon*, **F. Yang***, N. Aigerman, and S. Z. Kovalsky. "Differentiation Through Black-Box Quadratic Programming Solvers." *NeurIPS*, 2025.

(* Equal contribution)

Academic Activities

The Triangle Computational and Applied Mathematics Symposium (TriCAMS) Nov. 2023

Lightning Talk + Poster: Coupling Structural and Functional Brain Connectome

NSF Focused Research Group (FRG) Collaborative Research Meeting Nov. 2023

Presentation: Spatio-Temporal Analysis of Brain Imaging

2023 Summer Argonne Student Symposium (SASSy) Jul. 2023

Presentation: Statistical Model of Crystallographic Disorder

Teaching Experience

- TA for *Scientific Computation* (graduate level), *Optimization with Applications in Machine Learning*, *Numerical PDE*, *Linear Algebra*, *Discrete Mathematics*.
- Recitation Leader for *Calculus I, II, III*.

Computer skills

Python, PyTorch, MATLAB, Julia, R, JavaScript, Tableau