Xuheng Li

CONTACT

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EDUCATION

Bachelor of Science September 2017 - July 2021
School of Mathematical Sciences, Peking University. Beijing, China, 100871.
Major: Information and Computational Mathematics.

Doctor of Philosophy September 2021 - June 2027 (estimated)
Department of Computer Science, UCLA. Los Angeles, California, USA, 90095.
Major: Artificial Inteligence. Supervised by Professor Quanquan Gu.

PROFESSIONAL EXPERIENCE

Research Internship June 2024 - December 2024
Bytedance AI Lab.
Project: Trivialized momentum for protein conformation generation.

RESEARCH INTERESTS

My research interest lies broadly in machine learning, with a focus on the pretraining and inference of large language models. Specifically, I am curious about how the performance of high-dimensional models is affected by the underlying low-dimensional structure of the data and optimization algorithms.

PROJECTS

EurekaClaw March 2026 - Present
Automated research agent focusing on theoretical machine learning problems.

PUBLICATIONS

Dimension-Independent Convergence of Underdamped Langevin Monte Carlo in KL Divergence
Shiyuan Zhang*, Qiwei Di*, *Xuheng Li**, and Quanquan Gu. 2026. Under review. arxiv.

Mirror Diffusion Models for Mixed-Type EHR Time Series Generation
Xuheng Li, Shiyuan Zhang, Melika Emami, Mohit Yadav, Jun Han, Robert E. Tillman, and Quanquan Gu. 2026. Under review.

Best-of-Majority: Minimax-Optimal Strategy for Pass@k Inference Scaling
Qiwei Di*, Kaixuan Ji*, *Xuheng Li**, Heyang Zhao, and Quanquan Gu. 2025. Accepted by **ICLR 2026**. arxiv.

Understanding SGD with Exponential Moving Average: A Case Study in Linear

Regression
Xuheng Li, and Quanquan Gu. 2024. Under review. arxiv.

Risk Bounds of Accelerated SGD for Overparameterized Linear Regression
Xuheng Li, Yihe Deng, Jingfeng Wu, Dongruo Zhou, and Quanquan Gu. 2023. Accepted by **NeuIPS 2023 OPT Workshop** and **ICLR 2024**. arxiv.

Variance-Aware Feel-Good Thompson Sampling for Contextual Bandits
Xuheng Li, and Quanquan Gu. 2025. Accepted by **NeurIPS 2025**. arxiv.

Feel-Good Thompson Sampling for Contextual Dueling Bandits
Xuheng Li, Heyang Zhao, and Quanquan Gu. 2024. Accepted by **ICML 2024**. arxiv.

AWARDS

Outstanding Reviewer of NeurIPS 2025
Finalist of MCM/ICM 2020
Project: Markov chain model for soccer team formation.

TEACHING

Teaching Assistant for CS 161 at UCLA Fall 2022, Winter 2023
Fundamentals of Artificial Intelligence
Teaching Assistant for CS CM122 at UCLA Spring 2023
Algorithms in Bioinformatics
Teaching Assistant for CS 31 at UCLA Fall 2023, Winter 2024
Introduction to Computer Science I
Teaching Assistant for CS C121 at UCLA Spring 2024
Probabilistic Models in Computational Genomics

PROFICIENCIES

Programming:
- Python (including PyTorch)
- C/C++
- MatLab