

Diantong Li

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Education

The Chinese University of Hong Kong, Shenzhen, BS in Statistics Sept 2022 - Jul 2026

- **Related Courses:** Probability Theory, Real Analysis, Stochastic Process, Statistical Inference, Bayesian Statistics, Advanced Linear Algebra, Stochastic Simulation
- **Honors and Awards:** Academic Performance Scholarship (2023-2024, top1%; 2022-2023, top5%), Dean's List (2022-2025)

Research Interests

Data-driven Decision-making (Experimental Design, Drug Discovery)
Probabilistic Reasoning in Machine Learning
Deep Learning

Publications

Constrained Multi-objective Bayesian Optimization through Optimistic Constraints Estimation May 2025

Diantong Li, F. Zhang, C. Liu, Y. Chen

International Conference on Artificial Intelligence and Statistics (AISTATS), May 2025. [paper](#); [poster](#)

Research Experience

Constrained Multi-objective Bayesian Optimization Jul 2024 - May 2025

Advised by [Prof. Yuxin Chen](#), University of Chicago

Chicago, IL and Remote

This project focuses on developing a constrained multi-objective Bayesian optimization (CMOBO) algorithm. In real-world experiments, such as molecule search in drug discovery, researchers aim to optimize multiple black-box objectives while satisfying unknown constraints (e.g., medical safety thresholds). We developed a novel CMOBO algorithm that employs optimistic constraint estimation via upper confidence bounds, providing the first UCB-type high-probability bounds for Hypervolume regret and constraint violation. Our algorithm outperforms state-of-the-art methods in real-world molecule search and drug synthesis, achieving superior efficiency and robustness.

Few-shot Bayesian Optimization with Prior-fitted Neural Networks June 2025 - Present

Advised by [Prof. Chong Liu](#), State University of New York at Albany

Remote

We propose FSBO-MDP, a few-shot Bayesian optimization method that integrates Prior-Fitted Networks (PFNs) with a novel Markov Decision Process (MDP) prior. Unlike standard BO, our approach transfers procedural knowledge from related tasks by modeling expert optimization trajectories using reinforcement learning agents. This MDP-based prior captures both query-response patterns and decision-making strategies, enabling the PFN surrogate to make fast and informed predictions. We pre-train on synthetic function priors and fine-tune using sampled expert trajectories. Experiments on hyperparameter tuning and drug discovery benchmarks show that FSBO-MDP achieves faster convergence and superior sample efficiency compared to existing few-shot BO methods.

Industrial Experience

Anker Innovations × CUHK(SZ) Capstone Project:
Advertising and Optimization

Feb 2025 - June 2025

Advertising Algorithm Development Intern; Advised by [Prof. Zizhuo Wang](#)

Shenzhen, China

- Proposed a scalable model selection, evaluation and optimization advertising strategy based on deep causal learning
- Helped allocate advertising resource of each Anker's product in Amazon under a strict offline constraint, based

on a real-world advertisement dataset containing thousands of products across three global markets over a two-year span

- Led a team of 6 undergraduate students from different majors in CUHK(SZ). Won best capstone project presentation award (top 5 among 23 teams). A poster is available online

Teaching Experience

Undergraduate Student Teaching Fellowship	The Chinese University of Hong Kong, Shenzhen
Honors Probability and Statistics I	Fall 2024
Honors Probability and Statistics II	Spring 2025
Stochastic Process	Fall 2025

Skills

Languages: Python, R

Frameworks: PyTorch, BoTorch, GPyTorch, OR-Tools, CausalML, Gym

Machine Learning: Deep Learning, Transformer architecture, Reinforcement Learning, Bayesian Optimization