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, Statistical Inference, Bayesian Statistics, Stochastic Process, Advanced Linear Algebra, Stochastic Simulation, Design and Analysis of Algorithm, Machine Learning
- **Honors and Awards:** The Nobel Class Programme 2025 at CUHKSZ (one student per year); 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

Publications

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

Diantong Li, Fengxue Zhang, Chong Liu, Yuxin Chen

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

None To Optima in Few Shots: Bayesian Optimization with MDP Priors — September 2025

Diantong Li, Kyunghyun Cho, Chong Liu

preprint; *highlighted in an invited talk at NeurIPS 2025*

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 MDP Priors — June 2025 - Jan 2026

Advised by Prof. Chong Liu, State University of New York at Albany — Remote

We introduce the Procedure-inFormed BO (ProfBO) algorithm, which solves black-box optimization with remarkably few function evaluations. At the heart of our algorithmic design are Markov Decision Process (MDP) priors that model optimization trajectories from related source tasks, thereby capturing procedural knowledge on efficient optimization. We embed these MDP priors into a prior-fitted neural network and employ model-agnostic meta-learning for fast adaptation to new target tasks. Experiments on real-world Covid and Cancer benchmarks and hyperparameter tuning tasks demonstrate that ProfBO consistently outperforms state-of-the-art methods by achieving high-quality solutions with significantly fewer evaluations, making it ready for practical deployment.

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 CUHKSZ

Honors Probability and Statistics I	Fall 2024
Honors Probability and Statistics II	Spring 2025
Stochastic Process	Fall 2025

Other Services

Peer Advisor in The School of Data Science, CUHKSZ	Fall 2024
Reviewer	ICLR, 2026

Skills

Languages: Python, R

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

Machine Learning: Bayesian Optimization, Transformer models