

Diantong Li

diantongli@link.cuhk.edu.cn | <https://dancewithdiantong.github.io/>

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 CUHK SZ (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
Under Review at ICLR 2026. [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

CUHK SZ

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, CUHK SZ

Fall 2024

Reviewer

ICLR, 2026

Skills

Languages: Python, R

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

Machine Learning: Bayesian Optimization, Transformer models