

Yimeng Zeng

🏠 yimengz.org | ✉ yimengz@seas.upenn.edu

RESEARCH

I develop methods that combine generative modeling and Bayesian optimization (BO) to solve open-ended design problems in science. By pairing generative models (e.g., VAEs/LLMs) with Bayesian optimization, my methods find high-performing candidates more efficiently. Applications include biomedical discovery (antibody/peptide design) and data systems (query planning/code optimization), focusing on end-to-end, closed-loop pipelines that learn from real-world feedback.

EDUCATION

University of Pennsylvania

- Ph.D. in Computer Science 08/2022 - Now

Cornell University

- B.S. in Computer Science 08/2018 - 05/2022
- B.S. in Mathematics 08/2018 - 05/2022

Publications

See also at my Google Scholar page  * denotes equal contribution.

Refereed Conference & Journal Publications

- [C1] Natalie Maus, Kyurae Kim, **Yimeng Zeng**, Haydn Thomas Jones, Fangping Wan, Marcelo Der Torossian Torres, Cesar de la Fuente-Nunez, Jacob R. Gardner
Multi-Objective Coverage Bayesian Optimization (MOCOBO)
Advances in Neural Information Processing Systems (NeurIPS). 2025. [\[paper\]](#)
- [C2] Alexander Shypula, Aman Madaan, **Yimeng Zeng**, Uri Alon, Jacob Gardner, Milad Hashemi, Graham Neubig, Parthasarathy Ranganathan, Osbert Bastani, Amir Yazdanbakhsh
Automated High-Level Code Optimization for Warehouse Performance
IEEE Micro, “Top Picks” issue. 2025. [\[paper\]](#)
- [C3] Wentao Guo, Jikai Long, **Yimeng Zeng**, Zirui Liu, Xinyu Yang, Yide Ran, Jacob R. Gardner, Osbert Bastani, Christopher De Sa, Xiaodong Yu, Beidi Chen, Zhaozhuo Xu
Zeroth-Order Fine-Tuning of LLMs with Transferable Static Sparsity
Proceedings of the International Conference on Learning Representations (ICLR). 2025. *Also appeared at the ES-FOMO-II & WANT Workshops, ICML 2024.* [\[paper\]](#)
- [C4] Jeffrey Tao, Natalie Maus, Haydn Jones, **Yimeng Zeng**, Jacob R. Gardner, Ryan Marcus
Learned Offline Query Planning via Bayesian Optimization
Proceedings of the ACM SIGMOD International Conference on Management of Data (SIGMOD). 2025. [\[paper\]](#)
- [C5] Alexander Shypula, Aman Madaan, **Yimeng Zeng**, Uri Alon, Jacob Gardner, Milad Hashemi, Graham Neubig, Parthasarathy Ranganathan, Osbert Bastani, Amir Yazdanbakhsh
Learning Performance-Improving Code Edits
Proceedings of the International Conference on Learning Representations (ICLR). 2024. [\[paper\]](#) [\[code\]](#)

- [C6] Michael S. Yao, **Yimeng Zeng**, Hamsa Bastani, Jacob R. Gardner, James Gee, Osbert Bastani
Generative Adversarial Model-Based Optimization via Source Critic Regularization
 Advances in Neural Information Processing Systems (NeurIPS). 2024. [\[paper\]](#) [\[slides\]](#) [\[poster\]](#) [\[code\]](#)

Workshop Papers

- [W1] **Yimeng Zeng**, Jeffrey Tao, Haydn Thomas Jones, Natalie Maus, Osbert Bastani, Jacob R. Gardner, Ryan Marcus
Adversarial Query Synthesis via Bayesian Optimization
 NeurIPS ML for Systems Workshop. 2025. [\[paper\]](#)
- [W2] **Yimeng Zeng**, Hunter Elliott, Phillip Maffettone, Peyton Greenside, Osbert Bastani, Jacob R. Gardner
Antibody Design with Constrained Bayesian Optimization
 ICLR Workshop on Generative & Experimental Methods in Biology (GEMBio). 2024. *Oral.* [\[paper\]](#) [\[poster\]](#)

Preprints

- [P1] **Yimeng Zeng**, Natalie Maus, Haydn Thomas Jones, Jeffrey Tao, Fangping Wan, Marcelo Der Torossian Torres, Cesar de la Fuente-Nunez, Ryan Marcus, Osbert Bastani, Jacob R. Gardner
Large Scale Multi-Task Bayesian Optimization with Large Language Models
arXiv preprint. 2025. [\[paper\]](#)
- [P2] Marcelo D. T. Torres*, **Yimeng Zeng***, Fangping Wan*, Natalie Maus, Jacob Gardner, Cesar de la Fuente-Nunez
A Generative Artificial Intelligence Approach for Antibiotic Optimization
bioRxiv preprint. 2024. [\[paper\]](#) [\[code\]](#)
- [P3] Halley Young, **Yimeng Zeng**, Jacob Gardner, Osbert Bastani
Improving Structural Diversity of Black-Box LLMs via Chain-of-Specification Prompting
arXiv preprint. 2024. [\[paper\]](#)
- [P4] Natalie Maus*, **Yimeng Zeng***, Daniel Allen Anderson, Phillip Maffettone, Aaron Solomon, Peyton Greenside, Osbert Bastani, Jacob R. Gardner
Inverse Protein Folding Using Deep Bayesian Optimization
arXiv preprint. 2023. [\[paper\]](#)

TEACHING EXPERIENCE

- **Graduate Teaching Assistant, University of Pennsylvania**
 - CIS 5200 Introduction to Machine Learning 08/2023 - 12/2023
- **Undergraduate Teaching Assistant, Cornell University**
 - CS 4780 Intro to Machine Learning 08/2021 - 05/2022

ACADEMIC SERVICE

- **Reviewer:** NeurIPS'24, ACL ARR (June 2024), NeurIPS'25, ICLR'26

HONORS

- University of Pennsylvania Graduate Fellowship
- Cornell University Dean's List, College of Arts and Sciences 19FA, 20FA