

Yimeng Zeng

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RESEARCH

My research develops LLM-centric generative optimization methods, combining generative models with Bayesian optimization (BO) to solve open-ended design problems efficiently. I focus on end-to-end, closed-loop systems that propose candidates, evaluate them, and learn from feedback. Applications include biomedical discovery (antibody/peptide design) and systems performance optimization (query planning and code optimization).

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] **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
[Scaling Multi-Task Bayesian Optimization with Large Language Models](#)
Proceedings of the International Conference on Learning Representations (ICLR). 2026.
- [C2] 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 \[code\]](#)
Nature Machine Intelligence. (Pre-accepted). 2026.
- [C3] 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.
- [C4] 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.
- [C5] 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.
- [C6] Jeffrey Tao, Natalie Maus, Haydn Jones, **Yimeng Zeng**, Jacob R. Gardner, Ryan Marcus
[Learned Offline Query Planning via Bayesian Optimization \[code\]](#)

- [C7] 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 \[code\]](#)
Proceedings of the International Conference on Learning Representations (ICLR). 2024.
- [C8] Michael S. Yao, **Yimeng Zeng**, Hamsa Bastani, Jacob R. Gardner, James Gee, Osbert Bastani
[Generative Adversarial Model-Based Optimization via Source Critic Regularization \[slides\] \[poster\] \[code\]](#)
Advances in Neural Information Processing Systems (NeurIPS). 2024.

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.
- [W2] **Yimeng Zeng**, Hunter Elliott, Phillip Maffettone, Peyton Greenside, Osbert Bastani, Jacob R. Gardner
[Antibody Design with Constrained Bayesian Optimization \[poster\]](#)
ICLR Workshop on Generative & Experimental Methods in Biology (GEMBio). 2024. Oral.

Preprints

- [P1] Natalie Maus, **Yimeng Zeng**, Haydn Thomas Jones, Yining Huang, Gaurav Ng Goel, Alden Rose, Kyurae Kim, Hyun-Su Lee, Marcelo Der Torossian Torres, Fangping Wan, Cesar de la Fuente-Nunez, Mark Yatskar, Osbert Bastani, Jacob R. Gardner
[Purely Agentic Black-Box Optimization for Biological Design](#)
- [P2] Halley Young, **Yimeng Zeng**, Jacob Gardner, Osbert Bastani
[Improving Structural Diversity of Black-Box LLMs via Chain-of-Specification Prompting](#)
- [P3] 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](#)

TEACHING EXPERIENCE

- **Graduate Teaching Assistant, University of Pennsylvania**
 - CIS 5200 Introduction to Machine Learning 08/2023 - 12/2023
 - CIS 6200 Advanced Topics in Machine Learning 01/2026 - 05/2026
- **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, ICML'26

HONORS

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