Yimeng Zeng

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RESEARCH

I develop methods at the intersection of probabilistic machine learning, Bayesian optimization, and generative modeling. My work combines large language models with principled optimization for open-ended design problems, using generative models as priors in BO loops to enable sample-efficient search. Applications span natural sciences (peptide/protein sequence design) and systems challenges (database query optimization). I focus on building closed-loop discovery pipelines that integrate modeling, acquisition, and real-world feedback, emphasizing reliability, interpretability, and scalability.

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**] 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]

[**C2**] 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]

[**C3**] 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.

[**C4**] 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]

[**C5**] 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**, 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**] 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]

[**P2**] Halley Young, **Yimeng Zeng**, Jacob Gardner, Osbert Bastani
Improving Structural Diversity of Black-Box LLMs via Chain-of-Specification Prompting
arXiv preprint. 2024. [paper]

[**P3**] 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]

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

HONORS

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