Theo Sternlieb

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EXPERIENCE

Deep Learning Researcher July 2024 – Present
Dyno Therapeutics

- Led research integrating high-throughput binding affinity assay data with AlphaFold2 for protein-protein interaction prediction, achieving significant performance gains over sequence-based models.
- Fine-tuned structure prediction methods with a denoising diffusion probabilistic modeling (DDPM) objective to obtain structure-conditional generative models of peptide binders.
- Investigated performance of AlphaFold2 in the context of disordered and co-evolution free binding prediction, leading to new insights into computational prediction of short linear motif mediated interactions.

Machine Learning Engineer July 2022 – July 2024
Dyno Therapeutics

- Contributed tens of thousands of protein designs to high-throughput *in vivo* and *in vitro* libraries, accelerating evaluation of in-house models.
- Implemented and evaluated a number of model-based optimization methods for protein design enhancing performance on internal data.
- Constructed inference pipeline for large protein language models, enabling the machine learning team to scale to millions of *in silico* protein designs screened with AlphaFold2.

Research Assistant August 2020 – June 2022
Thayer Lab, Wesleyan University

- Developed graph generative models for small molecules, trained using self-supervised learning on molecular corpora, and fine-tuned with policy gradients based on docking simulation rewards against specific targets.
- Performed molecular dynamics simulation of P53-DNA complexes and developed self-supervised methods for classification of stable states.
- Led workshops introducing lab members to key concepts in deep learning and their implementation using TensorFlow.

EDUCATION

Wesleyan University Middletown, CT
Sep 2021 – May 2022
Master of Arts, Computer Science
GPA: 3.95/4.00

Wesleyan University Middletown, CT
Sep 2017 – May 2021
Bachelor of Arts, Mathematics
GPA: 3.50/4.00

TECHNICAL SKILLS

Languages and Frameworks
Python, PyTorch, TensorFlow, DGL, Bash

Protein Modeling
RFdiffusion, ProteinMPNN, PyMol, ESM2, Structure Prediction

TEACHING HISTORY

- **Special Topics in Computer Science: Artificial Intelligence (COMP360D)**, *Wesleyan University*, Teaching Assistant
- **Machine Learning (COMP343)**, *Wesleyan University*, Teaching Assistant

PAPERS

- **Sternlieb, Theodore**, Jakub Otwinowski, and Jeffrey Chan. "Low-n OpenFold fine-tuning improves peptide design without additional structures" (2024)
- **Sternlieb, Theodore**, Abhishaike Mahajan, Davian Ho, and Jeffrey Chan. "De Novo Short Linear Motif (SLiM) Discovery With AlphaFold-Multimer." (2023).
- Damani, Farhan, David H. Brookes, **Theodore Sternlieb**, [...]. "Beyond the training set: an intuitive method for detecting distribution shift in model-based optimization." arXiv preprint arXiv:2311.05363 (2023).
- **Sternlieb, Theodore Beck**. "Target Specific Drug Design with Deep Reinforcement Learning." PhD diss., Wesleyan University, 2022.