## **Pascal Sturmfels**

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#### **EDUCATION**

# Ph.D. in Computer Science, Institute for Protein Design, University of Washington

- I was supervised by David Baker. My research focused on developing deep learning models for protein design and structure prediction, and in particular predicting the structure of protein-ligand complexes. I was generally interested in applications in drug discovery, including docking and virtual screening.
- From 2018 to 2020 I worked in the AIMS Lab developing methods for explainable machine learning.

# **B.E in Computer Science, Minor in Mathematics**, University of Michigan

Fall 2017

June 2024

#### **EMPLOYMENT**

# Vilya, Deep Learning Scientist

September 2024 - Now

• Working on deep learning models for drug discovery, particularly structure prediction and virtual screening

#### Meta AI Research, Research Intern

Summer 2022

- Supervised by Alexander Rives and Adam Lerer
- Developed large language models for protein sequence diversification tasks

## Salesforce Research, Research Intern

Summer 2020

- Supervised by Nazneen Rajani, Jesse Vig and Ali Madani
- Worked on novel, self-supervised pre-training tasks for protein language models

#### MLD3 Lab, Research Assitant

September 2017 - May 2018

- Supervised by Jenna Wiens
- Designed new CNN architectures for predicting properties from MRI scans

#### Microsoft, Software Engineering Intern

Summer 2017

• Worked on the Core Services Engineering and Operations Team (CSEO)

#### **CAAR REU**, Research Assistant

Summer 2016

- Supervised by Samir Khuller
- Worked on approximation algorithms for online machine scheduling problems

### Pachter Lab, Research Assistant

May 2015 - July 2016

- Supervised by Lior Pachter and Harold Pimental
- Worked on data visualization tools for differential expression analysis.

# TEACHING EXPERIENCE

### Teaching Assistant, University of Washington

### • CSE 312: Foundations of Computing

Summer 2021

• CSE 427: Computational Biology

Spring 2021

• CSE 546: Machine Learning

Fall 2018

### Teaching Assistant, University of Michigan

• EECS 445: Machine Learning

Fall 2017

• EECS 376: Theory of Computation

Winter 2017

#### **PUBLICATIONS**

- [1] Krishna, Rohith, Jue Wang, Woody Ahern, **Pascal Sturmfels**, Preetham Venkatesh, Indrek Kalvet, Gyu Rie Lee et al. "Generalized biomolecular modeling and design with RoseTTAFold All-Atom." Science (2024).
- [2] **Sturmfels, Pascal**, Roshan Rao, Robert Verkuil, Zeming Lin, Ori Kabeli, Tom Sercu, Adam Lerer, and Alexander Rives. "Seq2MSA: A Language Model for Protein Sequence Diversification." Machine Learning for Structural Biology, NeurIPS Workshop (2022).
- [3] Rutherford, Saige, **Pascal Sturmfels**, Mike Angstadt, Jasmine Hect, Jenna Wiens, Marion I. van den Heuvel, Dustin Scheinost, Moriah Thomason, and Chandra Sripada. "Observing the origins of human brain development: automated processing of fetal fMRI." Neuroinformatics (2021): 1-13.

- [4] Beebe-Wang, Nicasia, Safiye Celik, Ethan Weinberger, Pascal Sturmfels, Phillip L. De Jager, Sara Mostafavi, and Su-In Lee. "Unified AI framework to uncover deep interrelationships between gene expression and Alzheimer's disease neuropathologies." Nature communications 12.1 (2021): 1-17.
- [5] Janizek, Joseph D.\*, **Pascal Sturmfels**\*, and Su-In Lee. "Explaining Explanations: Axiomatic Feature Interactions for Deep Networks." Journal of Machine Learning Research 22.104 (2021): 1-54.
- [6] Erion, Gabriel\*, Joseph D. Janizek\*, Pascal Sturmfels\*, Scott Lundberg, and Su-In Lee. "Improving performance of deep learning models with axiomatic attribution priors and expected gradients." Nature Machine Intelligence (2021): 1-12.
- [7] Evtimov, Ivan, **Pascal Sturmfels**, and Tadayoshi Kohno. "FoggySight: A Scheme for Facial Lookup Privacy." Proc. Priv. Enhancing Technol. 2021.3 (2021): 204-226.
- [8] **Sturmfels, Pascal**, Jesse Vig, Ali Madani, and Nazneen Fatema Rajani. "Profile Prediction: An Alignment-Based Pre-Training Task for Protein Sequence Models." Machine Learning for Structural Biology, NeurIPS Workshop (2020).
- [9] **Sturmfels, Pascal**, Scott Lundberg, and Su-In Lee. "Visualizing the impact of feature attribution baselines." Distill 5, no. 1 (2020): e22.
- [10] Khuller, Samir, Jingling Li, Pascal Sturmfels, Kevin Sun, and Prayaag Venkat. "Select and permute: An improved online framework for scheduling to minimize weighted completion time." Theoretical Computer Science 795 (2019): 420-431.
- [11] Sturmfels, Pascal, Saige Rutherford, Mike Angstadt, Mark Peterson, Chandra Sripada, and Jenna Wiens. "A Domain Guided CNN Architecture for Predicting Age from Structural Brain Images." In Machine Learning for Healthcare Conference, pp. 295-311. 2018.
- [12] Pimentel, Harold, **Pascal Sturmfels**, Nicolas Bray, Páll Melsted, and Lior Pachter. "The Lair: a resource for exploratory analysis of published RNA-Seq data." BMC bioinformatics 17, no. 1 (2016): 490.