Nikhil Shenoy

Email Website Google Scholar GitHub

About

I am currently a Senior Research Engineer at Recursion where I focus on developing ML methods to better understand physical interactions between molecules. I am also involved in designing strong research engineering practices to enable effective development, scaling, and deployment of models.

Work Experience

Recursion — **Toronto, Canada**

Senior Research Engineer 1 — *August 2025 – Current*

- Nesso-1: Led the development of a coarse-grained cofolding model for binding affinity prediction achieving >10× speedup over Boltz-2 with competitive out-of-distribution accuracy [Code: 200+ GitHub stars, Weights: 400k+ HF downloads].
- AquaGen: Co-developed an all-atom, explicit-solvent flow matching model for Boltzmann sampling on thousands of atoms, estimating hydration free energies 4–10× faster than GPU-based MD.

Machine Learning Engineer — *July 2024 – July 2025*

- Developed in-house expertise to work with protein structure models like AlphaFold, Boltz, etc. Enhanced conformational sampling abilities of these models by fine-tuning on molecular dynamics trajectories.
- Built scalable research infrastructure that reduced development time for different projects.

WadhwaniAI — **Mumbai, India**

Associate Machine Learning Scientist I — *August 2020 – September 2022*

- Cough Against Tuberculosis (TB): Built cough detection and unsupervised time-segment endpointing models for an audio-diagnostic TB triage tool; deployed across 21+ states with 400k+ patients screened.
- CottonAce: Developed a pest-monitoring model using object detection for Indian cotton farmers and compressed models via distillation for on-device Android inference. Recipient of the H&M Foundation Global Change Award [Code, Link].
- Cough Against Covid: Built an audio-diagnostic triage tool using cough sounds and symptoms; collected India's largest RT-PCR verified Covid-19 cough dataset and open-sourced the codebase.

Education

University of British Columbia — **September 2022 – July 2024**

M.Sc (Thesis) in Computer Science, GPA: 92.0% — *Vancouver, Canada*

Indian Institute of Technology, Delhi — **July 2016 – May 2020**

B.Tech in Biochemical Engineering and Biotechnology, GPA : 8.06 / 10.00 — *New Delhi, India*

Internships

Recursion — **Montreal, Canada**

Machine Learning Intern — *May 2023 – December 2023*

- ET-Flow: Improved molecular conformer generation with generative equivariant transformers [NeurIPS 2024, Code].
- Built openQDC, an open-source repository to access public QM datasets to train ML Potentials.
- Understand QM dataset biases to evaluate out-of-distribution performance of ML potentials [NeurIPS 2023 AI4Science].

Elucidata — **New Delhi, India**

Data Science Intern — *May 2019 – July 2019*

- Worked on classification models for breast cancer sub type classification. Used these classification models to classify other TCGA cancers into breast cancer subtypes to find out similarity.
- Built a Web App to perform Weighted Gene Co-Expression Analysis on RNA-seq data to visualise results. Additional features were designed to provide users with relevant insights across different cancers.

Computational Biology Lab, NTHU — **Hsinchu, Taiwan**

Research Intern — *May 2018 – July 2018*

- Performed drug-protein docking using Autodock Vina and extracted features using a python package PyMol. Used the features to predict the inhibitory response.