

ANKIT GUPTA

gupta.v.ankit@gmail.com • <http://www.ankitg.me>

EXPERIENCE

Reverie Labs

Co-Founder, CTO

Cambridge, MA

Nov 2017 — Present

Experienced AI/ML Entrepreneur and Startup Executive

- Co-Founder of Reverie Labs, pharmaceutical company using machine learning to drive kinase drug discovery
- Raised \$31M in funding from top investors, including Y-Combinator and First Round Capital
- Scaled team from 2 founders to 30 employees, actively hiring engineers, chemists, and executives across multiple roles.
- Advanced molecules using in-house AI/ML tools from virtual screening through lead opt and candidate nomination
- Wore many hats as a founder alongside hands-on engineering leadership, including managing budgets, handling HR and benefits, fostering relationships with investors and fundraising, and driving partnerships with big pharma companies.

Hands-On Technical Leader

- Directly oversaw team of engineers spanning infrastructure, machine learning, full-stack, and front-end. Managed and grew several individual contributors from new-grad to staff-level engineers, and developed new managers for subteams as the company grew. Set a culture of rapid iteration and product release to therapeutic teams.
- Defined the strategy and vision as a novel computationally-enabled pharma company, setting the roadmap for a hybrid research/engineering org that enabled creative breakthroughs while shipping code that was useful to therapeutic programs
- Recruited and retained elite machine learning talent (often against deep-pocketed competitors) by building state-of-the-art technology, fostering a culture of growth and ownership, and engaging with the broader academic community
- Led the development of a modern deep learning research/development org delivering dozens of production models for molecular potency/ADMET properties to in-house therapeutic programs in oncology
- Secured a multi-year partnership with Roche/Genentech to advance 3 therapeutic targets enabling multi-million dollar up-front revenue, and developed engineering culture and roadmap that enabled secure data sharing and collaboration.

Led Development of Modern AI-Enabled Software Stack

- Discovered multiple breakthrough AI/ML models, with deep expertise in graph neural networks and generative AI methods
- Oversaw the development of a modern multi-region, multi-account secure AWS Cloud environment, enabling massive-scale training and inference of ML models with 1000s of GPUs, and large-scale CPU workflows spanning 100,000s of cores
- Contributed extensively to the design and implementation of an AWS-hosted Kubernetes cluster running workloads spanning machine learning training, inference, computational chemistry simulations, and software automation.
- Led the development of systems for dataset/model registries, model versioning, automatic retraining and redeployment, and retrospective dashboards for automatic historical analysis of production models.
- Led the development of substantial CI/CD automation to enable a smooth developer experience even as a nimble startup, giving in-house developers a modern Dockerized workflow across all develop types, enabled by Github self-hosted runners.
- Managed the development of a in-house Django-based suite of generative molecular design technologies, enabling therapeutic teams to access computational scale to enable parallel molecular design.

Vicarious AI

Research Engineer (Deep Learning)

San Francisco Bay Area, CA

July 2017 — Nov 2017

- Worked as research engineer at 50-person ML/robotics company with \$130M+ in funding
- Designed and implemented large-scale deep learning models for visual perception

TECHNICAL SKILLS

Programming Languages

Python, C++, C, Java, Go, Typescript, SQL, HTML, CSS, MATLAB

Tools

AWS Cloud Infra, PyTorch, Tensorflow, Ray, Docker, Kubernetes, Git

EDUCATION

Harvard University, B.A./M.S. in Computer Science

Cambridge, MA

GPA: 3.94/4.0. Magna Cum Laude with Highest Honors. Inducted into Phi Beta Kappa.

Coursework includes: Deep Learning (CS 287), Machine Learning (CS 181, CS 281), Distributed Comp. (CS 262), Prob. Algorithms (CS 223), Parallel Comp. (CS 205), Data Struct./Alg. (CS 124), Probability (Stat 110), Real Analysis (Math 25)

- Conducted **deep learning thesis research**. Studying transcription factor binding. Published/presented work at ICML.
- Head Teaching Fellow for CS 181 (Machine Learning) - Taught section, wrote and graded problem sets, and held office hours. Taught four course-wide review sessions per semester.
- Teaching Fellow for CS 182 (Artificial Intelligence) - Taught section, graded problem sets, and held office hours

EXPERIENCE (CONTINUED)

Harvard University School of Engineering and Applied Sciences

Cambridge, MA

Researcher and Machine Learning Teaching Fellow

Jan 2016 — June 2017

- Short Paper “Dilated Convolutions for Modeling Long-Distance Genomic Dependencies” was accepted to the ICML 2017 Workshop on Computational Biology. Invited to give one of four contributed talks.
- Won Speaker Award and Best Poster Award at ICML 2017 workshop. Talk viewable at <https://youtu.be/HmCecphEvQg>.
- Taught sections, held office hours, and wrote and graded problem sets for Harvard’s undergraduate machine learning courses
- Held 8 course-wide exam review sessions across two semesters with 100+ students in attendance at each

Palantir and Google

Various

Software Engineering Internships

2015-2016

- Worked as full-stack developer on Palantir’s core Spark-based data analysis and visualization product
- Designed back-end for new data transformation prototype product that is used in production across the company
- Engaged closely with team of engineers to actively develop a product used across dozens of high-impact deployments
- Developed back-end software for Google’s content ad targeting teams, using internal parallel data processing tools
- Used text clustering machine learning models to diagnose the source of misclassifications of advertisements