

# ANKIT GUPTA

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## Experienced AI/ML Entrepreneur and Technology 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.
- Advanced molecules using in-house AI/ML tools from virtual screening through lead opt and candidate nomination.
- 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.
- Scaled team from 2 founders to 30 employees, actively hiring engineers, chemists, and executives across multiple roles.
- Wore many hats as a founder alongside hands-on engineering leadership, including managing budgets, handling HR, fostering relationships with investors and fundraising, and driving deep partnerships with big pharma companies.

## EXPERIENCE

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### Reverie Labs

Co-Founder, CTO

Cambridge, MA

Nov 2017 — Present

#### Hands-On Technical Leader

- 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.
- 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.
- 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.
- Managed multi-national data acquisition initiatives via partners in China, India, Ukraine, Europe, and Canada.

#### 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 Python-based suite of generative molecular design technologies with Django-based web tooling, 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

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### ML/AI

PyTorch, Tensorflow, Graph Convolutions, Transformers, Diffusion Models

### Software Tools

AWS Infra, Ray, Docker, Kubernetes, Terraform, Helm, Django, SQL, NoSQL, Git

### Programming Languages

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

## EDUCATION

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### Harvard University, B.A. in Computer Science

Cambridge, MA

### Harvard University, M.S. in Computer Science

Magna Cum Laude with Highest Honors. Inducted into Phi Beta Kappa.

- Published and presented **deep learning research at ICML**. Focus on modeling transcription factor binding.
- Head Teaching Fellow for CS 181 (Machine Learning) and CS182 (Artificial Intelligence) - Taught students, wrote problem sets, and held office hours.

## EXPERIENCE (CONTINUED)

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### 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*

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