

ASHKA SHAH

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EDUCATION

The University of Chicago

Ph.D. in Computer Science

Chicago, IL

October 2025 (Expected)

Harvey Mudd College

B.S. in Physics

Claremont, CA

May 2016

SKILLS

Languages: Python, PyTorch, Tensorflow, C++

Research: AI for Science, Causal Discovery, Knowledge Graphs, Optimal Experimental Design, Systems Biology

RESEARCH EXPERIENCE

The University of Chicago

Department of Computer Science, Advised by Rick Stevens

Chicago, IL

Fall 2019 – Present

- Parallel causal discovery using overlapping graph partitioning. Proof that divide-and-conquer strategy produces consistent results in infinite data limit. Empirical analysis of speed and accuracy with comparable algorithms ([Code](#)).
- Developed SP-GIES – a structure learner that achieves 4x speedup compared to existing algorithms. SP-GIES learns causal relationships of gene interaction networks using interventions ([Code](#)).
- Leveraged graph representations of enumerated drug libraries for efficient navigation of the chemical space using scaffold subgraphs.
- Investigated use of counterfactuals and adversarial examples in tabular RNA sequence model robustness.
- Implemented and trained deep learning image models to predict dock scores of COVID-19 protein targets for virtual screening tasks.

Flatiron Institute

Center for Computational Biology, Advised by Olga Troyanskaya

New York, NY

May 2023 – August 2023

- A case study on causal discovery with human tissue-specific gene expression data for inferring gene regulatory networks from functional networks ([Code](#)).

Argonne National Laboratory

Advised by Rick Stevens, Arvind Ramanathan

Chicago, IL

June 2020 – September 2020, June 2021 – September 2021

- Developed optimal experimental design algorithms for selecting interventional experiments for recovering causal mechanisms in gene regulatory networks.
- Implemented DNA Assembly protocols on Opentrons OT-2 pipetting robots for Argonne's Rapid Prototyping Laboratory.

WORK EXPERIENCE

Lawrence Livermore National Laboratory

National Ignition Facility Computation Software Engineer, Supervised by Jarom Nelson

Livermore, CA

June 2016 – Aug 2019

- Designed, developed and tested VBL (Virtual Beamline) laser propagation model of NIF laser system in C++ for use in high performance computing environments.

RELEVANT COURSEWORK

Probabilistic Graphical Models (Toyota Institute of Technology, Spring 2022)
Machine Learning (The University of Chicago, Spring 2020)
Biophysics of Biomolecules (The University of Chicago, Spring 2020)
Topics in Computer Architecture (The University of Chicago, Winter 2020)
Machine Learning in Medicine, (The University of Chicago, Fall 2019)
Argonne Training Program on Extreme-Scale Computing (Argonne National Laboratory, Summer 2020)

TEACHING

CMSC 35440 - Machine Learning in Biology and Medicine (The University of Chicago, Fall 2023)
CMSC 14100 - Introduction to Data Science Guest Lecture (The University of Chicago, Summer 2022)
CMSC 14100 - Introduction to Computer Science I (The University of Chicago, Fall 2019)

PUBLICATIONS

[Causal Discovery over High-Dimensional Structured Hypothesis Spaces with Causal Graph Partitioning](#) *ICML 2024 AI for Science Workshop, Best Paper Award*

[Causal Discovery and Optimal Experimental Design for Genome-Scale Biological Network Recovery](#) *PASC 2023*

[Scaffold-Induced Molecular Subgraphs \(SIMSG\): Effective Graph Sampling Methods for High-Throughput Computational Drug Discovery](#) *BMC Bioinformatics 2022*

[Probing Decision Boundaries in Cancer Data Using Noise Injection and Counterfactual Analysis](#) *Computational Approaches to Cancer Workshop at SC 2021*

[IMPECCABLE: Integrated Modeling Pipeline for COVID Cure by Assessing Better Leads](#) *ICPP 2021*

POSTERS

Hypothesis Ranking and Causal Discovery for Antimicrobial Resistance
The University of Chicago Data Science Institute AI + Science Summer School, August 2022

Addressing Challenges in Developing Virtual Beamline: A Large-Scale, High-Energy Parallel Laser Simulation Code
Grace Hopper Celebration Poster Session, Sept 2018

HONORS AND LEADERSHIP

Secretary of Energy Achievement Honor Award 2021 (National Virtual Biotech Lab Team)
Graduate Women in Computer Science Co-Chair 2020 – 2022 (The University of Chicago)
Crerar Fellowship 2019 (The University of Chicago)

VOLUNTEER WORK

South Side Science Festival (August 2022)
Editor at ACM's Student Magazine XRDS (2021 – 2022)
CS Education Week (Little Village High School, 2020)
Girls Who Code (2018 – 2019)