http://amyxlu.github.io github.com/amyxlu

EDUCATION

University of California, Berkeley

PhD Student, Department of Electrical Engineering and Computer Science

Berkeley, USA

Aug 2021 - Present

University of Toronto

Masters in Computer Science

Toronto, Canada

Jan 2019 - May 2020

University of Waterloo

Bachelors of Science, Honours Science, Bioinformatics Option

Waterloo, Canada

Sept 2014 - May 2018

RESEARCH EXPERIENCE

Google Brain

Mountain View, USA

Student Researcher — Research Host: Andreea Gane, Lucy Cowell

May 2022 - Present

- Protein sequence modelling: Understanding protein functions with machine learning.

UC Berkeley/Berkeley AI Research

Berkeley, USA

PhD Student — Advisor: Nilah Ioannidis

July 2021 - Present

- Biological sequence design: Developing methods for ML-guided protein design.

Insitro

South San Francisco, USA

July 2020 - July 2021

Machine Learning Engineer III

- Image profiling: Engineered representations of microscopy image phenotypes for drug discovery.
- Molecular design: Supported ML-guided design of small molecules through representation learning and chemoinformatics analyses.

University of Toronto/Vector Institute

Toronto, Canada

Masters Student — Advisors: Alan Moses, Marzyeh Ghassemi

Jan 2019 - May 2020

- Representation learning for proteins: Developed self-supervised representations for proteins using contrastive mutual information maximization (MLCB 2020, PLOS Computational Biology).
- Generalizability to distribution shifts: Benchmarked self-supervised computer vision methods for microscopy images to address generalization challenges to natural covariate shifts (NeurIPS 2019).
- ML for Health, algorithmic fairness: Quantitative and qualitative evaluation of bias in contextual word embeddings of clinical notes (*Spotlight*, ACM CHIL 2020).

Stanford University

Stanford, USA

Visiting Student Researcher — Advisor: Anshul Kundaje

Sept 2019 - Jan 2020

Regulatory genomics: Using domain adaptation methods to enable transcription factor binding prediction when
evaluating on holdout cell lines.

Harvard Medical School/Boston Children's Hospital

Boston, USA

 $Intern,\ Research\ Computing\ --\ Advisor:\ Piotr\ Sliz$

Jun 2018 - Jan 2019

- Exome variant prioritization: Understanding genotype-phenotype relationships in childhood epilepsy.

Interpreted important model features to seek novel disease-associated variants from whole exome (WES) data.

University of Waterloo

Waterloo, Canada

Undergraduate Thesis Student — Advisor: Andrew Doxey

Sept 2017 - May 2018

Chromatin accessibility: Prediction of accessible chromatin regions for femur growth regulation. Reconstructed
convolutional filters as a position-weighted matrix (PWM) with statistical matches in JASPAR, a database of
known motifs.

École polytechnique fédérale de Lausanne

Lausanne, Switzerland

Research Intern — Advisor: Matteo Dal Peraro

Jun 2017 - Sept 2017

 Molecular dynamics: Used molecular dynamics (MD) and GROMACS to simulate enzyme-membrane interaction mechanisms of NDM-1, an enzyme which confers antibiotic resistance.

PREPRINTS AND PUBLICATIONS

- AX Lu, AX Lu, I Pritišanac, T Zarin, JD Forman-Kay, AM Moses. Discovering molecular features of intrinsically disordered regions by using evolution for contrastive learning. PLOS Computational Biology.
- S Kolli, **AX Lu**, X Geng, A Kumar, S Levine. Data-Driven Optimization for Protein Design: Workflows, Algorithms and Metrics. *ICLR 2022 Workshop on Machine Learning for Drug Discovery workshop (MLDD)*.
- C Dallago, K Schütze, M Heinzinger, T Olenyi, M Littmann, **AX Lu**, KK Yang, S Min, S Yoon, JT Morton, B Rost. Using protein sequence representations from deep learning to visualize and predict protein sets. *Current Protocols*.
- AX Lu, H Zhang, M Ghassemi, AM Moses. Self-supervised contrastive learning of protein representations by mutual information maximization. *Machine Learning for Computational Biology (MLCB) 2020.*
- AX Lu, AX Lu, AM Moses. Evolution Is All You Need: Phylogenetic Augmentation for Contrastive Learning. Machine Learning for Computational Biology (MLCB) 2020.
- H Zhang*, **AX Lu***, M Abdalla, M McDermott, M Ghassemi. Hurtful Words: Quantifying Biases in Clinical Contextual Word Embeddings. <u>Spotlight</u>, ACM Conference on Health, Inference, and Learning (CHIL) 2020. *Equal Contribution.
- AX Lu, AX Lu, W Schormann, M Ghassemi, DW Andrews, AM Moses. The Cells Out of Sample (COOS) dataset and benchmarks for measuring out-of-sample generalization of image classifiers. *Neural Information Processing* Systems (NeurIPS) 2019.
- M Abdalla, H Zhang, **AX Lu**, I Chen, M Ghassemi. Quantifying Fairness in a Multi-Group Setting and its Impact in the Clinical Setting. *NeurIPS 2019 Workshop on Fair ML for Health*.
- AM Moses, AX Lu, AX Lu, M Ghassemi. Transfer Learning vs. Batch Effects: what can we expect from neural networks in computational biology? *Machine Learning for Computational Biology (MLCB) 2019*.
- AX Lu, AX Lu, AM Moses. Paired Cell Inpainting: A Multiple-Instance Extension of Self-Supervised Learning for Bioimage Analysis. ICML 2019 Workshop on Self-Supervised Learning.
- J Ban, M Tadrous, **AX Lu**, EA Cicinelli, SM Cadarette. Diffusion of indirect comparison meta-analytic methods to study drugs: a systematic review and co-authorship network analysis. *BMJ Open*.

Awards

- D. E. Shaw Graduate & Postdoc Women's Fellowship: Fellowship program for graduate & postdoc women in computational drug discovery.
- Paula Hawthorn Fellowship: UC Berkeley Computing, Data Science and Society departmental fellowship.
- NSERC Postgraduate Scholarships Doctoral program (PGS D) Award: Federal doctoral scholarship tenurable abroad, selected in the Committee for Computing Sciences.
- NSERC Canada Graduate Scholarships Doctoral (CGS D) Award: Federal doctoral scholarship tenurable only at a Canadian institution, selected in the Committee for Computing Sciences [DECLINED].
- Alexander Graham Bell Canada Graduate Scholarships Master's (CGS M) Award: Federal research scholarship for high-calibre Master's research students.
- NSERC Michael Smith Foreign Supplement: Supports high-calibre Canadian graduate students in pursuing research abroad.
- EPFL Scholarship of Excellence in Research: Sponsors students for research internship at EPFL.
- President's Scholarship of Distinction, Arebi Family Science Scholarship: University of Waterloo.
- Royal Conservatory of Music (RCM): ARCT Performer's Diploma in Piano.

SERVICE

- Research to the People, Core Team (formerly SVAI): Non-profit connecting patients of rare genomic diseases to the medical/AI research community and industry partners through collaborative research initiatives.
- Tosamaganga Hospital: Supported operations at a rural Tanzanian hospital.
- Residence Don: Organized events, responded to crises, and established rapport with diverse students. Leader for the Velocity Residence, a spin-off program of the Velocity start-up incubator.

REVIEWING

Machine Learning for Health: 2020, 2021, 2022 Machine Learning for Computational Biology: 2021 ICLR Workshop on AI4Science: 2022

ICML Workshop on AI4Science: 2022

NeurIPS Workshop on AI for Science: 2021, 2022

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NeurIPS Workshop on ML for Structural Biology: 2022 NeurIPS Workshop on Distribution Shifts: 2021, 2022 NeurIPS Workshop on Robustness in Sequence Modelling: 2022