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

I am interested in **developing machine learning methods for the unique challenges in computational biology**, especially in generalizability, representation learning, and fairness. I am currently exploring these interests at Insitro, a machine-learning driven drug discovery company led by Dr. Daphne Koller.

#### EDUCATION

#### University of Waterloo

Waterloo, Canada

Bachelors of Science, Honours Science, Bioinformatics Option

2014 - 2018

### University of Toronto, Vector Institute

Master's in Computer Science

Toronto, Canada 2019 - 2020

## RESEARCH EXPERIENCE

### Insitro

South San Francisco, USA

Machine Learning Engineer III

2020 - Present

- Research engineering, generalizability, image-based profiling: Engineering and researching generalizable and interpretable methods for high-throughput imaging and gene expression phenotypes.
- Molecular design, representation learning: Exploring problems in ML-guided molecular design through representation learning and uncertainty quantification.

#### Stanford University

Palo Alto, USA

Visiting Student Researcher — Domain Adaptation in Regulatory Genomics, Dr. Anshul Kundaje

2019 - 2019

• Domain adaptation, regulatory genomics, interpretability: Using domain adaptation methods to improve transcription factor binding prediction when evaluating for a different cell line.

# University of Toronto/Vector Institute

Toronto, Canada

Masters Student — Representation learning in genomics, Dr. Alan Moses & Dr. Marzyeh Ghassemi

2019 - 2020

- Self-supervised learning, representation learning for proteins: Developed a parameter-efficient representation for proteins using contrastive mutual information maximization (MLCB 2020; bioRxiv).
- Generalizability, microscopy imaging: Benchmarked self-supervised computer vision methods in a microscopy image dataset with covariate shift to highlight generalization failures in machine learning. (NeurIPS 2019).
- Algorithmic fairness, clinical decision support: Quantitative and qualitative evaluation of bias in contextual word embeddings on clinical notes; fairness definitions for multi-group settings. (Spotlight, ACM CHIL 2020).

## Harvard Medical School/Boston Children's Hospital

Boston, USA

Research Intern — Machine Learning in Clinical Genomics, Dr. Piotr Sliz

2018 - 2019

- Genotype-phenotype studies, clinical interpretability: Understanding disease genotype-phenotype relationships using machine learning models. Interpreted important model features to seek novel disease-associated variants from whole exome (WES) data.
- Variant filtering, pathway analyses: Applied standard filtering pipelines for false-positive variants. Explored classification from pathway- and variant-level features.
- Statistical genetics: Explored methods for capturing epistatic non-linearities and statistical dimensionality reduction.

### University of Waterloo

Waterloo, Canada

Undergraduate Thesis Student — Deep Learning in Regulatory Genomics, Dr. Andrew Doxey

2017 - 2018

- Chromatin accessibility prediction, interpretability: Trained a convolutional neural network to classify ATAC-seq accessible regions; reconstructed first-layer features as a position-weighted matrix (PWM) with statistical matches in JASPAR, a database of known motifs.
- Phylogenetics, metagenomic data mining: Used various bioinformatics pipeline tools (HMMER, BLAST, etc.) to understand biochemical properties of potentially uncharacterized toxins in metagenomic data.

# École polytechnique fédérale de Lausanne

Lausanne, Switzerland

Research Intern — Molecular Dynamics Simulations, Dr. Matteo Dal Parero

• Molecular dynamics: Used molecular dynamics (MD) and GROMACS to simulate enzyme-membrane mechanisms of bacterial "superbugs"

### University of Toronto

Toronto, Canada

Research Intern — Data Visualization in Pharmacoepidemiology, Dr. Suzanne Cadarette

2015 - 2017

• Data visualization, pharmacoepidemiology: Analysis and visualization of the social diffusion of methodological innovation in pharmacoepidemiology.

#### JOURNAL ARTICLES AND CONFERENCE PROCEEDINGS

- C Dallago, K Schtze, 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. Preprint.*
- AX Lu, AX Lu, AM Moses. Evolution Is All You Need: Phylogenetic Augmentation for Contrastive Learning. Machine Learning for Computational Biology (MLCB) 2020. Preprint.
- H Zhang\*, **AX Lu\***, M Abdalla, M McDermott, M Ghassemi. Hurtful Words: Quantifying Biases in Clinical Contextual Word Embeddings. Spotlight, ACM Conference on Health, Inference, and Learning (CHIL) 2020. \*Equal Contribution. Preprint.
- 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.* Preprint.
- 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*.
- 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*.

#### Workshop Papers and Posters

- C Dallago, K Schütze, M Heinzinger, T Olenyi, M Littmann, **AX Lu**, KK Yang, S Min, S Yoon, B Rost. Streamlining value of protein embeddings through bio\_embeddings. *NeurIPS 2020 Workshop on Learning Meaningful Representations of Life (LMRL)*.
- 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*.
- H Zhang\*, **AX Lu\***, M Abdalla, M McDermott, M Ghassemi. Hurtful Words: Quantifying Biases in Clinical Contextual Word Embeddings. Hurtful Words: Quantifying Biases in Clinical Contextual Word Embeddings. *NeurIPS 2019 Workshop on Machine Learning for Healthcare (ML4H).* \*Equal contribution.
- 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.
- AX Lu, S Rockowitz, A Poduri, P Sliz. From data to precision medicine: predictive machine learning models to uncover disease-associated variants. *Harvard Medical School BCMP Retreat 2019*.

#### Awards

- NSERC Postgraduate Scholarships Doctoral program (PGS D) Award: Federal doctoral scholarship tenurable abroad, selected in the Committee for Computing Sciences (\$63,000).
- NSERC Canada Graduate Scholarships Doctoral (CGS D) Award: Federal doctoral scholarship tenurable only at a Canadian institution, selected in the Committee for Computing Sciences (\$105,000) [DECLINED].
- Alexander Graham Bell Canada Graduate Scholarships Master's (CGS M) Award: Federal research grant (\$17,500).
- NSERC Michael Smith Foreign Supplement: "Supports high-calibre Canadian graduate students in pursuing research abroad" (\$6,000).
- Scholarship of Excellence in Research: Sponsors students for research internship at EPFL (CHF 4,500).
- University of Waterloo: Various entrance awards totaling \$6,000.
- Royal Conservatory of Music (RCM): ARCT Performer's Diploma in Piano.

#### SERVICE AND ACTIVITIES

- Program Committee: Reviewer, NeurIPS Workshop on Machine Learning for Health 2020.
- Research to the People (formerly SVAI): Core Team of Research to the People, a non-profit connecting patients of rare genomic diseases to the medical/AI research community and industry partners through collaborative research initiatives.
- Tosamaganga Hospital, Tanzania: 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 for the Velocity start-up incubator.

#### Teaching

- Teaching Assistant, Genetics: Taught weekly tutorial lectures for BIOL 239 at the University of Waterloo.
- Piano, music theory: Taught piano performance, ear training, RCM music history, and RCM Intermediate Rudiments.