# Alston Lo

alstonlo.github.io | 🖸 alstonlo | 🛅 alston-lo

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#### EDUCATION

Honours Bachelor of Science, University of Toronto (UofT)

Sep. 2019 - Jun. 2024

Math and Computer Science | cGPA: 4.00/4.00, Average: 96%

# **PUBLICATIONS**

- [1] **A. Lo**, R. Pollice, A. Nigam, A. D. White, M. Krenn, and A. Aspuru-Guzik, "Recent advances in the self-referencing embedded strings (SELFIES) library," *Digital Discovery*, vol. 2, pp. 897–908, 4 2023. DOI: 10.1039/D3DD00044C.
- [2] J. Bae, N. H. Ng, **A. Lo**, M. Ghassemi, and R. B. Grosse, "If influence functions are the answer, then what is the question?" In *Advances in Neural Information Processing Systems*, 2022. [Online]. Available: <a href="https://openreview.net/forum?id=hzbguA9zMJ">https://openreview.net/forum?id=hzbguA9zMJ</a>.
- [3] M. Krenn *et al.*, "SELFIES and the future of molecular string representations," *Patterns*, vol. 3, no. 10, p. 100588, 2022. DOI: 10.1016/j.patter.2022.100588.
- [4] W. D. Jeong\*, S. D. Jeong\*, K. R. Wang\*, and **A. Lo**\*, "siRNA-mediated silencing of antifungal resistance genes: A research protocol," *Undergraduate Research in Natural and Clinical Science and Technology Journal*, vol. 5, no. 8, pp. 1–7, 2021. DOI: 10.26685/urncst.292.

#### **PREPRINTS**

[1] A. Cheng\*, A. Lo\*, S. Miret, B. Pate, and A. Aspuru-Guzik, "Reflection-equivariant diffusion for 3D structure determination from isotopologue rotational spectra in natural abundance," 2023. arXiv: 2310.11609,

presented at MoML 2023, Accelerate 2023, and NeurIPS AI4Mat 2023 (spotlight, upcoming).

[2] A. Celaj *et al.*, "An RNA foundation model enables discovery of disease mechanisms and candidate therapeutics," *bioRxiv*, 2023. DOI: 10.1101/2023.09.20.558508,

presented at Oligonucleotide Therapeutics Society 2023 Annual Meeting.

\* Equal Contribution

#### Awards & Honors

Gold Medal, Best Model Award, and Nominations for Best Climate Crisis Project, Wiki, Integrated Human Practices, Entrepreneurship, and Presentation, iGEM	Oct. 2023
Qualcomm's Most Popular Project, EigenAI Conference, UTMIST	Sep. 2023
The James Scott Scholarship, UofT (\$500)	Feb. 2023
Dean's List Scholar, UofT	Dec. $2020 - Dec. 2022$
Gold Medal and Nomination for Best Conservation Project, iGEM	Oct. 2022
The Dickinson-Cartwright 3t0 Scholarship, UofT (\$500)	Nov. 2021
UofT In-Course Scholarships, UofT (\$1500)	Sep. 2021
Undergraduate Student Research Award, NSERC (\$7500)	May 2021
The Honourable Ray Lawson Scholarships, UofT (\$500)	Dec. 2020
The Joseph Alfred Whealy Scholarship, UofT (\$1500)	Sep. 2020
2 <sup>nd</sup> Place Research Proposal, Scinapse Undergraduate Case Competition	May 2020
The Elliott Scholarships, UofT (\$2000)	Sep. 2019
UofT Scholars Program Scholarship, UofT (\$7500)	Sep. 2019
7 <sup>th</sup> /3135 Place, Scholar with Distinction, UofT National Biology Competition (\$3000 scholar	arship) Apr. 2019

#### EXPERIENCE

# Research Intern, Deep Genomics, Toronto

May 2022 - Present

Full-time until May 2023, part-time afterwards

- Leveraged state-space models on long-range genomics tasks, achieving competitive performance to previous internal models, with only 17% as many parameters and 2.5× faster training speed
- Designed and implemented a tool that interfaces internal datasets with an accessible and reproducible API for training, supporting multiple ML frameworks

• Developed large genomics language models (200M+ parameters) in PyTorch and TensorFlow, for sequences with >100K tokens, and conducted distributed training on TPU pods and GPU clusters

# Machine Learning Research Assistant, The Matter Lab. UnfT

May 2020 - Present

Supervisors: Austin Cheng, Mario Krenn, and Prof. Alán Aspuru-Guzik

- Main developer for v1 onwards of their selfies library (see publications and projects)
- Trained variational autoencoders and applied disentanglement and dimensionality reduction techniques to investigate whether scientific insight can be extracted from the structured latent representations of molecules
- Formulated and researched equivariant diffusion models for *de novo* 3D-structure determination of molecules from their rotational spectra and crystal structure elucidation

#### Machine Learning Research Intern, Vector Institute, UofT

May 2021 - Jan. 2023

Supervisors: Juhan Bae and Prof. Roger Grosse, NSERC-funded

- Designed and implemented novel objectives for the efficient and scalable approximation of influence functions, which measure how training point(s) impact a deep model's predictions
- Assisted with empirical and theoretical analyses providing novel insights into influence functions

Researcher, Machine Intelligence Student Team, UofT

Project co-director | poster (presented at EigenAI conference) | samples

Sep. 2022 - Apr. 2023

• Developed a hybrid state-space Transformer diffusion model to compose classical piano performances, and trained the model on the MAESTRO dataset using mixed-precision and DDP parallelism

Project developer

Sep. 2023 – Present

• Formulating empirical analyses and improvements upon hashing approaches in neural graphics primitives

# Dry Lab Researcher, iGEM Toronto Club, UofT

• All work is done in a collaborative student-led effort and is presented at the International Genetically Engineered Machine (iGEM) competition

Team member | homepage

Apr. 2023 - Oct. 2023

• Constructed genome-scale metabolic models of methylotrophic bacteria and formulated flux balance analysis algorithms to discover gene knockout, overexpression, and addition targets that improve methanol consumption

Team member | homepage

Apr. 2022 – Oct. 2022

- Designed LAMP primers in silico for the rapid cell-free diagnosis of oak wilt fungal pathogen, using primer discovery and analysis tools such as PrimerExplorer, NEB Primer Design Tools, GLAPD, and Primer3
- Analyzed 48 oak wilt fungi genomic sequences compiled from the GenBank NCBI database to find regions of the oak wilt genome amenable for LAMP primer design

Team member (2020) and lead (2021)

Apr. 2020 - Jan. 2022

 Researched sequence- and structured-based ML techniques to design novel and improved plastic-degrading enzymes, with respect to thermostability and catalytic activity

#### Projects

# torch-influence $(50+ \bigstar, 5)$

Jul. 2022

- An open-source library that implements influence functions in PyTorch
- Designed a simple and minimal API that researchers can easily adapt into existing workflows, while also fixing a few mathematical errors found in existing implementations of influence functions

### selfies>=1.0.0 (550+ ★, 110+ 🎝)

Jun. 2020 - Aug. 2022

- An open-source library that implements SELF-Referencing Embedded Strings (SELFIES), which is a 100% robust string representation framework for molecules. The library has accrued over 300 stars since my joining
- Generalized v0 to a larger class of molecules and user-defined constraints
- Boosted conversion efficiency between SELFIES and SMILES by over 10-fold by formulating and implementing a novel translation algorithm
- Enhanced library quality-of-life by writing comprehensive documentation and tutorials hosted on ReadTheDocs, devising exhaustive unit-tests, and setting up CI workflows using tox

#### Selected Coursework

MGY441, Bioinformatics
MAT347, Groups, Rings and Fields

Dec. 2023

Dec. 2023

CSC412 <sup>†</sup> , Probabilistic Machine Learning	Apr. 2022
$\mathbf{CSC413}^{\dagger}$ , Neural Networks and Deep Learning	Apr. 2022
CSC420, Introduction to Image Understanding	Apr. 2022
APM462, Nonlinear Optimization	Apr. 2022
MAT357, Foundations of Real Analysis	Apr. 2022
MAT1841*, Mathematics of Massive Data Analysis: Fundamentals and Application	ns Dec. 2021
MAT327, Introduction to Topology	Dec. 2021
CSC498, Introduction to Reinforcement Learning	Dec. 2021
CSC265, Enriched Data Structures and Analysis	Dec. 2020
	* Graduate, † Cross-listed Graduate

# TECHNICAL SKILLS

Languages: Python, Java, C, R, Bash

Libraries: PyTorch, TensorFlow, JAX, NumPy, SciPy, scikit-learn, pandas, Matplotlib, RDKit, Biopython, WandB,

PyTorch Lightning, Deep Graph Library, PyTorch Geometric, Flax, Haiku

**Tools**: Git, Anaconda, Slurm, Google Cloud Platform, PyCharm **Training Methods**: GPU, TPU, distributed training, mixed-precision