JONATHAN WOO

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RESEARCH INTERESTS

Deep learning, drug discovery, protein engineering, AI for science, geometric deep learning, quantum mechanical modelling

EDUCATION

University of Toronto *Sept. 2020 - Apr. 2025*
Bachelor of Applied Science in Engineering Science, Major in Machine Intelligence Major GPA: 3.95/4.0
5x Dean's Honour List

RELEVANT COURSEWORK

- ECE367: Matrix Algebra & Optimization (A)
- ECE421: Introduction to Machine Learning (A+)
- ECE358: Foundations of Computing (A)
- ECE324: Software & Neural Networks (A+)
- ECE353: Systems Software (A+)
- ECE368: Probabilistic Reasoning (A+)
- ROB311: Artificial Intelligence (A+)
- STA410: Statistical Computation (A+)

RESEARCH EXPERIENCE

Undergraduate Thesis Student Toronto, Canada
Vector Institute — Chemspacelab *Sept. 2024 - Apr. 2025*
Supervisor(s): Anatole Von Lilienfeld

- Developed machine learning and symbolic regression models to optimize parameters for semi-empirical tight binding (xTB), achieving near-DFT accuracy while reducing computational complexity from $\mathcal{O}(n^4)$ to $\mathcal{O}(n^2)$.

Visiting Research Student Cambridge, USA
MIT, Harvard Medical School — Laboratory for Translational Engineering *Sept. 2023 - Aug. 2024*
Supervisor(s): Alvin Chan, Troy Kang, Giovanni Traverso

- Developed COMET, an SE(3)-Transformer for mRNA LNP drug discovery. Leveraged multitask contrastive learning, noise augmentation, and model ensembling to enhance prediction accuracy and robustness, significantly accelerating candidate identification.
- Led successful lead generation and optimization of novel formulations, achieving cell and organ selectivity, cryoprotection, lyoprotection, and thermostability in vitro and in vivo. Patented formulations with >100$\times$ efficacy than clinical baselines.
- Employed integrated gradients and analysis of latent embeddings to derive mechanistic insights into LNP design, enhancing the understanding of structure-function relationships. Uncovered novel insights to factors contributing to efficacy.
- Published LANCE, the largest LNP dataset, spanning extensive chemical space, a key resource for the research community.
- Contributed as a core team member to ARPA-H REO's $70M+ initiative, advancing metabolic disease treatment research.
- Built an innovative time series-based machine learning algorithm with a custom attention mechanism to balance impedance and optical sensors, demonstrating the capability of algorithmically characterizing embryonic stem cells.
- Pioneered an in-context learning paradigm for scientific discovery, enabling large language models (LLMs) to leverage scientific foundation models without the need for fine-tuning. This approach involved injecting foundation model embeddings directly into the LLM's text embedding space, enabling inference conditioned on both the training corpus and external model embeddings, starting with molecular property prediction.
- Developed an optimized pipeline and user-friendly interface for LLM inference, fine-tuning, in-context learning, and evaluation, leveraging multi-GPU parallelism across distributed clusters to drastically improve the research team's efficiency and scalability.

Computational Neuroscience Research Intern Remote
University of Toronto — CoNSens Laboratory *May - Dec. 2023*
Supervisor(s): Matthias Niemeier

- Developed a tool to visualize the activity of convolutional layers in CNNs, enabling the neuroscience team to analyze complex, long-range interactions.

Machine Learning Research Intern Chalk River, Canada
Canadian Nuclear Laboratories — Applied Physics Branch *May - Aug. 2022*
Supervisor(s): Jude Alexander, Oleg Kamaev

- Developed machine learning models to classify nuclear material using low resolution time-series gamma ray spectra. Attained a state-of-the-art 94% classification accuracy using a random forest classifier, effectively minimizing nuisance false alarms.
- Implemented training and inference parallelization with CUDA and HPC which reduced the average processing time by 80%, thereby accelerating testing and optimization.

AI Hardware Acceleration Research Intern Toronto, Canada
University of Toronto — Intelligent Sensory Microsystems Laboratory *Apr. 2021 - Apr. 2022*
Supervisor(s): Amirali Amirsoleimani, Roman Genov

- Formulated 4 novel algorithms and 3 metrics for memristor crossbar arrays (MCAs) - analog hardware deep learning accelerators enabling $\mathcal{O}(1)$ complexity of matrix-vector-multiplication - to predict device behaviour using physical properties such that manufacturers can alleviate the bottleneck of testing individual devices.

INDUSTRY EXPERIENCE

Isomorphic Labs — Research Engineer
Sept. 2025 - Present
AlphaFold

Software Engineer Intern — Hong Kong
The Trade Desk — *Jun. - Aug. 2023*

- Spearheaded the development of a client onboarding tool, alleviating a critical bottleneck and retiring an inefficient scripting process. This saved engineers on average 10 hours a week and reduced the total onboarding time by 3 weeks.
- Led the retrofitting of two microservices to GraphQL, maintained gRPC compatibility, and reduced 3-5 API calls into one.
- Refactored 5+ critical endpoints, unit tests, and end-to-end tests improving performance and long-term maintainability.

Machine Learning Developer — Toronto, Canada
Omni Research — beta.omnilabs.ai — *Sept. 2022 - Apr. 2023*

- Developed a ChatGPT-like interface and crafted prompts for GPT-3 retrieval-augmented generation (RAG), enabling a personalized chatbot with persistent browsing capabilities.
- Created 7 few-shot learning prompts and APIs to query GPT-3, enabling the automatic generation of explanations, counterarguments, and Tweets. Directly expanded the capabilities of the platform with 15% more users post-launch.

JOURNAL PUBLICATIONS

RNA Nanomedicine Stabilization with Deep Learning — *Under Review*
Science Advances
Jonathan W*, *Alvin C.*, Ameya R. K.*, et al. Giovanni Traverso*

Designing Lipid Nanoparticles Using a Transformer-Based Neural Network — *Aug 2025*
Nature Nanotechnology
Alvin C., Ameya R. K.*, Qing R. Q., Xisha H., **Jonathan W.**, et al. Giovanni Traverso*

Smart Needle System for Point-of-care Characterization of Cell Therapy — *Under Review*
Nature Biotechnology
Yiyuan Y., Ziliang K.*, Nabil S.*, Jong S. L.*, Ming Z.*, Fangzhou X., Injoo M., **Jonathan W.**, et al. Robert Langer, Giovanni Traverso*

Oesophageal Tissue Screening (OTiS) Platform — *Under Review*
Nature Biomedical Engineering
Christina K., Thomas Y., Alvin C., Nikhil L., Charmaine J. C., Shriya R., Yuebin H., **Jonathan W.**, et al. Giovanni Traverso*

CONFERENCE PUBLICATIONS

Can LLMs Reason Over Non-Text Modalities in a Training-Free Manner? A Case Study with In-Context Representation Learning — *Dec 2025*
2025 Conference on Neural Information Processing Systems (NeurIPS)
Tianle Z., Wanlong F.*, **Jonathan W.***, et al. Alvin Chan*

Modelling Tools for Enhancing Nuclear Border Security — *May 2024*
International Conference on Nuclear Security: Shaping the Future
Genevieve H., **Jonathan W.**, et al.*

Radioisotope Identification Using CLYC Detectors — *Dec 2022*
2022 21st IEEE International Conference on Machine Learning and Applications (ICMLA)
10.1109/ICMLA55696.2022.00214
David P. L., Jude A.*, (Acknowledgements) **Jonathan W.**, et al.*

PROJECTS

LLMs for Addiction Recovery & Therapy — *Sept. - Dec. 2024*
OpenRecovery

- Collaborated with a startup to transition model deployment from prompt-engineered in-context learning to fine-tuned large language models (LLMs) optimized via Direct Preference Optimization (DPO) using LoRA.
- Designed and implemented a scalable, automated evaluation pipeline utilizing LLM-as-a-Judge to assess approximately 1,000 conversations, creating a high-quality dataset of preference pairs for improved model training and evaluation.

Decision Transformer for Autonomous Highway Driving *Jan. - Apr. 2023*
github.com/caixunshiren/Highway-Decision-Transformer

- Developed an autonomous highway driving agent using Decision Transformers, outperforming top RL algorithms (Deep Q-Learning, PPO) with superior adaptability and decision-making in complex scenarios.
- Created simulation environment and scripts to collect 20000 episodes of training data. Formulated novel reward-functions to influence driving behaviours from aggressive to passive.

IMC Prosperity Global Trading Challenge - #7 Canada/Top 1% Worldwide *Apr. 2024*
github.com/Jonathan-Woo/prosperity

- Led the end-to-end software implementation of quantitative trading strategies, building and maintaining essential tools such as an order book, backtester, and real-time performance dashboards. Enhanced trading infrastructure by integrating low-latency data feeds, optimizing execution algorithms, and ensuring robust data integrity for accurate trade simulations and live trading.
- Utilized historical price data to rigorously backtest and fine-tune parameters across a suite of models, including ARIMA for time-series forecasting, pairs trading for correlated asset strategies, mean reversion for statistical arbitrage, and linear regression for predictive pricing models. Performed parameter optimization and sensitivity analysis to refine model accuracy and improve profitability across market regimes, aligning with risk management objectives.

SKILLS

Languages: English (native)

Programming Languages: Python, C, C++, C#, TypeScript, SQL, MATLAB, LaTeX

ML: TensorFlow, PyTorch, JAX, Scikit-learn, Hugging Face, LangChain, XGBoost, RDKit, PyMC, Pandas, NumPy, SciPy

Backend: Flask, Docker, Kubernetes, gRPC, REST, GraphQL

HPC: CUDA, SLURM

GRANTS & AWARDS

Hosinec Family Scholarships *Mar. 2023*
University of Toronto

- Academic merit, leadership, and financial need.

Shaikh And Hashemi Family Engineering Science Award *Oct. 2022*
University of Toronto

- Academic merit, leadership, and financial need.

Hok Chee Poon & Yim Hung Kwong Bursary *Dec. 2021*
University of Toronto

- Academic merit, leadership, and financial need.

Fu Siang Pang & Ying Au Yeung Bursary *Dec. 2021*
University of Toronto

- Academic merit, leadership, and financial need.

Class of 4t7 Scholarship *Dec. 2021*
University of Toronto

- Academic merit, leadership, and financial need.

Class of 2004 Grant *Dec. 2021*
University of Toronto

- Academic merit, leadership, and financial need.

Faculty of Applied Science and Engineering Admission Scholarship *Oct. 2020*
University of Toronto

Army, Navy and Air Force Veterans in Canada (ANAVETS) Cadet Medal of Merit *Aug. 2018*
Air Cadet League of Canada

- The ANAVETS Cadet Medal of Merit is awarded by the Army, Navy, and Air Force Veterans in Canada to recognize excellence among cadets in the Canadian Cadet Organization. One medal is presented at each Cadet Training Centre (CTC) to the top male and female cadets in specified courses. Recipients are selected based on overall achievement, leadership, instructional abilities, dress, deportment, motivation, and teamwork.