Luke Thompson

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Education

University of Sydney, PhD - Computer Science   Jul 2024 – Present

- Working on neural operators (one-shot PDE solvers) for quantum chemistry and rough path theory.
- Awarded a A$75K CSIRO industry PhD scholarship to continue my work on graph transformers (declined).

University of Sydney, Bachelor of Science (Honours) - Pharmacology   Feb 2020 – Jun 2024

- Mark: 86, First Class Honours (Transcript)
- **Thesis**: Graph Transformer Neural Networks for Mutagenicity Prediction.
  - Incorporated chemically-informed structural graph encodings and tuned for regulatory application with Bayesian uncertainty estimation techniques.

Publications

Taming the (Itô-)Lyon: Neural Operators for Rough Differential Equations   May 2025

Luke Thompson, Josiah Evans, Dai Shi, Andi Han, Lequan Lin, Junbin Gao

- First neural operator for learning the Itô-Lyons map from a rough stochastic process to a solution path.
- Implemented using custom Jax libraries and Equinox/Diffrax.

Expanding the Chaos: Neural Operator for Stochastic Differential Equations   May 2025

Dai Shi, Andi Han, Lequan Lin, *Luke Thompson*, Junbin Gao

- Contributed SDE simulation code for Langevin dynamics and various non-Markovian SDEs.
- Authored section regarding molecular applications.

ATOM: A Pretrained Neural Operator for Dynamics Learning - Submitted NeurIPS   May 2025

Luke Thompson, Dai Shi, Andi Han, Slade Matthews, Junbin Gao

- State-of-the-Art molecular dynamics (MD) forecasting with an efficiently trainable transformer architecture.
- Developed a custom form of RoPE for dynamics learning and leveraged equivariant deep-learning methods.
- Worked with CSIRO researchers to build a multitask MD dataset using HPC resources (total cost US$130 000).

AmesFormer: State-of-the-Art Mutagenicity Prediction with Graph Transformers   Sep 2024

Luke Thompson, Josiah Evans, Slade Matthews

- **First** of 26 models for carcinogenicity prediction from chemical structure on a leading benchmark dataset.
- Implemented using PyTorch, PyTorch-Geometric, and a custom Rust library via foreign function interfaces.

Experience

Casual Academic, The University of Sydney – Camperdown, NSW   June 2024 – Present

- Tutored several third-year classes covering classical ML (linear regression, logistic regression) for pharmacology.
- Led two capstone project groups focusing on medicinal chemistry and computational toxicity assessment.

Geographic Data Analyst, Kumon – Chatswood, NSW   Feb 2024 – Present

- Saved $28 800 per annum by bringing population time-series forecasting in-house using an ensemble of autoregressive models, achieving 93.9% accuracy 5 years out.
- Migrated four legacy Australia-wide Visual Basic systems to a high-performance Rust and PostgreSQL backend, in one case reducing latency from ~ 4 hours to ~ 30 s and achieving $> 99\%$ uptime.

Projects

QuickSig: JAX library for computing path signatures (stochastic calculus)   GitHub Link

- Implemented a novel Horner algorithm exploiting tensor algebra structures achieving SOTA GPU performance.
- Projects the log signature to the free Lie algebra via Duval's algorithm.

FastASX: High-frequency trading library   GitHub Link

- #1 Fastest open-source NASDAQ ITCH message parser. Zero-allocation, parallel, built with Rust.
- Maintains a limit order book and intraday stock directory.

Cold War: Iron Curtain (Link): My open-source cold war strategy game modification with **600 000 unique users**.

Eigen[2] (Link): A from-scratch Python numerical linear algebra library focusing on eigenpair computation. Includes QR, Cholesky, Rayleigh-quotient methods, and Krylov subspace methods, among others.

Awards and Presentations

ACTRA Student Prize (2024): I was awarded the student prize for AmesFormer and presented at the Annual Scientific meeting of the Australasian College of Toxicologists and Risk Assessors. Valued at $\approx$ \$2000.
Presentations: Federal Department of Climate Change, AICIS (federal chemical regulator).

Grants

- Participated in a US\$1M Gates Foundation grant to develop new antimicrobial therapies (pending).
- Pending application for a A\$600K Cancer Council Australia grant to study disease dynamics using graph ML approaches.

Technologies

Languages: Rust, Python (PyTorch, Torch-Geometric, SKLearn, Pandas, Riskfolio-lib), MATLAB, PostgreSQL, LaTeX.

Software: Microsoft Office suite (incl. Access), Dragon & related cheminformatics software.