

Anabel Yong

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Summary

MSc in Computational Statistics and Machine Learning from UCL, with a specialization in scalable Bayesian optimization for molecular design. Experienced in developing hardware-optimized ML models using PyTorch and JAX and efficient compute frameworks for molecular property prediction. Strong interest in hardware-aware AI algorithms, distributed ML, and efficient compute for drug discovery applications.

Publications

- **Yong, A., Paige, B., Tripp, A. (2024). Beyond Scalarization: Extending GP-BO to Pareto Optimization with Independent Tanimoto Kernel Gaussian Processes. (*Submitted to ICLR 2025*)**

Education

MSc Computational Statistics and Machine Learning, UCL (Distinction, Dean's List 2024) 2024

Modules: Probabilistic and Unsupervised Learning (Gatsby PhD module) (91%), ML Seminar (Marc Deisenroth- DeepMind Chair in AI (88%), Numerical Optimization in Machine Learning (81%), Statistical NLP

BSc Mathematics & Biology, University of Edinburgh (1st Class Honours) 2019 - 2023

Modules: Bioinformatics (95%), Introductory Machine Learning (80%), Numerical Optimisation, Data Structures & Algorithms

Work Experience

- **ML Engineer Intern, IgnotaLabs.AI, Austin Tripp, University of Cambridge & Brooks Paige, UCL** June 2024- Sept 2024
 - Developed a multi-objective Bayesian optimization algorithm (GP-MOBO) using Tanimoto Kernels for small molecule optimization.
 - Deployed a Python package (KERN-GP) for efficient kernel-based Gaussian Processes, enabling scalable, GPU-optimized molecular property modeling.
 - Built scalable ML pipelines with PyTorch, optimizing molecular simulations by 20% through distributed training
- **Research Assistant, Kustatscher Lab, University of Edinburgh x Technical University of Munich** Sept 2022 - July 2023
 - Optimised data pre-processing pipeline (published to PyPI), (Link to pgFDR) to improve protein detection accuracy, identifying over 7000 novel micropoteins for molecular analysis.
- **Statistical Genetics Intern, ZiHeng Yang Lab, UCL Centre of Computational Biology, UCL** March 2022 - May 2022
 - Implemented Bayesian MCMC algorithms to model ABO blood type frequencies, contributing to personalized medicine approaches by estimating key genetic parameters for population studies.
- **Research Assistant, Grima Lab, Department of Systems & Synthetic Biology, University of Edinburgh** June 2020 - Jan 2022
 - Implemented stochastic and deterministic models to predict mRNA decay kinetics, aiding in the understanding of gene regulation mechanisms and supporting drug efficacy studies in preclinical research.

Personal Projects (on Portfolio)

- **DoLa-based Decoding for Instruction-Following LLMs**
 - Evaluated and adapted DoLa contrastive decoding in T5 and FLAN-T5, enhancing instruction accuracy and reducing hallucinations for large language models (LLMs).

Skills

Programming: Python, C++, R, MATLAB, SQL, git, Linux

Machine Learning: PyTorch, JAX, TensorFlow, Botorch, GPytorch

Bioinformatics/Cheminformatics: RDKit, PyMOL, UniProt, MaxQuant

Cloud Computing & HPC: Google Cloud Platform (GCP), AWServices (AWS)