## Isaac Reid

ir337@cam.ac.uk isaac-reid.github.io

## Research interests

I am interested in problems at the interface of ML, statistical physics and applied mathematics, especially where theoretical results have proved elusive and applications are high impact. Recently, I've focussed on efficient Transformers for graph-structured data. I hold a Google PhD Fellowship in Algorithms and Theory.

#### Education

#### Machine Learning Group, University of Cambridge

Oct 2022 - present

PhD in Engineering

Supervisors: Dr Adrian Weller and Prof. Rich Turner

Advisor: Prof. Carl Rasmussen

Subject: Scalable and data-efficient machine learning. Ongoing collaboration with Prof. Krzysztof Choromanski

(Google DeepMind and Columbia University, New York).

#### Physics, University of Oxford

Oct 2017 - Jun 2021

Master of Physics, MPhys

Grade: First class, 92%, top of Oxford cohort (out of  $\sim 150$ )

Research project: Quantum entanglement barriers in dual-unitary circuits

Supervisor: Dr Bruno Bertini

# Publications and select preprints

### Linear Transformer Topological Masking with Graph Random Features

Preprint, under review

**Isaac Reid**, Avi Dubey, Deepali Jain, Will Whitney, Amr Ahmed, Joshua Ainslie, Alex Bewley, Mithun Jacob, Aranyak Mehta, David Rendleman, Connor Schenck, Richard E. Turner, René Wagner, Adrian Weller, Krzysztof Choromanski

Synopsis: Efficiently incorporating structural information into Transformer attention using graph random walks, for applications in computer vision and robotics

https://arxiv.org/abs/2410.03462

#### Optimal Time-Complexity Algorithms for Computing General Random Walk Kernels on Sparse Graphs

Preprint, under review

Krzysztof Choromanski\*, Isaac Reid\*, Arijit Sehanobish, Avi Dubey

Synopsis: By simulating correlated random walks on an ensemble of graphs, you can estimate the graph kernel between any given pair in linear time

https://arxiv.org/abs/2410.10368

#### Variance-Reducing Couplings for Random Features

Preprint, under review

Isaac Reid, Stratis Markou, Krzysztof Choromanski, Richard E. Turner, Adrian Weller

Synopsis: Variance reduction in Monte Carlo is really a multi-marginal optimal transport problem, and treating it as such gives us tools to sample more efficiently in Euclidean and discrete space

https://arxiv.org/abs/2405.16541

#### Repelling Random Walks

ICLR 2024

Isaac Reid, Eli Berger, Krzysztof Choromanski, Adrian Weller

Synopsis: A QMC scheme that correlates the directions of walkers on a graph, providing better sample efficiency and improving the concentration of a host of statistical estimators

https://arxiv.org/abs/2310.04854

#### **General Graph Random Features**

ICLR 2024

Isaac Reid\*, Krzysztof Choromanski\*, Eli Berger\*, Adrian Weller

Synopsis: A random feature mechanism to approximate arbitrary functions of a weighted adjacency matrix, unlocking kernel-based learning on very large graphs

https://arxiv.org/abs/2310.04859

#### Quasi-Monte Carlo Graph Random Features

NeurIPS 2023, accepted as spotlight paper

Isaac Reid, Krzysztof Choromanski, Adrian Weller

Synopsis: A QMC scheme that induces correlations between the lengths of terminating random walks on a graph, with possible applications in bioinformatics and graph-based Transformers

https://arxiv.org/abs/2305.12470

#### Simplex Random Features

ICML 2023, accepted with oral presentation

Isaac Reid, Krzysztof Choromanski, Valerii Likhosherstov, Adrian Weller

Synopsis: Derivation of an optimal random feature mechanism for unbiased approximation of the Gaussian kernel, motivated by a host of new analytical results and tested with Transformer experiments

https://arXiv.org/abs/2301.13856

#### **Entanglement Barriers in Dual-Unitary Circuits**

Phys. Rev. B 104, 014301 - Published 1 July 2021

Isaac Reid, Bruno Bertini

Synopsis: Exact characterisation of the dynamics of quantum entanglement arising after a quantum quench in a many-body, locally interacting system, including both the integrable and completely chaotic regimes <a href="https://arxiv.org/abs/2103.12794">https://arxiv.org/abs/2103.12794</a>

## **Teaching**

Engineering 2P7 Michaelmas 2023 - present

Synopsis: Supervisions in mathematics for engineers (vector calculus, linear algebra and probability)

#### Pembroke International Summer Programme

Jun-Aug 2023

Synopsis: Research project on density ratio estimation in machine learning

#### **Talks**

# Efficient Transformers – Machine Learning Group, Cambridge Nov 2024

Synopsis: Seminar on mathematical tricks for subquadratic attention

Quasi-Monte Carlo Graph Random Features – NeurIPS@Cambridge, Cambridge Dec 2023

Synopsis: Invited talk to accompany NeurIPS spotlight paper

Simplex Random Features – ICML 2023, Honolulu July 2023

Synopsis: Oral presentation to accompany paper

Simplex Random Features – Microsoft Research, Cambridge

Jun 2023

Synopsis: Research talk on ICML paper

Random Features for Kernel Approximation – Machine Learning Group, Cambridge

Mar 2023

Synopsis: Seminar on random feature methods and recent QMC schemes to improve their convergence

## Experience

## Research Associate, IQ Capital

Nov 2024 - present

1 day/week advising and investing in ML startups and supporting portfolio companies

#### Student Researcher, Google

May 2024 - Nov 2024

Project on efficient Transformers, working closely with Krzysztof Choromanski and Avi Dubey

#### Systems Engineer, Opsydia

Sep 2021 - Sep 2022

R&D engineer at deep-tech startup specialising in laser technology and adaptive optics, spun out of Oxford University Engineering Department

Research Intern, Max Planck Institute for Dynamics and Self-Organisation, Göttingen Summer 2020 Computational study of Bose-Einstein condensation in active matter, applying theoretical results from many-body quantum physics to classical clustering phenomena observed in Kob-Andersen particle dynamics Supervisors: Dr Benoit Mahault and Prof. Ramin Golestanian

#### Research Intern, Rudolf Peierls Centre for Theoretical Physics, Oxford

Summer 2019

Study of relationship between spectral properties of Hessian of loss function and Bayesian prior upon deep neural network initialisation, estimated using random sampling of weights and Gaussian processes Supervisor: Prof. Ard Louis

## Scholarships and awards

For performance in first year (88%)

Google PhD Fellowship in Algorithms and Theory Funding from Google for remainder of PhD	2024-2026
G-Research Grant Financial award to help fund attendance of ICML conference	July 2023
Trinity College External Studentship Full scholarship for a PhD in Machine Learning	2022-2025
Encaenia One of six undergraduate students invited to attend Oxford's historic Encaenia ceremony	Jun 2022
Gibbs Prize For submitting the highest scoring MPhys research project (87%)	2020-2021
Scott Prize For best overall performance in the MPhys (92%)	2017-2021
Scott Prize For best performance in the third year (92%)	2019-2020
Winton Capital Prize For best performance in the second year (93%)	2018-2019
Hertford College Academic Scholarship	2018-2021