Ryan-Rhys Griffiths

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Email: ryangriff123@gmail.com

Employment

Fields Model Initiative, San Francisco, CA, USA June 2025 - Present

Director of ML Research and Partnerships

- Post-training fully open models for mathematics
- fundraising in the non-profit sector
- Designing challenging STEM benchmarks for frontier models
- Paper accepted to NeurIPS 2026
- Google Scholar citations: 3512
- Google Scholar h-index: 21
- Google Scholar i10-index: 26
- Area Chair for ICML 2027
- Area Chair for NeurIPS 2025 and ICML 2026 Workshops on AI4Science
- Co-organizer of OPTIMAL: Optimisation and Post-Bayesian Inference in Machine Learning workshop at AISTATS 2026.
- EB-1A Green Card Holder

FutureHouse, Inc., San Francisco, CA, USA May 2024 - June 2025

AI Research Scientist

- Post-training and language agents for chemistry
- Technical Interviewer for AI research roles
- Paper Accepted to NeurIPS 2025
- Area Chair for ICML 2024 and NeurIPS 2025 AI4Science Workshops
- Outstanding Reviewer Award AISTATS 2025 (top 5%)
- Top Reviewer Award NeurIPS 2025 (top 8%)

Meta Research, Menlo Park, CA, USA Aug 2022 - May 2024

AI Research Scientist

- Organization: Central Applied Science
- Specialism: Bayesian Optimization, LLMs, Generative AI
- 2 Papers Accepted to NeurIPS 2023
- Outstanding Reviewer Award NeurIPS 2023 (top 10%)
- Area Chair for NeurIPS AI4Science Workshop

Huawei Noah's Ark Lab, London, UK Oct 2020 - Oct 2021

AI Research Scientist

- Department: AI Theory Group
- Director: Prof. Haitham Bou-Ammar
- Intermitted PhD for 1 year to work full-time as a research scientist at Huawei Noah's Ark Lab while waiting for my PhD papers to be published
- Specialism: Optimization, Bayesian Deep Learning, Reinforcement Learning
- 1st Place in the 2020 NeurIPS Black-Box Optimization Competition
- Papers published in JMLR and JAIR

Secondmind Labs, Cambridge, UK Oct 2017 - Oct 2018

Machine Learning Engineer

- Department: Multiagent Systems Group
- Manager: Dr. Alexis Boukouvalas
- Specialism: Bayesian Nonparametrics and Reinforcement Learning
- Paper published at ICML 2019

Education

University of Cambridge Oct 2018 - Aug 2022

PhD, Machine Learning and Physics

- PhD Thesis: *Applications of Gaussian Processes at Extreme Lengthscales: From Molecules to Black Holes*
- Department: Physics, Theory of Condensed Matter, Cavendish Laboratory
- Supervisor: Dr. Alpha Lee
- Specialism: Astronomical time series, Gaussian processes, ML4Science
- Papers published in NeurIPS, the Astrophysical Journal, Chemical Science, Accounts of Chemical Research and Machine Learning: Science and Technology
- Featured a 1-year break to work full-time as a Research Scientist at Huawei Noah's Ark Lab

University of Cambridge Oct 2016 - Oct 2017

MPhil, Machine Learning and Machine Intelligence

- MPhil Thesis: Constrained Bayesian Optimization for Automatic Chemical Design
- Department: Engineering, Machine Learning Group
- Supervisor: Prof. José Miguel Hernández-Lobato
- Paper published in Chemical Science
- Coursework: Distinction grades in Probabilistic Machine Learning, Reinforcement Learning, and Natural Language Processing
- 1st Place in Kaggle Classification Competition

Imperial College London Oct 2012 - Jun 2016

MSci, Chemistry, 1st Class

- MSci Thesis: A Theory of a Self-Assembling Electrovariable Smart Mirror
- Department: Chemistry, Theoretical Chemical Physics Group
- Supervisor: Prof. Alexei Kornyshev
- Paper published in the Journal of Electroanalytical Chemistry
- Constructed a mathematical model of a nanophotonic, electrochemical mirror-window system for novel sensing applications in renewable energy, trace analyte detection and counter-terrorism
- Extended Thomas-Fermi theory to account for the effect of finite penetration of a point charge into the body of a material
- Coursework: Organic, Inorganic and Physical Chemistry, ranked in the top 10 students in finals

Coursera/EdX

- 33 certifications with topics including Linear Algebra, Bayesian Methods for Machine Learning, Deep Learning, Statistical Learning, Algorithms and Data Structures, Computational Neuroscience, Natural Language Processing, LLMs, and Generative AI

Other Positions

Mila - Quebec AI Institute, Montreal, Canada Jan 2022 - Jun 2022

Visiting Machine Learning Researcher

- Worked with Prof. Jian Tang
- Specialism: Molecular Machine Learning, Sequence Design
- Recipient of a $25,000 Samsung AI fellowship

Oxia Palus, London, UK Oct 2019 - Present

Machine Learning Research Associate

- Oxia Palus is an AI art collective using machine learning to recover lost artwork
- Research has been featured in MIT Technology Review

University College London, UK Jun 2015 - Oct 2015

Machine Learning Research Student

- Department: CSML, Gatsby Unit
- Supervisors: Prof. John Shawe-Taylor and Dr. Guy Lever
- Supervised Learning on the Alzheimer's Disease Neuroimaging Initiative (ADNI) biomedical dataset

Imperial College London, UK Jun 2014 - Oct 2014

Theoretical Condensed Matter Physics Research Student

- Department: Chemistry, Theoretical Chemical Physics Group
- Supervisor: Prof. Alexei Kornyshev
- Built a mathematical model of an electroactuator system for use in voltage-controlled micro and nano-robotics
- Placement funded through an EPSRC vacation bursary award

Consulting Experience

Independent, London, UK Oct 2017 - Aug 2022

Machine Learning

- Designed and delivered a course on Probabilistic Machine Learning for quantitative researchers at G-Research, a London-based hedge fund
- Delivered a course on Python and Machine Learning for the Schmidt Data Science Residency Programme at Cambridge University.
- Designed and delivered a Deep Learning seminar series for JPMorgan.
- Designed and delivered a Data Science course for Morgan Stanley.
- Lead Instructor for the Deep Learning course at the STFC Data Intensive, Artificial Intelligence and Machine Learning Summer School featuring ca. 150 graduate students across UK universities.

Teaching Experience, University of Cambridge, UK Oct 2018 - Aug 2022

- Demonstrator for the Natural Sciences Tripos undergraduate course on Scientific Computing
- Mentored 12 PhD and postdoctoral associates working in STEM fields for 6-week research projects as part of the Schmidt Data Science Residency Programme

Publications

Refereed Journal Papers

[J1] Rankovic, B, **Griffiths RR**, and Schwaller, P, Large language models as uncertainty-calibrated optimizers for experimental discovery. Nature Machine Intelligence, 2026.

[J2] Grosnit A, Cowen-Rivers A, Tutunov R, **Griffiths RR**, Wang J, Bou-Ammar H. Are We Forgetting About Compositional Optimisers in Bayesian Optimisation. *Journal of Machine Learning Research*, 2021.

[J3] Cowen-Rivers A, Lyu W, Tutunov R, Wang Z, Grosnit A, **Griffiths RR**, Hao J, Wang J, Bou-Ammar H. HEBO: Pushing The Limits of Sample-Efficient Hyperparameter Optimisation. *Journal of Artificial Intelligence Research*, 2022.

[J4] Bourached A, **Griffiths RR**, Gray R, Jha A, Nachev P. Generative Model-Enhanced Human Motion Prediction. *Applied AI Letters*, 2021.

[J5] **Griffiths RR**, Aldrick A, Garcia-Ortegon M, Lalchand V, Lee, AA. Achieving Robustness to Aleatoric Uncertainty with Heteroscedastic Bayesian Optimisation. *Machine Learning: Science and Technology*, 2021.

[J6] **Griffiths RR**, Jiang J, Buisson D, Wilkins D, Gallo L, Ingram, A, Lee AA, Grupe D, Kara M, Parker ML, Alston W, Bourached A, Cann G, Young A, Komossa S. Modelling the Multiwavelength Variability of Mrk-335 using Gaussian Processes. *The Astrophysical Journal*, 2021.

[J7] **Griffiths RR**, Hernández-Lobato JM. Constrained Bayesian Optimization for Automatic Chemical Design using Variational Autoencoders. *Chemical Science*, 2020.

[J8] Zagar C, **Griffiths RR**, Podgornik R, Kornyshev AA. On the Voltage-Controlled Self-Assembly of NP Arrays at Electrochemical Solid/Liquid Interfaces. *Journal of Electroanalytical Chemistry*, 2020.

[J9] Cheng B, **Griffiths RR**, Wengert S, Kunkel C, Stenczel T, Zhu B, Deringer VL, Bernstein N, Margraf JT, Reuter K, Csanyi G. Mapping Materials and Molecules. *Accounts of Chemical Research*, 2020.

[J10] **Griffiths RR**, Greenfield JL, Thawani AR, Jamasb A, Moss HB, Bourached A, Jones P, McCorkindale W, Aldrick AA, Fuchter M, Lee AA. Data-Driven Discovery of Molecular Photoswitches with Multioutput Gaussian Processes. *Chemical Science*, 2022.

[J11] Rankovic, B, **Griffiths, RR**, Moss, HB and Schwaller, P. Bayesian optimisation for additive screening and yield improvements–beyond one-hot encoding. *Digital Discovery*, 2023.

[J12] Tkachenko, N, Frieder, S, **Griffiths, RR**, Nedopil, C. Analyzing Global Utilization and Missed Opportunities in Debt-for-Nature Swaps with Generative AI. *Frontiers in Artificial Intelligence*, 2024.

Refereed Conference Papers

[C1] Frieder S, Bayer J, Looi S, Loader J, Berner J, Collins KM, Juhasz A, Ruehle F, Welleck S, Poesia G, Mistreanu I, **Griffiths RR**, Weller A, Goyal A, Lukasiewicz T, Freer C, Buzzard K, Gowers WT, We Need to Improve Benchmarks in AI for Mathematics. *NeurIPS*, 2026. (Position Paper Track).

[C2] Narayanan S, Braza JD, **Griffiths RR**, Bou A, Wellawatte G, Ramos MC, Mitchener L, Rodriques SG, White AD, Training a Scientific Reasoning Model for Chemistry. *NeurIPS*, 2025. (Main Track - 24.5% Acceptance Rate).

[C3] **Griffiths RR**, Klarner L, Moss HB, Ravuri A, Truong S, Du Y, Stanton S, Tom G, Rankovic B, Jamasb A, Schwartz J, Deshwal A, Tripp A, Kell G, Frieder S, Bourached A, Chan A, Moss J, Guo C, Durholt JP, Chaurasia S, Park JW, Strieth-Kalthoff F, Lee AA, Cheng B, Aspuru-Guzik, A, Schwaller P, Tang J, GAUCHE: A Library for Gaussian Processes in Chemistry. *NeurIPS*, 2023 (Main Track - 26.1% Acceptance Rate).

[C4] Frieder S, Pinchetti L, Chevalier A, **Griffiths RR**, Salvatori T, Lukasiewicz T, Petersen PC, and Berner J, 2023. Mathematical capabilities of ChatGPT. *NeurIPS*, 2023. (Datasets and Benchmarks Track - 32.7% Acceptance Rate).

[C5] Grant J, Boukouvalas A, **Griffiths RR**, Leslie D, Vaikili S, Munoz de Cote E. Adaptive Sensor Placement for Continuous Spaces. *ICML*, 2019 (22.6% Acceptance Rate).

[C6] Kell G, **Griffiths RR**, Bourached A, Stork D. Extracting Associations and Meanings of Objects Depicted in Artworks through Bi-Modal Deep Networks, *Electronic Imaging*, 2022.

[C7] Stork D, Bourached A, Cann G, **Griffiths RR**, Computational Identification of Significant Actors in Paintings through Symbols and Attributes, *Electronic Imaging*, 2021.

[C8] Cann G, Bourached A, **Griffiths RR**, Stork D. Resolution Enhancement in the Recovery of Underdrawings Via Style Transfer by Generative Adversarial Deep Neural Networks, *Electronic Imaging*. 2021.

[C9] Bourached A, Cann G, **Griffiths RR**, Stork D. Recovery of Underdrawings and Ghost-Paintings via Style Transfer by Deep Convolutional Neural Networks: A Digital Tool for Art Scholars, *Electronic Imaging*, 2021.

[C10] Bourached A, Cann G, **Griffiths RR**, Eriksson J, Stork D., Style Transfer for Improved Visualization of Underdrawings and Ghost Paintings: An Application to a Work by Vincent van Gogh, *Electronic Imaging*, 2023.

Refereed Workshop Papers

[W1] Verma E, Chakraborty S, **Griffiths RR**. High-Dimensional Bayesian Optimization with Invariance. *ICML Workshop on Adaptive Experimental Design and Active Learning in the Real World*, 2022.

[W2] Aziz A, Kosasih EE, **Griffiths RR**, Brintrup A. Data Considerations in Graph Representation Learning for Supply Chain Networks. *ICML Workshop on Machine Learning for Data: Automated Creation, Privacy, Bias*, 2021

[W3] **Griffiths RR***, Moss H*. Gaussian Process Molecular Machine Learning with FlowMO. *NeurIPS Workshop on Machine Learning for Molecules*, 2020 (Contributed Talk - top 5%, * joint first authorship).

[W4] Bourached A, **Griffiths RR**, Gray R, Jha A, Nachev P. Generative Model-Enhanced Human Motion Prediction. *NeurIPS Workshop on Interpretable Inductive Biases and Physically-Structured Learning*, 2020.

[W5] **Griffiths RR**, Jones P, McCorkindale W, Aldrick AA, Jamasb A, Day B. Benchmarking Scalable Active Learning Strategies on Molecules. *ICLR Workshop on Fundamental Science in the Era of AI* 2020.

[W6] **Griffiths RR**, Thawani AR, Elijosius R. Enhancing the Diversity of Molecular Machine Learning Benchmarks: An Open-Source Dataset for Molecular Photoswitches. *ICLR Workshop on Fundamental Science in the Era of AI*, 2020.

[W7] **Griffiths RR**, Schwaller P, Lee AA. Dataset Bias in the Natural Sciences: A Case Study in Chemical Reaction Prediction and Synthesis Design. *NeurIPS Workshop on Critiquing and Correcting Trends in Machine Learning*, 2018.

[W8] **Griffiths RR**, Hernández-Lobato JM. Constrained Bayesian Optimization for Automatic Chemical Design. *NIPS Workshop on Bayesian Optimization for Science and Engineering*, 2017.

Technical Reports

[R1] **Griffiths RR**. A Theory of a Self-Assembling Electrovariable Smart Mirror. *arXiv*, 2017.

Preprints

[P1] Truong, S.T., Nguyen, D.Q., Neiswanger, W., **Griffiths RR**., Ermon, S., Haber, N. and Koyejo, S., Neural Nonmyopic Bayesian Optimization in Dynamic Cost Settings. *arXiv*, 2026.

[P2] Baird S, Ansari M, Afzal Z, Ai Q, Al-Feghali A, Alain M, Altamirano M, Andrews T, Anker AS, Ansari R, Appiah SA. **Griffiths RR** et al. Bayesian Optimization Hackathon for Chemistry and Materials. ChemRxiv, 2025.

[P3] Narayanan, S, Braza, JD, **Griffiths RR**, Ponnapati, M, Bou, A, Laurent, J, Kabeli, O, Wellawatte, G, Cox, S, Rodriques, SG, and White, AD, 2024. Aviary: Training Language Agents on Challenging Scientific Tasks, *arXiv*, 2024.

[P4] Kell, G, Roberts, A, Umansky, S, Khare, Y, Ahmed, N, Patel, N, Simela, C, Coumbe, J, Rozario, J, **Griffiths RR** and Marshall, IJ, 2024. RealMedQA: A pilot biomedical question answering dataset containing realistic clinical questions. *arXiv*, 2024.

[P5] **Griffiths RR***, Grosnit A*, Tutunov R*, Maraval AM*, Cowen-Rivers A, Yang L, Lin Z, Lyu W, Chen Z, Wang J, Peters J, Bou-Ammar H. High-Dimensional Bayesian Optimisation with Variational Autoencoders and Deep Metric Learning. *arXiv*, 2021. (* joint first authorship)

[P6] Bourached A, Gray R, **Griffiths RR**, Jha A, Nachev P. Hierarchical Graph-Convolutional Variational AutoEncoding for Generative Modelling of Human Motion. *arXiv*, 2021.

PhD Thesis

[T1] **Griffiths RR**, Applications of Gaussian Processes at Extreme Lengthscales: From Molecules to Black Holes. PhD Thesis, *University of Cambridge*, 2022.

Reviewing

• NeurIPS	2021, 2022, 2023, 2024, 2025, 2026
• ICLR	2025, 2026, 2027
• ICML	2025, 2026
• AISTATS	2024, 2025, 2026, 2027
• AAAI	2026, 2027
• Nature Machine Intelligence	2020, 2023
• Nature Communications Chemistry	2022
• npj Computational Materials	2022
• AutoML Conference	2023, 2024, 2025
• IEEE Intelligent Systems	2021
• IEEE Transactions on Evolutionary Computation	2020
• Neural Computation	2024
• Entropy	2022
• PeerJ Computer Science	2022
• Neuromorphic Computing and Engineering	2022
• Applied Artificial Intelligence	2022
• Applied Physics Reviews	2021
• Classical and Quantum Gravity	2023
• Journal of Physics: Condensed Matter	2021
• Plasma Physics and Controlled Fusion	2021, 2022
• Machine Learning: Science and Technology	2021, 2025
• The Journal of Chemical Physics	2024

- Chemical Science 2019, 2020, 2021, 2022, 2023, 2024
- Chemical Communications 2020, 2021, 2022
- RSC Advances 2020, 2021, 2022
- Journal of Computational Chemistry 2022
- Reaction Chemistry and Engineering 2021, 2022
- Current Opinion in Chemical Engineering 2022
- Digital Discovery 2022, 2024
- Environmental Research and Communications 2021
- Minerals 2022

Program Committee

- Area Chair for ICML 2027 2027
- Area Chair for NeurIPS Workshop on AI4Science 2023, 2025
- Area Chair for ICML Workshop on AI4Science 2024, 2026
- NeurIPS Workshop on Gaussian Processes 2022
- NeurIPS Workshop on AI4Science 2021, 2022
- ICLR Workshop on Deep Generative Models 2022
- NeurIPS Workshop on Machine Learning for Molecules 2020
- NeurIPS Workshop on Machine Learning for Healthcare 2020, 2021, 2022
- NeurIPS Workshop on Machine Learning and the Physical Sciences 2021

Invited Talks

- *Towards Foundation Models that Learn from Every Experiment, Warp Sciences, San Mateo, USA, 2026*
- *Bayesian Optimization over Generative Models of Materials and Molecules*, Meta, Fundamental AI Research (FAIR), San Francisco, USA, 2023
- *Applications of Gaussian Processes at Extreme Lengthscales: From Molecules to Black Holes*, Tecnológico de Monterrey, Monterrey, Mexico, 2023
- *GAUCHE: A Library for Gaussian Processes in Chemistry*, Evonik Industries AG, Essen, Germany, 2022
- *Applications of Gaussian Processes at Extreme Lengthscales: From Molecules to Black Holes*, EPFL, Lausanne, Switzerland, 2022
- *Modelling the Multiwavelength Variability of Markarian 335 using Gaussian Processes*, Institute of Astronomy, Cambridge, UK, 2020
- *Automatic Chemical Design*, Wolfson Research Event, Cambridge, UK, 2019
- *The Rise of Machine Learning and its Relevance for the Natural Sciences*, Goodenough College, London, UK, 2019
- *Constrained Bayesian Optimization for Automatic Chemical Design*, NIPS Workshop on Bayesian Optimization for Science and Engineering, Long Beach, USA, 2017

Technical Skills

- **LLM Tools/Platforms**: Claude Code, Codex, LangChain, ElevenLabs, Cursor, Higgsfield, Manus
- **Programming Languages**: Python, MATLAB/Octave
- **Technologies/Frameworks**: PyTorch, TensorFlow, JAX, Theano, GPflow, BoTorch, GPyTorch, Azure
- **Operating System Tools**: UNIX shell, bash scripting
- **Chemistry Software**: RDKit, DeepChem, Avogadro, Gaussian, ChemDraw, SciFinder, Reaxys, MarvinSketch, ChemSpider

Awards

- Top Reviewer NeurIPS 2025 (Top 8%, 1957 of 24,430 reviewers) — Oct 2025
- Top Reviewer AISTATS 2025 (Top 5%) — May 2025
- Assistant Professorship in AI, University of Bristol, UK (Courteously Declined) — Mar 2024
- Top Reviewer NeurIPS 2023 (10.2%, 1,197 of 11,725 reviewers) — Dec 2023
- MILA-Samsung Scholarship: $25,000 — Jan 2022
- Huawei Noah's Ark Lab Prize - Best PhD research scientist — Feb 2021
- G-Research Prize - Best draft PhD thesis: £5,000 — Mar 2020
- NeurIPS 2019 Travel Grant — Dec 2019
- EPSRC Vacation Bursary Award: £2,200 — Jul 2014

Interests and Achievements

Chess

- FIDE Master with 2 International Master Norms
- Former British Junior Champion (U18)
- Five-time Irish Junior Champion (U14, U16, U19)
- Board 3 for the Irish Men's Team at the 2012 Chess Olympiad in Istanbul
- Board 1 for Cambridge in the 2017 Varsity Match

Other

- Captain of the Wolfson College University Challenge (televised quiz show) Team for the 2019-20 season: Episode Link
- Long-distance running: RunBritain handicap of 2.2
- Latin Dance: Cuban Salsa, Bachata, Cross-Body Salsa.