

HENRY MOSS

henry.moss@secondmind.ai

RESEARCH INTERESTS

Bayesian optimisation & active learning: information-theory; batch design; multi-fidelity.

Gaussian processes: scalable models; multi-fidelity; structural kernels.

Experimental design: gene design; molecular search.

Natural Language Processing: text-to-speech, hyper-parameter optimisation, model selection.

CURRENT ROLE

Research Scientist, Secondmind, Cambridge.

2022 -

Senior Machine Learning Researcher, Secondmind, Cambridge.

2021 - 2022

EDUCATION

PhD in Machine Learning and Statistics, STOR-i CDT, Lancaster University.

2017 - 2021

- *General-purpose Information-theoretical Bayesian Optimisation*
 - Extended information-theoretical Bayesian optimisation for batch and multi-fidelity designs.
 - Developed Bayesian optimisation methods for high-cost string design problems.
- Supervision by Prof. David Leslie (Statistics) and Prof. Paul Rayson (Computer Science).

MRes in Statistics and Operational Research, STOR-i CDT, Lancaster University.

2016 - 2017

MA in Mathematics, Emmanuel College, University of Cambridge.

2013 - 2016

PUBLICATIONS

Published:

Picheny V., **Moss H. B.**, Durrande N. & Torossian L. Bayesian Quantile and Expectile Optimisation. In *Association of Uncertainty in Artificial Intelligence (UAI)*, 2022.

Moss H. B., Ober S. W. & Picheny V. Information-theoretic Inducing Point Placement for High-throughput Bayesian Optimisation. In *The International Conference on Machine Learning: Workshop on Real World Experimental Design and Active Learning (ICML: Real-ML Workshop)*, 2022.

Payeles A., **Moss H. B.** & Picheny V. A Penalisation Method for Batch Multi-objective Bayesian Optimisation with Application in Heat-exchanger Design. In *The International Conference on Machine Learning: Workshop on Real World Experimental Design and Active Learning (ICML: Real-ML Workshop)*, 2022

Griffiths R., Klarner L., **Moss H. B.**, Ravuri A., Truong S. T., Ranković B., Schwaller P., Du Y., Jamasb A. R., Schwartz J., Tripp A., Kell G., Bourached A., Chan A., Moss J. Guo G., Lee A. & Jiang Tang. GAUCHE: A Library for GAussian Processes and Bayesian Optimisation in CHEmistry. In *The International Conference on Machine Learning: AI for Science Workshop (ICML: AI4Science Workshop)*, 2022

Vakili S., **Moss H. B.**, Artmev A., Dutordoir V. & Picheny V. Scalable Thompson Sampling using Sparse Gaussian Process Models. In *The Conference on Neural Information Processing Systems (NeurIPS)*, 2021.

Moss H. B., Leslie D. S., Gonzalez J. & Rayson P. General-purpose Information-based Bayesian Optimisation. In *The Journal for Machine Learning Research (JMLR)*, 2021.

Moss H. B., Beck D., Leslie D. S., Gonzalez J. & Rayson P. Bayesian Optimisation over String spaces. In *The Conference on Neural Information Processing Systems (NeurIPS)*, 2020 (**spotlight**).

Moss H. B. & Griffiths R. Gaussian Process Molecule Property Prediction With FlowMO. In *The Conference on Neural Information Processing Systems: Machine Learning for Molecules Workshop (NeurIPS: ML4Molecules Workshop)*, 2020 (**selected talk**).

Moss H. B., Leslie D. S. & Rayson P. BOSH: Bayesian Optimisation by Sampling Hierarchically. In *The International Conference on Machine Learning: Workshop on Real World Experimental Design and Active Learning* (ICML: Real-ML Workshop), 2020.

Moss H. B., Leslie D. S. & Rayson P. MUMBO: Multi-task Max-value Bayesian Optimisation. In *The European Conference on Machine Learning and Principles and Practice of Knowledge Discovery in Databases* (ECML), 2020.

Moss H. B., Aggarwal V., Prateek N., Gonzalez J. & Barra-Chicote R. BOFFIN TTS: Few-shot Speaker Adaptation By Bayesian Optimisation. In *The International Conference on Acoustics, Speech and Signal Processing* (ICASSP), 2020.

Moss H. B., Moore A., Leslie D. S. & Rayson P. FIESTA: Fast IdEntification of State-of-The-Art Models Using Adaptive Bandit Algorithms. In *The Annual Meeting of the Association of Computational Linguists* (ACL), 2019.

Moss H. B., Leslie D. S. & Rayson P. Using J - K -fold Cross Validation to Reduce Variance when Tuning Natural Language Processing Models. In *The International Conference on Computational Linguistics* (COLING), 2018 (area chair favourite).

Under Review:

Moss H. B., Ober S. W. & Picheny V. Inducing Point Allocation for Sparse Gaussian Processes in High-throughput Bayesian Optimisation Loops.

Ranković B., Griffiths R., **Moss H. B.** & Schwaller P. Bayesian Optimisation-accelerated Additives Screening and Yield Improvements in Chemical Reactions.

Qing J., **Moss H. B.** & Couckuyt I. $\{PF\}^2$ ES: Parallel Feasible Pareto Frontier Entropy Search for Multi-Objective Bayesian Optimization under Unknown Constraints.

Payeles A., **Moss H. B.** & Picheny V. HIPPO: Highly Parallelisable Pareto Optimisation for Multi-Objective Bayesian Optimisation.

Griffiths R., Thawani A., Jamasb A., **Moss H. B.**, Bourached A., Jones P., McCorkindale W. & Aldrick A. A Case for Domain Expert Dataset Curation in Machine-Learning Enabled Chemistry.

Chang P., Verma P., John ST., **Moss H. B.**, Picheny V. & Solin A. Fantasizing with Dual GPs in Bayesian Optimization and Active Learning.

PRIZES

Extra Mile award: Embodying Secondmind’s “Delight Every Customer” value.	2022
NeurIPS spotlight paper: Top 3% of submissions at NeurIPS.	2020
ML4Molecules contributed talk: Top 5% of submissions at the ML4Molecules Workshop at NeurIPS.	2020
Nick Smith prize: Best second-year Statistics PhD student at Lancaster University.	2019
Area chair favourite: Nominated for overall best paper at COLING 2018.	2018

PRESENTATIONS

Lancaster Alumni Day: <i>Job Hunting and Building an Early Career</i> (panel Session).	2022
Secondmind Seminar: <i>Inducing Point Allocation for Sparse Gaussian Processes ...</i> (talk).	2022
Real-ML@ICML: <i>Information-theoretic Inducing Point ...</i> and <i>A penalisation method for ...</i> (posters).	2022
UAI: <i>Quantile and Expectile Optimisation</i> (poster).	2022
Secondmind: <i>Introduction to Multi-Fidelity Modelling</i> and <i>Introduction to Profile Optimisation</i> (talks).	2022
Univ. Cambridge ML@Computer-Lab and Univ. Bern: <i>GIBBON</i> (talk).	2022
Gaussian Process Summer School: <i>Overview of Secondmind’s Toolboxes</i> (talk).	2021
Secondmind: <i>Introduction to Information Theory</i> (talk).	2021
NeurIPS: <i>BOSS: Bayesian Optimisation over String Spaces</i> (talk).	2020
ML4Molecules@NeurIPS: <i>Gaussian Process Molecule Property Prediction with FlowMo.</i> (talk).	2020
ECML: <i>MUMBO: Multi-task Max-value Bayesian Optimisation</i> (talk).	2020
Microsoft Research Cambridge: <i>Bayesian Optimisation in Gene Design Loops</i> (talk).	2020
Mathematics of Data Science Conference and ICML: RealML Workshop: <i>BOSH</i> (talk).	2020

ICASSP, Amazon Research Cambridge and University of Melbourne: <i>BOFFIN TTS</i> (talk).	2020
Prowler.io, Sheffield, Lancaster and Manchester Universities; <i>MUMBO</i> (talk).	2019
Amazon Intern Colloquium: <i>Rapid Speaker Adaptation with Bayesian Optimisation</i> (poster).	2019
ACL: <i>FIESTA: Fast Identification of SOTA</i> (talk).	2019
Google NLP Summit: <i>Reliable and Efficient Hyper-parameter Tuning for NLP</i> (poster).	2019
STOR-i Forum and Lancaster Data Science Group: <i>A Crash Course in Bayes Opt</i> (talk).	2018
Microsoft AI Summer School and COLING: <i>Using J-K-fold Cross Validation ...</i> (poster)	2018
UCREL Summer School in Corpus-based NLP: <i>Instabilities in NLP models</i> (poster).	2017

INTERNSHIPS AND SUMMER SCHOOLS

Visiting researcher , School of Computing and Information Systems, University of Melbourne.	2020
• Derived Bayesian optimisation for sequence design under syntactic constraints.	
Amazon PhD internship , Text-To-Speech Team, Amazon Alexa, Cambridge.	2019
• Used Bayesian optimisation to fine-tune neural systems to synthesise new voices with limited data.	
Amazon Intern Colloquium , Amazon Research, Cambridge.	2019
Google NLP Summit , Google Research, Zurich.	2019
Microsoft AI Summer School , Microsoft Research, Cambridge.	2018
UCREL NLP Summer School , Lancaster University.	2017
Wellcome Sanger internship , University of Cambridge.	2016
• Designed a system to automatically flag promising compounds during image-based drug screening.	
Summer research internship , STOR-i CDT, Lancaster University.	2016
Equity analyst: Oil & Gas researcher at Redburn International.	2015

RESEARCH SUPPORT

Visiting researcher grant: Collaboration sponsorship from the University of Melbourne.	2020
STOR-i research fund: Support for visit to the University of Melbourne from Lancaster University.	2020
Workshop sponsorship: Support for Bayesian optimisation workshop from Amazon Research.	2019
Faculty of Science and Technology travel grant: Travel support from Lancaster University.	2018
STOR-i PhD scholarship: Full funding for MRes and PhD programme.	2016

OTHER RELEVANT EXPERIENCE

Workshop Organiser: Organised interdisciplinary workshop on Gaussian processes in Astronomy.	2022
Seminar Coordinator: Ran Secondmind's external speaker seminar series.	2022
Internship Coordinator: Ran Secondmind's summer internship programme.	2022
Statistical Consultant: UK Environment Agency: Flood Hydrology Road Map.	2022
Reviewer: Reviewed manuscripts for Neural Computation and NeurIPS.	2022
Reading Group Coordinator: Ran Secondmind's summer internal reading group.	2021
Internship Supervisor: Supervisor for two summer placement students.	2021
Program Committee: Committee member for the NeurIPS ML4Molecules Workshop.	2020 - 2021
Reviewer: Reviewed manuscripts for AISTATS and ECML.	2020
MSc Masterclass: Designed and taught short course on Bayesian optimisation.	2019 - 2021
Statistical Consultant: Natural Language Identification Project, Lancaster University.	2018
STOR-i Computing Team: Assist peers with coding and distributed computing.	2017 - 2019
Tutor: Undergraduate Mathematics and MSc Data Science.	2017 - 2019
Lancaster University Outreach: Interactive sessions with local secondary schools.	2016 - 2018

COMPUTING SKILLS

Python, Tensorflow, PyTorch, GPflow, Git, Maintainer of Trieste, Contributor to Emukit, GPy, GPyOpt, Cython, MXNet, R, C.