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 -

- Co-lead of a team of 4 engineers, designing an ML system for electric vehicle engine calibration.

Senior Machine Learning Researcher, Secondmind, Cambridge. 2021 - 2022

AWARDS

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

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., Scwartz 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.

PRESENTATIONS

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

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