

CURRICULUM VITAE

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Personal Details

José Miguel Hernández Lobato
Department of Engineering
Trumpington Street
University of Cambridge, CB2 1PZ, UK

Phone: +44 12237 62363
Email: jmh233@cam.ac.uk
Homepage: <http://jmhl.org>
Google scholar: [link](#)

Education

- Dec. 2010 Ph.D. in Computer Science. Universidad Autónoma de Madrid, Spain.
Research area: Machine Learning. Advisor: Prof. Alberto Suárez González.
- Jun. 2007 M.Sc. in Computer Science. Universidad Autónoma de Madrid, Spain.
- Jun. 2004 B.Sc. in Computer Science. Universidad Autónoma de Madrid, Spain.
Award to **best academic record on graduation**.

Professional History

- 2022 – now Professor of Machine Learning (grade 11).
Department of Engineering, University of Cambridge, UK.
- 2020 – now Senior scientific research advisor for Boltzbit Limited.
- 2020 – now Co-director of the Cambridge ELLIS unit.
- 2020 – now Faculty member of the Cambridge Center for AI in Medicine.
- 2018 – 2020 Visiting researcher.
Microsoft Research Cambridge, Cambridge, UK.
- 2021 – 2022 Associate Professor in Machine Learning.
Department of Engineering, University of Cambridge, UK.
- 2016 – 2021 University Lecturer in Machine Learning.
Department of Engineering, University of Cambridge, UK.
- 2017 – 2021 Turing Fellow.
Alan Turing Institute, London, UK.
- 2014 – 2016 Postdoctoral Researcher.
Harvard Intelligent Probabilistic Systems Group.
School of Engineering and Applied Sciences, Harvard University, USA.
- 2013 – 2014 Research Associate.
Wolfson College, Cambridge, UK.
- 2011 – 2014 Postdoctoral Researcher.
Computational and Biological Learning Group.
Engineering Department, Cambridge University, UK.
- 2010 – 2011 Teaching Assistant.
Machine Learning Group, Computer Science Department.

Universidad Autónoma de Madrid, Spain.

Membership of Professional Bodies

Since 2011 Member of the Spanish Association for Artificial Intelligence (AEPIA).
Since 2019 Member of the European Laboratory for Learning and Intelligent Systems (ELLIS).
Since 2020 Member of the EPSRC Peer Review Associate College.

PhD. and MPhil. Thesis Examination

2016 - now **PhD. Thesis examination:**

2022 Tim Georg Johann Rudner, University of Oxford (external).
2022 Adria Garriga Alonso. University of Cambridge (internal).
2022 Didrik Nielsen. University of Copenhagen (external).
2022 Alexander Camuto, University of Oxford (external).
2021 Matthew Willets, University of Oxford (external).
2021 Harshil Shah, University College London (external).
2021 Joseph Sakaya, University of Helsinki (external).
2020 Niels Bruun Ipsen, Technical University of Denmark (external).
2020 Alex Botev, University College London (external).
2020 Niki Kilbertus, University of Cambridge (internal).
2020 Vikas Verma, Aalto University, Finland (external).
2020 Matej Balog, University of Cambridge (internal).
2019 Juho Piironen, Aalto University (external).
2019 Gintare Karolina Dziugaite, University of Cambridge (internal).
2019 Xiaoyu Lu, University of Oxford (external).
2019 Stefan Depeweg, Technical University of Munich (external).
2019 Yin Cheng, University College London (external).
2018 Mortiz August, Technical University of Munich (external).
2018 Alex Navarro, University of Cambridge (internal).
2018 Petros-Pavlos Ypsilantis, King's College London (external).
2018 Diane Bouchacourt, University of Oxford (external).
2017 Yarin Gal, University of Cambridge (internal).
2017 Lavanya Sita Tekumalla, Indian Institute of Science, Bangalore (external).
2016 Tomi Peltola, Aalto University, Finland (external).

2016 - now **MPhil thesis examination: 27**

Pietro Galliani, Jonathan Gordon, Marton Havasi, Ryan-R Griffiths, Sergio Pascual Diaz, Mara Graziani, Omar Mahmood, Richard Shen, Sigurjon Ísaksson, Philip Ball, Frances Ding, Yuanzhao Zhang, Gergely Flamich, Riccardo Barbano, Ramona Comanescu, Justin Bunker, Efstratios Markou, David Lines, Javier Antorán, Tong Che, Wenlong Chen, James Branigan, Aliaksandra Shysheya, Rui Xia, Yuxin Chang, Igor Adamski, Ioannis Tsetis.

Peer Review Activities

Senior conference program committee:

2021 Neural Information Processing Systems (NeurIPS) Datasets and Benchmarks track.
2021 – 2022 International Conference on Learning Representations (ICLR).
2020 – 2022 Neural Information Processing Systems (NeurIPS).
2019 International conference on Uncertainty in Artificial Intelligence (UAI).
2019 – 2022 International Joint Conference on Artificial Intelligence (IJCAI).
2017 – 2022 International Conference on Machine Learning (ICML).
2018 – 2022 Artificial Intelligence and Statistics (AISTATS).
2020 – 2023 Association for the Advancement of Artificial Intelligence (AAAI).

Conference program committee:

2021 – 2022	International conference on Uncertainty in Artificial Intelligence (UAI).
2012 – 2019	International Conference on Machine Learning (ICML).
2013 – 2019	Neural Information Processing Systems (NeurIPS).
2017 – 2020	International Conference on Learning Representations (ICLR).
2018 – 2019	Association for the Advancement of Artificial Intelligence (AAAI).
2016 – 2017	Artificial Intelligence and Statistics (AISTATS).

Workshop reviewer:

2021	Neural Information Processing systems (NeurIPS).
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Panel member in grant proposal evaluation process:

2022	EPSRC Information and Communication Technologies (ICT) Prioritisation Panel
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Grant proposal reviewer:

2022	Member of EPSRC prioritization panel. Reviewed 9 proposals.
2022	National Science Center, Poland.
2022	EPSRC Access to high performance computing call.
2022	AI Singapore Research Programme.
2021	St. John's College Research Fellowships.
2021	Swiss National Science Foundation
2021	EPSRC grant proposal.
2021	Wellcome Trust. Hub for Innovative Technologies for Neglected Tropical Diseases.
2020	Swiss Data Science Center, EPFL and ETH Zurich, Switzerland.
2020	Peterhouse Research Fellowships.
2020	Fulbright Senior Award 2021-2022, Polish-U.S. Fulbright Commission.
2020	Starting Grant Call, European Research Council.
2020	Program Committee for the evaluation of ELLIS faculty, ELLIS society.
2020	Croucher Foundation awards, Hong Kong.
2020	KTH Royal Institute of Technology, Sweden.
2020	National Science Center, Poland.
2019	Swiss Data Science Center, EPFL and ETH Zurich, Switzerland.
2019	Turing AI Fellowships, Alan Turing Institute.
2019	AI Singapore Research Programme.
2019	Israel Science Foundation
2019	Early Career Research Fellowships, Churchill College, University of Cambridge.
2018	Biotechnology and Biological Sciences Research Council (BBSRC).
2018	AI Singapore Research Programme.
2018	Lise Meitner Post-doctoral Programme Austrian Science Fund.
2017	Croucher Foundation awards, Hong Kong.

Journal reviewer:

Since 2009	Nature Computational Science, Nature Communications, Nature Nanotechnology, IEEE Transactions on Pattern Analysis and Machine Intelligence, Journal of Machine Learning Research, Neural Computation, Journal of the Royal Statistical Society, Journal of Artificial Intelligence Research, Transactions on Knowledge and Data, Engineering, ACS Central Science, The Journal of Physical Chemistry, IEEE Transactions on Signal Processing, Entropy, Digital Signal Processing, Journal of Selected Topics in Signal Processing, Neurocomputing, Journal of Empirical Finance, IBM Journal of Research and Development.
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Awards

2021	Elected Fellow of the European Laboratory for Learning and Intelligent Systems (ELLIS, https://ellis.eu).
2020	Supervisor of the best 4th-year project in Division F of the Department of Engineering with title "Improving Ergodic Inference with High Entropy Distributions".

- 2020 Best Paper Runner-up award. ICML workshop on "Bridge between Perception and Reasoning: Graph Neural Networks & Beyond".
- 2019 Nominee best lecturer in part IIA (third year). Department of Engineering, University of Cambridge.
- 2016 Best paper award. NeurIPS Constructive Machine Learning workshop, Barcelona, Spain, 2016.
- 2012 First prize in the EMC Data Science competition, London, worth 1,200 £, London, UK.
- 2012 Madrid Mentoring Network Award for the business project "Sugerendo".
- 2012 Cink emprende award to the best business project "Sugerendo".
- 2011 Bancaja award to the best business project "Sugerendo".
- 2006 Second best poster presentation, Summer School on Pattern Recognition, Plymouth, UK.
- 2004 First prize and special prize in the programming contest for the region of Madrid (CUPCAM).
- 2004 Special prize to the **best academic record on graduation**, Universidad Autónoma de Madrid.

Grants

- 2022 – 2023 EPSRC Tier-2 capital grant.
Towards Large-scale Machine Learning Models That Know When They Don't Know.
Investigators: J.M. Hernández-Lobato (PI) and James Allingham (Co-investigator).
Budget: 50,000 GPU hours on Cambridge CDS3 supercomputer, worth £10,000.
- 2022 – 2024 Marie Skłodowska-Curie Action,
Investigators: J.M. Hernández-Lobato (PI), Vikas Verma (sponsored postdoc researcher).
Funding agency: European Commission.
Budget: 236,748 EUR.
- 2022 – 2023 AWS Cloud Credit for Research
Investigators: J.M. Hernández-Lobato (PI)
Funding agency: Amazon
Budget: 20,000 USD.
- 2022 – 2024 Margarita Salas Fellowship
Investigators: J.M. Hernández-Lobato (PI) and Pablo Morales Álvarez (sponsored postdoc researcher).
Funding agency: Spanish Ministry of Universities
Budget: 75,000 EUR.
- 2021 – 2022 Qualcomm Innovation Fellowship Award
Investigators: J.M. Hernández-Lobato (PI) and James Allingham (PhD student).
Budget: 40,000 USD.
- 2021 – 2022 EPSRC Tier-2 capital grant.
Reinforcement Learning for Molecular Design Guided by Quantum Mechanics.
Investigators: J.M. Hernández-Lobato (PI) and Gregor Simm (Co-investigator).
Budget: 100,000 GPU hours on Cambridge CDS3 supercomputer, worth £20,000.
- 2020 – 2025 EPSRC Turing AI Acceleration Fellowship.
Machine Learning for Molecular Design.
Investigators: J.M. Hernández-Lobato (PI)
Budget: £1.3m.
- 2020 – 2025 Industrial funding to support a Cambridge ELLIS unit.
Investigators: J.M. Hernández-Lobato (PI) and Carl E. Rasmussen (Co-PI).
Funding sources: Invenia Labs, ARM, Cambridge Innovation Capital, IQ Capital, Schlumberger, AstraZeneca, Microsoft and Prolwer.io.
Budget: 1m EUR.
- 2020 – 2021 EPSRC Tier-2 capital grant EP/P020259/1
Unsupervised Learning with Structured Latent Representations

- Investigators: J.M. Hernández-Lobato (PI) and Kristoffer Stensbo-Smidt (Co-investigator).
Budget: 200,000 GPU hours on Cambridge CDS3 supercomputer, worth £40,000.
- 2019 – 2024 EPSRC Prosperity Partnership.
Machine Learning for Tomorrow: Efficient, Flexible, Robust and Automated
Investigators: Richard E. Turner (PI) and J.M Hernández-Lobato (Co-investigator)
Budget: £3.7m (£2m EPSRC, £1.7m Microsoft Research).
- 2019 – 2023 Microsoft Research PhD Scholarship 2019
EPSRC Case studentship
Budget: £134,510
- 2018 – 2020 Accelerated Discovery of Transition Metal-Catalyzed Reactions Through Machine Learning
Investigators: J.M. Hernández-Lobato (PI), Gregor Simm (sponsored postdoc researcher).
Funding agency: Swiss national science foundation.
Budget: 75,000 CHF.
- 2018 – 2021 Donation for Cambridge-Tuebingen PhD studentship.
Investigators: J.M. Hernández-Lobato (PI).
Funding agency: Google DeepMind.
Budget: 142,047 GBP.
- 2018 – 2020 Marie Skłodowska-Curie Action,
Investigators: J.M. Hernández-Lobato (PI), Kristoffer Stensbo-Smidt (sponsored postdoc researcher).
Funding agency: European Commission.
Budget: 183,455 EUR.
- 2018 – 2021 Design Space Exploration of Heterogeneous SoCs using Multi-Objective Bayesian Optimization.
Investigators: J.M. Hernández-Lobato (PI), David Brooks (Harvard University).
Funding agency: Semiconductor Research Corporation (SRC).
Budget: 135,000 USD.
- 2017 – 2020 Multi-Objective Bayesian Optimization for SoC Design Space Exploration.
Investigators: David Brooks (PI, Harvard University) and J.M Hernández-Lobato.
Funding agency: Intel Corporation.
Budget: 104,346 USD.
- 2017 – 2020 Probabilistic Machine Learning for Device Data Analysis.
Investigators: J.M Hernández-Lobato(PI), Z. Ghahramani, Carl E. Rasmussen and Adrian Weller.
Funding agency: Samsung Electronics.
Budget: 1,366,528 GBP
- 2014 – 2016 Information Theoretic Bayesian Optimization.
Investigators: J.M. Hernández-Lobato(PI) and Ryan P. Adams.
Funding agency: Rafael del Pino Foundation.
Budget: 50,000 EUR.

Invited Talks

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| Sep 2022 | Invited Talk | Leverhulme Research Centre for Functional Materials Design Symposium
University of Liverpool. UK |
| Jun 2022 | Invited Talk | “Invariant Causal Representation Learning for Out-of-Distribution Generalization”,
Mini-Workshop “Causal RL ² ”, MPI-IS, Tubingen, Germany.
Virtual talk. |
| Jun 2022 | Invited Talk | Data-efficient Predictions of Molecular Properties using Meta learning and Gaussian |

Jun 2022	Invited tutorial	Processes. Open research event, Department of Chemistry, University of Cambridge Nordic Probabilistic AI school, Helsinki, Finland.
Jun 2022	Panelist	Selected as panelist for the ACM 75th Anniversary Celebration, San Francisco, USA.
Apr 2022	Invited Talk	Data-efficient Predictions of Molecular Properties using Meta learning and Gaussian Processes. ICLR 2022 Workshop on Machine Learning for Drug Discovery Virtual Talk.
Apr 2022	Invited talk	Improving Data-efficiency and Hyperparameter Tuning in Deep Learning Seminar at Max Planck Institute for Biogeochemistry, Jena, Germany.
Apr 2022	Invited talk	Scalable One-Pass Optimisation of High-Dimensional Weight-Update Hyperparameters by Implicit Differentiation Seminar at DLR Institute of Data Science, Jena, Germany.
Feb 2022	Invited Talk	Advances in Molecular Design with Deep Generative Models Seminar series "Artificial Intelligence in Chemistry and Beyond" Ecole Polytechnique Fédérale de Lausanne, EPFL, Switzerland. Virtual Talk.
Feb 2022	Invited Talk	Molecule Optimization with Deep Generative Models Virtual workshop on BO/AI for chemical formulations Center for Accelerated Formulations Engineering (CAFE) Cornell University, USA.
Feb 2022	Invited Talk	Molecule Optimization and Deep Generative Models AAAI-22 Workshop on AI to accelerate science and engineering. Virtual Talk.
Jan 2022	Invited Tutorial	Molecule optimization with deep generative models Lifting inference with kernel embeddings, winter school and workshop, Bern, Switzerland. Virtual Talk.
Nov 2021	Invited Talk	Probabilistic methods for increased robustness in machine learning Accenture / Turing Innovation Symposium. An Online Event.
Nov 2021	Invited Talk	Bootstrap your flow. Opening of the Cambridge Innovation Centre in Digital Molecular Technologies (iDMT), Cambridge, UK. An Online Event.
Nov 2021	Invited Talk	Probabilistic Methods for Increased Robustness in Machine Learning. 10th EdukCircle International Convention on Engineering and Computer Technology. An Online Event.
Oct 2021	Invited Talk	Probabilistic Methods for Increased Robustness in Machine Learning. Jena University, Germany.
Oct 2021	Invited Talk	Probabilistic Methods for Increased Robustness in Machine Learning. Universidad Autonoma de Madrid. Held virtually due to COVID-19.
July 2021	Invited talk	Probabilistic Methods for Increased Robustness in Machine Learning. Secondmind (ex Prowler.io) Cambridge, UK. Held virtually due to COVID-19.
Jun 2021	Invited Talk	Deconfounding Reinforcement Learning in Observational Settings. EDM'21 Workshop on Reinforcement Learning for Education. Max Planck Institute for Software Systems.

		Saarbrücken Germany. Held virtually due to COVID-19.
May 2021	Invited Talk	Advances in Molecular Design with Deep Generative Models Birmingham Artificial Intelligence meetup. Held virtually due to COVID-19.
Apr 2021	Invited Talk	Successor Uncertainties: Efficient Exploration in Model-free RL Center for Advanced Mathematics for Energy Research Applications (CAMERA), Lawrence Berkeley National Lab, Berkeley, CA, USA. Held virtually due to COVID-19.
Apr 2021	Invited Talk	Getting a CLUE: A Method for Explaining Uncertainty Estimates ICLR Seminar series Institute for Adaptive and Neural Computation, Edinburgh. Held virtually due to COVID-19.
Mar 2021	Invited Talk	Expressive yet Tractable Bayesian Deep Learning via Subnetwork Inference Bi-weekly ML research meeting. ARM Ltd, Cambridge, UK. Held virtually due to COVID-19.
Mar 2021	Invited Talk	Machine Learning for Molecular Design AI UK 2021 Alan Turing Institute, London. Held virtually due to COVID-19.
Mar 2021	Invited Talk	Generative Models for Synthesizable Molecules. EMBL-EBI Industry Programme Workshop on Machine Learning in Drug Discovery and Precision Medicine II, Hinxton, Cambridge, UK. Held virtually due to COVID-19.
Dec 2020	Invited Talk	Latent Space Optimization with Deep Generative Models. Indian Symposium on Machine Learning (IndoML). Held virtually due to COVID-19.
Dec 2020	Invited Talk	Latent Space Optimization with Deep Generative Models. NeurIPS workshop on Learning Meaningful Representations of Life. Held virtually due to COVID-19.
July 2020	Invited Talk	Efficient Missing-value Acquisition with Variational Autoencoders. Bi-weekly ML research meeting. ARM Ltd, Cambridge, UK. Held virtually due to COVID-19.
July 2020	Invited Talk	Latent Space Optimization with Deep Generative Models. ML/AI in (bio)chemical engineering conference. University of Cambridge. Held virtually due to COVID-19.
July 2020	Invited Talk	Efficient Missing-value Acquisition with Variational Autoencoders. ICML workshop on The Art of Learning with Missing Values. Held virtually due to COVID-19.
July 2020	Invited Talk	Latent Space Optimization with Deep Generative Models. ICML Workshop on Real-World Experiment Design & Active Learning Held virtually due to COVID-19.
Mar 2020	Invited Talk	Deep Generative Models of Molecules in 3D Space Machine learning in Physics, Chemistry and Materials discussion group University of Cambridge. Held virtually due to COVID-19.
Mar 2020	Invited Talk*	Advances in Compression via Probabilistic Machine Learning, SIAM Conference on Uncertainty Quantification, mini-symposium on "Uncertainty Quantification in Deep Learning", Munich, Germany. (Cancelled due to COVID-19 outbreak)
Feb 2020	Invited Talk	Advances in Machine Learning for Molecules, Conference on "AI powered Drug Discovery and Manufacturing"

		Massachusetts Institute of Technology (MIT), USA. (Cancelled due to COVID-19 outbreak)
Feb 2020	Invited Talk	Advances in Compression and Exploration via Probabilistic Machine Learning, IBM research in Cambridge, MA. USA. (Cancelled due to COVID-19 outbreak)
Dec 2019	Invited Talk*	A generative model for molecular distance geometry Joint workshop on "Deep structures", Helsinki, Finland
Nov 2019	Invited Talk	Advances in Compression and Exploration via Probabilistic Machine Learning, Schlumberger, Cambridge, UK.
Oct 2019	Invited Tutorial	Graph neural networks. Machine Learning Tutorial at Imperial College, London, UK.
Oct 2019	Invited Talk	Advances in Compression via Probabilistic Machine Learning, Workshop on Generative Models and Uncertainty Quantification Technical University of Denmark, Copenhagen, Denmark.
Aug 2019	Invited Talk	Advances in Compression and Exploration via Probabilistic Machine Learning, Invited talk at Max Plank Institute for Intelligent Systems, Tuebingen, Germany.
Aug 2019	Invited Talk	Advances in Compression and Exploration via Probabilistic Machine Learning, Invited talk at Machine Learning Lab, University of Freiburg, Germany.
July 2019	Invited Talk	Advances in Compression and Exploration via Probabilistic Machine Learning, Invited seminar at Facebook AI Research, Paris, France.
Jun 2019	Oral*	Variational Implicit Process International Conference on Machine Learning (ICML), Long Beach, USA.
May 2019	Invited Talk	Advances in Compression and Exploration via Probabilistic Machine Learning, Machine Learning Coffee Seminar, Aalto University, Finland.
Mar 2019	Invited Talk	Advances in Machine Learning for Molecules, Workshop Artificial Intelligence and Machine Learning in Cambridge Microsoft Research Cambridge
Feb 2019	Invited Talk	Advances in Machine Learning for Molecules, Cantab Capital Institute for the Mathematics of Information University of Cambridge
Nov 2018	Invited Talk	Advances in Machine Learning for Molecules, Decision Summit by PROWLER.io Department of Engineering University of Cambridge
Sep 2018	Invited Tutorial	Advances in Machine Learning for Molecules, Machine Learning Summer School, Universidad Autónoma de Madrid, Spain.
Jul 2018	Invited Talk	Advances in Machine Learning for Molecules, First International Conference on Machine Learning and Physics, Institute for Advanced Study, Tsinghua University, China.
Jul 2018	Oral	Decomposition of Uncertainty in Bayesian Deep Learning for Efficient and Risk-sensitive Learning, International Conference on Machine Learning (ICML), Stockholm, Sweeden.
Jun 2018	Invited Talk	Bayesian Optimization for Accelerated Exploration of Chemical Space, International Society for Bayesian Analysis (ISBA) World Meeting, University of Edinburgh, UK.

May 2018	Invited Talk	Bayesian Machine Learning for Efficient Optimization of Black-box Functions, Statistical Science Seminar, Gatsby Unit, University College London, UK.
May 2018	Oral	Uncertainty Decomposition in Bayesian Deep Learning, Conference for the Information Engineering Division, Department of Engineering, University of Cambridge, UK.
Nov 2017	Invited Talk	Grammar Variational Autoencoder, Machine Learning & Molecules Conference, Copenhagen Biocenter, Copenhagen, Denmark.
Sep 2017	Invited Talk	Grammar Variational Autoencoder, Artificial Intelligence in Bioscience Symposium, The British Library, London, UK.
Sep 2017	Invited Talk	Bayesian Semi-Supervised Learning with Deep Generative Models, ARM Summit, Robinson College, Cambridge, UK.
Aug 2017	Oral	Parallel Thompson Sampling for Large-scale Accelerated Exploration of Chemical Space, International Conference on Machine Learning, Sydney, Australia.
May 2017	Invited Talk	Parallel Thompson Sampling for Large-scale Accelerated Exploration of Chemical Space, Gaussian Process Approximations Workshop, Amazon Research Center, Berlin, Germany.
May 2017	Invited Talk	Bayesian Machine Learning for Efficient Optimization of Black-box Functions, ARM Ltd, Cambridge, UK.
Mar 2017	Oral	Learning and Policy Search in Stochastic Dynamical Systems with Bayesian Neural Networks, Artificial Intelligence and Machine Learning in Cambridge, Microsoft Research Cambridge, Cambridge, UK.
Mar 2017	Invited Talk	Learning and Policy Search in Stochastic Dynamical Systems with Bayesian Neural Networks, Fourth Edinburgh Deep Learning Workshop, University of Edinburgh, UK.
Jan 2017	Invited Talk	Bayesian Optimization for Accelerated Exploration of Chemical Space, International Symposium on Machine Learning Challenges in Complex Multiscale Physical Systems, TUM, Munich, Germany.
Dec 2016	Invited Talk	Alpha divergence minimization for Bayesian deep learning, NeurIPS workshop on Bayesian deep learning, Barcelona, Spain.
Sep 2016	Invited Talk	Approximate EP for Deep Gaussian Processes, Dagstuhl Seminar 16481, New Directions for Learning with Kernels and Gaussian Processes, Schloss Dagstuhl, Germany.
Sep 2016	Invited Talk	Bayesian Optimization for Accelerated Exploration of Chemical Space, IPAM Workshop: Machine Learning Meets Many-Particle Problems, Institute for Pure and Applied Mathematics, Los Angeles, California, USA.
Sep 2016	Invited Talk	Bayesian Machine Learning for Efficient Optimization of Black-box Functions,

		Seminar series machine learning group, Department of Engineering, University of Oxford, UK.
Jul 2016	Invited Talk	Bayesian Optimization of Genetic Programs, Foundry Annual Meeting. Broad Institute of MIT and Harvard, Cambridge, MA, USA.
Mar 2016	Invited Talk	Bayesian Machine Learning for Efficient Optimization of Black-box Functions, Seminar Series, University of Toronto, Toronto, Canada,
Mar 2016	Invited Talk	Bayesian Machine Learning for Efficient Optimization of Black-box Functions, Seminar Series, Edinburgh University, Edinburgh, UK.
Mar 2016	Invited Talk	Bayesian Machine Learning for Efficient Optimization of Black-box Functions, Seminar Series, Max Planck Institute for Intelligent Systems, Tübingen, Germany.
Mar 2016	Invited Talk	Bayesian Machine Learning for Efficient Optimization of Black-box Functions, Seminar Series, EPFL, Lausanne, Switzerland.
Feb 2016	Invited Talk	Bayesian Machine Learning for Efficient Optimization of Black-box Functions, Seminar Series, New York University, New York City, USA.
Jan 2016	Oral	Bayesian Machine Learning for Efficient Optimization of Black-box Functions, Amazon Research Center, Berlin, Germany.
May 2015	Invited Talk	Probabilistic Backpropagation for Scalable Learning of Bayesian Neural Networks. Workshop on Gaussian Process Approximations, Copenhagen, Denmark.
March 2015	Invited Talk	Bayesian Optimization and Information-based Approaches. Machine Learning Meetup, Boston, Massachusetts, USA.
May 2014	Invited Talk	Stochastic Variational Inference for Large Scale Machine Learning. Department of Computer Science, Universidad Autónoma de Madrid, Spain.
Feb 2014	Oral	An Introduction to Determinantal Point Processes. Machine Learning Group, Cambridge University, Cambridge, UK.
Feb 2014	Invited Talk	Gaussian Process Conditional Copulas. Microsoft Research, Cambridge, UK.
Oct 2013	Invited Talk	Gaussian Process Conditional Copulas with Applications to Financial Time Series. Oxford-Man Institute of Quantitative Finance, University of Oxford, UK.
Jun 2013	Oral	Gaussian Process Vine Copulas for Multivariate Dependence. Columbia University, New York, USA.
Apr 2013	Oral	An Introduction to Sum Product Networks. Department of Engineering, Cambridge University, UK.
Feb 2013	Invited Talk	Stochastic Variational Inference for Modeling Binary Matrices. Xerox Research, Bangalore, India.

Feb 2013	Oral	NetBox: a Probabilistic Method for Analyzing Market Basket Data. Infosys Limited, Bangalore, India.
Feb 2012	Invited Talk	Ensemble Methods and Optimal Ensemble Size. Toshiba Research Laboratory, Cambridge, UK.
Dec 2011	Oral	Expectation Propagation for the Estimation of Conditional Bivariate Copulas. NeurIPS Workshop on Copulas in Machine Learning, Granada, Spain.
Sep 2011	Oral	Modeling Transaction Data. Infosys Limited, Bangalore, India.
Sep 2011	Oral	Market Basket Analysis: An Introduction. Infosys Limited, Bangalore, India.
Jul 2011	Oral	Gaussianity Measures for Detecting the Direction of Causal Time Series. International Joint Conference on Artificial Intelligence, Barcelona, Spain.
Sep 2010	Oral	Hub Gene Selection Methods for the Reconstruction of Transcription Networks. European Conference on Machine Learning (ECML), Barcelona, Spain.
Jul 2009	Oral	Modeling Dependence in Financial Data with Semiparametric Archimedean Copulas. Workshop on Advances in Machine Learning for Computational Finance (AMLFCF), London, UK.

* = Given on my behalf by one of my PhD students / Postdoctoral researchers.

Research Co-workers

PhD Students

2021 – now	Shreyas Padhy	Cambridge Harding Scholarship and Cambridge ELLIS unit. (directly supervised by me)
2021 – now	Wenlin Chen	Cambridge International Scholarship and Huawei. (directly supervised by me)
2020 – now	Gergely Flamich	Funded directly by my personal research funds. (directly supervised by me)
2020 – now	Vincent Stimper	Amazon Studentship (directly supervised by me)
2019 – now	James Allingham	The Mikheev Charitable Trust and EPSRC International Doctoral Studentship (directly supervised by me)
2019 – now	Austin Tripp	Cambridge International Scholarship (directly supervised by me)
2019 – now	Javier Antoran	EPSRC iCASE studentship with Microsoft Research. (directly supervised by me)
2019 – now	Erik Daxberger	EPSRC studentship and a Qualcomm European research studentship

		(directly supervised by me)
2018 – now	Ross Clarke	EPSRC Doctoral Training Programme award (directly supervised by me)
2018 – 2022	Chao Ma Now research scientist at Microsoft Research.	CSC Scholarship and Microsoft Research (directly supervised by me)
2018 – now	Chaochao Lu	Cambridge-Tuebingen Fellowship (directly supervised by me)
2017 – 2020	Jonathan Gordon Now research scientist at Open AI.	Samsung Electronics collaboration grant (directly supervised by me)
2017 – 2021	Marton Havazi Now postdoc at MIT.	EPSRC Doctoral Training Programme award (directly supervised by me)
2017 – now	Wenbo Gong Now research scientist at Microsoft Research.	CSC Cambridge International Scholarship (directly supervised by me)
2016 – 2021	David Janz Now research assistant and then postdoc at Amii.	Microsoft Research Scholarship (directly supervised by me)
2016 – 2021	John Bradshaw Now postdoc at Cambridge and then MIT.	Cambridge-Tuebingen Fellowship Co-supervised together with Z. Ghahramani
2015 – 2019	Stefan Depeweg Now research scientist at Siemens.	Collaborator at Technical University of Munich (co-supervised with Thomas Runkler).

Research Associates (Postdocs)

2022 – now	Emile Mathieu	UKRI Prosperity Partnership	Co-supervised with Rich Turner.
2022 – now	Sukriti Singh	UKRI Turing AI Fellowship	Directly supervised by me
2021 – 2021	John Bradshaw Now postdoc at MIT.	Samsung Electronics collaboration grant	Directly supervised by me
2018 – 2022	Gregor Simm Now researcher at Microsoft Research Amsterdam	Swiss national science foundation award	Directly supervised by me
2018 – 2020	Yichuan Zhang Now director at Boltzbit Limited.	Samsung Electronics collaboration grant	Directly supervised by me
2018 – 2020	Eric Nalisnick. Now assistant professor at University of Amsterdam.	Samsung Electronics collaboration grant	Directly supervised by me
2018 – 2020	Kristoffer Stensbo-Smidt Now postdoc at Technical University of Denmark (DTU) with Jes Frelsen	Marie Sklodowska-Curie Action	Directly supervised by me
2016 – 2018	Matthew Kusner. Now associate professor at UCL.	Turing Research Fellow	Collaborator
2016 – 2018	Brooks Paige. Now associate professor at UCL.	Turing Research Fellow	Collaborator

Research Coordinators

May 2021 – now Kimberly Cole Role: support with administrative tasks in group.

Research Assistants

Oct 2019 – Oct 2020	Gergely Flamich	Graduate, MPhil in Machine Learning and Machine Intelligence, University of Cambridge.	Directly supervised by me
Sep 2019 – Mar 2020	Rajan Troll	Undergraduate, BA in Mathematics, University of Cambridge.	Directly supervised by me

Visiting Researchers

March 2020 – now	Ignacio Peis	Visiting Graduate Student, Universidad Carlos III de Madrid, (research stay held remotely due to covid19).	Directly supervised by me
Feb 2020 – Jul 2020	Jiayu Yao	Visiting Graduate Student, School of Engineering and Applied Sciences, Harvard University.	Directly supervised by me
Sep 2019 – Dec 2019	Maximilian Vording	Visiting Graduate Student, Department of Applied Mathematics and Computer Science, Technical University of Denmark	Directly supervised by me
Sep 2019 – May 2020	Pablo Morales Alvarez	Visiting Graduate Student, Department of Computational Science and Artificial Intelligence, Universidad de Granada	Directly supervised by me
Feb 2019 – May 2019	Daniel Ramos	Visiting Academic Fellow, Department of Computer Science, Universidad Autónoma de Madrid	Directly supervised by me
Feb 2019 – Apr 2019	Alonso Marco Valle	Visiting Graduate Student, Department of Engineering, University of Cambridge	Directly supervised by me
May 2018 – Aug 2018	Alejandro Catalina Feliú	Visiting Graduate Student, Department of Engineering, University of Cambridge.	Directly supervised by me
Aug 2017 – Nov 2017	Moritz August	Visiting Graduate Student, Department of Engineering, University of Cambridge.	Directly supervised by me
Sep 2017 – Dec 2017	Juan José Murillo-Fuentes	Visiting Academic Fellow, Department of Engineering, University of Cambridge.	Directly supervised by me

Press coverage

2021	My work was mentioned in “La inteligencia artificial conquista la última frontera: el diseño de sus propios chips”, an article in the Spanish newspaper “EL País”.
2021	Interview at The TWIML AI Podcast. https://twimlai.com/
2020	J. M. Hernández (Cambridge): "La conexión entre empresas y la universidad acelera la IA", article in Spanish newspaper “El Español”.

Lecture Courses

2021 Lent	MPhil	MPhil in MLMI	MLMI7: Reinforcement learning and decision making	4 lectures
2021 Lent	MPhil	MPhil in MLMI	MLMI4: Advanced machine learning	4 lectures
2021 Lent	Undergraduate	Part IIA	3F8: Inference	8 lectures
2020 Michaelmas	Undergraduate	Part IIB	4F13: Probabilistic Machine Learning	8 lectures
2020 Michaelmas	Undergraduate	Part IIB	4F10: deep learning and structured data	4 lectures
2020 Lent	MPhil	MPhil in MLMI	MLMI7: Reinforcement learning and decision making	4 lectures
2020 Lent	MPhil	MPhil in MLMI	MLMI4: Advanced machine learning	4 lectures
2020 Lent	Undergraduate	Part IIA	3F8: Inference	8 lectures
2019 Michaelmas	Undergraduate	Part IIB	4F10: deep learning and structured data	6 lectures
2019 Lent	MPhil	MPhil in MLMI	MLMI7: Reinforcement learning and decision making	4 lectures
2019 Lent	MPhil	MPhil in MLMI	MLMI4: Advanced machine learning	4 lectures
2019 Lent	Undergraduate	Part IIA	3F8: Inference	8 lectures
2018 Michaelmas	Undergraduate	Part IA	Exposition	16 hours
2018 Michaelmas	Undergraduate	Part IIB	4F10: deep learning and structured data	4 lectures
2018 Lent	MPhil	MPhil in MLMI	MLSALT4: Advanced machine learning	9 lectures
2018 Lent	Undergraduate	Part IIA	3F8: Inference	14 lectures
2017 Michaelmas	Undergraduate	Part IIB	4F10: deep learning and structured data	4 lectures (prepared new material)
2017 Lent	MPhil	MPhil in MLMI	MLSALT4: Advanced machine learning	4 lectures (prepared new material)
2017 Lent	Undergraduate	Part IIA	3F8: Inference	4 lectures (prepared new material)
2016 Michaelmas	MPhil	MPhil in MLMI	MLSALT1:	4 lectures

introduction to machine learning (prepared new material)

Labs

2017 Michaelmas	MPhil	MPhil in MLMI	MLSALT1: Introduction to machine learning	Lab leader and 4 hours demonstration
2016 Michaelmas	MPhil	MPhil in MLMI	MLSALT1: Introduction to machine learning	Lab leader and 4 hours demonstration

Projects Taught

2021	MPhil in MLMI	Laurence Midgley	Annealed Importance Sampling and Alpha Divergences for Improved Boltzman Generators
2021	MPhil in MLMI	Kristopher Miliadiou	Efficient Data Compression with Deep Generative Models
2021	MPhil in MLMI	Chelsea Murray	Depth Uncertainty Networks for Active and Meta Learning
2021	MPhil in MLMI	Ginte Petrulionyte	Improving Deep Ensembles for Better Deep Uncertainty Quantification
2021	MPhil in MLMI	Wenlin Chen	Importance-Weighted Training for Identifiable Deep Generative Models
2021	Part IIB (4th-year)	Joe Xu	Information theoretic exploration in reinforcement learning with successor uncertainties
2021	Part IIB (4th-year)	Hannan Saddiq	Robust optimization in latent space with Bayesian variational auto encoders
2020	MPhil in MLMI	Wenlong Chen	Improved Ergodic Inference via Kernelised Stein Discrepancy, cosupervised with Wenbo Gong
2020	MPhil in MLMI	James Branigan	Self-Supervised Learning with Contrastive Predictive Coding, cosupervised with Javier Antoran
2020	MPhil in MLMI	Ioannis Tsetis	Information-Theoretic Exploration with Successor Uncertainties, co-supervised with Robert Pinsler
2020	Part IIB (4th-year)	Andrew Campbell	Improving Ergodic Inference
2020	Part IIB (4th-year)	Aleksandra Dokic	Refining the Variational Posterior Through Iterative Optimization
2019	MPhil in MLMI	Javier Antoran	Understanding Uncertainty in Bayesian Neural Networks, cosupervised with Tameem Adel
2019	MPhil in MLMI	Gergely Flamich	Compression without Quantization, cosupervised with Marton Havazi

2019	MPhil in MLMI	Ramona Comanescu	Sum-Product Copulas, cosupervised with Robert Peharz
2019	MPhil in MLMI	Riccardo Barbano	Investigating Inference in Bayesian Neural Networks via Active Learning, cosupervised with Jonathan Gordon and Robert Pinsler
2019	Part IIB (4th-year)	Basil Mustafa	Attention-based generative models of molecules
2019	Part IIB (4th-year)	Clifford Wilmot	Improved inference in deep Gaussian process models
2019	Part IIB (4th-year)	Mike Zheng	Efficient reinforcement learning with generative models and Bayesian inference
2018	MPhil in MLMI	Richard Shen	Automatic Chemical Design with Molecular Graph Variational Autoencoders
2018	MPhil in MLMI	Omar Mahmood	New Methods for Molecule Generation and Optimisation
2018	MPhil in Engineering	Johannes Harbrecht	Not finished yet.
2018	Part IIB (4th-year)	Luka Bojovic	Neural networks with optimal accuracy and speed in their predictions
2018	Part IIB (4th-year)	William Tai	Alpha divergence minimization in deep probabilistic programs
2018	Part IIB (4th-year)	Peter Choy	Distributed neuroevolution for meta reinforcement learning
2017	MPhil in MLMI	Marton Havasi	Designing Neural Network Hardware Accelerators Using Deep Gaussian Processes
2017	MPhil in MLMI	Jonathan Gordon	Bayesian deep generative models for semi-supervised and active learning
2017	MPhil in MLMI	Ryan-Rhys Griffiths	Constrained Bayesian Optimization for Automatic Chemical Design
2014	Part IIB (4th-year)	Kee Chong Tan	The Automated Statistician
2013	Part IIB (4th-year)	Menglun Li	Machine Learning for Recommender Systems
2013	Part IIB (4th-year)	Mina Spasic	Machine Learning for Recommender Systems

PhD advisor / evaluation of first-year reports

Andrew Foong

Marc Girona-Mata

Toby Howison

Valerii Likhoshesterov

Alberto Pepe

Robert Pinsler

James Requeima

Jonathan So

Ryan-Rhys Griffiths

Dan Jarrett

Ahmad Khan

Yassir Fathullah
 Aliaksandra Shysheya
 Hao Sun

Teaching Administration

2021 Lent	MPhil in MLMI	MLMI7: Reinforcement Learning and Decision Making	Module Leader
2021 Lent	Part IIA	3F8: Inference	Lab leader
2020 Michaelmas	Part IIB	4F13: Deep learning and structured data	Module leader
2020 Lent	Part IIA	3F8: Inference	Lab leader
2019 Michaelmas	Part IIB	4F10: Deep learning and structured data	Module leader
2019 Lent	Part IIA	3F8: Inference	Lab leader
2018 Lent	Part IIA	3F8: Inference	Module and lab leader
2018 Lent	MPhil in MLMI	MLSALT4: Advanced machine learning	Module leader
2017 Michaelmas	MPhil in MLMI	MLSALT1: Introduction to machine learning	Lab leader
2017 Lent	Part IIA	3F8: Inference	Lab leader
2016 Michaelmas	MPhil in MLMI	MLSALT1: Introduction to machine learning	Lab leader

Course Design

2018/2019	Part IIA	Project SF3: Machine Learning	Together with Dr. Rich E. Turner and Gabor Csanyi
2016/2017	Part IIA	Module 3F8: Inference	Together with Dr. Rich E. Turner
2016/2017	Mphil in MLMI	Module MLMI4: Advanced machine learning	Together with Dr. Rich E. Turner and Adrian Weller.
2016/2017	Mphil in MLMI	Module MLMI1: Introduction to Machine Learning	Together with Dr. Rich E. Turner

Undergraduate Supervisions

2021 Lent	Part IIA	3F8: Inference	Supervised 3 groups (12 hours).
2020 Lent	Part IIA	3F8: Inference	Supervised 3 groups (12 hours).
2019 Lent	Part IIA	3F8: Inference	2 hours group supervisions
2018 Lent	Part IIA	3F8: Inference	Supervised 3 groups (12 hours)
2017 Lent	Part IIA	3F8: Inference	6 hours group supervisions

Significant Teaching Developments or Innovations

2017	Together with Dr. Richard Turner, I put into practice a new supervision system for the module "3F8: Inference", where students received three large group supervisions given by the course lecturers, with 15-20 students attending each one. In addition, the students received three small group supervisions, including a revision supervision. The collected feedback indicates that the students prefer the new
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supervision system, which is cheaper to run.

Examining and Assessment Duties

2019 Lent	MPhil in MLMI	MLMI7: Reinforcement Learning and Decision Making	Report marking.
2021 Lent	Part IIA	3F8: Inference	Lab marking
2021 Lent	Part IIA	3F8: Inference	Full technical report marking
2021 Lent	Part IB	Paper 6: Information Engineering [Signals/Comms]	Assessor. Prepared exam and marked about 300 scripts.
2020 Michaelmas	Part IIB	4F13: Probabilistic Machine Learning	Principal assessor. Managed the marking of 480 reports submitted by 160 students with the help of PhD students.
2020 Michaelmas	Part IIA	3F8: Inference	Second assessor
2020 Michaelmas	Part IIB	4F10: Deep learning and structured data	Second assessor
2020 Lent	Part IB	4F10: Deep Learning and Structured Data	Principal assessor Prepared the exam but did not mark due to covid19.
2019 Lent	MPhil in MLMI	MLMI7: Reinforcement Learning and Decision Making	Report marking.
2020 Lent	Part IIA	3F8: Inference	Lab marking
2020 Lent	Part IIA	3F8: Inference	Full technical report marking
2020 Lent	Part IB	Paper 6: Information Engineering [Signals/Comms]	Assessor Prepared the exam but did not mark due to covid19.
2019 Lent	MPhil in MLMI	MLMI7: Reinforcement Learning and Decision Making	Report marking.
2019 Lent	Part IIA	3F8: Inference	Lab marking
2019 Lent	Part IIA	3F8: Inference	Full technical report marking
2019 Lent	Part IB	Paper 6: Information Engineering [Signals/Comms]	Assessor. Prepared exam and marked about 300 scripts.
2019 Michaelmas	Part IIA	3F8: Inference	Second assessor
2019 Michaelmas	Part IIB	4F10: deep learning and structured data	Second assessor
2018 Lent	Part IIA	3F8: Inference	Principal assessor
2018 Lent	Part IIA	3F8: Inference	Lab marking
2018 Lent	Part IIA	3F8: Inference	Full technical report marking
2018 Lent	MPhil in MLMI	MLSALT4: Advanced machine learning	Principal assessor
2018 Lent	MPhil in MLMI	MLSALT4: Advanced machine learning	Course work assessor
2018 Michaelmas	Part IIB	4F10: deep learning and structured data	Second assessor
2017 Michaelmas	MPhil in MLMI	MLSALT1: Introduction to machine learning	Course work assessor
2017 Michaelmas	Part IIB	4F10: deep learning and structured data	Second assessor
2017 Lent	Part IIA	3F8: Inference	Second assessor

2017 Lent	Part IIA	3F8: Inference	Lab marking
2017 Lent	Part IIA	3F8: Inference	Full technical report marking
2016 Michaelmas	MPhil in MLMI	MLSALT1: Introduction to machine learning	Course work assessor

External Teaching

2020 – 2021	Taught a lecture on graph neural networks on the Summer School on Machine Learning in Bioinformatics, Moscow (held virtually due to covid19).
2020	Taught 2 lectures on Approximate inference and on Bayesian optimization within the 2019-2020 Microsoft AI residency programme.
2019	Taught 2 lectures on Approximate inference and on Bayesian linear regression within the 2018-2019 Microsoft AI residency programme.
2018	Taught two lectures on graph neural networks on the International Machine Learning Summer School in Madrid.

Recognition of Teaching Quality

2019	Nominee best lecturer in part IIA (third year). Department of Engineering, University of Cambridge.
2018	Mark of 8.1 out of 10 in teaching quality, Machine Learning Summer School, Madrid.

Administrative Contributions to the Department/University

2022	Organization of the 2022 ELLIS Machine Learning Summer School in Cambridge. Raised 8.5k GBP in funding from industry for the organization of the school.
2020 – now	Director of the Cambridge ELLIS unit.
2021	Chaired the 4 th year project presentation session for students supervised by members of the Computational and Biological learning group at the Department of Engineering.
2020	Helped with mocked panel interview for UKRI FLF proposal by Cengiz Oztireli.
2020	Helped with mocked panel interview for UKRI Turing Fellowship proposal by Adrian Weller.
2021	Helped with mocked panel interview for UKRI Turing Fellowship proposal by Ferenc Huszar.
2020	Wrote a successful proposal for the creation of a Cambridge-based unit within the European Laboratory for Learning and Intelligent Systems (ELLIS), attracting 1m € in initial funding from industrial sponsors.
2020	Participated as a core researcher member in the formation of the “Cambridge Centre for AI in Medicine”, helping to define goals, outcomes and operations.
2020	University Lectureship Long-listing, shortlisting. Interviewing and panel. University Lecturer in Machine Learning and/or Computer Vision. Done twice since the initial positions had to be re-advertised.
2020, 2021	Participation in the University Mentoring Scheme for Postdocs. About 1.5 hours introductory session plus 3 – 5 meetings with mentee over nine months.
2021 – 2022	Acted as Complaint Officer for the University of Cambridge. 2021 – Three cases considered. 2022 – Two cases considered.
2020 – 2022	Acted as Examination Review Officer for the University of Cambridge. 2020 – Two cases considered. 2021 – One case considered. 2022 – One case considered.

2020	Attended briefing session to become decision-makers to consider student complaints and/or examination reviews and and/or reviews of other University decisions.
2019 – 2020	Shortlisted and interviewed applicants to the MLMI MPhil programme 2019: shortlisted among 100 applications, interviewed 16 applicants. 2020: shortlisted among 10 applicants, interviewed 2 applicants for Gates funding. 2020: shortlisted among 100 applicants, interviewed 14 applicants for university funding.
2019	Represented The Machine Learning Group from the University of Cambridge at initial European meetings to set up a society for a cross-national European Laboratory for Learning and Intelligent Systems (ELLIS, https://ellis.eu) which includes the creation of a research network, a pan-European PhD program and a focal point for industrial engagements.
2018	Representative from the Department of Engineering for the Center for Doctoral Training (CDT) on Automated Chemical Synthesis Enabled by Digital Molecular Technologies. Collaborated in the successful application process for the CDT. Currently an academic member of the CDT.
2018 – now	Internal examiner for the MPhil programme in Machine Learning and Machine Intelligence.
2018 – now	Contact person for the AI partnership between Microsoft Research-Cambridge and the University of Cambridge by which Microsoft supports PhD students and postdocs at the University, while its researchers teach at the university and supervise student projects.
2017, 2018	Chair for the Information Engineering Division Conference. Organised and managed the conference which included choosing venue, inviting speakers, arranging the schedule, etc.
2017	Wrote Successful Case for New University Lectureship in Computer Vision and Robotics that was supported by the Department. The post was filled.
2017	Interviewed applicants to the MLMI MPhil programme (9 students).
2016 – 2020	Fellow at the Alan Turing Institute (ATI):
2016 – 2018	- Participated on the shortlisting and interviews of applicants to the ATI PhD programme with affiliation with the University of Cambridge.
2019	- Managed at the Departmental side the extension of the contract for Dr. Brooks Paige, an ATI Research Fellow with University of Cambridge affiliation.
2017 – now	Contact person for the Cambridge - Tuebingen PhD programme in Machine Learning. Participation in the short-listing, interviews and recruitment of new students.
2017 – now	Member of the Cambridge Big-Data Strategic Initiative.
2017	Member of the Argentine tango society at Wolfson college, Cambridge. Participated in the instruction and organisation of Argentine tango lessons at Wolfson college.

Non-Departmental Administration

2021--2022	External evaluation of applicants for the faculty recruitment process at Saarland University, Germany. 3 applicants evaluated in 2021 and 3 other applicants evaluate in 2022. Conference session chairing:
2022	- ICLR session on Probabilistic Models, Vision.
2021	- ICML session on Deep Generative Models.
2020	- NeurIPS session on COVID/Applications/Composition.
2021	Participation in the selection of new ELLIS units. Evaluated 1 proposal to assess whether it satisfied the required international quality standards.
2020	Participation in the selection of Fellows and Scholars in ELLIS units. Evaluated 3 profiles to assess whether they satisfied the required international quality standards.

2020	Co-organizer of the 2020 NeurIPS data science competition “Diagnostic Questions: Predicting Student “Responses and Measuring Question Quality”, where participants compete to obtain the best score on a machine learning task of interest to the NeurIPS community.
2020 – now	Coordinator of the Cambridge unit within the European Laboratory for Learning and Intelligent Systems (ELLIS). The unit is formed by 11 academics from the University of Cambridge and has a research budget of 1.2m € per year.
2018	Co-organizer of the 2018 Machine Learning Summer School in Madrid. Raised 10k USD from industry for the organization of the school.
2018, 2019	Co-organizer of the Pizza + AI seminar series in Cambridge. Monthly event between Microsoft Research staff and Machine Learning Group researchers.
2017 – 2019	Organization of the CamAIML workshop in Cambridge. Annual event between Microsoft Research staff and Machine Learning Group researchers.
2021	Co-organizer of NeurIPS workshop on Deep Generative Models and Downstream Applications.
2017 – 2019	Co-organizer of NeurIPS workshop on Bayesian Deep Learning.
2017, 2018, 2020	Co-organizer of NeurIPS workshop on Machine Learning for Molecules and Materials.
2017	Co-organizer of NeurIPS workshop on Bayesian Optimization for Science and Engineering.

LIST OF PUBLICATIONS

Three Selected Recent Publications

2018	*Gómez-Bombarelli R., *Wei J., *Duvenaud D., *Hernández-Lobato J. M., Sánchez-Lengeling B., Sheberla D., Aguilera-Iparraguirre J., Hirzel T., Adam R. P. and Aspuru-Guzik A. Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules, ACS Central Science, 2018, 4 (2), 268–276. Impact Factor: 14.5. Google scholar h5-median: 137. Pages: 9. Citations in Google scholar: 1445 (*joint first authors)
2017	Kusner M. J., Paige B. and Hernández-Lobato J. M. Grammar Variational Autoencoder, In 34th International Conference on Machine Learning (ICML),1945–1954. ERA conference ranking: A*. Google scholar h5-median: 370. Citations in Google scholar: 488
2017	Depeweg S., Hernández-Lobato J. M., Doshi-Velez F. and Udluft S. Learning and Policy Search in Stochastic Dynamical Systems with Bayesian Neural Networks, In 5th International Conference on Learning Representations (ICLR). ERA conference ranking: A*. Google scholar h5-median: 470. Pages: 14. Citations in Google scholar: 125

Patents

2020	Nowozin S., Zhang C., Koenigstein K., Ma C., Hernández-Lobato J. M. and Gong W. Data retrieval, United States Patent Application 2020015022 A1. Assignee: Microsoft Technology Licensing. Pages: 17.
2020	Zhang C., Nowozin S., Patel A., Belgrave D., Palla K., Thieme A., Buchan I., Ma C., Tschitschek S., Hernández-Lobato J. M. Gathering data in a communication system, United States Patent Application 20200104702 A1. Assignee: Microsoft Technology Licensing. Pages: 23.
2020	Zhang C., Nowozin S., Patel A., Belgrave D., Palla K., Thieme A., Buchan I., Ma C., Tschitschek S.,

- Hernández-Lobato J. M.
Gathering data in a communication system,
United States Patent Application 20200105381 A1. Assignee: Microsoft Technology Licensing.
Pages: 17.
- 2020 Zhang C., ZAYKOV Y. K., Li Y. Hernandez-Lobato J. M., Popkesh A.-L. and S. C. Overweg
Interpretable neural network,
United States Patent Application 2020/0349441 A1. Assignee: Microsoft Technology Licensing.
Pages:19.
- 2019 Shastri L., Gharamani Z., Hernández-Lobato J. M., Kanagasabapathi B. and Raj K. S. A. A. D.
Method and system for mining frequent and in-frequent items from a large transaction database.
United States Patent Application 20150178303 A1. Assignee: INFOSYS LIMITED.
Pages: 8.

Refereed Journal Papers

- 2021 Havasi M., Snoek J., Tran D., Gordon J. and Hernández-Lobato J. M.
Sampling the Variational Posterior with Local Refinement
Entropy, 23 (11), 1475.
Impact Factor: 2.4. Google scholar h5-median: 81
Pages: 17.
- 2020 Gordon J. and Hernández-Lobato J. M.
Combining Deep Generative and Discriminative Models for Bayesian Semi-Supervised Learning,
Pattern Recognition, Volume 100, 107156
Impact Factor: 7.7, Google scholar h5-median: 141.
Pages: 10.
- 2019 Griffiths, R.-R. and Hernández Lobato, J. M.
Constrained Bayesian Optimization for Automatic Chemical Design using Variational Autoencoders,
Chemical Science, Volume 11, Issue 2, 577–586.
Impact factor: 9.3, Google scholar h5-median: 165.
Pages: 10
- 2019 Bhardwaj K., Havasi M., Yao Y., Brooks D. M., Hernández-Lobato J. M and Wei G.-Y.
Determining Optimal Coherency Interface for Many-Accelerator SoCs Using Bayesian Optimization,
IEEE Computer Architecture Letters, 18(2):119–123.
Impact factor: 1.2, Google scholar h5-median: 29
Pages: 4.
- 2018 *Gómez-Bombarelli R., *Wei J., *Duvenaud D., *Hernández-Lobato J. M., Sánchez-Lengeling B.,
Sheberla D., Aguilera-Iparraguirre J., Hirzel T., Adam R. P. and Aspuru-Guzik A.
Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules,
ACS Central Science, 2018, 4 (2), 268–276.
Impact Factor: 14.5. Google scholar h5-median: 137.
Pages: 9.
- 2016 Hernández-Lobato J. M., Gelbart A. M., Hoffman M. W., Adams R. and Ghahramani Z.
A General Framework for Constrained Bayesian Optimization using Information-based Search,
Journal of Machine Learning Research, 17(160):1–53.
Impact Factor: 4.1. Google scholar h5-median: 165.
Pages: 54.
- 2015 Hernández-Lobato J. M., Hernández-Lobato D. and Suárez A.
Expectation Propagation in Linear Regression Models with Spike-and-slab Priors,
Machine Learning, 99(3):437–487.
Impact Factor: 2.9. Google scholar h5-median: 74.
Pages: 51.
- 2013 Hernández-Lobato D., Hernández-Lobato J. M. and Dupont P.
Generalized Spike-and-Slab Priors for Bayesian Group Feature Selection Using Expectation
Propagation,
Journal of Machine Learning Research, 14:1891–1945.
Impact Factor: 4.1. Google scholar h5-median: 165.
Pages: 55.

- 2011 Hernández-Lobato J. M. and Suárez A.
Semiparametric Bivariate Archimedean Copulas.
Computational Statistics & Data Analysis, 55(6), 2038–2058.
Impact Factor: 1.6. Google scholar h5-median: 50.
Pages: 21.
- 2011 Hernández-Lobato J. M., Hernández-Lobato D. and Suárez A.
Network-based Sparse Bayesian Classification,
Pattern Recognition, 44(4), 886–900.
Impact Factor: 7.7,. Google scholar h5-median: 141.
Pages: 15.
- 2010 Hernández-Lobato D., Hernández-Lobato J. M. and Suárez A.
Expectation Propagation for Microarray Data Classification,
Pattern Recognition Letters, 31(12), 1618–1626, 2010.
Impact Factor: 2.8. Google scholar h5-median: 93.
Pages: 9.
- 2008 Hernández-Lobato D. and Hernández-Lobato J. M.
Bayes Machines for Binary Classification,
Pattern Recognition Letters, 29(10), 1466–1473.
Impact Factor: 2.8. Google scholar h5-median: 93.
Pages: 8.

Refereed Conference Proceedings

- 2021 Notin P., Hernández-Lobato J. M. and Gal Y.
Improving black-box optimization in VAE latent space using decoder uncertainty,
In Advances in Neural Information Processing Systems 32 (NeurIPS).
ERA conference ranking: A*. Google scholar h5-median: 422.
Pages: 12.
- 2021 Ma C. and Hernández-Lobato J. M.
Functional Variational Inference based on Stochastic Process Generators,
In Advances in Neural Information Processing Systems 32 (NeurIPS).
ERA conference ranking: A*. Google scholar h5-median: 422.
Pages: 13.
- 2021 Wang Z., Lamb A., Saveliev E., Zaykov Y., Cameron P., Hernandez-Lobato J. M., Turner R. E.,
Baraniuk R. G., Peyton Jones S., Barton C., Woodhead S. and Zhang C.
Diagnostic Questions: The NeurIPS 2020 Education Challenge,
NeurIPS 2020 Competition and Demonstration Track,
Proceedings of Machine Learning Research, 133, 191–205.
Pages: 14.
- 2021 Campbell A., Chen W., Stimper V., Hernández-Lobato J. M. and Zhang Y.
A Gradient Based Strategy for Hamiltonian Monte Carlo Hyperparameter Optimization,
In 38th International Conference on Machine Learning (ICML), 1238–1248.
ERA conference ranking: A*. Google scholar h5-median: 370.
Pages 9.
- 2021 Gong W., Zhang K., Li Y. and Hernández-Lobato J. M.
Active Slices for Sliced Stein Discrepancy,
In 38th International Conference on Machine Learning (ICML), 3766–3776.
ERA conference ranking: A*. Google scholar h5-median: 370.
Pages 9.
- 2021 Daxberger E., Nalisnick E., Allingham J., Antoran J. and Hernández-Lobato J. M.
Bayesian Deep Learning via Subnetwork Inference,
In 38th International Conference on Machine Learning (ICML), 2510–2521.
ERA conference ranking: A*. Google scholar h5-median: 370.
Pages 9.
- 2021 Nalisnick E., Gordon J. and Hernández-Lobato J. M.
Predictive Complexity Priors,
In 24th International Conference on Artificial Intelligence and Statistics (AISTATS), 694–702.

- ERA conference ranking: A. Google scholar h5-median: 101.
Pages 9.
- 2021 Morales-Alvarez P., Hernández-Lobato D., Molina R. and Hernández-Lobato J. M.
Activation-level uncertainty in deep neural networks,
In 9th International Conference on Learning Representations (ICLR).
ERA conference ranking: A*. Google scholar h5-median: 470.
Pages 9.
- 2021 Simm G. N. C., Pinsler R., Csányi G. and Hernández-Lobato J. M.
Symmetry-Aware Actor-Critic for 3D Molecular Design,
In 9th International Conference on Learning Representations (ICLR).
ERA conference ranking: A*. Google scholar h5-median: 470.
Pages 9.
- 2021 Gong W., Li Y. and Hernández-Lobato J. M.
Sliced Kernelized Stein Discrepancy,
In 9th International Conference on Learning Representations (ICLR).
ERA conference ranking: A*. Google scholar h5-median: 470.
Pages 9.
- 2021 Antoran J. , Bhatt U., Adel T., Weller A. and Hernández-Lobato J. M.
Getting a CLUE: A Method for Explaining Uncertainty Estimates,
In 9th International Conference on Learning Representations (ICLR).
ERA conference ranking: A*. Google scholar h5-median: 470.
Pages 9.
- 2021 Wang Z., Tschitschek S., Woodhead S., Hernández-Lobato J. M.,
Peyton Jones S., Baraniuk R. G. and Zhang C.
Educational Question Mining At Scale: Prediction, Analysis and Personalization,
In 35th AAAI Conference on Artificial Intelligence, 15669–15677.
ERA conference ranking: A.
Pages: 9.
- 2020 Ma C., Tschitschek S., Turner R. E., Hernández-Lobato J. M. and Zhang C.
VAEM: a Deep Generative Model for Heterogeneous Mixed Type Data,
In Advances in Neural Information Processing Systems 31 (NeurIPS).
ERA conference ranking: A*. Google scholar h5-median: 422.
Pages: 10.
- 2020 Bradshaw J., Paige B., Kusner M. J., Segler M. H. S. and Hernández-Lobato J. M.
Barking up the right tree: an approach to search over molecule synthesis DAGs,
In Advances in Neural Information Processing Systems 31 (NeurIPS).
ERA conference ranking: A*. Google scholar h5-median: 422.
Pages: 10.
- 2020 Antoran J., Allingham J. and Hernández-Lobato J. M.
Depth Uncertainty in Neural Networks,
In Advances in Neural Information Processing Systems 31 (NeurIPS).
ERA conference ranking: A*. Google scholar h5-median: 422.
Pages: 10.
- 2020 Flamich G., and Havasi M. and Hernández-Lobato J. M.
Compressing Images by Encoding Their Latent Representations with Relative Entropy Coding,
In Advances in Neural Information Processing Systems 31 (NeurIPS).
ERA conference ranking: A*. Google scholar h5-median: 422.
Pages: 10.
- 2020 Tripp A., Daxberger E. and Hernández-Lobato J. M.
Sample-Efficient Optimization in the Latent Space of Deep Generative Models via Weighted Retraining,
In Advances in Neural Information Processing Systems 31 (NeurIPS).
ERA conference ranking: A*. Google scholar h5-median: 422.
Pages: 10.
- 2020 Simm G. N., Pinsler R. and Hernández-Lobato J. M.
Reinforcement Learning for Molecular Design Guided by Quantum Mechanics,

- In 37th International Conference on Machine Learning (ICML), 8959–8969.
ERA conference ranking: A*. Google scholar h5-median: 370.
Pages: 11.
- 2020 Simm G. N., and Hernández-Lobato J. M.
A Generative Model for Molecular Distance Geometry,
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