CURRICULUM VITAE

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Personal Details

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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

2025 – now	Full Professor of Machine Learning (grade 12). Department of Engineering, University of Cambridge, UK.
2024 – now	Chief AI officer for Angstrom AI Inc.
2024 – 2024	Advisor for Epsilico.
2024 – now	Advisor for Atinary Inc.
2023 – now	Advisor for Omnix Inc.
2022 – 2025	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 – now	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:**

2025 Gary Tom, University of Toronto (external).
2025 Jannik Kossen, University of Oxford (external).
2025 Francisco Vargas, University of Cambridge (internal).
2025 Julius Kunze, University College London (external).
2025 Laurens Sluijterman, Radboud University, The Netherlands (external).
2024 Weiyang Liu, University of Cambridge (internal).
2024 Marcin Tomczak, University of Cambridge (internal).
2024 Tim Bakker, University of Amsterdam (external).
2024 Sheh Zaidi, University of Oxford, (external).
2024 Pieter-Jan Hoedt, Johannes Kepler University Linz, Austria, (external).
2023 Julius von Kügelgen, University of Cambridge, (internal).
2023 Vidhi Lalchand, University of Cambridge, (internal).
2023 Cristian Bodnar, University of Cambridge, (internal).
2022 Evan A. Ott, University of Texas at Austin, USA (external).
2022 Vaden Masrani, University of British Columbia, Canada (external).
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, Universisty 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:** 53

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, Chelsea Murray, Eli Persky, Ginte Petrulionyte, Javier Abad, Kristopher Miltiadou, Laurence Midgley, Wenlin Chen, Adrian Black, David Goldfarb, Federico Barbero, Haoran Peng, Maximiliaan Bronckers. Jonas Scholz. John Boom, Richard Bergna, Jiajun He, Szilvia Ujváry, Ilaria Sartori, Mohd Sadiq, Pablo Monteagudo, Fengzhe Zhang, Tony AuYeung, Yuxuan Ou, Jingyi Zhao, Jose Miguel Lara Rangel, Krisztina Sinkovics

Peer Review Activities

Senior area chair for conferences:

2024 – 2025 Artificial Intelligence and Statistics (AISTATS).
2025 International Conference on Learning Representations (ICLR).
2025 International Joint Conference on Artificial Intelligence (IJCAI).

Area chair for conferences:

2021 Neural Information Processing Systems (NeurIPS) Datasets and Benchmarks track.
2021 – 2024 International Conference on Learning Representations (ICLR).
2020 – 2025 Neural Information Processing Systems (NeurIPS).
2019, 2023 – 2025 International conference on Uncertainty in Artificial Intelligence (UAI).
2019 – 2024 International Joint Conference on Artificial Intelligence (IJCAI).
2017 – 2024 International Conference on Machine Learning (ICML).
2018 – 2025 Artificial Intelligence and Statistics (AISTATS).
2020 – 2025 Association for the Advancement of Artificial Intelligence (AAAI).

Reviewer for conferences:

2021 – 2023 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).

Panel member in grant proposal evaluation process:

2024 Academic Review of Schmidt Science Fellows. Reviewed 15-25 applications.
2023 Academic Review of Schmidt Science Fellows. Reviewed 15-25 applications.
2023 EPSRC Foundational AI Outlines Panel. Reviewed 20 outline proposals.
2022 EPSRC Prioritisation Panel. Reviewed 9 proposals.
2022 Academic Review of Schmidt Science Fellows. Reviewed 15-25 applications.

Grant proposal reviewer:

2024 Starting Grant Call, European Research Council.
2023 Swiss National Science Foundation.
2023 Workshop proposal for CECAM (Centre Européen de Calcul Atomique et Moléculaire).

2023	Starting Grant Call, European Research Council.
2023	Veni Proposal, Dutch Research Council.
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 editor roles:

2023	Guest editor for the journal Proceeding of the National Academy of Sciences.

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.

Awards

2023	Elected Fellow member of the ELLIS research program on Molecule Discovery. https://ellis.eu/programs/machine-learning-for-molecule-discovery
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

2025 – 2028 Developing better treatments for Mycobacterium abscessus
Funding agency: Cystic Fibrosis Trust
Investigators: Andres Floto (PI), David Spring (Co-I), Miguel Hernandez Lobato (Co-I), Vitor Silva E Costa Mendes (Co-I)
Budget: £800k

2025 – 2029 Home PhD studentship.
Investigators: J.M Hernández-Lobato (PI)
Funding agency: AstraZeneca.
Budget: £92k.

2024 – 2029 AI Hub in Generative Models
Funding agency: EPSRC
Investigators: David Barber (PI) and J.M. Hernández-Lobato (coPI)
Budget: £12m (£884k for Cambridge)

2024 – 2028 Home PhD studentship.
INEOS Oxbridge Doctoral Initiative on Antimicrobial Resistance.
Budget: £92k

2024 – 2028 Siemens PhD Studentship 2024
EPSRC iCase studentship
Budget: £140,000

2023 – 2024 EPSRC Tier-2 capital grant.
Generative models for the Boltzmann distribution of molecules.
Investigators: J.M. Hernández-Lobato (PI), Laurence Midgley and Jihao Andreas Li (Co-investigators).
Budget: 20,000 GPU hours on Cambridge CDS3 supercomputer, worth £5,000.

2022 – 2026 Advances in Deep Learning for Molecular Property Prediction
Investigators: J.M Hernández-Lobato (PI)
Funding agency: AstraZeneca.
Budget: 160,144 GBP

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 Sklodowska-Curie Action,
Investigators: J.M. Hernández-Lobato (PI), Vikas Verma (sponsored postdoc researcher).
Funding agency: European Comission first and then funding matched by EPSRC.
Budget: £204,000.

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
Inverstigators: 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 Sklodowska-Curie Action,
Investigators: J.M. Hernández-Lobato (PI), Kristoffer Stensbo-Smidt (sponsored postdoc researcher).
Funding agency: European Comission.
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

Jun 2025	Invited talk	8th Machine Learning and AI in Bio(Chemical) Engineering Conference, Department of Chemical Engineering and Biotechnology, University of Cambridge, UK.
Jun 2025	Invited tutorial	Summer School and Conference on the Mathematical Foundations of AI. University of Bristol. UK.
Jun 2025	Invited talk	IDP2Biomed Training School. Computational and Experimental Methods for characterizing the conformational properties of IDPs. Department of Chemistry, University of Cambridge, UK
Jun 2025	Invited tutorial	2025 Summer School on Machine Learning for Healthcare and Biology. University of Manchester, UK.
Jun 2025	Invited talk	Machine Learning for Molecular Simulations and Sampling. Online reading group. University of Cambridge, UK.
May 2025	Invited talk	Plenary speaker at BISP14, the 14th Workshop on Bayesian Inference in Stochasic Processes, CNR IMATI, Milan, Italy.
March 2025	Invited talk	AI Hub in Generative Models Launch event. Francis Crick Institute, London, UK.
Feb 2025	Invited talk	Stat-ML day, Jesus College, University of Oxford, UK.
Dec 2024	Invited talk	CDT in Digital and Automated Materials's Winter School on Robotics & AI for Materials Chemistry, University of Liverpool, Liverpool, UK.
Dec 2024	Invited talk	RT-UQ / Samourai workshop at IHP in Paris, France.
Oct 2024	Invited talk	Joint workshop CCAIM and Boehringer Ingelheim
Oct 2024	Invited talk	Manchester AI-Fun/ELLIS seminar series.
Oct 2024	Invited talk	AI for Good webinar series, "AI for Earth and Sustainability Science,"
Oct 2024	Invited talk	Structured Learning Workshop. Chalmers University of Technology, Gothenburg, Sweden.
Sep 2024	Invited tutorial	iDMT summer school, University of Cambridge, UK.
Sep 2024	Invited talk	Workshop on Bayesian Artificial Intelligence at Lancaster University.
Sep 2024	Invited talk	CCAIM AI and Machine Learning for Healthcare Summer School Online event.
Jul 2024	Invited talk	INS Colloquia, Shanghai Jiao Tong University, Shanghai, China.

Jul 2024	Invited panelist	ICML Workshop on Structured Probabilistic Inference & Generative Modeling, Vienna, Austria.
Jul 2024	Keynote talk	keynote of a session of ‘Learning & Decision-Making’ at Leeds Annual Statistical Research (LASR) conference on New Faces of Statistical Learning and Beyond. Unviersity of Leeds, UK. Cancelled due to last minute family commitments.
Jul 2024	Invited talk	Deep Generative Models. ELLIS summer school on Probabilistic Machine Learning, Cambridge, UK.
Jul 2024	Keynote talk	Relative Entropy Coding. Satellite workshop, 'Learn to Compress', at the International Symposium on Information Theory (ISIT), Athens, Greece, 2024.
Jun 2024	Invited talk	ELISE Wrap Up and ELLIS Community Conference in Helsinki, Finland. Online talk.
Jun 2024	Invited tutorial	Deep Generative Models. ELLIS summer school on Machine Learning for Healthcare and Biology, Manchester, UK.
May 2024	Invited talk	QIF Europe 2024 Finalists event - Invited talk
April 2024	Invited talk	Normalizing Flows for Molecular Modeling. Generative AI in Life Science Conference. Copenhagen, Denmark.
April 2024	Invited talk	Scalable Gaussian process inference with stochastic gradient descent. Seminar at Max Planck Institute for Biogeochemistry, Jena, Germany.
April 2024	Invited talk	Meta-learning Adaptive Deep Kernel Gaussian Processes Online webinar for Atinary Inc.
Mar 2024	Invited talk	SIAM Conference on Uncertainty Quantification (UQ24). Minisymposium Invitation on Uncertainty Quantification for Neural Networks. Given by one of my PhD students on my behalf.
Jan 2024	Invited talk	Scaling up Gaussian Processes with Stochastic Gradient Descent IDMT2 lecture series. Department of Chemistry. University of Cambridge.
Dec 2023	Invited talk	Normalizing Flows for Molecular Modeling Workshop on ML in Quantum Matter, Imperial College, London.
Dec 2023	Invited panellist	UK-China Workshop: Exchanges and Collaboration on AI and Data Governance. British Embassy, Beijing, China.
Nov 2023	Keynote talk	Flexible and Scalable Optimization of Hyperparameters with Hypergradients. AutoML Fall School 2023, Munich, Germany.
Nov 2023	Invited talk	Normalizing Flows for Molecular Modeling. UCL DeepMind/ELLIS CSML Seminar Series, London, UK.
Nov 2023	Invited panellist	Machine Learning: Portents and Possibilities workshop. Møller Institute, Cambridge, United Kingdom.
Oct 2023	Invited talk	Normalizing Flows for Molecular Modeling. Huawei Thames Summit & European Innovation Star Workshop, Cambridge UK.
Oct 2023	Invited talk	Missing Data Acquisition with Deep Generative Models. AI in Medicine joint Cambridge-Singapore one day Symposium, Cambridge, UK.
Jul 2023	Invited talk	Advances in Molecular Design with Deep Generative Models Shanghai AI Lab, Shanghai, China.

Jul 2023	Invited talk	Normalizing flows for molecular modelling. Cambridge ELLIS Summer School in Probabilistic Machine Learning. Department of Computer Science and Technology, University of Cambridge.
Jul 2023	Keynote talk	Relative Entropy Coding. ICML workshop on Neural Compression: From Information Theory to Applications, ICML, Hawaii, USA.
Jun 2023	Invited tutorial	ELLIS summer school on Machine Learning for Healthcare and Biology, Manchester, UK.
Jun 2023	Invited tutorial	Machine Learning Summer School ML4Science, Kraków, Poland.
May 2023	Invited talk	Deep Generative Models for Improved Molecular Simulations. Turing AI Fellows workshop, Museum of Natural Sciences, London.
May 2023	Invited talk	Causality and the Cambridge Machine Learning Group. Launch of the Centre for Causality. MRC Biostatistics Unit, University of Cambridge
May 2023	Invited talk	Relative Entropy Coding. London Symposium of Information Theory (LSIT), Imperial College London.
April 2023	Invited talk	Meta-learning Adaptive Deep Kernel Gaussian Processes for Molecular Property The mathematical and statistical foundation of future data-driven engineering, Data Driven Optimisation, workshop. Isaac Newton Institute, Cambridge, UK.
Mar 2023	Invited talk	Methods for approximate Bayesian inference. DL for Infectious Diseases workshop (Feb 2023), by Cambridge Infectious Diseases IRC & Cambridge Centre for AI in Medicine. Sydney-Sussex College, Cambridge, UK.
Mar 2023	Invited talk	Deep Generative Models for Improved Molecular Simulations. AI UK, national showcase of AI and data science research, Queen Elizabeth II Centre in Westminster, London.
Jan 2023	Invited Talk	Introduction to the Cambridge Machine Learning Group. Collaboration Day for Interdisciplinary Data Science and AI Research. Centre for Mathematical Sciences, Wilberforce Road, Cambridge, UK.
Nov 2022	Invited Panellist	NeurIPS tutorial on Advances in Bayesian Optimization. New Orleans, USA.
Nov 2022	Invited Panellist	ELLIS workshop on machine learning for molecules. Online event.
Nov 2022	Invited Talk	Meta-learning Adaptive Deep Kernel Gaussian Processes for Molecular Property Prediction. AstraZeneca Journal Club. Virtual talk.
Nov 2022	Keynote talk	Meta-learning Adaptive Deep Kernel Gaussian Processes for Molecular Property Prediction. Huawei workshop in Cambridge, UK.
Nov 2022	Invited Talk	Advances in Compression and Exploration via Probabilistic Machine Learning Seminar at DLR Institute of Data Science, Jena, Germany.
Sep 2022	Invited Talk	Meta-learning Adaptive Deep Kernel Gaussian Processes for Molecular Property Prediction. Leverhulme Research Centre for Functional Materials Design Symposium University of Liverpool. UK
Sep 2022	Invited Tutorial	Uncertainty in healthcare. Machine learning in healthcare summer school. Cambridge Center for AI in Medicine. Cambridge, 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 Processes. Open research event, Department of Chemistry, University of Cambridge
Jun 2022	Invited tutorial	Nordic Probabilistic AI school, Helsinki, Finland.

Jun 2022	Panellist	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 Dagsthul, 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, Tubingen, 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 (AMLCF), London, UK.

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

Research Co-workers

PhD Students

2024 – now	Richard Bergna	Siemens iCASE studentship. (directly supervised by me)
2024 – now	Jiajun He	Cambridge International Scholarship. (directly supervised by me)
2023 – now	Sergio Calvo Ordonez	PhD student at Oxford cosupervised by me and Prof Alvaro Cartea at Oxford.
2023 – now	Laurence Midgley	Synthec CDT studentship (co-supervised with Gabor Csanyi)
2022 – now	Timothy Hargreaves	EPSRC Doctoral Training Programme award (co-supervised with Hong Ge)
2022 – now	Julien Horwood	CCAIM studentship. (directly supervised by me)
2022 – now	Jihao Andreas Lin	Harding Distinguished Postgraduate Scholarship (supervised by me together with Bernhard Schölkopf)
2021 – now	Shreyas Padhy	Cambridge Harding Scholarship and Cambridge ELLIS unit. (directly supervised by me)
2021 – now	Wenlin Chen	Cambridge International Scholarship and

		Huawei. (supervised by me together with Bernhard Schölkopf)
2020 – 2024	Gergely Flamich Now Postdoc at Imperial College, London.	Funded directly by my personal research funds. (directly supervised by me)
2020 – 2024	Vincent Stimper Now research scientist at Isomorphic Labs (Google DeepMind's spin-off for drug discovery).	Amazon Studentship (directly supervised by me)
2019 – 2024	James Allingham Now research scientist at Google DeepMind.	The Mikheev Charitable Trust and EPSRC International Doctoral Studentship (directly supervised by me)
2019 – 2024	Austin Tripp Now research scientist at Recursion.	Cambridge International Scholarship (directly supervised by me)
2019 – 2024	Javier Antoran Now postdoc at Cambridge Machine Learning group and co-founder of Angstrom AI.	EPSRC iCASE studentship with Microsoft Research. (directly supervised by me)
2018 – 2024	Ross Clarke Now research engineering at Boltzbit.	EPSRC Doctoral Training Programme award (directly supervised by me)
2019 – 2023	Erik Daxberger Now research scientist at Apple.	EPSRC studentship and a Qualcomm European research studentship (directly supervised by me)
2018 – 2022	Chao Ma Now research scientist at Microsoft Research.	CSC Scholarship and Microsoft Research (directly supervised by me)
2018 – 2022	Chaochao Lu Now research scientist and PI at the Shanghai AI Lab, which is China's national institute for data science and artificial intelligence.	Cambridge-Tuebingen Fellowship (directly supervised by me together with Bernhard Schölkopf)
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 Harvard and then Research Engineer at Meta.	EPSRC Doctoral Training Programme award (directly supervised by me)
2017 – 2022	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 (Directly supervised by me)
2015 – 2019	Stefan Depeweg Now research scientist at Siemens.	Collaborator at Technical University of Munich (co-supervisied with Thomas Runkler).

Research Associates (Postdocs)

2024 – now	Zixing Song	EPSRC grant: AI Hub on Generative Models.	Directly supervised by me and Mark Girolami.

2024 – now	Jaiver Antoran	EPSRC postdoctoral grant	Directly supervised by me
2022 – 2024	Emile Mathieu Now research scientist at Xaria.	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 Frellsen	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 2024 – now	Toby Elles	Role: support with administrative tasks in group and ELLIS unit Cambridge.
Nov 2024 – May 2024	Catarina Lopes	Role: support with administrative tasks in group and ELLIS unit Cambridge.
May 2021 – Nov 2024	Kimberly Cole Now promoted to main administrator to div-F Information Engineering	Role: support with administrative tasks in group and ELLIS unit Cambridge.

Research Assistants

Nov 2023 – April 2024	Richard Bergna	Graduate, MPhil in Machine Learning and Machine Intelligence, University of Cambridge.	Directly supervised by me
Nov 2023 – Oct 2024	Jiajun He	Graduate, MPhil in Machine Learning and Machine Intelligence, University of Cambridge.	Directly supervised by me
Oct 2022 – Sep 2023	Laurence Midgley	Graduate, MPhil in Machine Learning and Machine Intelligence, University of Cambridge.	Directly supervised by me
Oct 2019 – Sep 2020	Gergely Flamich	Graduate, MPhil in Machine Learning and Machine Intelligence, University of	Directly supervised by me

		Cambridge.	
Sep 2019 – Mar 2020	Rajan Troll	Undergraduate, BA in Mathematics, University of Cambridge.	Directly supervised by me

Visiting Researchers

Mar 2025 – Now	Louis Grenioux	Visiting Graduate Student, Ecole Polytechnique, France.	Directly supervised by me
Jan 2025 – now	Xiuyuan Hu	Visiting Graduate Student, Tsinghua University, China.	Directly supervised by me
Sep 2024 – Dec 2024	Rissanen Severi	Visiting Graduate Student, Aalto University, Finland.	Directly supervised by me
Sep 2024 – Dec 2024	Antonio Almudeva Atienza	Visiting Graduate Student, Universidad de Zaragoza, Spain.	Directly supervised by me
Jun 2024 – Nov 2024	Joanna Sliwa	Visiting Graduate Student, Tuebingen University, Germany.	Directly supervised by me
Jun 2024 – Nov 2024	Weinlin Chen	Visiting Graduate Student, Computer Science and Technology at Guangdong University of Technology, China	Directly supervised by me
Oct 2023 – Dec 2023	Tobias Pielok	Visiting Graduate Student, Ludwig Maximilian University of Munich, Germany.	Directly supervised by me
Oct 2023 – Dec 2023	Javier Garcia Barcos	Visiting Graduate Student, Universidad de Zaragoza, Spain.	Directly supervised by me
Oct 2023 – Dec 2023	Luis Antonio Ortega Andres	Visiting Graduate Student, Universidad de Autonoma de Madrid, Spain.	Directly supervised by me
Apr 2023 – Mar 2024	Xuexin Chen	Visiting Graduate Student, Computer Science and Technology at Guangdong University of Technology, China	Directly supervised by me
Oct 2022 – Dec 2022	Daniel Fernandez Sanchez	Visiting Graduate Student, Universidad de Autonoma de Madrid, Spain.	Directly supervised by me
Sep 2022 – Dec 2022	Javier Garcia Barcos	Visiting Graduate Student, Universidad de Zaragoza, Spain.	Directly supervised by me
Sep 2021 – Dec 2021	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

Startups that originated from my lab

2024	Angstrom AI	Co-founded by myself PhD student Laurence Midgley, my postdoc Javier Antoran and my colleague Gabor Csanyi.
2020	Boltzbit	Co-founded by my former postdoc Yichuan Zhang (current CEO at Boltzbit).

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

2024 Lent	MPhil	MPhil in MLMI	MLMI4: Advanced machine learning	5 lectures
2024 Lent	Undergraduate	Part IIA	3F8: Inference	8 lectures

2023 Michaelmas	Undergraduate	Part IIB	4F10: deep learning and structured data	4 lectures
2023 Lent	MPhil	MPhil in MLMI	MLMI4: Advanced machine learning	5 lectures
2023 Lent	Undergraduate	Part IIA	3F8: Inference	16 lectures
2022 Michaelmas	Undergraduate	Part IIB	4F10: deep learning and structured data	4 lectures
2022 Michaelmas	MPhil	MPhil in MLMI	MLMI1: Introduction to machine learning	10 lectures
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: introduction to machine learning	4 lectures (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

2024	MPhil in MLMI	Pablo Monteagudo	Controlled Sampling in Diffusion Models
2024	MPhil in MLMI	Fengzhe Zhang	Efficient and Unbiased Sampling of Molecular Energy Functions via Consistency Models
2024	MPhil in MLMI	Tony AuYeung	(B)EnDEM: (Bootstrap) Energy-Based Denoising Energy Matching for Sampling from Boltzmann Densities
2024	MPhil in MLMI	Yuxuan Ou	Generative Models for Synthesizable Lipids
2024	MPhil in MLMI	Jingyi Zhao	Generative Models for Synthesizable Lipids
2024	Part IIB (4th-year)	Baiyu Su	Improving Hypergradient Methods for Meta Learning
2024	Part IIB (4th-year)	Cameron Mackenzie	Data Compression with Variational Implicit Neural Representations
2024	Part IIB (4th-year)	Yiduo Hao	Efficient Uncertainty Quantification in Transformers
2024	M.Phil in ACS	Paulina Kulyte	Improving Antibody Design with Force-Guided Sampling in Diffusion Models (Co-supervised with Pietro Lio)
2023	MPhil in MLMI	Szilvia Ujvary	PAC-Bayes with Channel Simulation

2023	MPhil in MLMI	Mohd Sadiq	Value Functions for Chemical Retrosynthesis
2023	MPhil in MLMI	Ilaria Sartori	Value Functions for Chemical Retrosynthesis
2023	MPhil in MLMI	Jiajun He	Data Compression with Variational Implicit Neural Representations
2023	MPhil in MLMI	Richard Bergna	Graph Neural Stochastic Differential Equations
2023	Part IIB (4th-year)	Bryan Ang	Data efficient prediction of molecular properties
2023	Part IIB (4th-year)	Tom Ryan	Applying efficient high dimensional sampling techniques to the linearized Laplace method
2023	Part IIB (4th-year)	Yitak Lee	Efficient neural network compression
2022	MPhil in MLMI	Adrian Salovaara Black	Deep Reinforcement Learning for 3D Molecular Design
2022	MPhil in MLMI	Haoran Peng	Outlier Detection with Hierarchical VAEs and Hamiltonian Monte Carlo
2021	MPhil in MLMI	Laurence Midgley	Annealed Importance Sampling and Alpha Divergences for Improved Boltzman Generators
2021	MPhil in MLMI	Kristopher Militiadou	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 Likhosherstov

Alberto Pepe

Robert Pinsler

James Requeima

Jonathan So

Ryan-Rhys Griffiths

Dan Jarrett

Ahmad Khan

Yassir Fathullah

Aliaksandra Shysheya

Hao Sun

Ross Viljoen

Evgeny Saveliev

Tristan Trebaol

Max Zhu

Yichao Liang

Kevin Ly

Tamas Stenczel

Cristiana-Diana Diaconu

Dmitrii Krasheninnikov

Harry Wang

Teaching Administration

2024 Lent	Part IIA	3F8: Inference	Lab leader
2023 Lent	Part IIA	3F8: Inference	Module Leader
2022 Michaelmas	MPhil in MLMI	MLMI1: Introduction to machine learning	Module Leader
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

2024 Lent	Part IIA	3F8: Inference	Supervised 3 groups (12 hours).
2023 Lent	Part IIA	3F8: Inference	Supervised 2 groups (8 hours).
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 supervision system, which is cheaper to run.

Examining and Assessment Duties

2024 Lent	Part IIA	3F8: Inference	Lab marking
2024 Lent	Part IIA	3F8: Inference	Full technical report marking
2023 Lent	Part IIA	3F8: Inference	Principal assessor. Prepared exam and marked about 115 scripts.
2022 Michaelmas	MPhil in MLMI	MLMI1: Introduction to machine learning	Principal assessor. Prepared exam and marked about 40 scripts.
2022 Easter	Part IB	Paper 6: Information Engineering [Signals/Comms]	Assessor. Marked about 300 scripts.
2019 Lent	MPhil in MLMI	MLMI7: Reinforcement Learing 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 Learing 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 Learing 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

2024	6 hours training program on machine learning For IN ThoughtBridge Co.
2024	24 hours course on Reinforcement Learning for CL-global.
2024	9 lectures on machine learning and artificial intelligence for Looker China.
2024	18 lectures on machine learning and artificial intelligence for Looker China.
2023	6 hours training program on machine learning For IN ThoughtBridge Co.
2023	7 hours of Cambridge admission mock interviews for Teachdeme.
2023	15 hour training program on machine learning for Teachdeme.
2023	18 lectures on machine learning and artificial intelligence for Looker China.
2023	6 hour research program on peptide design for CL-global.

2023	30 hour course on Advanced Machine Learning for CL-global.
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

2024	Mark of 8.8 out of 10 given by students on teaching survey, Machine Learning Summer School, Cambridge.
2023	Mark of 8.0 out of 10 given by students on teaching survey, AutoML Fall School, Munich.
2023	Mark of 8.3 out of 10 given by students on teaching survey, Machine Learning Summer School, Cambridge.
2022	Mark of 8.0 out of 10 given by students on teaching survey, Machine Learning Summer School, Cambridge.
2019	Nominee best lecturer in part IIA (third year). Department of Engineering, University of Cambridge.
2018	Mark of 8.1 out of 10 given by students on teaching survey, Machine Learning Summer School, Madrid.

Administrative Contributions to the Department/University

2024	Chair of Information Subject Group Committee Meeting (ISGC).
2023	Affiliated member of the Cambridge Center for Causality.
2022	Representative from Engineering ML group at the Cambridge Centre for Data-Driven Discovery (C2D3). Attended 9 committee meetings a year.
2022	Helped with hosting the visit of 60 students from WASP (Wallenberg AI, Autonomous systems, and Software Program, https://wasp-sweden.org/) to the Department of Engineering. Gave a research talk and description of the machine learning group.
2024	Organization of the 2024 ELLIS Machine Learning Summer School in Cambridge. Raised 5k GBP in funding from industry for the organization of the school.
2023	Organization of the 2023 ELLIS Machine Learning Summer School in Cambridge. Raised 13.5k GBP in funding from industry for the organization of the school.
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 Easter 2023 Easter 2023 Michaelmas 2024 Michaelmas 2024 Easter	Chaired the 4th year project presentation session for students supervised by members of the Computational and Biological learning group at the Department of Engineering.
2024	Helped with mocked panel interview for EPSRC Open Fellowship proposal by Cecilia Mascolo.
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.
2024	University Professorship Long-listing, shortlisting. University Assistant Professor in Machine Intelligence.
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 – 2024	Participation in the University Mentoring Scheme for Postdocs. About 1.5 hours introductory session plus 3 – 5 meetings with mentee over nine months. List of mentees: Johannes Pausch, Chao Li, Zhong-Qiu Yu, Yan Liang, Slawomir Tadeja.
2022	Participated in a mentoring session for participants of the 2022 CCAIM summer school on machine learning for healthcare.
2021 – 2023	Acted as Complaint Officer for the University of Cambridge. 2021 – Three cases considered. 2022 – Two cases considered. 2023 – One case considered.
2020 – 2024	Acted as Review Officer for the University of Cambridge. 2020 – Two cases considered. 2021 – One case considered. 2022 – Eight cases considered. 2023 – Nine cases considered. 2024 – Six cases 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 – 2024	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. - 2022: interviewed 3 applicants for Gates funding. - 2023: shortlisted among 100 applicants, interviewed 16 applicants. - 2024: shortlisted among 10 applicants, interviewed 2 applicants for Gates funding. - 2024: shortlisted among 120 applicants, interviewed 16 applicants.
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 – 2021, 2024	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 (now C2D3).
2017	Member of the Argentine tango society at Woflson college, Cambridge. Participated in the instruction and organisation of Argentine tango lessons at Wolfson college.

Non-Departmental/University Administration

2025	Co-organizer of NeurIPS workshop “Is Probabilistic Inference Still Relevant in the Era of Foundation Models?”.
2025	External evaluator of applicant for promotion to full professor, University of Oxford. Two applications evaluated.
2022 – 2023, 2024 – now	Director of the ELLIS research program on “Machine Learning for Molecule Discovery”.
2021 – 2022	Coorganizer of the ELLIS workshop on machine learning for molecules.
2024	Tenure Review of Assistant Professor, Singapore Management University, School of Computing and Information Systems.
2024	Review on our candidates' eligibility for the position of Full Professor (W3) of Machine Learning in Science, University of Tubingen, Germany.
2024	External evaluator of applicants for promotion to tenured faculty at Singapore Management University. 1 applicant evaluated in 2024.
2024	External evaluator of applicants for promotion to tenured faculty at the Max Planck Institute for Software Systems. 1 applicant evaluated in 2024.
2024	External evaluator of applicants for promotion to tenured Associate Professor, Department of Chemical Engineering, Massachusetts Institute of Technology (MIT). 1 applicant evaluated in 2024.
2023	External evaluator of applicants for promotion to non-tenured Associate Professor, Department of Chemical Engineering, Massachusetts Institute of Technology (MIT). 1 applicant evaluated in 2023.
2023	External evaluator of applicants for promotion to tenured faculty at Computer Science department at UNC Chapel Hill. 1 applicant evaluated in 2023.
2024	External evaluation of applicant for the faculty recruitment process at Institute of Science and Technology Austria (ISTA).
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 Probablistic 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, 2024	Participation in the selection of Fellows and Scholars in ELLIS units. 2023 – Evaluated 3 profiles to assess whether they satisfied the quality standards. 2024 – Evaluated 1 profiles to assess whether they satisfied the 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 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: 3380 (*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. Pages 10. **Citations in Google scholar: 1079**
2018	Depeweg S., Hernández-Lobato* J. M., Doshi-Velez F. and Udluft S. Decomposition of Uncertainty in Bayesian Deep Learning for Efficient and Risk-sensitive Learning, In 35th International Conference on Machine Learning (ICML), 1192–1201. ERA conference ranking: A*. Google scholar h5-median: 370. Pages: 10. **Citations in Google scholar: 435 (*main academic supervisor)**

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., Tschiatschek 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., Tschiatschek 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

2024 Singh S. and Hernández-Lobato J. M.
Data-Driven Insights on Transition Metal-Catalyzed Asymmetric Hydrogenation of Olefins,
The Journal of Organic Chemistry, Volume 89, Issue 17, 12467–12478.
Impact Factor: 3.3, Google Scholar h5-median: 74.
Pages: 12.

Chen W., Horwood J., Heo J. and Hernández-Lobato J. M.
2024 Leveraging Task Structures for Improved Identifiability in Neural Network Representations,
Transactions of Machine Learning Research.
Impact Factor: (Not available), Google Scholar h5-median: (Not available).
Pages: 24.

2024 Singh S. and Hernández-Lobato J. M.
Deep Kernel Learning for Reaction Outcome Prediction and Optimization,
Communications Chemistry, 7, 136.
Impact Factor: 6.58, Google Scholar h5-median: (Not available).
Pages: 9.

2024 Barbano R., Antoran J., Leuschner J., Hernández-Lobato J. M., Jin B. and Kereta Z.
Image Reconstruction via Deep Image Prior Subspaces,
Transactions of Machine Learning Research.
Impact Factor: (Not available), Google Scholar h5-median: (Not available).
Pages: 17.

2024 P. Morales-Álvarez, A. Schmidt, J.M. Hernández-Lobato, R. Molina
Introducing instance label correlation in multiple instance learning. Application to cancer detection on histopathological images,
Pattern Recognition, 0031-3203, 146, 110057.
Impact Factor: 7.19, Google Scholar h5-median: 164.
Pages: 11.

2023 Antoran J., Barbano R., Leuschner J., Hernández-Lobato J. M. and Jin B.
Uncertainty Estimation for Computed Tomography with a Linearised Deep Image Prior,
Transactions of Machine Learning Research.
Impact Factor: (Not available), Google Scholar h5-median: (Not available).
Pages: 19.

2023 Daxberger E., Swaroop S., Osawa K., Yokota R., Turner R. E., Hernández-Lobato J. M. and Khan M. E.
Improving Continual Learning by Accurate Gradient Reconstructions of the Past,
Transactions of Machine Learning Research.
Impact Factor: (Not available), Google Scholar h5-median: (Not available).
Pages: 16.

2022 Stimper V., Liu D., Campbell A., Berenz V., Ryll R., Schölkopf B and Hernández-Lobato J. M.
normflows: A PyTorch Package for Normalizing Flows,
Journal of Open Source Software, 8(86), 5361.
Impact Factor: 4.6, Google Scholar h5-median: 159.
Pages: 4.

2022 García-Ortegón M., Simm G. N. C., Tripp A. J., Hernández-Lobato J. M., Bender A. and Bacallado S.
DOCKSTRING: Easy Molecular Docking Yields Better Benchmarks for Ligand Design,
Journal of Chemical Information and Modeling, 62, 15, 3486–3502.
Impact Factor: 5.6, Google Scholar h5-median: 145.
Pages: 17.

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

2024 Lin J. A., Padhy S., Mlodozeniec B. K., Antoran J. and Hernández-Lobato J. M.
Improving Linear System Solvers for Hyperparameter Optimisation in Iterative Gaussian Processes,
In Advances in Neural Information Processing Systems 37 (NeurIPS).
ERA conference ranking: A*. Google Scholar h5-median: 614.
Pages: 31.

2024 Shysheya A., Diaconu C., Bergamin F., Perdikaris P., Hernández-Lobato J. M., Turner R. E. and Mathieu E.
On conditional diffusion models for PDE simulations,
In Advances in Neural Information Processing Systems 37 (NeurIPS).
ERA conference ranking: A*. Google Scholar h5-median: 614.
Pages: 45.

2024 He J., Flamich G., Hernández-Lobato J. M.
Accelerating Relative Entropy Coding with Space Partitioning,
In Advances in Neural Information Processing Systems 37 (NeurIPS).
ERA conference ranking: A*. Google Scholar h5-median: 614.
Pages: 35.

2024 Allingham J. U., Mlodozeniec B. K, Padhy S., Antoran J., Krueger D., Turner R. E., Nalisnick E. and Hernández-Lobato J. M.
A Generative Model of Symmetry Transformations,
In Advances in Neural Information Processing Systems 37 (NeurIPS).
ERA conference ranking: A*. Google Scholar h5-median: 614.
Pages: 36.

2024 Papamarkou T., Skoularidou M., Palla K., Aitchison L., Arbel J., Dunson D., Filippone M., Fortuin V., Hennig P., Hernández-Lobato J. M., Hubin A., Immer A., Karaletsos T., Khan M. E., Kristiadi A., Li Y., Mandt S., Nemeth C., Osborne M. A., Rudner T. G. J., Rügamer D., Teh Y. W., Welling M., Wilson A. G. and Zhang R.
Position Paper: Bayesian Deep Learning in the Age of Large-Scale AI,
In 41st International Conference on Machine Learning (ICML), PMLR 235:39556–39586.
ERA conference ranking: A*. Google Scholar h5-median: 424.
Pages: 31.

2024 Clarke R. M. and Hernández-Lobato J. M.
Studying K-FAC Heuristics by Viewing Adam through a Second-Order Lens,
In 41st International Conference on Machine Learning (ICML), PMLR 235:9000–9032.
ERA conference ranking: A*. Google Scholar h5-median: 424.
Pages: 33.

2024 Chen X., Cai R., TingHuang Z., Zhu Y., Horwood J., Hao Z., Li Z. and Miguel Hernández-Lobato J. M.
Feature Attribution with Necessity and Sufficiency via Dual-stage Perturbation Test for Causal Explanation,
In 41st International Conference on Machine Learning (ICML), PMLR 235:6486–6502.
ERA conference ranking: A*. Google Scholar h5-median: 424.
Pages: 17.

2024 Chen W., Zhang M., Paige B., Hernández-Lobato J. M. and Barber D.
Diffusive Gibbs Sampling,
In 41st International Conference on Machine Learning (ICML), PMLR 235:7731–7747.
ERA conference ranking: A*. Google Scholar h5-median: 424.
Pages: 17.

2024 Lin J. A., Padhy S., Antoran J., Tripp A., Terenin A., Szepesvari C., Hernández-Lobato J. M. and Janz D.
Stochastic Gradient Descent for Gaussian Processes Done Right,
In 12th International Conference on Learning Representations (ICLR).
ERA conference ranking: A*. Google Scholar h5-median: 584.
Pages: 18.

2024 He J., Flamich G., Guo Z. and Hernández-Lobato J. M.
RECOMBINER: Robust and Enhanced Compression with Bayesian Implicit Neural Representations,
In 12th International Conference on Learning Representations (ICLR).
ERA conference ranking: A*. Google Scholar h5-median: 584.
Pages: 27.

2024 Tripp A., Maziarz K., Lewis S., Segler M. and Hernández-Lobato J. M.
Retro-fallback: retrosynthetic planning in an uncertain world,
In 12th International Conference on Learning Representations (ICLR).
ERA conference ranking: A*. Google Scholar h5-median: 584.
Pages: 58.

2023 Tripp A., Bacallado S., Singh S. and Hernández-Lobato J. M.
Tanimoto Random Features for Scalable Molecular Machine Learning,
In Advances in Neural Information Processing Systems 36 (NeurIPS), 33656–33686.
ERA conference ranking: A*. Google Scholar h5-median: 614.
Pages: 31.

2023 Guo Z., Flamich G., He J., Zhibo Chen Z., and Hernández-Lobato J. M.
Compression with Bayesian Implicit Neural Representations,
In Advances in Neural Information Processing Systems 36 (NeurIPS),
1938–1956.
ERA conference ranking: A*. Google Scholar h5-median: 614.
Pages: 19.

2023 Flamich G., Markou S. and Hernández-Lobato J. M.
Faster Relative Entropy Coding with Greedy Rejection Coding,
In Advances in Neural Information Processing Systems 36 (NeurIPS),
50558–50569.
ERA conference ranking: A*. Google Scholar h5-median: 614.
Pages: 12.

2023 Lin J. A., Antoran J., Padhy S., Janz D., Hernández-Lobato J. M. and Terenin A.
Sampling from Gaussian Process Posteriors using Stochastic Gradient Descent,
In Advances in Neural Information Processing Systems 36 (NeurIPS),
36886–36912.
ERA conference ranking: A*. Google Scholar h5-median: 614.
Pages: 27.

2023 Midgley L. I., Stimper V., Antoran J., Mathieu E., Schölkopf B. and Hernández-Lobato J. M.
SE(3) Equivariant Augmented Coupling Flows,
In Advances in Neural Information Processing Systems 36 (NeurIPS),
79200–79225.
ERA conference ranking: A*. Google Scholar h5-median: 614.
Pages: 26.

2023 Antoran J., Padhy S., Barbano R., Nalisnick E., Janz D. and Hernández-Lobato J. M.

Sampling-based inference for large linear models, with application to linearised Laplace,
In 11th International Conference on Learning Representations (ICLR).
ERA conference ranking: A*. Google Scholar h5-median: 584.
Pages: 34.

2023 Midgley L. I., Stimper V., Simm G. N. C., Schölkopf B. and Hernández-Lobato J. M.
Flow Annealed Importance Sampling Bootstrap,
In 11th International Conference on Learning Representations (ICLR).
ERA conference ranking: A*. Google Scholar h5-median: 584.
Pages: 45.

2023 Chen W., Tripp A. and Hernández-Lobato J. M.
Meta-learning Adaptive Deep Kernel Gaussian Processes for Molecular Property Prediction,
In 11th International Conference on Learning Representations (ICLR).
ERA conference ranking: A*. Google Scholar h5-median: 584.
Pages: 25.

2022 Peis I., Ma C. and Hernández-Lobato J. M.
Missing Data Imputation and Acquisition with Deep Hierarchical Models and Hamiltonian Monte Carlo,
In Advances in Neural Information Processing Systems 35 (NeurIPS),
35839–35851.
ERA conference ranking: A*. Google Scholar h5-median: 614.
Pages: 13.

2022 Flamich G., Markou S. and Hernández-Lobato J. M.
Fast Relative Entropy Coding with A* coding,
In 39th International Conference on Machine Learning (ICML), PMLR 162:6548–6577.
ERA conference ranking: A*. Google Scholar h5-median: 424.
Pages: 30.

2022 Antoran J., Janz D., Allingham J., Daxberger E., Barbano R., Nalisnick E., and Hernández-Lobato J. M.
Adapting the Linearised Laplace Model Evidence for Modern Deep Learning,
In 39th International Conference on Machine Learning (ICML), PMLR 162:796–821.
ERA conference ranking: A*. Google Scholar h5-median: 424.
Pages: 26.

2022 Huang B., Lu C., Leqi L., Hernandez-Lobato J. M., Glymour C., Schölkopf C. and Zhang K.
Action-Sufficient State Representation Learning for Control with Structural Constraints,
In 39th International Conference on Machine Learning (ICML), PMLR 162:9260–9279.
ERA conference ranking: A*. Google Scholar h5-median: 424.
Pages: 20.

2022 Lu C., Wu Y., Hernández-Lobato J. M and Schölkopf B.
Invariant Causal Representation Learning for Out-of-Distribution Generalization,
In 10th International Conference on Learning Representations (ICLR).
ERA conference ranking: A*. Google Scholar h5-median: 584.
Pages: 32.

2022 Ross C. M. , Oldewage E. T. and Hernández-Lobato J. M.
Scalable One-Pass Optimisation of High-Dimensional Weight-Update Hyperparameters by Implicit Differentiation,
In 10th International Conference on Learning Representations (ICLR).
ERA conference ranking: A*. Google Scholar h5-median: 584.
Pages: 41.

2022 He W., Mao X., Ma C., Huang Y., Hernández-Lobato J. M. and Chen T.
BSODA: A Bipartite Scalable Framework for Online Disease Diagnosis,
In the ACM Web Conference, (WWW), 2511–2521.
ERA conference ranking: A*. Google Scholar h5-median: 169.
Pages: 11.

2022 Murray C., Allingham J. U., Antorán J. and Hernández-Lobato J. M.
Addressing Bias in Active Learning with Depth Uncertainty Networks… or Not,
In Proceedings on “I (Still) Can’t Believe It’s Not Better!” at NeurIPS 2021 Workshops, PMLR 163:59–63.

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