Agustinus Kristiadi

Assistant Professor / Vector Faculty Affiliate

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Introduction

In machine learning, conferences are the most prestigious venues for publication. Top conferences include NeurIPS (previously NIPS), ICML, ICLR, AISTATS, and UAI. They are highly selective, with an acceptance rate of around 25%, and have peer-reviewing processes similar to journals (JMLR, TMLR).

The first or joint-first author (the latter is marked with a '*') of a paper is the lead author. The last or joint-last author is usually the one who came up with the idea and directed the project. They are all considered to be the core authors of the paper.

Academic Experience

07/2025 - Present	**Vector Institute**, Toronto, Canada *Faculty Affiliate*
07/2025 - Present	**Western University**, London, Canada *Assistant Professor* Tenure-track. Department of Computer Science.
02/2023 - 06/2025	**Vector Institute**, Toronto, Canada *Distinguished Postdoctoral Fellow* Advised by Alán Aspuru-Guzik and Pascal Poupart.
06/2019 - 01/2023	**University of Tübingen**, Tübingen, Germany *Ph.D., Computer Science* Advised by Philipp Hennig and Matthias Hein. Grade: magna cum laude.
04/2017 - 04/2019	**University of Bonn**, Bonn, Germany *M.Sc., Computer Science* Advised by Asja Fischer and Jens Lehmann. Grade: 1.1/1.0 cum laude (3.9/4.0 GPA equivalent).
08/2009 - 01/2013	**Atma Jaya University**, Yogyakarta, Indonesia *B.Eng., Informatics Engineering* Grade: 3.9/4.0 cum laude.

Honors & Awards

2025	**Spotlight Paper**, NeurIPS Top 4% of all submissions. Awarded to the paper titled "FlashMD: Long-Stride, Universal Prediction of Molecular Dynamics".
2023	**Best PhD Thesis**, German Research Foundation (DFG) Annual award valued EUR 2,000 by the Theoretical Foundations of Deep Learning (FoDL) program of DFG.
2023	**Spotlight Paper**, NeurIPS Top 4% of all submissions. Awarded to the paper titled "The Geometry of Neural Nets' Parameter Spaces Under Reparametrization".
2021	**Spotlight Paper**, NeurIPS

Top 3% of all submissions. Awarded to the paper titled "An Infinite-Feature Extension for Bayesian ReLU Nets That Fixes Their Asymptotic Overconfidence".

2021 | **Long-Talk Paper**, UAI
Top 6% of all submissions. The paper titled "Learnable Uncertainty under Laplace Approximations" was selected as a long-talk (cf. lightning-talk) presentation at the conference.

2021 | **Best Reviewer**, ICML
Awarded to the top 10% of all reviewers.

Funding

2025 - 2030 | **Start-Up Grant**, Western University
Awarded. CAD 100,000.

Thesis Publications

1. **Kristiadi, Agustinus**. *Low-cost Bayesian methods for fixing neural networks' overconfidence.* PhD thesis, University of Tübingen, 2023.

2. **Kristiadi, Agustinus**. *Predictive uncertainty quantification with compound density networks.* Master's thesis, University of Bonn, 2019.

3. **Kristiadi, Agustinus**. *Parallel particle swarm optimization for image segmentation.* Bachelor's thesis, Universitas Atma Jaya Yogyakarta, 2013.

Journal Publications

1. Sun, Yan; Chen, Lianghong; Jing, Zihao; Li, Yan Yi; Kim, Dongkyu; Gao, Jing-Yan; Noroozi, Reza; Yi, Grace; Feugmo, Conrard Tetsassi; Klinkova, Anna; Sask, Kyla; **Kristiadi, Agustinus**; Wang, Boyu; Gillies, Elizabeth; Lu, Kun Ping; Shi, HaoTian Harvey; Hu, Pingzhao. *Generative AI for the design of molecules: advances and challenges.* Journal of Chemical Information and Modeling, 2025.

2. **Kristiadi, Agustinus**; Pranowo. *Deep convolutional level set method for image segmentation.* Journal of ICT Research & Applications, 11(3), 2017.

Conference Publications

1. Bigi, Filippo; Chong, Sanggyu; **Kristiadi, Agustinus**; Ceriotti, Michele. *FlashMD: Long-stride, universal prediction of molecular dynamics.* Conference on Neural Information Processing Systems (NeurIPS), 2025. **(Spotlight; top 4%.)**

2. Rashid, Ahmad; Wu, Ruotian; Grosse, Julia; **Kristiadi, Agustinus**; Poupart, Pascal. *A critical look at tokenwise reward-guided text generation.* In Conference on Language Modeling (COLM), 2025.

3. Rashid, Ahmad; Wu, Ruotian; Fan, Rongqi; Li, Hongliang; **Kristiadi, Agustinus**; Poupart, Pascal. *Towards cost-effective reward guided text generation.* In International Conference on Machine Learning (ICML), 2025.

4. **Kristiadi, Agustinus**; Strieth-Kalthoff, Felix; Skreta, Marta; Poupart, Pascal; Aspuru-Guzik, Alán; Pleiss, Geoff. *A sober look at LLMs for material discovery: Are they actually good for Bayesian optimization over molecules?* In International Conference on Machine Learning (ICML), 2024.

5. Lin, Wu; Dangel, Felix; Eschenhagen, Runa; Neklyudov, Kirill; **Kristiadi, Agustinus**; Turner, Richard E; Makhzani, Alireza. *Structured inverse-free natural gradient: memory-efficient and numerically-stable KFAC for large neural nets.* In International Conference on Machine Learning (ICML), 2024.

6. Papamarkou, Theodore; Skoularidou, Maria; Palla, Konstantina; Aitchison, Laurence; Arbel, Julyan; Dunson, David; Filippone, Maurizio; Fortuin, Vincent; Hennig, Philipp; Hubin, Aliaksandr; Immer, Alexander; Karaletsos, Theofanis; Khan, Mohammad Emtiyaz; **Kristiadi, Agustinus**; Li, Yingzhen; Mandt, Stephan; Nemeth, Christopher; Osborne, Michael A.; Rudner, Tim G. J.; Rügamer, David; Teh, Yee Whye; Welling, Max; Wilson, Andrew Gordon; Zhang, Ruqi. *Position paper: Bayesian deep learning in the age of large-scale AI.* In International Conference on Machine Learning (ICML), 2024.

7. Rashid, Ahmad; Hacker, Serena; Zhang, Guojun; **Kristiadi, Agustinus**; Poupart, Pascal. *Preventing arbitrarily high confidence on far-away data in point-estimated discriminative neural networks.* In International Conference on Artificial Intelligence and Statistics (AISTATS), 2024.

8. **Kristiadi, Agustinus**; Dangel, Felix; Hennig, Philipp. *The geometry of neural nets' parameter spaces under reparametrization.* In Conference on Neural Information Processing Systems (NeurIPS), 2023. **(Spotlight; top 4%.)**

9. **Kristiadi, Agustinus**; Eschenhagen, Runa; Hennig, Philipp. *Posterior refinement improves sample efficiency in Bayesian neural networks.* In Conference on Neural Information Processing Systems (NeurIPS), 2022.

10. Hobbhahn, Marius; **Kristiadi, Agustinus**; Hennig, Philipp. *Fast predictive uncertainty for classification with Bayesian deep networks.* In Conference on Uncertainty in Artificial Intelligence (UAI), 2022.

11. **Kristiadi, Agustinus**; Hein, Matthias; Hennig, Philipp. *Being a bit frequentist improves Bayesian neural networks.* In International Conference on Artificial Intelligence and Statistics (AISTATS), 2022.

12. Rendsburg, Luca; **Kristiadi, Agustinus**; Hennig, Philipp; Luxburg, Ulrike. *Discovering inductive bias with Gibbs priors: A diagnostic tool for approximate Bayesian inference.* In International Conference on Artificial Intelligence and Statistics (AISTATS), 2022.

13. Daxberger, Erik; **Kristiadi, Agustinus**; Immer, Alexander; Eschenhagen, Runa; Bauer, Matthias; Hennig, Philipp. *Laplace redux–effortless Bayesian deep learning.* In Conference on Neural Information Processing Systems (NeurIPS), 2021.

14. **Kristiadi, Agustinus**; Hein, Matthias; Hennig, Philipp. *An infinite-feature extension for Bayesian ReLU nets that fixes their asymptotic overconfidence.* In Conference on Neural Information Processing Systems (NeurIPS), 2021. **(Spotlight; top 3%.)**

15. **Kristiadi, Agustinus**; Hein, Matthias; Hennig, Philipp. *Learnable uncertainty under Laplace approximations.* In Conference on Uncertainty in Artificial Intelligence (UAI), 2021. **(Long Talk; top 6%.)**

16. **Kristiadi, Agustinus**; Hein, Matthias; Hennig, Philipp. *Being Bayesian, even just a bit, fixes overconfidence in ReLU networks.* In International Conference on Machine Learning (ICML), 2020.

17. **Kristiadi, Agustinus**; Khan, Mohammad Asif; Lukovnikov, Denis; Lehmann, Jens; Fischer, Asja. *Incorporating literals into knowledge graph embeddings.* In International Semantic Web Conference (ISWC), 2019.

18. Chaudhuri, Debanjan; **Kristiadi, Agustinus**; Lehmann, Jens; Fischer, Asja. *Improving response selection in multi-turn dialogue systems.* In Conference on Computational Natural Language Learning (CoNLL), 2018.

19. **Kristiadi, Agustinus**; Pranowo; Mudjihartono, Paulus. *Parallel particle swarm optimization for image segmentation.* In Digital Enterprise and Information Systems, 2013.

Workshop Publications

1. Cinquin, Tristan; Pleiss, Geoff; **Kristiadi, Agustinus**. *Limits of PRM-guided tree search for mathematical reasoning with LLMs.* In Workshop on Mathematical Reasoning and AI, 2025.

2. Cinquin, Tristan; Lo, Stanley; Strieth-Kalthoff, Felix; Aspuru-Guzik, Alán; Pleiss, Geoff; Bamler, Robert; Rudner, Tim G.J.; Fortuin, Vincent; **Kristiadi, Agustinus**. *What actually matters for materials discovery: Pitfalls and recommendations in Bayesian optimization.* In AI for Accelerated Materials Discovery Workshop, 2025.

3. Cordero, Andres Guzman; Thiede, Luca; Tom, Gary; Aspuru-Guzik, Alán; Strieth-Kalthoff, Felix; **Kristiadi, Agustinus**. *Dimension deficit: Is 3D a step too far for optimizing molecules?* In AI for Accelerated Materials Discovery Workshop, 2024.

4. Schmid, Stefan P; Rajaonson, Ella Miray; Ser, Cher Tian; Haddadnia, Mohammad; Leong, Shi Xuan; Aspuru-Guzik, Alán; **Kristiadi, Agustinus**; Jorner, Kjell; Strieth-Kalthoff, Felix. *If optimizing for general parameters in chemistry is useful, why is it hardly done?* In AI for Accelerated Materials Discovery Workshop, 2024.

5. Grosse, Julia; Wu, Ruotian; Rashid, Ahmad; Hennig, Philipp; Poupart, Pascal; **Kristiadi, Agustinus**. *Uncertainty-guided optimization on large language model search trees.* In Symposium on Advances of Approximate Bayesian Inference (AABI), 2024.

6. **Kristiadi, Agustinus**; Strieth-Kalthoff, Felix; Ganapathi Subramanian, Sriram; Fortuin, Vincent; Poupart, Pascal; Pleiss, Geoff. *How useful is intermittent, asynchronous expert feedback for Bayesian optimization?* In Symposium on Advances of Approximate Bayesian Inference (AABI), 2024.

7. Rashid, Ahmad; Wu, Ruotian; Grosse, Julia; **Kristiadi, Agustinus**; Poupart, Pascal. *A critical look at tokenwise reward-guided text generation.* In ICML 2024 Workshop on Foundation Models in the Wild, 2024.

8. **Kristiadi, Agustinus**; Immer, Alexander; Eschenhagen, Runa; Fortuin, Vincent. *Promises and pitfalls of the linearized Laplace in Bayesian optimization.* In Symposium on Advances of Approximate Bayesian Inference (AABI), 2023.

9. Eschenhagen, Runa; Daxberger, Erik; Hennig, Philipp; **Kristiadi, Agustinus**. *Mixtures of Laplace approximations for improved post-hoc uncertainty in deep learning.* In NeurIPS Workshop of Bayesian Deep Learning, 2021.

10. **Kristiadi, Agustinus**; Däubener, Sina; Fischer, Asja. *Predictive uncertainty quantification with compound density networks.* In NeurIPS Workshop of Bayesian Deep Learning, 2019.

Preprint Publications

1. **Kristiadi, Agustinus**. *Introduction to the analysis of probabilistic decision-making algorithms.* arXiv preprint arXiv:2508.21620, 2025.

2. Dangel, Felix; Eschenhagen, Runa; Ormaniec, Weronika; Fernandez, Andres; Tatzel, Lukas; **Kristiadi, Agustinus**. *Position: Curvature matrices should be democratized via linear operators.* arXiv preprint arXiv:2501.19183, 2025.

3. Carvalho, Gustavo Sutter Pessurno; Abdulrahman, Mohammed; Wang, Hao; Subramanian, Sriram Ganapathi; St-Aubin, Marc; O'Sullivan, Sharon; Wan, Lawrence; Ricardez-Sandoval, Luis; Poupart, Pascal; **Kristiadi, Agustinus**. *Simplifying Bayesian optimization via in-context direct optimum sampling.* arXiv preprint arXiv:2505.23913, 2025.

4. Sliwa, Joanna; Schneider, Frank; Bosch, Nathanael; **Kristiadi, Agustinus**; Hennig, Philipp. *Efficient weight-space Laplace-Gaussian filtering and smoothing for sequential deep learning.* arXiv preprint arXiv:2410.06800, 2024.

5. Wenger, Jonathan; Dangel, Felix; **Kristiadi, Agustinus**. *On the disconnect between theory and practice of overparametrized neural networks.* arXiv preprint arXiv:2310.00137, 2023.

Talks

1. *Uncertainty-aware foundation models for efficient decision-making in science.* AI Lecture Series, Ruhr University of Bochum. September 2025.

2. *Probabilistic decision-making algorithms for a better world.* First-Year Seminar in Science, University of British Columbia. March 2025.

3. *Probabilistic inference and decision-making with foundation models for Bayesian optimization.* Waterloo AI Seminars, University of Waterloo. October 2024.

4. *Probabilistic inference and decision-making with and for foundation models.* Machine Learning and Friends Lunch, UMass Amherst. October 2024.

5. *Probabilistic inference and decision-making with and for foundation models.* Seminar, Sander Lab, Harvard Medical School. October 2024.

6. *Uncertainty-guided optimization on LLM search trees.* Vector Research Day, Vector Institute. June 2024.

7. *Gaussian processes, the linearized Laplace, and sequential decision making.* Seminar, Pascal Poupart's Group, University of Waterloo. April 2024.

8. *Bayesian optimization with LLMs and expert feedback for material discovery.* Seminar, The Matter Lab, University of Toronto. March 2024.

9. *The geometry of neural nets' parameter spaces under reparametrization.* Math Machine Learning Seminar, University of California, Los Angeles. January 2024.

10. *The geometry of neural nets' parameter spaces under reparametrization.* ELLIS Reading Group on Mathematics of Deep Learning. December 2023.

11. *Bayesian deep learning: past, present, and future.* Theoretical Foundations of Deep Learning meeting. November 2023.

12. *The linearized Laplace and the geometry of NNs' parameter spaces.* Seminar, Pascal Poupart's Group, University of Waterloo. February 2023.

13. *Low-cost Bayesian methods for fixing neural nets' overconfidence.* LIFEPLAN Seminar. December 2022.

14. *Fisher SAM: information geometry and sharpness aware minimisation.* Seminar, Ferenc Huszár's Group, University of Cambridge. September 2022.

15. *Low-cost Bayesian methods for fixing neural nets' overconfidence.* Seminar, Vector Institute. August 2022.

16. *Posterior refinement improves sample efficiency in Bayesian neural networks.* Seminar, Søren Hauberg's Group, Technical University of Denmark. June 2022.

17. *Low-cost Bayesian methods for fixing neural nets' overconfidence.* Seminar, Roger Grosse's Group, University of Toronto. May 2022.

18. *Low-cost Bayesian methods for fixing neural nets' overconfidence.* Seminar, Arno Solin's Group, Aalto University. April 2022.

19. *Modern arts of Laplace approximations.* Seminar, Jörg Stückler's Group, Max Planck Institute for Intelligent Systems. September 2021.

Teaching

Winter 2026	**CS 9840: Probabilistic Generative AI**, Western University *Graduate computer science course. Main instructor.*
Winter 2022/23	**Numerics for Machine Learning**, University of Tübingen *Graduate course. Teaching assistant.*
Winter 2021/22	**Data Literacy**, University of Tübingen *Graduate course. Teaching assistant.*
Summer 2021	**Probabilistic Machine Learning**, University of Tübingen *Graduate course. Teaching assistant.*
Winter 2020/21	**Data Literacy**, University of Tübingen *Graduate course. Teaching assistant.*
Summer 2020	**Probabilistic Machine Learning**, University of Tübingen *Graduate course. Teaching assistant.*
Winter 2019/20	**Data Literacy**, University of Tübingen *Graduate course. Teaching assistant.*
2012	**Advanced Data Structure**, Atma Jaya University *Undergraduate course. Teaching assistant.*
2011	**Database**, Atma Jaya University *Undergraduate course. Teaching assistant.*

Supervision

09/2025 - Present	**MSc Thesis**, Western University *Paul Moore* Co-supervision with Lucian Ilie.
09/2025 - Present	**MSc Thesis**, Western University *Nouran Sakr* Co-supervision with Yalda Mohsenzadeh.

09/2025 - Present	**BSc Honours Thesis**, Western University *Xueying Hou*
09/2025 - Present	**BSc Honours Thesis**, Western University *Jacob Colton*
09/2025 - 12/2025	**MSc Directed Study**, Western University *Lyuhu Wang*
09/2025 - 12/2025	**MSc Directed Study**, Western University *Zijian Yang*

Internal Services

02/2026	**Western University** *PhD Thesis Examiner of Gezheng Xu*
12/2025	**Western University** *PhD TSP Chair of Gad Gad*
08/2025	**Western University** *MSc Thesis Examiner of Alana Deng*
07/2025	**Western University** *PhD TSP Examiner of Gezheng Xu*
02/2025 - 04/2025	**Vector Scholarship in AI** *Adjudication Committee*
02/2023 - 04/2023	**Vector Scholarship in AI** *Adjudication Committee*

External Services

2026 - Present	**Symposium on Probabilistic Machine Learning (ProbML)** *Organizing Committee* Program Chair: ProbML 2026.
02/2024 - 02/2025	**Indigenous and Black Engineering and Technology PhD Project (IBET)** *Mentor*
2024 - Present	**Symposium on Advances in Approximate Bayesian Inference (AABI)** *Organizing Committee* Website Chair: AABI 2024, 2025.
2023 - 2025	**Symposium on Advances in Approximate Bayesian Inference (AABI)** *Program Committee* Area Chair: AABI 2024, 2025.
2022 - Present	**Transaction on Machine Learning Research (TMLR)** *Program Committee* Reviewer: 2022–Present.
2023 - Present	**International Conference on Learning Representations (ICLR)** *Program Committee* Reviewer: ICLR 2023, 2024.

2022 - Present	**Artificial Intelligence and Statistics (AISTATS)**
	Program Committee
	Reviewer: AISTATS 2022. Area Chair: AISTATS 2025, 2026.

2021 - Present	**Neural Information Processing Systems (NeurIPS)**
	Program Committee
	Reviewer: NeurIPS 2021, 2022, 2024, 2025.

2021 - Present	**Uncertainty in Artificial Intelligence (UAI)**
	Program Committee
	Reviewer: UAI 2021.

2021 - Present	**International Conference on Machine Learning (ICML)**
	Program Committee
	Reviewer: ICML 2021, 2022, 2023, 2024. Area Chair: ICML 2025.

Other Experience

| 09/2017 - 04/2019 | **University of Bonn**, Bonn, Germany |
| | *Student Research Assistant (Part Time)* |

| 10/2016 - 02/2017 | **Atma Jaya University**, Yogyakarta, Indonesia |
| | *Student Research Assistant (Part Time)* |

| 04/2013 - 12/2015 | **GDP Labs**, Jakarta, Indonesia |
| | *Software Engineer* |

| 07/2012 | **Astra International**, Jakarta, Indonesia |
| | *Software Engineer Intern* |

| 01/2011 - 12/2011 | **Atma Jaya University**, Yogyakarta, Indonesia |
| | *Teaching Assistant (Part Time)* |

Open-Source Softwares

1. ULTS: Uncertainty-guided tree search. https://github.com/JuliaGrosse/ults.

2. Pub Ready Plots: Publication-ready plotting library. https://github.com/wiseodd/pub-ready-plots.

3. Lapeft-Bayesopt: Discrete Bayesian optimization with large language models and the Laplace approximation. https://github.com/wiseodd/lapeft-bayesopt.

4. Laplace-Bayesopt: Bayesian optimization with the Laplace approximation. https://github.com/wiseodd/laplace-bayesopt.

5. Laplace-Torch: Laplace approximations for deep neural networks. https://github.com/aleximmer/laplace.