

Agustinus Kristiadi — Curriculum Vitae

Department of Computer Science

Middlesex College, University of Western Ontario, London ON N6A 5B7 – Canada

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Research Interests

Probabilistic Machine Learning – Uncertainty Quantification – Decision-Making Under Uncertainty – AI4Science

Experience

Department of Computer Science, Western University

London, Canada

Assistant Professor

Jul 2025 –

Tenure track

Vector Institute

Toronto, Canada

Distinguished Postdoctoral Fellow

Feb 2023 – Jun 2025

Advisors: Alán Aspuru-Guzik and Pascal Poupart

Research in probabilistic foundation models, decision-making, and AI for chemistry

University of Tübingen

Tübingen, Germany

Ph.D., Computer Science

Jun 2019 – Jan 2023

International Max Planck Research School for Intelligent Systems

Advisor: Philipp Hennig

Co-advisor: Matthias Hein

Thesis: Low-Cost Bayesian Methods for Fixing Neural Networks' Overconfidence

The winner of 2023's "Theoretical Foundations of Deep Learning Learning Best Thesis Award"

Grade: *Magna cum laude*

University of Bonn

Bonn, Germany

M.Sc., Computer Science

Apr 2017 – Apr 2019

Advisor: Asja Fischer

Co-advisor: Jens Lehmann

Thesis: Predictive Uncertainty Quantification with Compound Density Networks

Grade: 1.1/1.0 *cum laude* (3.9/4.0 GPA equivalent)

Atma Jaya University, Yogyakarta

Yogyakarta, Indonesia

B.Eng., Informatics Engineering

Aug 2009 – Jan 2013

Advisor: Pranowo

Co-advisor: Paulus Mudjihartono

Thesis: Parallel Particle Swarm Optimization for Image Segmentation

Grade: 3.9/4.0 *cum laude*

Awards

- Best PhD thesis award from the Theoretical Foundations of Deep Learning program by DFG (German Research Foundation) — €2000
- Spotlight paper at NeurIPS 2023 — Top 4% of submissions

- Spotlight paper at NeurIPS 2021 — Top 3% of submissions
- Long-talk paper at UAI 2021 — Top 6% of submissions
- Best reviewers (top 10%) at ICML 2021

Publications

In machine learning, conferences are 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.

The first or joint-first author (the latter is marked with a ‘*’) of a paper is the lead author. The 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.

Thesis

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.

Conference

4. 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. [\[Link\]](#).
5. **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. [\[Link\]](#).
6. Lin, Wu; Dangel, Felix; Eschenhagen, Runa; Neklyudov, Kirill; **Kristiadi, Agustinus**; Turner, Richard E; Makhzani, Alireza. Structured inverse-free natural gradient: Memory-efficient & numerically-stable KFAC for large neural nets. In *International Conference on Machine Learning (ICML)*, 2024. [\[Link\]](#).
7. 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. [\[Link\]](#).
8. 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. [\[Link\]](#).
9. **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%)** [\[Link\]](#).
10. **Kristiadi, Agustinus**; Eschenhagen, Runa; Hennig, Philipp. Posterior refinement improves sample efficiency in

- Bayesian neural networks. In *Conference on Neural Information Processing Systems (NeurIPS)*, 2022. [\[Link\]](#).
11. Hobbhahn, Marius; **Kristiadi, Agustinus**; Hennig, Philipp. Fast predictive uncertainty for classification with Bayesian deep networks. In *Conference on Uncertainty in Artificial Intelligence (UAI)*, 2022. [\[Link\]](#).
 12. **Kristiadi, Agustinus**; Hein, Matthias; Hennig, Philipp. Being a bit frequentist improves Bayesian neural networks. In *International Conference on Artificial Intelligence and Statistics (AISTATS)*, 2022. [\[Link\]](#).
 13. 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. [\[Link\]](#).
 14. 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. [\[Link\]](#).
 15. **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%)** [\[Link\]](#).
 16. **Kristiadi, Agustinus**; Hein, Matthias; Hennig, Philipp. Learnable uncertainty under Laplace approximations. In *Conference on Uncertainty in Artificial Intelligence (UAI)*, 2021. **Long Talk (top 6%)** [\[Link\]](#).
 17. **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. [\[Link\]](#).
 18. **Kristiadi***, **Agustinus**; Khan*, Mohammad Asif; Lukovnikov, Denis; Lehmann, Jens; Fischer, Asja. Incorporating literals into knowledge graph embeddings. In *International Semantic Web Conference (ISWC)*, 2019. [\[Link\]](#).
 19. 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. [\[Link\]](#).
 20. **Kristiadi, Agustinus**; Pranowo, ; Mudjihartono, Paulus. Parallel pinproceedings swarm optimization for image segmentation. In *Digital Enterprise and Information Systems*, 2013. [\[Link\]](#).

Journal.....

21. **Kristiadi, Agustinus**; Pranowo, . Deep convolutional level set method for image segmentation. *Journal of ICT Research & Applications*, 11(3), 2017. [\[Link\]](#).

Workshop.....

22. Cinquin, Tristan; Lo, Stanley; Strieth-Kalthoff, Felix; Aspuru-Guzik, Alán; Pleiss, Geoff; Bamler, Robert; Rudner, Tim GJ; Fortuin, Vincent; **Kristiadi, Agustinus**. What actually matters for materials discovery: Pitfalls and recommendations in Bayesian optimization. In *AI for Accelerated Materials Discovery Workshop ICLR 2025*, 2025. [\[Link\]](#).
23. 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 NeurIPS 2024*, 2024. [\[Link\]](#).
24. 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 NeurIPS 2024*, 2024. [\[Link\]](#).
25. 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, 2024. [\[Link\]](#).

26. **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*, 2024. [\[Link\]](#).
27. 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. [\[Link\]](#).
28. **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*, 2023. [\[Link\]](#).
29. 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. [\[Link\]](#).
30. **Kristiadi, Agustinus**; Däubener, Sina; Fischer, Asja. Predictive uncertainty quantification with compound density networks. In *NeurIPS Workshop of Bayesian Deep Learning*, 2019. [\[Link\]](#).

Preprint

31. Bigi, Filippo; Chong, Sanggyu; **Kristiadi, Agustinus**; Ceriotti, Michele. FlashMD: Long-stride, universal prediction of molecular dynamics. *arXiv preprint arXiv:2505.19350*, 2025. [\[Link\]](#).
32. 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. [\[Link\]](#).
33. 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. [\[Link\]](#).
34. Wenger, Jonathan; Dangel, Felix; **Kristiadi, Agustinus**. On the disconnect between theory and practice of overparametrized neural networks. *arXiv preprint arXiv:2310.00137*, 2023. [\[Link\]](#).

Other Relevant Experience

University of Bonn

Student Research Assistant (Part Time)

Research in knowledge graphs and natural language processing

Bonn, Germany

Sep 2017 – Apr 2019

Atma Jaya University, Yogyakarta

Research Assistant (Part Time)

Research in Computer vision

Yogyakarta, Indonesia

Oct 2016 – Feb 2017

GDP Venture

Software Engineer

Data analytics and full-stack application development

Jakarta, Indonesia

Apr 2013 – Dec 2015

Astra International

Software Engineer Intern

Full-stack application development

Jakarta, Indonesia

Jul 2012

Atma Jaya University, Yogyakarta

Teaching Assistant (Part Time)

Yogyakarta, Indonesia

Jan 2011 – Dec 2011

Teaching “Advance Data Structure” and “Database” courses

Teaching Experience

Mentorship

Tristan Cinquin

Vector Institute

Intern

2025

Probabilistic decision-making for reasoning in large language models

Andrés Guzmán Cordero

Vector Institute

Intern

2024

Investigating 3D representations of molecules for Bayesian optimization

Ken Mangouh Nsiempba

Vector Institute

IBET PhD project

2024

Navigating life as a PhD student

Serena Hacker

Vector Institute

Intern

2023

Research in robustness of neural networks, resulting in [an AISTATS publication](#)

Madhav Iyengar

University of Tübingen

Master's student

2022

Student research project in Bayesian neural networks

Naman Deep Singh

University of Tübingen

Master's student

2022

Student research project in Bayesian neural networks

Tobias Ludwig

University of Tübingen

Master's student

2021

Student research project in Bayesian neural networks

Runa Eschenhagen

University of Tübingen

Master's student

2021

Student research project in Bayesian neural networks, resulting in [a workshop publication](#)

Marius Hobbhahn

University of Tübingen

Master's student

2020

Mater's thesis in Bayesian deep learning, resulting in [a UAI publication](#)

Teaching assistantship

Numerics for Machine Learning

University of Tübingen, 2022/2023

Data Literacy

University of Tübingen, 2021/2022

Probabilistic Machine Learning

University of Tübingen, 2021

Data Literacy

University of Tübingen, 2020/2021

Probabilistic Machine Learning

University of Tübingen, 2020

Data Literacy

University of Tübingen, 2019/2020

Advanced Data Structure

Atma Jaya University, 2012

Database

Atma Jaya University, 2011

Services

Community Services

- Organizer of the AABI symposium, co-located with ICML 2024
- IBET PhD mentor 2024
- Speaker at the Black in AI mentorship session, NeurIPS 2023
- Adjudication committee for Vector Scholarship in AI 2023

Peer-Reviewing

As area chair: AISTATS 2024, AABI Symposium 2024, AABI Symposium 2025

As reviewer: JMLR, TMLR, NeurIPS 2020, ICML 2021, UAI 2021, NeurIPS 2021, AISTATS 2022, ICML 2022, NeurIPS 2022, ICML 2023, ICLR 2023, ICML 2024, NeurIPS 2024, ICLR 2024, ICML 2025, NeurIPS 2025

Open-Source Softwares

- Uncertainty-guided likelihood-tree search for optimizing LLM's output log-likelihood:
<https://github.com/JuliaGrosse/ults>
- Publication-ready plotting library:
<https://github.com/wiseodd/pub-ready-plots>
- Discrete Bayesian optimization with LLMs and the Laplace approximation:
<https://github.com/wiseodd/lapeft-bayesopt>
- BoTorch interface for the Laplace approximated neural net surrogate:
<https://github.com/wiseodd/laplace-bayesopt>
- Easy Laplace approximation for deep neural networks:
<https://github.com/aleximmer/Laplace>

Talks

Probabilistic Decision-Making Algorithms For A Better World

First-Year Seminar in Science, University of British Columbia

March 2025

Probabilistic Inference and Decision-Making with Foundation Models for Bayesian Optimization

Waterloo AI Seminars, University of Waterloo

October 2024

Probabilistic Inference and Decision-Making With and for Foundation Models

Machine Learning and Friends Lunch, UMass Amherst

October 2024

Probabilistic Inference and Decision-Making With and for Foundation Models

Seminar, Sander Lab, Harvard Medical School

October 2024

Uncertainty-Guided Optimization on LLM Search Trees

Vector Research Day, Vector Institute

June 2024

Gaussian Processes, The Linearized Laplace, and Sequential Decision Making

Seminar, Pascal Poupart's Group, University of Waterloo

April 2024

Bayesian Optimization With LLMs and Expert Feedback for Material Discovery

Seminar, The Matter Lab, University of Toronto

March 2024

The Geometry of Neural Nets' Parameter Spaces Under Reparametrization <i>Math Machine Learning Seminar, University of California, Los Angeles</i>	January 2024
The Geometry of Neural Nets' Parameter Spaces Under Reparametrization <i>ELLIS Reading Group on Mathematics of Deep Learning</i>	December 2023
Bayesian Deep Learning: Past, Present, and Future <i>Theoretical Foundations of Deep Learning meeting</i>	November 2023
The Linearized Laplace and the Geometry of NNs' Parameter Spaces <i>Seminar, Pascal Poupart's Group, University of Waterloo</i>	February 2023
Low-Cost Bayesian Methods for Fixing Neural Nets' Overconfidence <i>LIFEPLAN Seminar</i>	December 2022
Fisher SAM: Information Geometry and Sharpness Aware Minimisation <i>Seminar, Ferenc Huszár's Group, University of Cambridge</i>	September 2022
Low-Cost Bayesian Methods for Fixing Neural Nets' Overconfidence <i>Seminar, Vector Institute</i>	August 2022
Posterior Refinement Improves Sample Efficiency in Bayesian Neural Networks <i>Seminar, Søren Hauberg's Group, Technical University of Denmark</i>	June 2022
Low-Cost Bayesian Methods for Fixing Neural Nets' Overconfidence <i>Seminar, Roger Grosse's Group, University of Toronto</i>	May 2022
Low-Cost Bayesian Methods for Fixing Neural Nets' Overconfidence <i>Seminar, Arno Solin's Group, Aalto University</i>	April 2022
Modern Arts of Laplace Approximations <i>Seminar, Jörg Stückler's Group, Max Planck Institute for Intelligent Systems</i>	September 2021

Media Appearances

FoDL Best Thesis Award <i>Theoretical Foundations of Deep Learning [Link]</i>	November 2023
Painless Uncertainty for Deep Learning <i>Machine Learning for Science [Link]</i>	July 2021

Languages

English (IELTS 8.0 / C1 equivalent), German (A2), Indonesian (native), Javanese (native)