Agustinus Kristiadi — Curriculum Vitae

Department of Computer Science
Middlesex College, Room MC 362, University of Western Ontario, London ON N6A 5B7
Canada
agustinus@kristia.de • agustinus.kristia.de • Google Scholar
agustinus-kristiadi • akristiadi7 • wiseodd

Research Interests

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

Experience

Western University — **London, Canada**
Assistant Professor — *Jul 2025 –*
Tenure-track, Department of Computer Science

Vector Institute — **London, Canada**
Faculty Affiliate — *Jul 2025 –*

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; Grosse, Julia; ***Kristiadi****, ***Agustinus***; Poupart*, Pascal. A critical look at tokenwise reward-guided text generation. In *Conference on Language Modeling (COLM*, 2025. [Link].
5. 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].
6. ***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].
7. 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].
8. 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].
9. 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].

10. ***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].

11. ***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].

12. 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].

13. ***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].

14. 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].

15. 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].

16. ***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].

17. ***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].

18. ***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].

19. ***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].

20. 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].

21. ***Kristiadi***, ***Agustinus***; Pranowo, ; Mudjihartono, Paulus. Parallel pinproceedings swarm optimization for image segmentation. In *Digital Enterprise and Information Systems*, 2013. [Link].

Journal

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

Workshop

23. 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].

24. 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].

25. 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].

26. 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].

27. ***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].

28. 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].

29. ***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].

30. 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].

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

Preprint

32. Bigi, Filippo; Chong, Sanggyu; ***Kristiadi***, ***Agustinus***; Ceriotti, Michele. FlashMD: Long-stride, universal prediction of molecular dynamics. *arXiv preprint arXiv:2505.19350*, 2025. [Link].

33. 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. [Link].

34. 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].

35. 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].

36. 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 — **Bonn, Germany**
Student Research Assistant (Part Time) — *Sep 2017 – Apr 2019*
Research in knowledge graphs and natural language processing

Atma Jaya University, Yogyakarta — **Yogyakarta, Indonesia**
Research Assistant (Part Time) — *Oct 2016 – Feb 2017*

Research in Computer vision

GDP Venture **Jakarta, Indonesia**
Software Engineer *Apr 2013 – Dec 2015*
Data analytics and full-stack application development

Astra International **Jakarta, Indonesia**
Software Engineer Intern *Jul 2012*
Full-stack application development

Atma Jaya University, Yogyakarta **Yogyakarta, Indonesia**
Teaching Assistant (Part Time) *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
Math Machine Learning Seminar, University of California, Los Angeles — *January 2024*

The Geometry of Neural Nets' Parameter Spaces Under Reparametrization
ELLIS Reading Group on Mathematics of Deep Learning — *December 2023*

Bayesian Deep Learning: Past, Present, and Future
Theoretical Foundations of Deep Learning meeting — *November 2023*

The Linearized Laplace and the Geometry of NNs' Parameter Spaces
Seminar, Pascal Poupart's Group, University of Waterloo — *February 2023*

Low-Cost Bayesian Methods for Fixing Neural Nets' Overconfidence
LIFEPLAN Seminar — *December 2022*

Fisher SAM: Information Geometry and Sharpness Aware Minimisation
Seminar, Ferenc Huszár's Group, University of Cambridge — *September 2022*

Low-Cost Bayesian Methods for Fixing Neural Nets' Overconfidence
Seminar, Vector Institute — *August 2022*

Posterior Refinement Improves Sample Efficiency in Bayesian Neural Networks
Seminar, Søren Hauberg's Group, Technical University of Denmark — *June 2022*

Low-Cost Bayesian Methods for Fixing Neural Nets' Overconfidence
Seminar, Roger Grosse's Group, University of Toronto — *May 2022*

Low-Cost Bayesian Methods for Fixing Neural Nets' Overconfidence
Seminar, Arno Solin's Group, Aalto University — *April 2022*

Modern Arts of Laplace Approximations
Seminar, Jörg Stückler's Group, Max Planck Institute for Intelligent Systems — *September 2021*

Media Appearances

FoDL Best Thesis Award
Theoretical Foundations of Deep Learning [Link] — *November 2023*

Painless Uncertainty for Deep Learning
Machine Learning for Science [Link] — *July 2021*

Languages

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