

# GEOFF PLEISS, CURRICULUM VITAE

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## ACADEMIC POSITIONS AND EDUCATION

- 2023– UNIVERSITY OF BRITISH COLUMBIA (Vancouver, BC, Canada)  
**Assistant Professor**, Department of Statistics (2023–)  
Associate Member, Department of Computer Science (2023–)  
Centre for Artificial Intelligence Decision-Making and Action (CAIDA)  
Artificial Intelligence Methods for Scientific Impact (AIM-SI) Cluster
- 2023– VECTOR INSTITUTE (Toronto, ON, Canada)  
**CIFAR AI Chair** (2024–)  
Faculty Member (2023–)
- 2020–2023 COLUMBIA UNIVERSITY (New York, NY, USA)  
**Postdoctoral Research Scientist**, Zuckerman Institute  
Supervisor: John P. Cunningham
- 2015–2020 CORNELL UNIVERSITY (Ithaca, NY, USA)  
**Ph.D., Computer Science** (2020)  
**M.S., Computer Science** (2018)  
Committee: Kilian Q. Weinberger (chair), Andrew Gordon Wilson, Karthik Sridharan  
Dissertation: A Scalable and Flexible Framework for Gaussian Processes via Matrix-Vector Multiplication
- 2009–2013 OLIN COLLEGE OF ENGINEERING (Needham, MA, USA)  
**B.Sc., Engineering** (2013)  
Concentration: Computing with Applied Mathematics

## OTHER RELEVANT EXPERIENCE

- 2019–2020 ASAPP, INC. (Ithaca, NY, USA)  
**Research Intern**
- 2018 MICROSOFT, INC. (Redmond, WA, USA)  
**Research Intern**
- 2013–2015 PIVOTAL INC. (New York, NY, USA)  
**Software Engineer**

## HONOURS AND AWARDS

2023	AISTATS Top Reviewer (top 10%)
2022	NeurIPS “I Can’t Believe It’s Not Better” Workshop – Most Surprising Result Award
2022	AISTATS Top Reviewer (top 10%)
2020	NeurIPS Top Reviewer (top 10%)
2019	NeurIPS Top Reviewer (top 50%)
2017	National Science Foundation Graduate Research Fellowship (honorable mention)
2016	National Science Foundation Graduate Research Fellowship (honorable mention)
2012	Barry M. Goldwater Scholarship (honorable mention)
2009–2013	Olin Merit Scholarship (full-tuition recipient)

## PUBLICATIONS

### Citation Statistics

*All statistics are based on Google Scholar, with manual corrections for errors.*

Total citations of all publications: 10000+

Total citations of top-three most cited publications: 7000+

Publications (including technical reports) with 100+ citations: 11

Publications (including technical reports) with 10+ citations: 25

### Preprints Under Submission

- [U1] Agustinus Kristiadi, Felix Strieth-Kalthoff, Marta Skreta, Pascal Poupart, Alán Aspuru-Guzik, and **Geoff Pleiss**. A sober look at LLMs for material discovery: Are they actually good for Bayesian optimization over molecules? *arXiv preprint arXiv:2402.05015*, 2024.
- [U2] Jinsoo Yoo, Yunpeng Liu, Frank Wood, and **Geoff Pleiss**. Layerwise proximal replay: A proximal point method for online continual learning. *arXiv preprint arXiv:2402.09542*, 2024.
- [U3] Alexandre Bouchard-Côté, Trevor Campbell, **Geoff Pleiss**, and Nikola Surjanovic. MCMC-driven learning. *arXiv preprint arXiv:2402.09598*, 2024.

### Refereed Conference Publications

*In machine learning, conferences are considered prestigious venues for publication. All venues listed here are highly selective (acceptance rate 20 – 30%) and have peer-reviewing and refereeing processes similar to journals.*

*\* denotes equal author contribution (shared first-authorship).*

- [C1] Kaiwen Wu, Jonathan Wenger, Hadyn Jones, **Geoff Pleiss**, and Jacob R. Gardner. Large-scale Gaussian processes via alternating projection. In *Artificial Intelligence and Statistics*, 2024.
- [C2] Andres Potapczynski\*, Marc Anton Finzi\*, **Geoff Pleiss**, and Andrew Gordon Wilson. CoLA: Exploiting compositional structure for automatic and efficient numerical linear algebra. In *Neural Information Processing Systems*, 2023.

- [C3] Alexandre Capone, Sandra Hirche, and **Geoff Pleiss**. Sharp calibrated Gaussian processes. In *Neural Information Processing Systems*, 2023.
- [C4] Jonathan Wenger, **Geoff Pleiss**, Marvin Pförtner, Philipp Hennig, and John P. Cunningham. Posterior and computational uncertainty in Gaussian processes. In *Neural Information Processing Systems*, 2022.
- [C5] Taiga Abe\*, E. Kelly Buchanan\*, **Geoff Pleiss**, Richard Zemel, and John P. Cunningham. Deep ensembles work, but are they necessary? In *Neural Information Processing Systems*, 2022.
- [C6] Luhuan Wu, **Geoff Pleiss**, and John P. Cunningham. Variational nearest neighbor Gaussian processes. In *International Conference on Machine Learning*, 2022.
- [C7] Jonathan Wenger, **Geoff Pleiss**, Philipp Hennig, John P. Cunningham, and Jacob R. Gardner. Preconditioning for scalable Gaussian process hyperparameter optimization. In *International Conference on Machine Learning*, 2022. [LONG ORAL PRESENTATION—TOP 2% OF SUBMISSIONS].
- [C8] **Geoff Pleiss** and John P. Cunningham. The limitations of large width in neural networks: A deep Gaussian process perspective. In *Neural Information Processing Systems*, 2021.
- [C9] Anthony L. Caterini\*, Gabriel Loaiza-Ganem\*, **Geoff Pleiss**, and John P. Cunningham. Rectangular flows for manifold learning. In *Neural Information Processing Systems*, 2021.
- [C10] Andres Potapczynski\*, Luhuan Wu\*, Dan Biderman\*, **Geoff Pleiss**, and John P. Cunningham. Bias-free scalable Gaussian processes via randomized truncations. In *International Conference on Machine Learning*, 2021.
- [C11] Luhuan Wu\*, Andrew Miller\*, Lauren Anderson, **Geoff Pleiss**, David Blei, and John P. Cunningham. Hierarchical inducing point Gaussian process for inter-domain observations. In *Artificial Intelligence and Statistics*, 2021.
- [C12] **Geoff Pleiss**, Martin Jankowiak, David Eriksson, Anil Damle, and Jacob R. Gardner. Fast matrix square roots with applications to Gaussian processes and Bayesian optimization. In *Neural Information Processing Systems*, 2020.
- [C13] **Geoff Pleiss**, Tianyi Zhang, Ethan Elenberg, and Kilian Q. Weinberger. Identifying mislabeled data using the area under the margin ranking. In *Neural Information Processing Systems*, 2020.
- [C14] Martin Jankowiak, **Geoff Pleiss**, and Jacob R. Gardner. Deep sigma point processes. In *Uncertainty in Artificial Intelligence*, 2020.
- [C15] Martin Jankowiak, **Geoff Pleiss**, and Jacob R. Gardner. Parametric Gaussian process regressors. In *International Conference on Machine Learning*, 2020.
- [C16] Yurong You\*, Yan Wang\*, Wei-Lun Chao\*, Divyansh Garg, **Geoff Pleiss**, Bharath Hariharan, Mark Campbell, and Kilian Q. Weinberger. Pseudo-lidar++: Accurate depth for 3d object detection in autonomous driving. In *International Conference on Learning Representations*, 2020.
- [C17] Ke Wang\*, **Geoff Pleiss**\*, Jacob R. Gardner, Stephen Tyree, Kilian Q. Weinberger, and Andrew Gordon Wilson. Exact Gaussian processes on a million data points. In *Neural Information Processing Systems*, 2019.
- [C18] Jacob R. Gardner\*, **Geoff Pleiss**\*, David Bindel, Kilian Q. Weinberger, and Andrew Gordon Wilson. GPyTorch: Blackbox matrix-matrix Gaussian process inference with GPU acceleration. In *Neural Information Processing Systems*, 2018. [SPOTLIGHT PRESENTATION—TOP 4% OF SUBMISSIONS].
- [C19] **Geoff Pleiss**, Jacob R. Gardner, Andrew Gordon Wilson, and Kilian Q. Weinberger. Constant time predictive distributions for Gaussian processes. In *International Conference on Machine Learning*, 2018.

- [C20] Jacob R. Gardner, **Geoff Pleiss**, Ruihan Wu, Andrew Gordon Wilson, and Kilian Q. Weinberger. Product kernel interpolation for scalable Gaussian processes. In *Artificial Intelligence and Statistics*, 2018.
- [C21] **Geoff Pleiss\***, Manish Raghavan\*, Felix Wu, Jon Kleinberg, and Kilian Q. Weinberger. On fairness and calibration. In *Neural Information Processing Systems*, 2017.
- [C22] Chuan Guo\*, **Geoff Pleiss\***, Yu Sun\*, and Kilian Q. Weinberger. On calibration of modern neural networks. In *International Conference on Machine Learning*, 2017.
- [C23] Paul Upchurch\*, Jacob Gardner\*, **Geoff Pleiss**, Kavita Bala, Robert Pless, Noah Snavely, and Kilian Q. Weinberger. Deep feature interpolation for image content changes. In *Computer Vision and Pattern Recognition*, 2017.
- [C24] Gao Huang\*, Yixuan Li\*, **Geoff Pleiss**, Zhuang Liu, John E. Hopcroft, and Kilian Q. Weinberger. Snapshot ensembles: Train 1, get  $M$  for free. In *International Conference on Learning Representations*, 2017.

### Journal Publications

- [J1] Taiga Abe, E. Kelly Buchanan, **Geoff Pleiss**, and John P. Cunningham. Pathologies of predictive diversity in deep ensembles. *Transactions on Machine Learning Research*, 2024. [FEATURED PAPER—TOP 2% OF SUBMISSIONS].
- [J2] Jordan Venderley, Michael Matty, Krishnanand Mallayya, Matthew Krogstad, Jacob Ruff, **Geoff Pleiss**, Varsha Kishore, David Mandrus, Daniel Phelan, Lekhanath Poudel, and others. Harnessing interpretable and unsupervised machine learning to address big data from modern x-ray diffraction. *Proceedings of the National Academy of Sciences*, 119(24), 2022.
- [J3] Gao Huang\*, Zhuang Liu\*, **Geoff Pleiss**, Laurens van der Maaten, and Kilian Q. Weinberger. Convolutional networks with dense connectivity. *Transactions on Pattern Analysis and Machine Intelligence*, 2019.
- [J4] James Knighton, **Geoff Pleiss**, Elizabeth Carter, Steven Lyon, M. Todd Walter, and Scott Steinschneider. Potential predictability of regional precipitation and discharge extremes using synoptic-scale climate information via machine learning: An evaluation for the eastern continental United States. *Journal of Hydrometeorology*, 20(5):883–900, 2019.

### Technical Reports and Workshop Proceedings

- [R1] E. Kelly Buchanan, **Geoff Pleiss**, Yixin Wang, and John P. Cunningham. The effects of ensembling on long-tailed data. In *NeurIPS “Heavy Tails in ML: Structure, Stability, Dynamics” Workshop*, 2023.
- [R2] Taiga Abe\*, E. Kelly Buchanan\*, **Geoff Pleiss**, and John P. Cunningham. The best deep ensembles sacrifice predictive diversity. In *NeurIPS “I Can’t Believe It’s Not Better!” Workshop*, 2022. [ORAL PRESENTATION].
- [R3] Martin Jankowiak and **Geoff Pleiss**. Scalable cross validation losses for Gaussian process models. *arXiv preprint arXiv:2105.11535*, 2021.
- [R4] Elliott Gordon-Rodriguez, Gabriel Loaiza-Ganem, **Geoff Pleiss**, and John P. Cunningham. Uses and abuses of the cross-entropy loss: Case studies in modern deep learning. In *NeurIPS “I Can’t Believe It’s Not Better!” Workshop*, 2020. [ORAL PRESENTATION].
- [R5] **Geoff Pleiss\***, Danlu Chen\*, Gao Huang, Tongcheng Li, Laurens van der Maaten, and Kilian Q. Weinberger. Memory-efficient implementation of DenseNets. *arXiv preprint arXiv:1707.06990*, 2017.

## SELECTED OPEN SOURCE

### Co-Founder and Maintainer

- 2018– GPyTorch  
<https://gpytorch.ai>
- 2022– LinearOperator  
<https://linear-operator.readthedocs.io>
- 2023– CoLA (Compositional Linear Algebra)  
<https://cola.readthedocs.io/>

## PATENTS

- [P1] Tianyi Zhang, Sam Altschul, Kilian Weinberger, Michael Griffiths, and Geoffrey Michael Pleiss.  
Trend detection via machine learning models, September 19 2023. US Patent 11,763,230.

## GRANTS

- 2024 NSERC Discovery (PI)
- 2024 NSERC Early Career Supplement (PI)

## INVITED TALKS

- June 2024 Adaptive Experimentation Workshop, Meta Inc. (New York, NY, USA)  
*Title TBD*
- May 2024 AI In Medicine Meeting, Karolinska Institute (Stockholm, Sweden)  
*Foundation Models for Science: A Case Study on Combining LLMs and Black-Box Optimization for Materials Discovery*
- April 2024 Academic Seminar, Two Sigma Investments LP (New York, NY, USA)  
*Towards Reliable Neural Networks: What's Within Grasp and What's Out of Reach?*
- Dec. 2023 Vector Distinguished Talk Series, Vector Institute (Toronto, ON, Canada)  
*Troubling Trajectories for Uncertainty Quantification and Decision Making with Neural Networks*
- Spring 2022 Job talk, various universities  
*Bridging The Gap Between Deep Learning and Probabilistic Modeling*
- Nov. 2021 New York University (New York, NY, USA)  
*Understanding Neural Networks through Gaussian Processes, and Vice Versa*
- Oct. 2021 Artificial Intelligence Seminar, University College London (Virtual)  
*Understanding Neural Networks through Gaussian Processes, and Vice Versa*
- Dec. 2020 Machine Learning for Nuclear Data Workshop (Virtual)  
*GPyTorch: A Scalable and Flexible Framework for Gaussian Processes via Matrix-Vector Multiplication*
- May 2020 Columbia University (Virtual)  
*GPyTorch: A Scalable and Flexible Framework for Gaussian Processes via Matrix-Vector Multiplication*

- Nov. 2019      Computer Science Colloquium, Cornell University (Ithaca, NY, USA)  
*From  $N = 1,000$  to  $N = 1,000,000$ : Scaling Gaussian Process Inference with Matrix Multiplication and GPU Acceleration*
- May 2019      Symposium on Bayesian Optimization, Uber AI (San Francisco, CA, USA)  
*From  $N = 1,000$  to  $N = 1,000,000$ : Scaling Gaussian Process Inference with Matrix Multiplication and GPU Acceleration*

## CONTRIBUTED TALKS

- Aug. 2024      Joint Statistical Meeting (Portland, OR, USA)  
*Task-Aware Scalable Gaussian Processes*
- June 2024      Statistical Society of Canada Annual Meeting (St. John's, NL, Canada)  
*Ensembles in the Age of Overparameterization: Promises and Pathologies*
- Feb. 2024      SIAM UQ Conference (Trieste, Italy)  
*Blurring the Distinction Between Data Collection and Computation in Gaussian Processes*
- Dec. 2018      Neural Information Processing Systems (Montreal, QC, Canada)  
*GPyTorch: Blackbox Matrix-Matrix Gaussian Process Inference with GPU Acceleration*
- July 2018      International Conference on Machine Learning (Stockholm, Sweden)  
*Constant Time Predictive Distributions for Gaussian Processes*
- Aug. 2017      International Conference on Machine Learning (Sydney, Australia)  
*On Calibration of Modern Neural Networks*

## TEACHING

### University of British Columbia

- Fall 2023      STAT 520P — Topics in Bayesian Analysis and Decision Theory: Bayesian Optimization

## ADVISING AND SUPERVISION

### Doctoral Thesis Pre-Examiner

- Paul E. Chang, Aalto University (Spring 2024)

## PROFESSIONAL SERVICE

### Area Chair

- International Conference on Machine Learning (2022–2024)  
 International Conference on Learning Representations (2024)  
 International Joint Conference on Artificial Intelligence (2023)  
 Neural Information Processing Systems (2022–2023)

### **Organizing Committee Member**

NeurIPS Workshop on Gaussian Processes, Spatiotemporal Modeling, and Decision-Making Systems (2022)

Virtual Seminar on Gaussian Processes, Spatiotemporal Modeling, and Decision-Making Systems (2022–2023)

### **Panelist**

Scientific Software Development Panel: Dagstuhl Seminar on Probabilistic Numerical Methods (2021)

### **Conference Reviewer**

AAAI Conference on Artificial Intelligence (2017)

Artificial Intelligence and Statistics (2019–2024)

International Conference on Learning Representations (2022)

International Conference on Machine Learning (2019–2021)

Neural Information Processing Systems (2018–2021)

Uncertainty in Artificial Intelligence (2018)

### **Journal Reviewer**

Bernoulli (2022)

Journal of Machine Learning Research (2019–2022)

SIAM/ASA Journal on Uncertainty Quantification (2024)

Transactions on Machine Learning Research (2022–2023)

Transactions on Pattern Analysis and Machine Intelligence (2020–2021)

### **Workshop Reviewer**

NeurIPS “I Can’t Believe It’s Not Better” Workshop (2023)

NeurIPS “Your Model is Wrong: Robustness and Misspecification in Probabilistic Modeling” Workshop (2021)

## **MEDIA APPEARANCES**

May 2023      “The Ensembles Podcast”

## **OUTREACH**

Fall 2020      LatinX in AI NeurIPS mentorship program

Spring 2018      Cornell “Expand Your Horizons” (STEM workshop for middle school girls)

Spring 2017      Cornell “GRASSHOPR” (After-school CS class at local middle school)

Spring 2016      Cornell “Expand Your Horizons”

Spring 2016      “Code4Kids” (After-school CS class at local elementary school)