

Zelda E. Mariet

Modeling uncertainty in machine learning

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PROFESSIONAL EXPERIENCE

Senior Research Scientist Google DeepMind

Reliable Deep Learning team | *Modeling uncertainty in neural networks and LLMs.* 2019–

- **Understanding why diversity improves robustness in neural network ensembles.** Generalized the bias-variance decomposition to classification losses and derived an exact, computationally trivial definition of ensemble diversity which resolves a longstanding issue¹ in understanding ensembles of classifiers.
- **Plex: Reliability via pretrained large models.** Developed models with state-of-the-art performance across a variety of vision, language, and decision-making tasks involving uncertainty.

AI for Science team | *Machine learning for drug discovery.*

- **ML-guided nanobody design targeting COVID-19.** Used ML to design nanobodies that neutralize SARS-CoV-2, including variants not seen during training, such as Delta and Omicron.

Software Engineering Intern Google Research

- *Generative models for negatively dependent measures (2018).* *Summers 2016–2018*
- *Theory and applications of high-dimensional time series forecasting (2017).*
- *Ranking optimization for Google Maps (2016).*

EDUCATION

PhD (computer science), advised by Suvrit Sra MIT

*Theory and applications of negatively dependent measures for ML. **Minor:** physical cosmology.* 2014–2019

Master of Science MIT

Thesis: modeling diversity with determinantal point processes. 2014–2016

Master of Science & Bachelor of Science Ecole polytechnique (France)

Specialization in Mathematics and Computer Science. 2011–2014

SELECTED PUBLICATIONS & PATENTS

- High-throughput ML-guided design of diverse single-domain antibodies against SARS-CoV-2. *Angermueller, Mariet, et al.* Under review
- [Ensembling mixture-of-experts neural networks.](#) *Patent #US20230107409A1* pending, 2023
- [Population-based black-box optimization.](#) *Patent #US20230083892A1* pending, 2023
- [Ensembles of classifiers: a bias-variance perspective.](#) *Gupta, Smith, Adlam, Mariet* TMLR 2022
- [Sparse MoEs meet efficient ensembles.](#) *Allingham et al.* TMLR 2022
- [Faster & More Reliable Tuning of Neural Networks: Bayesian Optimization with Importance Sampling.](#) *Ariafar, Mariet, Brooks, Dy, Snoek* AISTATS 2021

¹“Understanding ensemble diversity remains a holy grail problem” (*Ensemble Methods: Foundations and Algorithms*, Zhi-Hua Zhou, 2012)

- Distilling ensembles improves uncertainty estimates. *Mariet, Jenatton, Wenzel, Tran* AABI 2021
- Population-based black-box optimization for biological sequence design. *Angermueller, Belanger, Gane, Mariet, Dohan, Murphy, Colwell, Sculley* ICML 2020
- Foundations of sequence-to-sequence modeling for time series. *Mariet, Kuznetsov* AISTATS 2019
- Learning DPPs by sampling inferred negatives. *Mariet, Gartrell, Sra* AISTATS 2019
- Exponentiated strongly Rayleigh distributions. *Mariet, Sra, Jegelka* NeurIPS 2018
- Maximizing induced cardinality under a DPP. *Gillenwater, Kulesza, Vassiltiskii, Mariet* NeurIPS 2018
- Elementary symmetric polynomials for optimal experimental design. *Mariet, Sra* NeurIPS 2017
- Kronecker determinantal point processes. *Mariet, Sra* NIPS 2016
- Diversity networks: neural network compression using DPPs. *Mariet, Sra* ICLR 2016
- Fixed-point algorithms for learning determinantal point processes. *Mariet, Sra* ICML 2015

INVITED TALKS

- ML-guided nanobody design targeting COVID-19. *Gaussian Process Seminar Series* 2023
- Ensembling over classifiers: a bias-variance perspective. *ASU Lyons Seminar* 2022
- Modeling Negative Dependence at Scale. *UAI Tractable Probabilistic Modeling workshop* 2021

HOSTED WORKSHOPS

- Duality Principles for Modern Machine Learning (DP4ML 2023) ICML 2023
- Negative Dependence and Submodularity for Machine Learning (NegDepML 2020) ICML 2020
- Negative Dependence in Machine Learning (NegDepML 2019) ICML 2019

TEACHING EXPERIENCE

- **Harvard instructor:** Topics in Machine Learning (CS282r) 2022
- **CSRMP mentor** to 7 undergrad & grad students from underrepresented communities 2022
- **MIT Teaching Assistant:** Machine Learning graduate course (6.867) 2016
- **Math instructor** at GEPPM, a French non-profit for underprivileged students 2011–2012

AWARDS & COMMUNITY SERVICE

- Women in Machine Learning (WiML) mentor 2022
- Google PhD Fellowship in machine learning 2018
- Criteo Faculty Research Award program 2017
- Accepted to the Corps des Mines after graduating from Ecole polytechnique 2014
- Silver medal, SWERC international algorithmics contest 2013
- NeurIPS/ICML reviewer awards 2019, 2020, 2022

Area Chair: AISTATS, IJCAI **Reviewer:** NeurIPS, ICML, ICLR, TMLR, JMLR

SPOKEN LANGUAGES

English/French: bilingual **Japanese:** JLPT N3 **German:** strong skills