Marvin Schmitt

Computer Scientist · Psychologist · Researcher

mail.marvinschmitt@gmail.com · www.marvinschmitt.com · marvinschmitt · @MarvinSchmittML

Education

since 12/2021 **PhD, Computer Science and Simulation Science**
University of Stuttgart, Germany
- Working title: Towards Trustworthy Amortized Bayesian Inference with Deep Learning
- Advisors: Prof. Dr. Paul-Christian Bürkner (TU Dortmund), Prof. Dr. Andreas Bulling (University of Stuttgart)
- ELLIS PhD student, research visit at Aalto University, Finland, hosted by Prof. Dr. Aki Vehtari, 03/2024–08/2024

2020 – 2022 **MSc, Data and Computer Science**
Heidelberg University, Germany
- Grade 1.0 / 4.0 (A+; best: 1.0)
- Master thesis: Visualization of Distribution and Uncertainty of Posterior Model Probabilities

2018 – 2021 **MSc, Psychology**
Heidelberg University, Germany
- Grade 1.0 / 4.0 (A+; best: 1.0)
- Master thesis: Model Misspecification in Bayesian Parameter Estimation Tasks with Invertible Neural Networks

2014 – 2018 **BSc, Psychology**
Heidelberg University, Germany
- Grade 1.2 / 4.0 (A; best: 1.0)
- Bachelor thesis: Influence of Suggestive Questions on Usability Tests

Experience

since 12/2021 **PhD Researcher**
Cluster of Excellence SimTech, University of Stuttgart, Germany
- Authored 10 publications within 2 years, thereof 8 as first author and 3 preprints (detailed list below).
- Delivered 10 research talks and 5 poster presentations at international machine learning venues
- Defined, implemented, and evaluated machine learning algorithms for robust simulation-based inference
- Shaped the lab's research agenda by initiating 3 collaborations with labs in Germany, Finland, and the U.S.
- Supported budgeting third-party funding across 3 years (travel and student assistant funds)
- Contributed to securing 353 000 EUR of competitive third-party funding for a research software engineering project
- Supervised 4 graduate student assistants and 1 Master's project, managed recruiting process with 20+ applicants

since 12/2021 **Open Source Developer**
BayesFlow package for amortized Bayesian workflows in Python
- Developed an open-source Python package for amortized Bayesian workflows with generative neural networks
- Advanced publicity for the library, as evidenced by a 14x increase in GitHub stars and 3 535 downloads on PyPI
- Designed a testing infrastructure with pytest, automated package documentation with sphinx, and CI/CD pipeline

2017 – 2019 **Network Officer**
Marsilius-Kolleg Center for Advanced Study, Heidelberg University, Germany
- Supported outreach and public relations of state-of-the-art research at Heidelberg University
- Assisted in preparing and conducting interdisciplinary scientific symposia
- Maintained the website and digital knowledge base in Imperia CMS with HTML, CSS, PHP, and JavaScript

2018 **Research Intern**
Quantitative Research Methods in Psychology, Heidelberg University, Germany
- Developed an algorithm to derive expectation measures from eye-tracking data
- Implemented machine learning methods to improve eye-tracking based usability research

Honors & Awards

2024 **Mobility grant (3 000 EUR),** European Lighthouse on Secure and Safe AI (ELSA; EU Horizon)
2023 **Mobility grant (5 000 EUR),** European Network of Excellence Centers (ELISE; EU Horizon)
since 2023 **Associated IMPRS-IS student,** International Max Planck Research School for Intelligent Systems, Germany
2023 **Academic research grant (1 000 EUR),** Google Cloud Program
2023 **Best paper honorable mention,** German Conference on Pattern Recognition
2019 – 2021 **Scholarship holder (Studienstiftung),** German Academic Scholarship Foundation
2018 **Teaching certificate,** Heidelberg University
2014 **Award for remarkable social commitment,** Auguste-Viktoria-Gymnasium, Trier, Germany

Teaching

Taught statistical inference and probability theory to 800+ undergrad, grad, and PhD students across 4 lectures, 4 seminars, 6 exercises, and 7 tutorials (each of which for 90-120 minutes per week over 12 weeks), 4 days of workshops, 140+ exams. Received excellent teaching evaluation with an average score of 1.5, median of 1.0 (lower is better, best: 1.0).

Winter 2023	**Exercise (TA),** Applied Bayesian Data Analysis at TU Dortmund University
Winter 2023	**Workshop (Independent),** Scientific Python for PhD researchers at RTG Statistical Modeling in Psychology
Summer 2022	**Workshop (Independent),** Bayesian statistics with R and brms for PhD researchers at FGME conference, Konstanz
Summer 2022	**Lecture & Exercise (Independent),** Statistical Inference at Fresenius UAS, Heidelberg
Summer 2022	**Exercise (TA),** Bayesian Statistics and Probabilistic Machine Learning at University of Stuttgart
Winter 2021/22	**Lecture & Exercise (Independent),** Statistical Inference at Fresenius UAS, Heidelberg
Winter 2021/22	**Seminar (Independent),** Introduction to Statistics with R for PhD researchers at Heidelberg University
Summer 2021	**Exercise (Independent),** Descriptive Statistics & Probability Theory at Fresenius UAS, Heidelberg
Summer 2021	**Lecture & Exercise (Independent),** Statistical Inference at Fresenius UAS, Heidelberg
Winter 2020/21	**Seminar (TA),** Statistics with R at Heidelberg University
Winter 2020/21	**Lecture & Exercise (Independent),** Statistical Inference at Fresenius UAS, Heidelberg
Summer 2020	**Seminar (TA),** Programming with R at Heidelberg University
2020	**Seminar (Co-Leader),** Communication Techniques at Fresenius UAS, Wiesbaden
2017	**Workshop (Co-Leader),** Group Coaching at Fresenius UAS, Frankfurt
2016–2019	**Exercise (Tutor),** Descriptive Statistics, Probability Theory & Statistical Inference at Heidelberg University

Selected Involvement

since 2022	**Reviewer,** ICML (2022), AISTATS (2022, 2023), NeurIPS workshops (AABI2022, DGM4H2023, UniReps2023), PNAS
2023	**Member,** Society of SimTech, University of Stuttgart, Germany
2022	**Academic consultant in industry,** Axem Neurotechnology
2022	**Participant,** 1st SimTech summer school: Knowledge-driven machine learning and its applications
2016 – 2021	**Elected representative,** Examination board M.Sc. & Diploma Psychology (break 10/2016 – 09/2017)
2016 – 2021	**Elected representative,** Institute council (Fachrat) Psychology
2016 – 2020	**Member,** Student council (Fachschaft) Psychology

Talks and Presentations

2024	**Conference workshop (co-lead),** *Amortized Bayesian inference*, Bayes on the Beach, Australia
2024	**Talk (contributed),** *Towards reliable amortized Bayesian inference*, Bayes on the Beach, Australia
2023	**Research talk (invited),** *Jointly Amortized Bayesian Inference*, Machine and Human Intelligence group, University of Helsinki & Finnish Center for Artificial Intelligence (FCAI), Finland
2023	**Presentation,** *Leveraging Self-Consistency for Data-Efficient Amortized Bayesian Inference*, NeurIPS workshop for Unifying Representations in Neural Models (UniReps)
2023	**Oral,** *Detecting Model Misspecification in Amortized Bayesian Inference with Neural Networks*, German Conference on Pattern Recognition, Heidelberg, Germany, paper awarded with an honorable mention
2023	**Poster,** *Meta-Uncertainty in Bayesian Model Comparison*, SimTech, University of Stuttgart, Germany
2023	**Talk (contributed),** *Amortized Simulation-Based Inference: Tooling Session*, ELLIS Doctoral Symposium, Helsinki, Finland
2023	**Journal club moderator,** *Probabilistic Machine Learning*, ELLIS Doctoral Symposium, Helsinki, Finland
2023	**Poster,** *Meta-Uncertainty in Bayesian Model Comparison*, AISTATS 2023, Valencia, Spain
2023	**Talk (invited),** *Detecting Model Misspecification in Amortized Bayesian Inference with Neural Networks*, Bayes Comp conference, Levi, Finland
2023	**Poster,** *Detecting Model Misspecification in Amortized Bayesian Inference with Neural Networks*, Bayes Comp conference, Levi, Finland
2022	**Poster,** *Model Misspecification in Simulation-Based Inference*, ELLIS Unit Stuttgart, Germany
2022	**Talk (invited),** *What is AI?*, Writing workshop for AI short stories, Cyber Valley, Tübingen, Germany
2022	**Poster,** *Model Misspecification in Simulation-Based Inference*, SimTech, University of Stuttgart, Germany
2022	**Talk (invited),** *Where Does AI begin?*, Cyber Valley Office hours (general public audience), Tübingen, Germany
2022	**Talk (invited),** *Validating synthetic training data in probabilistic machine learning*, Blue Yonder Group Inc., Karlsruhe, Germany

Skills

Languages	German (native), English (fluent), French (basic), Latin (basic), Norwegian (basic)
Programming	Python, R, occasionally: C++, Java, JavaScript, HTML, CSS
Data Science	Python (Tensorflow/keras, PyTorch, sklearn, scipy, numpy, pandas, pytest), R (brms, lme4, afex, tidyverse), Stan
Visualization	Python (matplotlib, seaborn), R (ggplot2, plotly, rgl, shiny, gganimate), OpenGL
Documentation	LaTeX (KOMA, tikZ), git, Imperia, Markdown, RMarkdown, Jupyter, sphinx, roxygen, Quarto

Publications

* indicates equal contribution. The full publication list is also available via Google Scholar (link).

Selected Publications

[1] **Schmitt, M.**, Bürkner, P.-C., Köthe, U., and Radev, S. T. (2024). *Detecting Model Misspecification in Amortized Bayesian Inference with Neural Networks*, pp. 541–557. Springer Nature Switzerland. preprint published in December 2021, awarded with best paper honorable mention at GCPR 2023

Relevance: Back in 2021, this paper's preprint was the first work to recognize the importance of model misspecification for neural amortized Bayesian inference and propose a robust detection criterion for potentially unfaithful inference. This paper was awarded the Best Paper Honorable Mention at the German Conference on Pattern Recognition (GCPR) 2023.

[2] Radev*, S. T., **Schmitt*, M.**, Schumacher, L., Elsemüller, L., Pratz, V., Schälte, Y., Köthe, U., and Bürkner, P.-C. (2023). BayesFlow: Amortized Bayesian workflows with neural networks. *Journal of Open Source Software*, 8(89):5702

Relevance: All new amortized Bayesian inference methods of our lab are implemented in our open source library BayesFlow (www.bayesflow.org). The library is modular and adheres to contemporary software engineering best practices to ensure highest quality for users.

[3] **Schmitt, M.**, Radev, S. T., and Bürkner, P.-C. (2023). Meta-Uncertainty in Bayesian Model Comparison. In *Proceedings of The 26th International Conference on Artificial Intelligence and Statistics (AISTATS)*, volume 206 of *PMLR*, pp. 11–29

Relevance: Meta-uncertainty is a novel framework to combine Bayesian and frequentist notions of uncertainty with connections to overconfidence and reproducibility. Due to its high computational cost, the framework significantly benefits from amortized Bayesian methods for practicality.

[4] **Schmitt, M.**, Ivanova, D. R., Habermann, D., Koethe, U., Bürkner, P.-C., and Radev, S. T., (2023). Leveraging self-consistency for data-efficient amortized Bayesian inference. Previously published as an extended abstact in NeurIPS UniReps: the First Workshop on Unifying Representations in Neural Models

Relevance: In applied modeling scenarios, researchers often only have access to small amounts of data. This might impede the performance of machine learning algorithms that typically require lots of training data. This paper proposes a method to make amortized Bayesian inference more data-efficient by leveraging symmetries in the probabilistic joint model of data and parameters.

[5] Radev, S. T., **Schmitt, M.**, Pratz, V., Picchini, U., Köthe, U., and Bürkner, P.-C. (2023). JANA: Jointly Amortized Neural Approximation of Complex Bayesian Models. In Evans, R. J. and Shpitser, I. (eds.), *Proceedings of the 39th Conference on Uncertainty in Artificial Intelligence*, volume 216 of *Proceedings of Machine Learning Research*, pp. 1695–1706. PMLR

Relevance: This paper combines neural posterior and likelihood approximation, enabling amortized marginal likelihood and posterior predictive estimation. This is relevant for model evaluations and applied downstream tasks in the Bayesian workflow. This paper was selected for a spotlight at the Conference on Uncertainty in Artificial Intelligence (UAI) 2023.

All Publications

[1] **Schmitt*, M.**, Ewendt*, F., Kluttig, A., Mikolajczyk, R., Kraus, F. B., Wätjen, W., Bürkner, P.-C., Stangl, G. I., and Föller, M. (2024). Smoking is associated with increased eryptosis, suicidal erythrocyte death, in a large population-based cohort. *Nature Scientific Reports*, 14(1)

[2] **Schmitt*, M.**, Pratz*, V., Köthe, U., Bürkner, P.-C., and Radev, S. T., (2023). Consistency models for scalable and fast simulation-based inference. arXiv:2312.05440

[3] **Schmitt, M.**, Radev, S. T., and Bürkner, P.-C., (2023). Fuse it or lose it: Deep fusion for multimodal simulation-based inference. arXiv:2311.10671

[4] Elsemüller, L., Olischläger, H., **Schmitt, M.**, Bürkner, P.-C., Köthe, U., and Radev, S. T., (2023). Sensitivity-aware amortized Bayesian inference. arXiv:2310.11122

[5] **Schmitt, M.**, Ivanova, D. R., Habermann, D., Koethe, U., Bürkner, P.-C., and Radev, S. T., (2023). Leveraging self-consistency for data-efficient amortized Bayesian inference. Previously published as an extended abstact in NeurIPS UniReps: the First Workshop on Unifying Representations in Neural Models

[6] **Schmitt, M.**, Bürkner, P.-C., Köthe, U., and Radev, S. T. (2024). *Detecting Model Misspecification in Amortized Bayesian Inference with Neural Networks*, pp. 541–557. Springer Nature Switzerland. preprint published in December 2021, awarded with best paper honorable mention at GCPR 2023

[7] Radev*, S. T., **Schmitt*, M.**, Schumacher, L., Elsemüller, L., Pratz, V., Schälte, Y., Köthe, U., and Bürkner, P.-C. (2023). BayesFlow: Amortized Bayesian workflows with neural networks. *Journal of Open Source Software*, 8(89):5702

[8] Radev, S. T., **Schmitt, M.**, Pratz, V., Picchini, U., Köthe, U., and Bürkner, P.-C. (2023). JANA: Jointly Amortized Neural Approximation of Complex Bayesian Models. In Evans, R. J. and Shpitser, I. (eds.), *Proceedings of the 39th Conference on Uncertainty in Artificial Intelligence*, volume 216 of *Proceedings of Machine Learning Research*, pp. 1695–1706. PMLR

[9] **Schmitt, M.**, Radev, S. T., and Bürkner, P.-C. (2023). Meta-Uncertainty in Bayesian Model Comparison. In *Proceedings of The 26th International Conference on Artificial Intelligence and Statistics (AISTATS)*, volume 206 of *PMLR*, pp. 11–29

[10] Ewendt*, F., **Schmitt*, M.**, Kluttig, A., Kühn, J., Hirche, F., Kraus, F. B., Ludwig-Kraus, B., Mikolajczyk, R., Wätjen, W., Bürkner, P.-C., Föller§, M., and Stangl§, G. I. (2023). Association between vitamin D status and eryptosis – results from the German National Cohort Study. *Annals of Hematology*