

# Marvin Schmitt

MACHINE LEARNING SCIENTIST · ELLIS PHD STUDENT

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## 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 program, co-advised by Prof. Dr. Aki Vehtari (Aalto University, Finland)
- Expected graduation: 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 9 publications within 24 months, thereof 7 as first author and 3 preprints (detailed list below).
- Delivered 9 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 Finland and the U.S.
- Supported budgeting Cyber Valley 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 student**, International Max Planck Research School for Intelligent Systems (IMPRS-IS), 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**, German Academic Scholarship Foundation (Studienstiftung d. dt. Volkes)

2018

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

## SELECTED INVOLVEMENT

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

## TALKS AND PRESENTATIONS

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

## SKILLS

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

## SELECTED PUBLICATIONS

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- [1] **Schmitt, M.**, Habermann, D., Bürkner, P.-C., Koethe, U., and Radev, S. T. (2023). Leveraging self-consistency for data-efficient amortized Bayesian inference. In *NeurIPS UniReps: the First Workshop on Unifying Representations in Neural Models*
- [2] **Schmitt, M.**, Bürkner, P.-C., Köthe, U., and Radev, S. T. (2023). Detecting Model Misspecification in Amortized Bayesian Inference with Neural Networks. *45th German Conference on Pattern Recognition (GCPR)*. Awarded with a best paper honorable mention
- [3] 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
- [4] 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
- [5] **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

## ALL PUBLICATIONS

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

- [1] **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
- [2] **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
- [3] Elsemüller, L., Olischläger, H., **Schmitt, M.**, Bürkner, P.-C., Köthe, U., and Radev, S. T., (2023). Sensitivity-aware amortized Bayesian inference. arXiv:2310.11122
- [4] **Schmitt, M.**, Habermann, D., Bürkner, P.-C., Koethe, U., and Radev, S. T. (2023). Leveraging self-consistency for data-efficient amortized Bayesian inference. In *NeurIPS UniReps: the First Workshop on Unifying Representations in Neural Models*
- [5] **Schmitt, M.**, Bürkner, P.-C., Köthe, U., and Radev, S. T. (2023). Detecting Model Misspecification in Amortized Bayesian Inference with Neural Networks. *45th German Conference on Pattern Recognition (GCPR)*. Awarded with a best paper honorable mention
- [6] 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
- [7] 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
- [8] **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
- [9] Ewendt\*, F., **Schmitt\*, M.**, Kluttig, A., Kühn, J., Hirche, F., Kraus, F. B., Ludwig-Kraus, B., Mikolajczyk, R., Wätjen, W., Bürkner, P.-C., Föller<sup>§</sup>, M., and Stangl<sup>§</sup>, G. I. (2023). Association between vitamin D status and eryptosis – results from the German National Cohort Study. *Annals of Hematology*