# Marvin Schmitt

MACHINE LEARNING SCIENTIST · FLLIS PHD STUDENT

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# EDUCATION

# since 12/2021

# **PhD**, Computer 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.
- $\bullet \ \ Supported \ budgeting \ a \ total \ of \ 242\ 000\ EUR\ Cyber\ Valley\ funding\ across\ 3\ years\ (travel\ and\ student\ assistant\ funds)$
- $\bullet \ \ Contributed to securing 353\,000\,EUR\,of competitive third-party funding for a research software engineering project$
- 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
- $\bullet \ \ \text{Designed a testing infrastructure with pytest, automated package documentation with sphinx, and CI/CD pipeline}$

# 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

2014

#### **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

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	<b>Exercise (Tutor),</b> Descriptive Statistics, Probability Theory & Statistical Inference at Heidelberg University

# Advised Students

since 12/2023	<b>Pritom Gogoi,</b> Research assistant (MSc), University of Stuttgart, Germany
since 12/2023	Leona Odole, Research assistant (MSc), TU Dortmund University, Germany
since 09/2023	Adya Maheshwari, Research assistant (MSc), TU Dortmund University, Germany
since 05/2023	Yuga Hikida, Research assistant (MSc), TU Dortmund University, Germany
08/2022 - 04/2023	Rebecca Kohlhaas, Student project (MSc), University of Stuttgart, Germany

# Selected Involvement

since 2022	<b>Reviewer,</b> ICML (2022), AISTATS (2022, 2023), NeurIPS workshops (AABI2022, DGM4H2023, UniReps2023)
2023	Member, Society of SimTech, University of Stuttgart, Germany
2022	Academic Consultant, Axem Neurotechnology
2022	<b>Participant,</b> 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 \_\_\_\_\_

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> Leveraging Self-Consistency for Data-Efficient Amortized Bayesian Inference, NeurIPS workshop for Unifying Representations in Neural Models (UniReps), New Orleans, US
2023	<b>Oral,</b> 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, 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	<b>Talk (invited),</b> Detecting Model Misspecification in Amortized Bayesian Inference with Neural Networks, Bayes Comp conference, Levi, Finland
2023	<b>Poster,</b> 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 Al?, 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 Al begin?, Cyber Valley Office hours (general public audience), Tübingen, Germany
2022	<b>Talk (invited),</b> 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

# SELECTED PUBLICATIONS

[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

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§, M., and Stangl§, G. I. (2023). Association between vitamin D status and eryptosis results from the German National Cohort Study. *Annals of Hematology*