Nathanael Bosch

☐ nathanael.bosch@protonmail.com
☐ nathanaelbosch.github.io
☐ nathanaelbosch

Research Interests

Probabilistic machine learning *for* and *with* **dynamical systems:** state-space models and differential equations, Bayesian filtering and smoothing, scientific machine learning, probabilistic numerics. Gaussian processes, control.

Professional Experience

École polytechnique fédérale de Lausanne (EPFL)

Lausanne, Switzerland

Postdoctoral Researcher

2025/10 - today

Supervised by Michael Herbst, in the Mathematics for Materials Modelling group.

Gradient-accelerated Bayesian optimization for inverse materials design.

Amazon Web Services

Berlin, Germany

Applied Scientist Intern

2024/08 - 2025/01

Automatic machine learning for time series forecasting. With Oleksandr Shchur and Caner Türkmen.

University of Tübingen

Tübingen, Germany

Research Assistant

2020/05 - 2024/06

Supervised by Philipp Hennig, in the Methods of Machine Learning group.

Researching and developing probabilistic numerical solvers for differential equations.

Max Planck Institute for Intelligent Systems, Embodied Vision Group

Tübingen, Germany

Student Assistant 2019/03 - 2019/10 Master's thesis project on "Learning Gaussian Process Dynamics Models from Visual Observations for Control".

Supervised by Jörg Stückler.

Horváth&Partners Munich, Germany

Data Science Intern

2016/05 - 2016/07

Basket analysis of a large quantity of real-world retail sales data. Methods and results were published as part of a german business analytics book ("Strategische Unternehmensführung mit Advanced Analytics").

Education

University of Tübingen

Tübingen, Germany

Ph.D. Computer Science

2020/05 - 2025/02

International Max Planck Research School for Intelligent Systems (IMPRS-IS)

Passed Magna Cum Laude (with great distinction).

Doctoral thesis: "A Flexible and Efficient Framework for Probabilistic Numerical Simulation and Inference".

Advisor: Philipp Hennig.

Technical University of Munich

Munich, Germany

M.Sc. Data Engineering and Analytics

2018/04 - 2019/10

Passed with Distinction. German Grade 1.3, American GPA 3.7

Master thesis: "Learning Gaussian Process Dynamics Models from Visual Observations for Control".

Technical University of Munich

Munich, Germany

M.Sc. Mathematics

2016/10 - 2018/10

Passed with High Distinction. German Grade 1.2, American GPA 3.8. Master thesis: "Evolutionary Games for Global Function Minimization".

Technical University of Munich

Munich, Germany

B.Sc. Mathematics

2012/10 - 2016/06

Passed with Distinction. German Grade 1.8, American GPA 3.2.

Bachelor thesis: "Different Noise Models in Variable Density Compressed Sensing".

Landesgymnasium für Hochbegabte

Schwäbisch Gmünd, Germany

Abitur German Grade 1.4, American GPA 3.6. 2007/09 - 2012/06

Publications

<u>NB</u>, Oleksandr Shchur, Nick Erickson, Michael Bohlke-Schneider, and Ali Caner Turkmen. "Multi-layer Stack Ensembles for Time Series Forecasting". International Conference on Automated Machine Learning, **AutoML**, 2025.

Ori Press et al. "AlgoTune: Can Language Models Speed Up General-Purpose Numerical Programs?" Conference on Neural Information Processing Systems, **NeurIPS**, 2025.

Dingling Yao, Filip Tronarp, and <u>NB</u>. "Propagating Model Uncertainty through Filtering-based Probabilistic Numerical ODE Solvers". International Conference on Probabilistic Numerics, **ProbNum**, 2025.

Jonas Beck, <u>NB</u>, Michael Deistler, Kyra L. Kadhim, Jakob H. Macke, Philipp Hennig, and Philipp Berens. "Diffusion Tempering Improves Parameter Estimation with Probabilistic Integrators for Ordinary Differential Equations". International Conference on Machine Learning, **ICML**, 2024.

Amon Lahr, Filip Tronarp, <u>NB</u>, Jonathan Schmidt, Philipp Hennig, and Melanie N. Zeilinger. "Probabilistic ODE Solvers for Integration Error-aware Numerical Optimal Control". Learning for Dynamics & Control Conference, **L4DC**, 2024.

<u>NB</u>. "ProbNumDiffEq.jl: Probabilistic Numerical Solvers for Ordinary Differential Equations in Julia". Journal of Open Source Software, **JOSS**, 2024.

NB, Adrien Corenflos, Fatemeh Yaghoobi, Filip Tronarp, Philipp Hennig, and Simo Särkkä. "Parallel-in-Time Probabilistic Numerical ODE Solvers". Journal of Machine Learning Research, JMLR, 2024.

<u>NB</u>, Philipp Hennig, and Filip Tronarp. "Probabilistic Exponential Integrators". Conference on Neural Information Processing Systems, **NeurIPS**, 2023.

Nicholas Krämer*, <u>NB*</u>, Jonathan Schmidt*, and Philipp Hennig. "Probabilistic ODE Solutions in Millions of Dimensions". International Conference on Machine Learning, **ICML**, 2022.

NB, Filip Tronarp, and Philipp Hennig. "Pick-and-Mix Information Operators for Probabilistic ODE Solvers". International Conference on Artificial Intelligence and Statistics, **AISTATS**, 2022.

Filip Tronarp*, <u>NB*</u>, and Philipp Hennig. "Fenrir: Physics-Enhanced Regression for Initial Value Problems". International Conference on Machine Learning, **ICML**, 2022.

<u>NB</u>, Philipp Hennig, and Filip Tronarp. "Calibrated Adaptive Probabilistic ODE Solvers". International Conference on Artificial Intelligence and Statistics, **AISTATS**, 2021.

<u>NB*</u>, Jan Achterhold*, Laura Leal-Taixé, and Jörg Stückler. "Planning from Images with Deep Latent Gaussian Process Dynamics". Learning for Dynamics & Control Conference, **L4DC**, 2020.

Preprints

Joanna Sliwa, Frank Schneider, <u>NB</u>, Agustinus Kristiadi, and Philipp Hennig. "Efficient Weight-Space Laplace-Gaussian Filtering and Smoothing for Sequential Deep Learning". arXiv, 2024.

Software

ProbNumDiffEq.jl

Maintainer

Probabilistic Numerical Differential Equation solvers via Bayesian filtering and smoothing in Julia; compatible with the popular Differential Equations.jl / SciML ecosystem. Package presented at the JuliaCon 2024 in Eindhoven.

TuePlots.jl

Maintainer

A light-weight library to help create better plots for scientific publications, by taking care of the annoying bits like figure size, font size, and setting the correct font, with minimal overhead.

^{*} indicates equal contribution.

Teaching Experience

University of Tübingen

Tübingen, Germany

Teaching assistant / Co-lecturer: "Probabilistic Machine Learning"

Course mainly taught by Philipp Hennig. In addition to the regular teaching assistant duties, I gave one full M.Sc.-level lecture on "Hidden Markov Models".

University of Tübingen

Tübingen, Germany

Co-lecturer: "Numerics of Machine Learning"

2022 / 2023

Gave two full M.Sc.-level lectures on "Ordinary Differential Equations" and "Probabilistic Numerical ODE Solvers", as part of a course taught by Philipp Hennig and multiple other PhD students from the Methods of Machine Learning group. This also included preparing and grading homework assignments.

Uppsala University

Uppsala, Sweden

Guest lecturer: "Probabilistic Numerics for Ordinary Differential Equations"

2021

Gave a single guest lecture as a part of a seminar on "A computational introduction to stochastic differential equations", organized and taught by Zheng Zhao.

University of Tübingen

Tübingen, Germany

Teaching assistant: "Data Literacy" Course taught by Philipp Hennig.

2021 / 2022

University of Tübingen

Seminar: "Machine learning for and with dynamical systems"

Tübingen, Germany

Jointly organized with Nicholas Krämer and Philipp Hennig.

University of Tübingen

Tübingen, Germany

Teaching assistant: "Time Series" Course taught by Filip Tronarp.

2020 / 2021

Technical University of Munich

Munich, Germany

Teaching assistant: "Principles of Mathematics 2"

Mathematics course, aimed at B.Sc. Engineering Science students.

abiturma GbR Course instructor Munich and Stuttgart, Germany

Intensive five-day preparation course for the german Abitur in mathematics.

2016 & 2017

Supervision

Fabrice van der Lehr, Master's thesis

2024

"Bayesian Filtering for Black Box Simulators"; co-supervised with Tobias Weber.

Sofiya Garkot, Essay rotation

2023 / 2024

"Exploring Probabilistic Solvers for Hodgkin-Huxley Models"; co-supervised with Jonas Beck.

Thomas Albrecht, Master's thesis

2021 / 2022

"Bayesian Physics-Informed Neural Networks via Laplace Approximations".

Felix Böhm, Bachelor's thesis

2021 / 2022

"Inferring ODE Parametric Latent Forces via Neural ODEs".

Dingling Yao, Master's thesis

"Uncertainty Propagation in Probabilistic Ordinary Differential Equation Solvers"; co-supervised with Filip Tronarp.

Joanna Sliwa, Essay rotation

2021

"Physics-Informed Neural Networks"; co-supervised with Nicholas Krämer.

Invited talks

Probabilistic Numerics Workshop (ProbNum24)

London, United Kingdom

Talk: "Robust Parameter Inference in ODEs via Physics-Enhanced Gaussian Process Regression" 2024/07

Probabilistic Numerics Spring School

Southampton, United Kingdom

Practical session: "Probabilistic Numerics for ODEs"

2024/04

International Conference on Scientific Computing and Machine Learning

Talk: "Probabilistic Numerical Solvers for Differential Equations"

Kyoto, Japan

2024/03

SIAM Conference on Uncertainty Quantification

Talk: "Probabilistic Numerics for Ordinary Differential Equations"

Trieste, Italy 2024/02

Statistics PhD seminar, University of Edinburgh

Talk: "Probabilistic Numerics for Ordinary Differential Equations"

Edinburgh, United Kingdom (virtual) 2023/05

Probabilistic Numerics Spring School

Practical session: "Probabilistic Numerics for ODEs"

Tübingen, Germany 2023/03

Institute for Dynamic Systems and Control, ETH Zurich

Talk: "ODE Solvers as Gauss-Markov Regression"

2023/01

Zurich, Switzerland

Sensor informatics and medical technology group, Aalto University

Talk: "Solving Differential Equations with Bayesian Filtering and Smoothing"

Aalto, Finnland 2022/05

Dagstuhl Seminar on Probabilistic Numerical Methods

Talk: "ProbNumDiffEq.jl: Fast and Practical ODE Filters in Julia"

Wadern, Germany

Review services

International Conference on Machine Learning (ICML)

2022, 2023, 2024

Conference on Neural Information Processing Systems (NeurIPS)

2021, 2022, 2023

International Conference on Artificial Intelligence and Statistics (AISTATS)
Transactions on Machine Learning Research (TMLR)

2021, 2022, 2023, 2024 2022 – 2023

International Conference on Probabilistic Numerics (ProbNum)

2025

Al4DifferentialEquations in Science (ICLR workshop)

2024

Technical skills

Working knowledge: Julia, Python, jax, NumPy/SciPy, PyTorch, git/GitHub, LATEX, Unix, GNU Emacs.

Basic knowledge: C/C++, SLURM, MATLAB, R, SQL.

Language skills

German: Native speaker French: Near native English: Fluent

Spanish: Good working knowledge **Russian**: Basic communication skills

Scholarships

Leadership Talent Academy

2025

Selected participant in the University of Tübingen's Leadership Talent Academy, a 3-month program of intensive weekend modules and coaching sessions focused on developing leadership skills and personal growth.

German Academic Scholarship Foundation

2013 - 2019

Recipient of the German Academic Scholarship Foundation, providing financial and academic support to selected students.

Siemens Mentoring Program

2017 - 2018

Selected participant in the Siemens Mentoring Program, pairing students with Siemens professionals for career development and mentorship.

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