

Yannik Schälte

Curriculum Vitae

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📅 1993-12-31



Experience

- 09.2021–present **Post-Doctoral Researcher and Team Leader**, *University of Bonn, Life & Medical Sciences Institute*, Bonn.
At the interface of machine learning and mathematical modeling. E.g. likelihood-free inference, high-dimensional optimization, non-linear mixed-effect modeling.
- 09.–10.2022 **Visiting Researcher**, *University of Oxford*, Oxford, United Kingdom.
Mathematical Institute. Multi-fidelity and neural likelihood-free inference.
- 07.–08.2022 **Visiting Researcher**, *MILA - Quebec Artificial Intelligence Institute*, Montréal, Canada.
Generative modeling in Systems Biology.
- 08.2017–09.2021 **PhD Candidate**, *Helmholtz Center Munich*, Munich.
Institute of Computational Biology. Development of statistical inference methods for deterministic and stochastic models of complex biochemical systems. Software development.
- 04.–08.2017 **Teaching Assistant**, *University of Bielefeld*, Bielefeld.
Analysis tutor.
- 02.–03.2017 **Software Development Intern**, *Diamant Software*, Bielefeld.
Using Microsoft SQL Server Reporting Services for an accounting solution via C# and OData REST services.
- 06.–08.2012 **Technology Consulting Intern**, *Itelligence*, Bielefeld.
Department for technology consulting. Development of tutorials; creation of a Java web interface and a logging framework.
- 01.2010 **Banking Intern**, *Commerzbank*, Bielefeld.
Private customer service.

Education

- 2017–2021 **PhD in Mathematics**, *Technical University of Munich*, Grade: *Summa cum laude*.
Computational Biology. Thesis: *Efficient accurate and robust statistical inference for deterministic and stochastic models of biochemical systems*, with Prof. Jan Hasenauer.
- 2015–2017 **MSc in Mathematics**, *University of Bielefeld*, Grade: *1.0 (A+ with distinction)*.
Exchange semester at University of Stockholm and Royal Technical University of Stockholm. Thesis: *Connections between Random Matrices, Branching Random Walks and the Riemann Zeta Function with special emphasis on Maximum Statistics*, with Prof. Holger Kösters.
- 2012–2015 **BSc in Mathematics**, *University of Bielefeld*, Grade: *1.1 (A+ with distinction)*.
Minor in Computer Sciences. Thesis: *Elliptic Functions*, with Prof. Michael Spieß.

2004–2012 **Abitur**, *Gymnasium Heepen*, Bielefeld, Grade: 1.0 (A+ with distinction).
Bilingual English-German.

Awards and Scholarships

- 2022 **Add-On Fellowship for Interdisciplinary Life Science**, *Joachim Herz Stiftung*.
- 2020 **Ian Lawson Van Toch Memorial Award for Outstanding Student Paper**, *ISMB conference, Montréal, Canada*.
- 2020 **Prize for best social event organizer**, *Helmholtz Center Munich, Institute of Computational Biology* :).
- 2020 **DAAD travel scholarship**.
- 2016–2017 **Erasmus+ exchange scholarship**.
- 2017 **Award for the best MSc Mathematics degree**, *University of Bielefeld*.
- 2015 **Award for the best BSc Mathematics degree**, *University of Bielefeld*.
- 2013, 2014, **Studienfonds OWL excellence scholarship**.
- 2016 In cooperation with Diamant Software, Gauselmann, and the Zierold Foundation.
- 2012 **Abitur awards**.
For Physics (DPG) and Mathematics (DMV), e-follows scholarship, and Dr.-Wilhelm-Döpelheuer award for the best Abitur at Gymnasium Heepen.

Skills

Languages

- Native German
- Professional English (C1, Cambridge CAE, or C2, DAAD)
- Basic Swedish (A2), French, Spanish (B1), Latin (Latinum)

Computer skills

- Advanced Python
- Basic \LaTeX , R, Matlab, Web, Java, Android, HPC

Certifications

- 2022 **Deep Learning Specialization**, *Coursera / DeepLearning.AI*.
Neural Networks and Deep Learning; Hyperparameter Tuning, Regularization and Optimization; Structuring Machine Learning Projects; Convolutional Neural Networks; Sequence Models. Credential ID: AF2QMAR8WD3A
- 2019 **Zertifikat Hochschullehre der Bayerischen Universitäten**, *Technical University of Munich*.
Certificate University Teaching of the Bavarian Universities

Volunteering

- 2018–2021 **Campaign Coordinator**, *Stadtradeln*.
Organization of the participation of the Helmholtz Center Munich at the campaign “Stadtradeln” (<https://city-cycling.org>), to promote environment-friendly and healthy mobility by bike. 05.-06.2018, 07.2019, 10.2020, 06.2021.

- 03.–08.2017 **Refugee Teacher**, *Hotspot Heepen*.
Extra tuition for refugee children. Mainly German, Physics and Mathematics (primary and grammar school level).
- 2014–2015 **Ministry Service Organizer**, *Catholic Church Bielefeld East*.
Organization of mass service, events and excursions; development of a Church Service Scheduler used in dozens of parishes in Germany, Austria and Switzerland (<https://yannikschaelte.github.io/MiniPlaner>).

Selected Presentations

- 01.2021 **Invited lecture: *Parameter inference in Computational Biology***, *Open-SourceEconomics Scientific Computing Seminar*, Bonn, Germany.
- 11.2020 **Invited talk: *pyABC: Statistical inference without a likelihood?***, *Open-SourceEconomics Meetup*, Bonn, Germany.
- 07.2020 **Conference talk: *Efficient Exact Inference for Dynamical Systems with Noisy Measurements using Sequential Approximate Bayesian Computation***, *ISMB Conference*, Montréal, Canada.
- 05.2019 **Conference talk: *(py)ABC: it's easy***, *New Vistas Conference*, Vigo, Spain.
- 10.2018 **Invited lecture: *Approximate Bayesian Computation for Parameter Estimation of Complex Stochastic Models***, *CRM SNS Workshop*, Pisa, Italy.
- 08.2018 **Conference talk: *Evaluation of Derivative-Free Optimizers for Parameter Estimation in Systems Biology***, *FOSBE Conference*, Chicago, USA.
- 07.2018 **Conference talk: *pyABC - A framework for distributed likelihood-free inference***, *SBMC Conference*, Bremen, Germany.

Teaching and Supervision

Teaching

- 2022 **Graduate seminar *Bridging the Gap Between Mathematical Modeling and Machine Learning***, *University of Bonn*, Lecturer.
- 2022 **Graduate seminar *Statistical Learning for Biomedical Data Analysis***, *University of Bonn*, Lecturer.
- 2019 **Lecture *Statistical Inference for Dynamical Systems***, *Technical University of Munich*, Lecturer and tutor.
- 2017 **Lecture *Analysis 1***, *University of Bielefeld*, Tutor.

Supervision

- 2022 **BSc thesis *Zijian Wang***, *University of Bonn*.
Title: *Missing data handling in invertible neural networks*.
- 2020 **MSc thesis *Felipe Reck***, *University of Bonn*.
Title: *Acceleration of ABC-SMC methods using improved parallelization and proposal generation*.
- 2019 **BSc thesis *Philipp Städter***, *Technical University of Munich*.
Title: *Assessment and Prediction of ODE Solver Performance for Biological Processes*.

2018 **MSc thesis Lukas Sandmeir**, *Technical University of Munich*.

Title: *Parameter Estimation for Rule-Based Models with Approximate Bayesian Computation*.

Publications

- [1] Zijian Wang, Jan Hasenauer*, and **Yannik Schälte***. “Missing data in amortized simulation-based neural posterior estimation”. In: *bioRxiv* (2023), pp. 2023–01.
- [2] Emad Alamoudi, Jörn Starruß, Nils Bundgaard, Robert Müller, Felipe Reck, Frederik Graw, Lutz Brusch, Jan Hasenauer, and **Yannik Schälte**. “Massively Parallel Likelihood-Free Parameter Inference for Biological Multi-Scale Systems”. In: vol. 51. Publication Series of the John von Neumann Institute for Computing (NIC). Jülich: Forschungszentrum Jülich GmbH Zentralbibliothek, Verlag, 2022, pp. 355–365.
- [3] **Yannik Schälte**. “Efficient accurate and robust statistical inference for deterministic and stochastic models of biochemical systems”. Dissertation. München: Technische Universität München, 2022.
- [4] **Yannik Schälte**, Emmanuel Klinger, Emad Alamoudi, and Jan Hasenauer. “pyABC: Efficient and robust easy-to-use approximate Bayesian computation”. In: *arXiv preprint arXiv:2203.13043* (2022).
- [5] **Yannik Schälte** and Jan Hasenauer. “Informative and adaptive distances and summary statistics in sequential approximate Bayesian computation”. In: *bioRxiv* (2022).
- [6] Katja Radon, Abhishek Bakuli, Peter Pütz, Ronan Le Gleut, Jessica Michelle Guggenbuehl Noller, Laura Olbrich, Elmar Saathoff, Mercè Gari, **Yannik Schälte**, Turid Frahnöw, Roman Wölfel, Michael Pritsch, Camilla Rothe, Michel Pletschette, Raquel Rubio-Acero, Jessica Beyerl, Dafni Metaxa, Felix Forster, Verena Thiel, Noemi Castelletti, Friedrich Riess, Maximilian Diefenbach, Günther Fröschl, Jan Brugger, Simon Winter, Jonathan Frese, Kerstin Puchinger, Isabel Brand, Inge Kroidl, Andreas Wieser, Michael Hoelscher, Jan Hasenauer, and Christiane Fuchs. “From first to second wave: Follow-up of the prospective COVID-19 cohort (KoCo19) in Munich (Germany)”. In: *BMC infectious diseases* 21.1 (2021), pp. 1–15.
- [7] Simon Syga, Diana David-Rus, **Yannik Schälte**, Michael Meyer-Hermann, Haralampos Hatzikirou, and Andreas Deutsch. “Inferring the effect of interventions on COVID-19 transmission networks”. In: *Scientific reports* 11.1 (2021), pp. 1–11.
- [8] Fabian Fröhlich, Daniel Weindl, **Yannik Schälte**, Dilan Pathirana, Łukasz Paszkowski, Glenn Terje Lines, Paul Stapor, and Jan Hasenauer. “AMICI: High-performance sensitivity analysis for large ordinary differential equation models”. In: *Bioinformatics* 37.20 (2021), pp. 3676–3677.
- [9] Karina Durso-Cain, Peter Kumberger, **Yannik Schälte**, Theresa Fink, Harel Dahari, Jan Hasenauer, Susan L Uprichard, and Frederik Graw. “HCV spread kinetics reveal varying contributions of transmission modes to infection dynamics”. In: *Viruses* 13.7 (2021), p. 1308.
- [10] Jakob Vanhoefer, R Marta, Dilan Pathirana, **Yannik Schälte**, and Jan Hasenauer. “yaml2sbml: Human-readable and-writable specification of ODE models and their conversion to SBML”. In: *Journal of Open Source Software* 6.61 (2021), p. 3215.
- [11] Philipp Städter*, **Yannik Schälte***, Leonard Schmiester*, Jan Hasenauer, and Paul L Stapor. “Benchmarking of numerical integration methods for ODE models of biological systems”. In: *Scientific reports* 11.1 (2021), pp. 1–11.

- [12] Lorenzo Contento, Noemi Castelletti, Elba Raimundez, Ronan Le Gleut, **Yannik Schälte**, Paul Stapor, Ludwig Christian Hinske, Michael Hoelscher, Andreas Wieser, Katja Radon, Christiane Fuchs, and Jan Hasenauer. “Integrative modelling of reported case numbers and seroprevalence reveals time-dependent test efficiency and infection rates”. In: *medRxiv* (2021).
- [13] Laura Olbrich*, Noemi Castelletti*, **Yannik Schälte***, Mercè Gari*, Peter Pütz, Abhishek Bakuli, Michael Pritsch, Inge Kroidl, Elmar Saathoff, Jessica Michelle Guggenbuehl Noller, Volker Fingerle, Ronan Le Gleut, Leonard Gilberg, Isabel Brand, Philine Falk, Alisa Markgraf, Flora Deák, Friedrich Riess, Maximilian Diefenbach, Tabea Eser, Franz Weinauer, Silke Martin, Ernst-Markus Quenzel, Marc Becker, Jürgen Durner, Philipp Girtl, Katharina Müller, Katja Radon, Christiane Fuchs, Roman Wölfel, Jan Hasenauer, Michael Hoelscher, and Andreas Wieser. “Head-to-head evaluation of seven different seroassays including direct viral neutralisation in a representative cohort for SARS-CoV-2”. In: *Journal of General Virology* (2021).
- [14] **Yannik Schälte**, Emad Alamoudi, and Jan Hasenauer. “Robust adaptive distance functions for approximate Bayesian inference on outlier-corrupted data”. In: *bioRxiv* (2021).
- [15] Laura Olbrich*, Noemi Castelletti*, **Yannik Schälte***, Mercè Gari*, Peter Pütz, Abhishek Bakuli, Michael Pritsch, Inge Kroidl, Elmar Saathoff, Jessica Michelle Guggenbuehl Noller, Volker Fingerle, Ronan Le Gleut, Leonard Gilberg, Isabel Brand, Philine Falk, Alisa Markgraf, Flora Deák, Friedrich Riess, Maximilian Diefenbach, Tabea Eser, Franz Weinauer, Silke Martin, Ernst-Markus Quenzel, Marc Becker, Jürgen Durner, Philipp Girtl, Katharina Müller, Katja Radon, Christiane Fuchs, Roman Wölfel, Jan Hasenauer, Michael Hoelscher, and Andreas Wieser. “A Serology Strategy for Epidemiological Studies Based on the Comparison of the Performance of Seven Different Test Systems – The Representative COVID-19 Cohort Munich”. In: *medRxiv* (2021).
- [16] Leonard Schmiester*, **Yannik Schälte***, Frank T Bergmann, Tacio Camba, Erika Dudkin, Janine Egert, Fabian Fröhlich, Lara Fuhrmann, Adrian L Hauber, Svenja Kemmer, et al. “PEtab – Interoperable specification of parameter estimation problems in systems biology”. In: *PLoS computational biology* 17.1 (2021), e1008646.
- [17] Michael Pritsch, Katja Radon, Abhishek Bakuli, Ronan Le Gleut, Laura Olbrich, Jessica Michelle Guggenbuehl Noller, Elmar Saathoff, Noemi Castelletti, Mercè Gari, Peter Pütz, **Yannik Schälte**, Turid Frahnöw, Roman Wölfel, Camilla Rothe, Michel Pletschette, Dafni Metaxa, Felix Forster, Verena Thiel, Friedrich Riess, Maximilian Diefenbach, Günther Fröschl, Jan Brugger, Simon Winter, Jonathan Frese, Kerstin Puchinger, Isabel Brand, Inge Kroidl, Jan Hasenauer, Christiane Fuchs, Andreas Wieser, and Andreas Hoelscher. “Prevalence and Risk Factors of Infection in the Representative COVID-19 Cohort Munich”. In: *International journal of environmental research and public health* 18.7 (2021), p. 3572.
- [18] **Yannik Schälte** and Jan Hasenauer. “Efficient exact inference for dynamical systems with noisy measurements using sequential approximate Bayesian computation”. In: *Bioinformatics* 36.Supplement_1 (2020), pp. i551–i559.
- [19] Leonard Schmiester*, **Yannik Schälte***, Fabian Fröhlich, Jan Hasenauer, and Daniel Weindl. “Efficient parameterization of large-scale dynamic models based on relative measurements”. In: *Bioinformatics* 36.2 (2020), pp. 594–602.
- [20] **Yannik Schälte**, Paul Stapor, and Jan Hasenauer. “Evaluation of derivative-free optimizers for parameter estimation in systems biology”. In: *IFAC-PapersOnLine* 51.19 (2018), pp. 98–101.

(*equal contribution)