

DARIUS SCHAUB

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Objective

My goal is to contribute to the understanding of biological life and to solving the stabilization problem underlying medicine. This includes advancements in multi-modal representation learning and data-driven complex systems modeling and control. Moreover, I aim to use data-driven models to gain mechanistic insights that extend our current biomedical knowledge, while also effectively integrating existing knowledge into the modeling approach.

Education

University Medical Center Hamburg-Eppendorf, Center for Biomedical AI

Dec. 2022 – Present

Ph.D. student in the lab of Prof. Stefan Bonn

Hamburg, Germany

- Focus: data-driven modeling of cell-cell interactions for deciphering disease mechanisms

Harvard Medical School, Channing Division of Network Medicine

Feb. 2021 – Jun. 2023

Remote visiting student in the lab of Prof. Yang-Yu Liu

Boston, MA

- Focus: deep reinforcement learning, combinatorial optimization, graph neural networks, multi-omics integration, microbiome modeling
- Successful participation in the VDAART disease outcome prediction challenge hosted by the Channing Division of Network Medicine

University of Hamburg & Hamburg University of Technology

Oct. 2019 – Jun. 2022

Master of Science in Industrial Mathematics

Hamburg, Germany

- Grade 1.05 (passed with distinction)
- Relevant courses: partial differential equations, systems theory, mathematics of neural networks, machine learning, optimization
- Projects: mathematical data analysis on the approximate inverse for linear problems, "Project: Machine Learning" in image classification as team leader
- Thesis: *Solving the traveling salesman problem via deep reinforcement learning* (supervised by Prof. Yang-Yu Liu)

University of Hamburg

Oct. 2017 – Sep. 2019

Bachelor of Science in Nanoscience

Hamburg, Germany

- Grade 1.35 (excellent)
- Relevant courses: quantum/statistical/solid-state physics, optimization, numerical mathematics, statistics
- Thesis: *Ionization dynamics of H₂O - a Matrix Product State study* (supervised by Prof. Daniela Pfannkuche)

University of Hamburg

Oct. 2015 – Sep. 2017

Bachelor of Science in Chemistry

Hamburg, Germany

- Successfully attended 80% of the B.Sc. Chemistry curriculum, including courses in biochemistry and organic chemistry

Experience

SICK AG

Jan. 2020 – Nov. 2022

Data Science working student

Hamburg, Germany

- Achieved an 80% reduction in scheduled maintenances by predicting sensor contamination
- Developed and deployed a predictive maintenance and time-series forecasting framework for various sensor species (scikit-learn, unittest, TypeScript)
- Gained experience with rare event prediction, time series forecasting, anomaly detection, and software engineering best practices (CI/CD)

SICK AG

Oct. 2020 – Dec. 2020

Data Science intern

Hamburg, Germany

- Tested various machine learning algorithms for predicting device errors and maintenance events (scikit-learn)

- Supervised exercise classes for mathematical courses in the chemistry department

Publications

- [1] **Darius P Schaub**^{*}, Behnam Yousefi^{*}, Nico Kaiser, Robin Khatri, Victor G Puelles, Christian F Krebs, Ulf Panzer, Stefan Bonn, “PCA-based spatial domain identification with state-of-the-art performance,” *Bioinformatics*, vol. 41, no. 1, btaf005, Jan. 1, 2025, ISSN: 1367-4811. DOI: 10.1093/bioinformatics/btaf005. [Online]. Available: <https://doi.org/10.1093/bioinformatics/btaf005>.
- [2] Sina Abdollahi, **Darius P. Schaub**, Madalena Barroso, Nora C. Laubach, Wiebke Hutwelker, Ulf Panzer, Søren W. Gersting, Stefan Bonn, “A comprehensive comparison of deep learning-based compound-target interaction prediction models to unveil guiding design principles,” *Journal of Cheminformatics*, vol. 16, no. 1, p. 118, Oct. 28, 2024, ISSN: 1758-2946. DOI: 10.1186/s13321-024-00913-1. [Online]. Available: <https://doi.org/10.1186/s13321-024-00913-1>.
- [3] Jonas Engesser^{*}, Robin Khatri^{*}, **Darius P. Schaub**^{*}, Yu Zhao, Hans-Joachim Paust, Zeba Sultana, Nariaki Asada, Jan-Hendrik Riedel, Varshi Sivayoganathan, Anett Peters, Anna Kaffke, Saskia-Larissa Jauch-Speer, Thiago Goldbeck-Strieder, Victor G. Puelles, Ulrich O. Wenzel, Oliver M. Steinmetz, Elion Hoxha, Jan-Eric Turner, Hans-Willi Mittrücker, Thorsten Wiech, Tobias B. Huber, Stefan Bonn, Christian F. Krebs, Ulf Panzer, “Immune profiling-based targeting of pathogenic T cells with ustekinumab in ANCA-associated glomerulonephritis,” *Nature Communications*, vol. 15, no. 1, p. 8220, Sep. 19, 2024, ISSN: 2041-1723. DOI: 10.1038/s41467-024-52525-w. [Online]. Available: <https://www.nature.com/articles/s41467-024-52525-w>.
- [4] Zeba Sultana, Robin Khatri, Behnam Yousefi, Nikhat Shaikh, Saskia L. Jauch-Speer, **Darius P. Schaub**, Jonas Engesser, Malte Hellmig, Arthur L. Hube, Varshi Sivayoganathan, Alina Borchers, Anett Peters, Anna Kaffke, Hans-Joachim Paust, Thiago Goldbeck-Strieder, Ulrich O. Wenzel, Victor Puelles, Elion Hoxha, Thorsten Wiech, Tobias B. Huber, Ulf Panzer, Stefan Bonn, Christian F. Krebs, “Spatio-temporal interaction of immune and renal cells determines glomerular crescent formation in autoimmune kidney disease.” (Dec. 21, 2024), [Online]. Available: <http://biorxiv.org/lookup/doi/10.1101/2024.12.18.629206>, pre-published.
- [5] Xu-Wen Wang, Tong Wang, **Darius P. Schaub**, Can Chen, Zheng Sun, Shanlin Ke, Julian Hecker, Anna Maaser-Hecker, Oana A. Zeleznik, Roman Zeleznik, Augusto A. Litonjua, Dawn L. DeMeo, Jessica Lasky-Su, Edwin K. Silverman, Yang-Yu Liu, Scott T. Weiss, “Benchmarking omics-based prediction of asthma development in children,” *Respiratory Research*, vol. 24, no. 1, p. 63, Feb. 26, 2023, ISSN: 1465-993X. DOI: 10.1186/s12931-023-02368-8. [Online]. Available: <https://doi.org/10.1186/s12931-023-02368-8>.

Conferences, Hackathons, and Summer schools

scverse Hackathon, Paris, France

Mar. 2025

- Accelerated point filter implementation in the spatialdata package by several orders of magnitude

ESSB Conference, Berlin, Germany

Dec. 2024

- Discussed spatial domain identification methods and nomenclature

scverse Conference, Munich, Germany

Sep. 2024

- Presented a poster on the paper “PCA-based spatial domain identification with state-of-the-art performance”

Oxford Machine Learning Summer School, Oxford, UK

Jun. 2023

- Winner of the MLx Cases team challenge among 30 competing teams, with the task to classify histology images of breast carcinoma under limited data constraints (PyTorch)
- Learned about and gained hands-on experience with state-of-the-art deep learning approaches to various medical and biological problem settings both from ML and clinical experts (self-supervised learning, geometric deep learning, causal ML, bayesian deep learning)

Skills and interests

Languages/Frameworks: Python (professional), PyTorch (professional), TensorFlow (advanced), C/C++ (intermediate), TypeScript (basic), SQL (basic)

Technologies: Linux, Github, Gitlab, Docker, Kubernetes, Jira

Other interests: science-fiction, fitness, nutrition, dancing, politics, philosophy, learning

^{*}Equal contribution.