

Charlotte Bunne

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Academic Positions

EPFL School of Computer and Communication Sciences and School of Life Sciences TENURE-TRACK ASSISTANT PROFESSOR Group: Artificial Intelligence for Personalized Medicine	<i>Lausanne, Switzerland</i> starting fall 2024
Genentech and Stanford University POSTDOCTORAL RESEARCHER Advisors: Aviv Regev and Jure Leskovec	<i>San Francisco, USA</i> 2023 - 2024

Education

Eidgenössische Technische Hochschule (ETH) Zurich PHD IN COMPUTER SCIENCE • Doctoral Committee: Andreas Krause, Marco Cuturi, Lucas Pelkmans, and Jure Leskovec	<i>Zurich, Switzerland</i> 2019 - 2023
Massachusetts Institute of Technology (MIT) VISITING STUDENT IN COMPUTER SCIENCE • Advisors: Stefanie Jegelka and David Alvarez-Melis	<i>Cambridge, USA</i> 2018
Eidgenössische Technische Hochschule (ETH) Zurich M.S. IN COMPUTATIONAL BIOLOGY AND BIOINFORMATICS • ETH Medal for best thesis (awarded to top 2.5% of all ETH graduates) • Willi-Studer Prize for best GPA and graduated with distinction • Selected into the Excellence Scholarship & Opportunity Program (ESOP)	<i>Zurich, Switzerland</i> 2016 - 2019
Heidelberg University B.S. IN BIOSCIENCES • Major in Bioinformatics and graduated among top 2% of class • Selected as Fellow of the German Academic Scholarship Foundation (Studienstiftung d. dt. Volkes)	<i>Heidelberg, Germany</i> 2013 - 2016

Research and Work Experience

2022 - 2023	Broad Institute of MIT and Harvard , Graduate Researcher • Supervisors: Anne Carpenter and Shantanu Singh	Cambridge, USA
2022	Apple , Research Intern • Machine Learning Group of Samy Bengio and Marco Cuturi	Paris, France
2020	Google Research , Research Intern • Brain Team of Jean-Philippe Vert and Marco Cuturi	Zurich, Switzerland
2019 - now	ETH AI Center , Graduate Researcher • Supervisor: Andreas Krause	Zurich, Switzerland
2018	MIT CSAIL , Research Assistant • Supervisors: Stefanie Jegelka and David Alvarez-Melis	Cambridge, USA
2017 - 2018	IBM Research , Software Engineering Intern • Cognitive Computing and Industry Solutions Group of Maria Gabrani	Zurich, Switzerland
2015 - 2016	German Cancer Research Center (DKFZ) , Research Assistant • Supervisors: Roland Eils and Thomas Höfer	Heidelberg, Germany

Fellowships and Awards

SELECTED AWARDS

2022	Outstanding Reviewer Award , AISTATS Conference	
2021	Best Paper Award , ICML Time Series Workshop	<i>1/35 Papers</i>
2020	Best Paper Award , ICML Workshop on Graph Representation Learning & Beyond	<i>1/73 Papers</i>
2019	ETH Medal , ETH Zurich	<i>Top 2.5% of All ETH Graduates</i>

- Willi Studer Prize**, ETH Zurich
- 2018 **Best Paper Award**, NeurIPS Workshop on Relational Representation Learning
- 2014 **Grand Prize**, iGEM Competition
- 2012 **Grand Prize**, iGEM High School Competition

Best GPA of Cohort
1/52 Papers
1/245 Teams, 3 Special Prizes
1/40 Teams, 5 Special Prizes

SELECTED FELLOWSHIPS

- 2020 **Generation Google Scholarship**, Google
 Scholarship of 7000 \$ and recognition for PhD studies.
- 2018 **Master Thesis Grant**, Zeno Karl Schindler Foundation
 12,000 \$ awarded in support for my Master thesis.
- Fellowship for Graduate Studies Abroad**, Dr. Jürgen Ulderup Scholarship
 Academic scholarship in support for graduate studies abroad.
- 2016 - 2019 **Excellence Scholarship and Opportunity Award**, ETH Zurich
 Excellence scholarship of the ETH Foundation covering the full study and living costs, i.e., ~35,000 \$.
- 2016 - 2019 **Fellow of German Academic Scholarship Foundation**, Studienstiftung d. dt. Volkes
 Germany's *most prestigious* academic scholarship throughout my undergraduate and graduate studies.
- 2015 - 2017 **STEM Excellence Award**, Manfred Lautenschläger Stiftung
 Scholarship of 3000 \$ and recognition for Bachelor studies.
- 2010 - 2013 **Fellowship for Gifted Student**, Life Science Lab of the German Cancer Research Center
 Science education of mathematically, scientifically, and technically particularly gifted high school students.

HONORS

- 2022 **Participant of Heidelberg Laureate Forum**, ETH Representative Heidelberg, Germany
 Recipient of Rhein-Neckar Grant
 Competitive selection of participating researchers in math and computer science.
- 2020 **Participant of Global Young Scientists Summit**, ETH Representative Singapore, SG
 Competitive selection of participating young researchers in science, mathematics, and technology.

Press and Outreach

- 2023 **ETH Press**, "[Predictions of the effect of drugs on individual cells are now possible.](#)"
- 2022 **MIT Press**, "[Artificial intelligence system rapidly predicts how two proteins will attach.](#)"
- 2014 **DKFZ News**, "[Ring of Fire wins the world championship in synthetic biology.](#)"
- 2014 **F.A.Z.**, "[The Ring of Fire from Heidelberg.](#)"

Professional Activities, Leadership, and Service

CONFERENCE AND WORKSHOP ORGANIZATION

- 2023 **Workshop Organizer**, [Workshop on Diffusion Models](#) New Orleans, USA
 A NeurIPS workshop on recent advances and future research directions of powerful diffusion generative models.
- 2023 **Workshop Organizer**, [New Frontiers in Learning, Control, and Dynamical Systems](#) Honolulu, USA
 A new interdisciplinary ICML workshop discussing the interaction between control theory, and deep learning.
- since* **Founding Conference Organizer**, [Molecular ML Conference \(MoML\)](#) Cambridge, USA
 Yearly conference on machine learning for molecular modeling, molecular interactions, and therapeutic design.
- since* **Workshop Organizer**, [Optimal Transport and Machine Learning Workshop](#) New Orleans, USA
- 2021 Bi-yearly NeurIPS workshop on recent advances and developments of optimal transport in machine learning.
- 2018 **Founding Conference Organizer**, [Women in Data Science Conference \(WiDS\)](#) Zurich, Switzerland
 Yearly technical conference featuring women's work in data science and adjacent engineering areas.

PEER REVIEW

Nature Communications, Neural Information Processing Systems (NeurIPS), International Conference on Machine Learning (ICML), International Conference on Learning Representations (ICLR), International Conference on Artificial Intelligence and Statistics (AISTATS), Molecular Machine Learning (MoML) Conference, and various workshops.

OPEN SOURCE CONTRIBUTIONS

- Python Library [OTT](#) for Optimal Transport Tools in JAX
- Python Library [PyCytominer](#) for Data Processing for Perturbation Profiling

SERVICE

2021-2023	Association Member , Global Shapers Project coordination in the youth group of the World Economics Forum (WEF).	Zurich, Switzerland
2017 - 2018	Association Member , CorrelAid Data analytics consulting for non-profit organizations (NGO).	Konstanz, Germany

Publications

* authors contributed equally; † mentored student

Most recent publications via [Google Scholar](#).

CONFERENCE AND JOURNAL PUBLICATIONS

Conference publications are archival and selectively refereed in Computer Science (acceptance rates ~20 %).

Charlotte Bunne*, Stefan Stark*, Gabriele Gut*, ..., Lucas Pelkmans, Andreas Krause, Gunnar Rätsch. *Learning Single-Cell Perturbation Responses using Neural Optimal Transport*. *Nature Methods*, 2023.

Selected as **Research Briefing** in *Nature Methods*.

Also presented at NeurIPS Workshop on Optimal Transport and Machine Learning, 2021.

Vignesh Ram Somnath**†, Matteo Pariset**†, Ya-Ping Hsieh, Maria Rodriguez Martinez, Andreas Krause, and **Charlotte Bunne**. *Aligned Diffusion Schrödinger Bridges*. *Uncertainty in Artificial Intelligence (UAI)*, 2023.

Charlotte Bunne*, Ya-Ping Hsieh*, Marco Cuturi, Andreas Krause. *The Schrödinger Bridge between Gaussian Measures has a Closed Form*. *International Conference on Artificial Intelligence and Statistics (AISTATS)*, 2023.

Oral Presentation at AISTATS (**Top 1.9 %** of Submitted Papers).

Presented at ICML Workshop on Continuous Time Methods for Machine Learning, 2022.

Charlotte Bunne, Andreas Krause, Marco Cuturi. *Supervised Training of Conditional Monge Maps*. *Advances in Neural Information Processing Systems (NeurIPS)*, 2022.

Also presented at ICML Workshop on Interpretable Machine Learning in Healthcare (IMLH), 2022.

Philippe Schwaller, Alain C. Vaucher, Ruben Laplaza, **Charlotte Bunne**, Andreas Krause, Clemence Corminboeuf, and Teodoro Laino. *Machine Intelligence for Chemical Reaction Space*. *WIREs Computational Molecular Science*, 2022.

Selected for **Featured Cover** of Volume 12, Issue 5

Charlotte Bunne, Laetitia Meng-Papaxanthos, Andreas Krause, and Marco Cuturi. *Proximal Optimal Transport for Population Dynamics*. *International Conference on Artificial Intelligence and Statistics (AISTATS)*, 2022.

Best Paper Award and **Contributed Talk** at ICML Time Series Workshop, 2021.

Octavian-Eugen Ganea*, Xinyuan Huang**†, **Charlotte Bunne**, ..., and Andreas Krause. *Independent SE(3)-Equivariant Models for End-to-End Rigid Protein Docking*. *International Conference on Learning Representations (ICLR)*, 2021.

Spotlight Talk at ICLR and Ranked and Top 15 among 3326 Submissions (**Top 0.4 %**).

Also **Contributed Talk** at ELLIS Machine Learning for Molecule Discovery Workshop, 2021.

Charlotte Bunne*, Vignesh Ram Somnath*, and Andreas Krause. *Multi-Scale Representation Learning on Proteins*. *Advances in Neural Information Processing Systems (NeurIPS)*, 2021.

Also presented at ICML Computational Biology Workshop, 2021.

Vignesh Ram Somnath†, **Charlotte Bunne**, Connor W. Coley, Andreas Krause, and Regina Barzilay. *Learning Template-Free Models for Retrosynthesis*. *Advances in Neural Information Processing Systems (NeurIPS)*, 2021.

Best Paper Award and **Contributed Talk** at ICML Workshop on Graph Representation Learning and Beyond

Matteo Manica*, **Charlotte Bunne***, Roland Mathis*, ..., María Rodríguez Martínez. *COSIFER: A Python Package for the Consensus Inference of Molecular Interaction Networks*. *Bioinformatics*, 2020.

Charlotte Bunne, David Alvarez-Melis, Andreas Krause, and Stefanie Jegelka. *Learning Generative Models across Incomparable Spaces*. *International Conference on Machine Learning (ICML)*, 2019.

Best Paper Award and **Contributed Talk** at NeurIPS Workshop on Relational Representation Learning, 2018.

Max Waldhauer, Silvan N. Schmitz, ..., **Charlotte Bunne**, ..., Roland Eils. *Backbone circularization of Bacillus subtilis family 11 xylanase increases its thermostability and its resistance against aggregation*. *Molecular BioSystems*, 2015.

PREPRINTS AND UNDER SUBMISSION

Matteo Pariset⁺, Ya-Ping Hsieh, **Charlotte Bunne**, Andreas Krause, Valentin De Bortoli. *Unbalanced Diffusion Schrödinger Bridges*. In Submission (arXiv:2306.09099), 2023.

Charlotte Bunne^{*}, Frederike Lübeck^{**}, Gabriele Gut, Jacobo Sarabia del Castillo, Lucas Pelkmans, David Alvarez-Melis. *Neural Unbalanced Optimal Transport via Cycle-Consistent Semi-Couplings*. Preprint (arXiv:2209.15621), 2023. Spotlight Presentation at NeurIPS Workshop on Learning Meaningful Representations of Life, 2022.

Marco Cuturi, Laetitia Meng-Papaxanthos, Yingtao Tian, **Charlotte Bunne**, Geoff Davis, Olivier Teboul. *Optimal Transport Tools (OTT): A JAX Toolbox for All Things Wasserstein*. In Submission (arXiv:2201.12324), 2022.

Mathieu Chevalley⁺, **Charlotte Bunne**, Andreas Krause, Stefan Bauer. *Invariant Causal Mechanisms through Distribution Matching*. Preprint (arXiv:2206.11646), 2022.

Lisa Buchauer, Muhammad Amir Khan, ..., **Charlotte Bunne**, ..., Thomas Höfer, Hai-Kun Liu. *Exponential Growth of Glioblastoma In Vivo Driven by Rapidly Dividing and Outwardly Migrating Cancer Stem Cells*. Preprint, 2019.

Presentations

TALK SERIES

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|---------|--|----------------|
| 07/2023 | Conference Tutorial , Optimal Transport in Learning, Control, and Dynamical Systems | Honolulu, USA |
| | Tutorial at the International Conference on Machine Learning (ICML) | |
| 11/2022 | Invited Talk , Neural Optimal Transport for Inferring Single-Cell Perturbation Responses | Cambridge, USA |
| | Models, Inference & Algorithms (MIA) Initiative at the Broad Institute | |
| 06/2022 | Invited Talk , Optimal Transport Modeling of Single-Cell Dynamics | virtual |
| | Molecular Modeling And Drug Discovery Talks Series of Valence Discovery and Mila - Quebec AI Institute | |
| 06/2020 | Invited Talk , Learning across Incomparable Spaces (in Biomedical Applications) | virtual |
| | Data Science Seminar at the German Cancer Research Center | |

CONFERENCE AND WORKSHOP TALKS

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| 11/2023 | Invited Talk , Machine Learning-Guided Treatment Outcome Prediction and Planning | Barcelona, Spain |
| | Artificial Intelligence meets Cancer Research Symposium | |
| 09/2023 | Invited Talk , Neural Optimal Transport for Treatment Outcome Prediction | Copenhagen, DK |
| | Conference on Generative Models and Uncertainty Quantification | |
| 07/2023 | Invited Talk , Neural Optimal Transport for Single-Cell Biology | Toronto, Canada |
| | Human Cell Atlas General Meeting | |
| 06/2023 | Invited Talk , Neural Optimal Transport for Inferring Single-Cell Perturbation Responses | Zurich, Switzerland |
| | Workshop on Emerging Topics in Applications of Optimal Transport | |
| 04/2023 | Invited Talk , Optimal Transport Modeling of Population Dynamics | Munich, Germany |
| | Workshop on Optimal Transport, Mean-Field Models, and Machine Learning at TUM-IAS | |
| 09/2022 | Invited Talk , Optimal Transport Modeling of Population Dynamics | San Diego, USA |
| | SIAM Conference on Mathematics of Data Science | |
| 03/2022 | Invited Talk , Optimal Transport Modeling of Single-Cell Dynamics | Lausanne, CH |
| | AMLD Conference Track 'AI in the Molecular World' | |
| 07/2021 | Contributed Talk , Proximal Optimal Transport Modeling of Population Dynamics | virtual |
| | ICML Time-Series Workshop | |
| 07/2021 | Contributed Talk , Multi-Scale Representation Learning on Proteins | virtual |
| | ICML Computational Biology Workshop | |
| 12/2018 | Contributed Talk , Learning Generative Models across Incomparable Spaces | Montreal, Canada |
| | NeurIPS Workshop on Relational Representation Learning (R2L) | |

SEMINARS AT UNIVERSITIES

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|---------|---|---------------------|
| 01/2023 | Invited Talk , Neural Optimal Transport for Inferring Single-Cell Perturbation Responses | Heidelberg, Germany |
| | Seminar at the German Cancer Research Center | |
| 12/2022 | Invited Talk , Neural Optimal Transport for Inferring Single-Cell Perturbation Responses | Palo Alto, USA |
| | Machine Learning Seminar at Stanford University | |
| 12/2022 | Invited Talk , Neural Optimal Transport for Inferring Single-Cell Perturbation Responses | Boston, USA |
| | Machine Learning Seminar at Dana-Farber Cancer Institute | |

- 09/2022 **Invited Talk**, Modeling (Combination) Therapy Outcomes using Optimal Transport
Computational Health Center at Helmholtz Munich Munich, Germany
- 08/2022 **Invited Talk**, Optimal Transport Modeling of Single-Cell Dynamics
Imaging Platform of the Broad Institute Cambridge, USA
- 06/2022 **Invited Talk**, Optimal Transport Modeling of Population Dynamics
StatEcoML Seminar of ENSAE - CREST Paris, France
- 06/2022 **Invited Talk**, Dynamic Models for Cell Dynamics and Protein Modeling
AI for Science Group at Humboldt University of Berlin Berlin, Germany
- 06/2022 **Invited Talk**, Optimal Transport Modeling of Population Dynamics in Single-Cell Biology
Berlin Institute of Health (BIH) Berlin, Germany

SEMINARS AT INDUSTRY RESEARCH LABS

- 12/2022 **Invited Talk**, Neural Optimal Transport for Inferring Single-Cell Perturbation Responses
Genentech San Francisco, USA
- 12/2022 **Invited Talk**, Neural Optimal Transport for Population Dynamics
Apple Cupertino, USA
- 11/2022 **Invited Talk**, Modeling (Combination) Therapy Outcomes using Optimal Transport
Microsoft Research Cambridge, USA
- 03/2022 **Invited Talk**, Optimal Transport Modeling of Population Dynamics
MIT-IBM Watson AI Lab virtual
- 09/2021 **Invited Talk**, Proximal Optimal Transport Modeling of Population Dynamics
Diff-Everything Workshop at Google Research virtual
- 11/2019 **Invited Talk**, Learning Generative Models across Incomparable Spaces
IBM Research Zurich, Switzerland

Teaching

UNIVERSITY COURSES AT ETH ZURICH

All taught classes consist of lectures, tutorials, and practical projects.

- Spring 2023 **Teaching Assistant**, Introduction to Machine Learning Zurich, Switzerland
- Fall 2022 **Teaching Assistant**, Probabilistic Artificial Intelligence
- Fall 2021 **Head Teaching Assistant**, Introduction to Machine Learning
- Spring 2021 **Head Teaching Assistant**, Introduction to Machine Learning (~1000 Students)
- Fall 2020 **Teaching Assistant**, Probabilistic Artificial Intelligence
- Spring 2020 **Teaching Assistant**, Introduction to Machine Learning
- Fall 2019 **Teaching Assistant**, Probabilistic Artificial Intelligence
- Spring 2019 **Teaching Assistant**, Fairness, Explainability, & Accountability for Machine Learning

SCIENCE EDUCATION AT THE GERMAN CANCER RESEARCH CENTER

Science education of mathematically, scientifically, and technically particularly gifted high school students.

- 2012-2016 **Mentor**, Synthetic Biology Group Heidelberg, Germany
Courses on concepts in *in silico* and *in vitro* bioengineering, project design, and scientific communication.
- 2014-2015 **Mentor**, Biophysics Group
Courses on concepts in theoretical biology and physics, project design, and scientific communication.

Mentoring

- 2023-now **Alexander Hägele**, Master Student, ETH Zurich and Apple
Co-supervision with Marco Cuturi (Apple) and Andreas Krause (ETH Zurich).
- 2023-now **Yunshu Ouyang**, Master Student, Broad Institute of MIT and Harvard
Co-supervision with Jiaqi Zhang and Caroline Uhler (MIT).
- 2022-2023 **Matteo Pariset**, Master Student, EPFL
Resulting paper accepted at UAI 2023 and awarded best thesis prize at EPFL.

- 2022-2023 **Frederike Lübeck**, Master Student, Harvard University
Co-supervision with David Alvarez Melis (Harvard). Resulting paper got spotlight at NeurIPS workshop.
- 2020-2021 **Mathieu Chevalley**, Master Student,
Co-supervision with Stefan Bauer (TUM).
- 2020-2021 **Xinyuan Huang**, Master Student, ETH Zurich
Co-supervision with Octavian Ganea (MIT). Resulting paper got a spotlight presentation (top 0.4%) at ICLR 2022.
- 2019-2020 **Kenza Amara**, Master Student, ETH Zurich
Co-supervision with David Dao (ETH).
- 2019-2020 **Vignesh Ram Somnath**, Master Student, Massachusetts Institute of Technology (MIT)
Co-supervision with Regina Barzilay. Resulting publication received *Best Paper Award* at ICML Workshop 2020.

Languages and Skills

Computer Skills

Languages: *Python, MATLAB, R, Git, SQL, L^AT_EX*
Libraries: *JAX, PyTorch, TensorFlow, SciKit*

Languages

German and English: Native and Fluent
French: Conversant