

Charlotte Bunne

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Education

Eidgenössische Technische Hochschule (ETH) Zurich

Zurich, Switzerland

PHD IN COMPUTER SCIENCE

2019 - 2023 (expected)

- Advisors: Andreas Krause and Marco Cuturi

Massachusetts Institute of Technology (MIT)

Cambridge, USA

VISITING STUDENT IN COMPUTER SCIENCE

2018

- Advisors: Stefanie Jegelka and David Alvarez-Melis

Eidgenössische Technische Hochschule (ETH) Zurich

Zurich, Switzerland

M.S. IN COMPUTATIONAL BIOLOGY AND BIOINFORMATICS

2016 - 2019

- **ETH Medal** for best thesis (awarded to top 2.5% of all ETH graduates)
- **Willi-Studer Prize** for best GPA and graduated (*summa cum laude*)
- Selected into the **Excellence Scholarship & Opportunity Program** (ESOP)

Heidelberg University

Heidelberg, Germany

B.S. IN BIOSCIENCES

2013 - 2016

- Major in Bioinformatics and graduated among top 2% of class
- Selected as Fellow of the **German Academic Scholarship Foundation** (Studienstiftung d. dt. Volkes)

Research and Work Experience

08/2022 - now **Broad Institute of MIT and Harvard**, Graduate Researcher Cambridge, USA

- Supervisors: Anne Carpenter and Shantanu Singh

02 - 07/2022 **Apple**, Research Intern Paris, France

- Machine Learning Group of Samy Bengio and Marco Cuturi

09 - 12/2020 **Google Research**, Research Intern Zurich, Switzerland

- Brain Team of Jean-Philippe Vert and Marco Cuturi

03/2019 - now **ETH AI Center**, Graduate Researcher Zurich, Switzerland

- Supervisor: Andreas Krause

04 - 12/2018 **MIT CSAIL**, Research Assistant Cambridge, USA

- Supervisors: Stefanie Jegelka and David Alvarez-Melis

10/2017 - 03/2018 **IBM Research**, Software Engineering Intern Zurich, Switzerland

- Cognitive Computing and Industry Solutions of Maria Gabrani

01/2015 - 08/2016 **German Cancer Research Center (DKFZ)**, Research Assistant Heidelberg, Germany

- Supervisors: Roland Eils and Thomas Höfer

Fellowships and Awards

SELECTED AWARDS

2022 **Outstanding Reviewer Award**, AISTATS Conference

2021 **Best Paper Award**, ICML Time Series Workshop

1/35 Papers

2020 **Best Paper Award**, ICML Workshop on Graph Representation Learning & Beyond

1/73 Papers

2019 **ETH Medal**, ETH Zurich

Top 2.5% of All ETH Graduates

Willi Studer Prize, ETH Zurich

Best GPA of Cohort

2018 **Best Paper Award**, NeurIPS Workshop on Relational Representation Learning

1/52 Papers

2014 **Grand Prize**, iGEM Competition

1/245 Teams, 3 Special Prizes

2012 **Grand Prize**, iGEM High School Competition

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

- 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**, [New Frontiers in Learning, Control, and Dynamical Systems](#) Kigali, Rwanda (tentative)
A new workshop at ICLR (tentative) discussing the interaction between control theory and deep learning.
- 2022 **Founding Conference Organizer**, [Molecular ML Conference \(MoML\)](#) Cambridge (MA), USA
Yearly conference on machine learning for molecular modeling, molecular interactions, and therapeutic design.
- 2021 **Workshop Organizer**, [NeurIPS Optimal Transport and Machine Learning Workshop](#) virtual
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 the work women are doing 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 Artificial Intelligence and Statistics (AISTATS), Women in Machine Learning Workshop (WiML), Molecular Machine Learning (MoML) Conference.

OPEN SOURCE CONTRIBUTIONS

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

SERVICE

2021-now	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](#).

PREPRINTS AND UNDER SUBMISSION

Charlotte Bunne^{*}, Frederike Lübeck^{**}, Gabriele Gut, Jacobo Sarabia del Castillo, Lucas Pelkmans, David Alvarez-Melis. *Neural Unbalanced Optimal Transport via Cycle-Consistent Semi-Couplings*. Under Review, 2022.

Charlotte Bunne^{*}, Stefan Stark^{*}, Gabriele Gut^{*}, ..., Lucas Pelkmans, Andreas Krause, Gynnar Rätsch. *Learning Single-Cell Perturbation Responses using Neural Optimal Transport*. Under Review at *Nature Methods*, 2022.
Also presented at NeurIPS Workshop on Optimal Transport and Machine Learning, 2021.

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.

Charlotte Bunne^{*}, Ya-Ping Hsieh^{*}, Marco Cuturi, Andreas Krause. *Recovering Stochastic Dynamics via Gaussian Schrödinger Bridges*. In Submission (arXiv:2202.05722), 2022.
Presented at ICML Workshop on Continuous Time Methods for Machine Learning, 2022.

Mathieu Chevalley[†], **Charlotte Bunne**, Andreas Krause, Stefan Bauer. *Invariant Causal Mechanisms through Distribution Matching*. In Submission (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.

CONFERENCE AND JOURNAL PUBLICATIONS

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

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)*, 2021.
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.

Presentations

TALK SERIES

- 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

- 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
- 12/2022 **Contributed Talk**, Supervised Training of Conditional Monge Maps New Orleans, USA
NeurIPS Main Conference Track
- 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'
- 03/2022 **Contributed Talk**, Proximal Optimal Transport Modeling of Population Dynamics virtual
AISTATS Main Conference Track
- 12/2021 **Contributed Talk**, Multi-Scale Representation Learning on Proteins virtual
NeurIPS Main Conference Track
- 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
- 17/2019 **Contributed Talk**, Learning Generative Models across Incomparable Spaces Long Beach, USA
ICML Main Conference
- 12/2018 **Contributed Talk**, Learning Generative Models across Incomparable Spaces Montreal, Canada
NeurIPS Workshop on Relational Representation Learning (R2L)

SEMINARS AT UNIVERSITIES

- 12/2022 **Invited Talk**, Neural Optimal Transport for Inferring Single-Cell Perturbation Responses Palo Alto, USA
Machine Learning Seminar at Stanford University
- 09/2022 **Invited Talk**, Modeling (Combination) Therapy Outcomes using Optimal Transport Munich, Germany
Computational Health Center at Helmholtz Munich
- 08/2022 **Invited Talk**, Optimal Transport Modeling of Single-Cell Dynamics Cambridge, USA
Imaging Platform of the Broad Institute
- 06/2022 **Invited Talk**, Optimal Transport Modeling of Population Dynamics Paris, France
StatEcoML Seminar of ENSAE - CREST
- 06/2022 **Invited Talk**, Dynamic Models for Cell Dynamics and Protein Modeling Berlin, Germany
AI for Science Group at Humboldt University of Berlin
- 06/2022 **Invited Talk**, Optimal Transport Modeling of Population Dynamics in Single-Cell Biology Berlin, Germany
Berlin Institute of Health (BIH)
- 10/2021 **Invited Talk**, Optimal Transport Modeling of Single-Cell Dynamics Zurich, Switzerland
Department of Molecular Life Sciences at University of Zurich

SEMINARS AT INDUSTRY RESEARCH LABS

- 12/2022 **Invited Talk**, Neural Optimal Transport for Inferring Single-Cell Perturbation Responses San Francisco, USA
Genentech
- 12/2022 **Invited Talk**, Neural Optimal Transport for Population Dynamics Cupertino, USA
Apple
- 11/2022 **Invited Talk**, Modeling (Combination) Therapy Outcomes using Optimal Transport Cambridge, USA
Microsoft Research

03/2022	Invited Talk , Optimal Transport Modeling of Population Dynamics MIT-IBM Watson AI Lab	virtual
02/2022	Invited Talk , Multi-Scale Representation Learning on Proteins NEC Laboratories	virtual
09/2021	Invited Talk , Proximal Optimal Transport Modeling of Population Dynamics Diff-Everything Workshop at Google Research	virtual
03/2021	Invited Talk , Machine Learning on Proteins Internal All-Hands Meeting at UBS	Zurich, Switzerland
11/2019	Invited Talk , Learning Generative Models across Incomparable Spaces IBM Research	Zurich, Switzerland

Teaching

UNIVERSITY COURSES AT ETH ZURICH

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

Fall 2022	Teaching Assistant , Probabilistic Artificial Intelligence	Zurich, Switzerland
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 Courses on concepts in <i>in silico</i> and <i>in vitro</i> bioengineering, project design, and scientific communication.	Heidelberg, Germany
2014-2015	Mentor , Biophysics Group Courses on concepts in theoretical biology and physics, project design, and scientific communication.	

Mentoring

2022-now	Frederike Lübeck , Master Student, Harvard University Ongoing co-supervision with David Alvarez Melis. Resulting paper currently in submission.
2022-now	Matteo Pariset , Master Student, EPFL Ongoing co-supervision with Martin Jaggi.
2022-now	Athina Nisioti , Master Student, ETH Zurich Ongoing supervision.
2020-2021	Mathieu Chevalley , Master Student, Co-supervision with Stefan Bauer.
2020-2021	Xinyuan Huang , Master Student, ETH Zurich Co-supervision with Octavian Ganea. Resulting paper got a spotlight presentation (top 0.4%) at ICLR 2022.
2019-2020	Vignesh Ram Somnath , Master Student, Massachusetts Institute of Technology (MIT) Co-supervision with Regina Barzilay. Resulting publication received <i>Best Paper Award</i> 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: Native
English: Fluent
French: Conversant