

# Charlotte Bunne

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## Academic Positions

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

## Education

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

## Research and Work Experience

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

## Fellowships and Awards

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### SELECTED AWARDS

2024	<b>Best Paper Award</b> , ICML AI for Science Workshop	<i>1/148 Papers</i>
2024	<b>SIB Remarkable Outputs 2023 Award</b> , SIB Swiss Institute of Bioinformatics	
2024	<b>Finalist of the German Thesis Award</b> , Körber Stiftung	<i>11/719 Theses</i>
2021	<b>Best Paper Award</b> , ICML Time Series Workshop	<i>1/35 Papers</i>
2020	<b>Best Paper Award</b> , ICML Workshop on Graph Representation Learning & Beyond	<i>1/73 Papers</i>

- 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

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- 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

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### CONFERENCE AND WORKSHOP ORGANIZATION

- 2024 **Workshop Organizer**, [Workshop on Machine Learning for Genomics Explorations](#) Vienna, Austria  
 An ICLR workshop bridging the gap between machine learning and genomics, with focus on target identification.
- 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.
- 2022 **Founding Conference Organizer**, [Molecular ML Conference \(MoML\)](#) Cambridge, USA  
 Yearly conference on machine learning for molecular modeling, molecular interactions, and therapeutic design.
- 2021 **Workshop Organizer**, [Optimal Transport and Machine Learning Workshop](#) New Orleans, USA  
 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.

### OPEN SOURCE CONTRIBUTIONS

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

## PROFESSIONAL SERVICE

**Editorial Board Member** of the Machine Learning: Science and Technology (MLST) IOP Publishing journal.

**Reviewer of Journals and Proceedings** in 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, Nature Communications, and various workshops.

## Publications

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\* 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**, Geoffrey Schiebinger, Andreas Krause, Aviv Regev, Marco Cuturi. *Optimal transport for single-cell and spatial omics*. *Nature Reviews Methods Primer*, 2024.

Jayoung Ryu, Romain Lopez, **Charlotte Bunne**, Aviv Regev. *Cross-modality Matching and Prediction of Perturbation Responses with Labeled Gromov-Wasserstein Optimal Transport*. *Machine Learning in Computational Biology*, 2024. **Best Paper Award** and **Contributed Talk** at ICML AI for Science Workshop, 2024.

Puck Gerwen, Ksenia Briling, **Charlotte Bunne**, Vignesh Ram Somnath, Ruben Laplaza, Andreas Krause, Clemence Corminboeuf. *3DReact: Geometric Deep Learning for Chemical Reactions*. *Journal of Chemical Information and Modeling*, 2023.

**Charlotte Bunne**<sup>\*</sup>, Stefan Stark<sup>\*</sup>, Gabriele Gut<sup>\*</sup>, ..., 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<sup>\*\*</sup>, Matteo Pariset<sup>\*\*</sup>, Ya-Ping Hsieh, Maria Rodriguez Martinez, Andreas Krause, and **Charlotte Bunne**. *Aligned Diffusion Schrödinger Bridges*. *Uncertainty in Artificial Intelligence (UAI)*, 2023.

**Charlotte Bunne**<sup>\*</sup>, Ya-Ping Hsieh<sup>\*</sup>, 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<sup>\*</sup>, Xinyuan Huang<sup>\*\*</sup>, **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**<sup>\*</sup>, Vignesh Ram Somnath<sup>\*</sup>, 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<sup>†</sup>, **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<sup>\*</sup>, **Charlotte Bunne**<sup>\*</sup>, Roland Mathis<sup>\*</sup>, ..., 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

Erik Serrano, ..., **Charlotte Bunne**, ..., Anne E. Carpenter, Beth A. Cimini, Shantanu Singh, Gregory P. Way. *Reproducible image-based profiling with Pycytominer*. *In Submission (arXiv:2311.13417)*, 2024.

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

**Charlotte Bunne**<sup>\*</sup>, Frederike Lübeck<sup>\*\*</sup>, 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<sup>+</sup>, **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

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### TALK SERIES

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|---------|--|------------------|
| 06/2024 | <b>Lecture</b> , Personalized Medicine through Generative Modeling<br>ML for Drug Discovery Summer School of Recursion and Valence Labs  | Montreal, Canada |
| 07/2023 | <b>Conference Tutorial</b> , <a href="#">Optimal Transport in Learning, Control, and Dynamical Systems</a><br>Tutorial at the International Conference on Machine Learning (ICML)  | Honolulu, USA    |
| 11/2022 | <b>Invited Talk</b> , Neural Optimal Transport for Inferring Single-Cell Perturbation Responses<br>Models, Inference & Algorithms (MIA) Initiative at the Broad Institute          | Cambridge, USA   |
| 06/2022 | <b>Invited Talk</b> , Optimal Transport Modeling of Single-Cell Dynamics<br>Molecular Modeling And Drug Discovery Talks Series of Valence Discovery and Mila - Quebec AI Institute | virtual          |
| 06/2020 | <b>Invited Talk</b> , Learning across Incomparable Spaces (in Biomedical Applications)<br>Data Science Seminar at the German Cancer Research Center                                | virtual          |

### CONFERENCE AND WORKSHOP TALKS

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|---------|---|---------------------|
| 06/2024 | <b>Invited Talk</b> , Predicting Patient Treatment Outcomes using Generative Models<br>CVPR Workshop on Computer Vision for Microscopy Image Analysis (CVMI)        | Seattle, USA        |
| 04/2024 | <b>Invited Talk</b> , Predicting Patient Treatment Outcomes using Generative Models<br>AMLD Workshop on AI in Genomics  | Lausanne, CH        |
| 11/2023 | <b>Invited Talk</b> , Machine Learning-Guided Treatment Outcome Prediction and Planning<br>Artificial Intelligence meets Cancer Research Symposium                  | Barcelona, Spain    |
| 09/2023 | <b>Invited Talk</b> , Neural Optimal Transport for Treatment Outcome Prediction<br>Conference on Generative Models and Uncertainty Quantification                   | Copenhagen, DK      |
| 07/2023 | <b>Invited Talk</b> , Neural Optimal Transport for Single-Cell Biology<br>Human Cell Atlas General Meeting  | Toronto, Canada     |
| 06/2023 | <b>Invited Talk</b> , Neural Optimal Transport for Inferring Single-Cell Perturbation Responses<br>Workshop on Emerging Topics in Applications of Optimal Transport | Zurich, Switzerland |
| 04/2023 | <b>Invited Talk</b> , Optimal Transport Modeling of Population Dynamics<br>Workshop on Optimal Transport, Mean-Field Models, and Machine Learning at TUM-IAS        | Munich, Germany     |
| 09/2022 | <b>Invited Talk</b> , Optimal Transport Modeling of Population Dynamics<br>SIAM Conference on Mathematics of Data Science   | San Diego, USA      |
| 03/2022 | <b>Invited Talk</b> , Optimal Transport Modeling of Single-Cell Dynamics<br>AMLD Conference Track 'AI in the Molecular World'                                       | Lausanne, CH        |

- 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

- 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 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)

### SEMINARS AT INDUSTRY RESEARCH LABS

- 06/2024 **Invited Talk**, Predicting Patient Treatment Outcomes using Generative Models Santa Clara, USA  
NVIDIA
- 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 virtual  
MIT-IBM Watson AI Lab
- 09/2021 **Invited Talk**, Proximal Optimal Transport Modeling of Population Dynamics virtual  
Diff-Everything Workshop at Google Research
- 11/2019 **Invited Talk**, Learning Generative Models across Incomparable Spaces Zurich, Switzerland  
IBM Research

## Teaching

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### 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

## Supervision

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- since 2024 **Johann Wenckstern**, PhD Student, EPFL  
EPFL EDIC Fellowship.
- since 2024 **Eeshaan Jain**, PhD Student, EPFL  
EPFL EDIC Fellowship.
- since 2024 **Siba Smarak Panigrahi**, PhD Student, EPFL  
EPFL EDIC Fellowship.
- 2023-2024 **Johann Wenckstern**, Master Student, ETH Zurich  
Co-supervision with the Unispital Zürich.
- 2023 **Alexander Hägele**, Master Student, ETH Zurich and Apple  
Co-supervision with Marco Cuturi (Apple) and Andreas Krause (ETH Zurich).
- 2023 **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

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### Computer Skills

Languages: *Python, MATLAB, R, Git, SQL, L<sup>A</sup>T<sub>E</sub>X*  
Libraries: *JAX, PyTorch, TensorFlow, SciKit*

### Languages

German and English: Native and Fluent  
French: Conversant