

Umberto Lupo

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Professional experience

- 6/2025 – present: **Senior AI Scientist**, *de novo* antibody design
[Absci](#), Switzerland
 - *In silico* screening of designed antibodies for on-target binding
 - *In silico* modelling of antibody-antigen interactions
 - Co-first author in [Origin-1: a generative AI platform for de novo antibody design against novel epitopes](#)
- 7/2024 – 5/2025: **AI Scientist II**, *de novo* antibody design
[Absci](#), Switzerland
- 7/2020 – 6/2024: **Post-doctoral Researcher**, machine learning & computational biology
[Bitbol Lab](#), [EPFL](#), Switzerland
 - **Protein language models** applied to protein-protein interactions, multimer structure prediction, *de novo* protein sequence generation & phylogenetic analysis
 - **Novel differentiable techniques** in discrete optimization applied to protein sequence data and LMs
 - Publications in high-impact journals & conferences (**poster + contributed talk @ ICML 2022 Workshop on Computational Biology**, **poster @ NeurIPS 2022 Workshop in Machine Learning for Structural Biology**, **spotlight @ MLCB 2022**)
 - **Keynote speaker** at the “[NLP in Biology and Chemistry](#)” Symposium, Bern (March 2024). Talk title: “Language model approaches for disentangling protein-protein interactions at different scales”
 - Supervisor: student projects/internships (6) and master theses (1)
 - Conference organization:
 1. Main organizer, “[Biological Evolution Across Scales](#)”, Bernoulli Center, EPFL (2023)
 2. Organizing committee, [ICML '24 Workshop “Translational ML for Health and Industrial Applications”](#), Vienna, Austria (2024, in preparation)
- 9/2018 – 6/2020: **Research Scientist & Open-Source Developer**
[L2F/Giotto-AI](#), Lausanne, Switzerland
 - Co-creator, lead developer & lead maintainer:  [giotto-tda](#) Python library for topological ML (★930, **spotlight talk @ NeurIPS 2020 Workshop “Topological Data Analysis and Beyond”**)
 - Co-creator & maintainer:  [giotto-ph](#) C++/Python library for multi-core topological computations
 - Maintainer:  [pyflagser](#) C++/Python library
 - **Elevated codebases** to meet scikit-learn standards. High unit/integration test coverage (98%), CI/CD across multiple Python versions and OSs, clear and accurate documentation, code style compliance
 - Research: data analysis/visualization algorithms, algebraic topology and differential geometry in ML
 - **Academic/industrial grants**:
 - [Conception & grant writing] [Novel connections between topological data analysis and deep learning](#), *Innosuisse federal grant*, 1M CHF, 2020–2022
 - [Execution] [Topological warning signals for time series](#), *Innosuisse federal grant*, 560k CHF, 2019–2020
 - Supervised interns (1), student projects (4) and master theses (1)

- Conceived & organized the first-ever “**AI & Topology**” track, Applied Machine Learning Days 2020
- 5/2018 – 8/2018: **Machine Learning Engineer**
L2F, Lausanne, Switzerland
 - Bespoke software for a large corporate client in the insurance sector. Delivered a **web platform** hosting business analytics, data visualization solutions and forecasts
- 3/2017 – 5/2017: **Post-doctoral Researcher**, quantum field theory and black hole physics
Albert Einstein Center for Fundamental Physics, University of Bern, Switzerland
- 10/2015 – 10/2016: **Content Developer & Mentor**, **Isaac Physics**
University of Cambridge, UK
 - Created **teaching and learning material** in mathematics, physics and chemistry to enhance problem-solving skills
 - Ran **masterclasses** for A-level teachers and students across England

Education

- 10/2011 – 9/2015: **PhD in Mathematics**
University of York, UK
Title: **Aspects of (quantum) field theory in curved spacetimes, particularly in the presence of boundaries**
Awards: **Anand Ramachandran Memorial Prize** for the best PhD thesis in Mathematics
Funding: University of York **teaching scholarship**
- 10/2010 – 6/2011: **Master of Advanced Studies** in Applied Mathematics and Theoretical Physics
University of Cambridge, UK
- 10/2007 – 6/2010: **BSc (Hons) in Mathematics and Physics**
University of Warwick, UK
Awards: **Undergraduate research project scholarship**. Used to write image-recognition software for microscope images of free-standing chemically modified graphene (**publication**)

Publications

- Levine, U.*, King, J. E.*, Stern, J.*, Grayson, D.*, Wang, R.*, Yin, R.*, **Lupo, U.***, Kulyte, P.*, Brand, R. M.*, Bertin, T.*, Pfingsten, R.*, Cejovic, J.* *et al* (2026)
Origin-1: a generative AI platform for de novo antibody design against novel epitopes
Biorxiv
- **Lupo, U.**, Sgarbossa, D., Milighetti, M. and Bitbol, A.-F. (2025)
DiffPaSS—high-performance differentiable pairing of protein sequences using soft scores
Bioinformatics 41(1), btae738
 github.com/Bitbol-Lab/DiffPaSS ★8
- **Lupo, U.**, Sgarbossa, D. and Bitbol, A.-F. (2024)
Pairing interacting protein sequences using masked language modeling
Proc. Natl. Acad. Sci. U.S.A. 121(27) e2311887121
 github.com/Bitbol-Lab/DiffPALM ★24
- Sgarbossa, D., **Lupo, U.** and Bitbol, A.-F. (2023)
Generative power of a protein language model trained on multiple sequence alignments
eLife 12(e79854)
 github.com/Bitbol-Lab/Iterative_masking ★26

- Dietler, N., **Lupo, U.** and Bitbol, A.-F. (2023)
[Impact of phylogeny on structural contact inference from protein sequence data](#)
J. R. Soc. Interface 20(20220707)
- **Lupo, U.**, Sgarbossa, D. and Bitbol, A.-F. (2022)
[Protein language models trained on multiple sequence alignments learn phylogenetic relationships](#)
Nat Commun 13(6298)
 github.com/Bitbol-Lab/Phylogeny-MSA-Transformer ★17
- Myers, A. *et al* (2022)
[ICLR 2022 Challenge for Computational Geometry & Topology: Design and Results](#)
Proceedings of Machine Learning Research 196, 269–276
- **Lupo, U.**, Medina-Mardones, A. and Tauzin, G. (2022)
[Persistence Steenrod Modules](#)
J Appl. and Comput. Topology 13(6298)
 github.com/Steenroder/steenroder ★8
- Miolane, N., Caorsi, M., **Lupo, U.** *et al* (2021)
[ICLR 2021 Challenge for Computational Geometry & Topology: Design and Results](#)
arXiv preprint
- Burella Pérez, J., Hauke, S., **Lupo, U.**, Caorsi, M., Dassatti, A. (2021)
[giotto-ph: A Python Library for High-Performance Computation of Persistent Homology of Vietoris–Rips Filtrations](#)
arXiv preprint
 github.com/giotto-ai/giotto-ph ★51
- Tauzin, G., **Lupo, U.**, Tunstall, L., Burella Pérez, J., Caorsi, M., Medina-Mardones, A. M., Dassatti, A., Hess, K. (2021)
[giotto-tda: A Topological Data Analysis Toolkit for Machine Learning and Data Exploration](#)
JMLR, 22(39)
 github.com/giotto-ai/giotto-tda ★930
 github.com/giotto-ai/pyflagser ★13
- **Lupo, U.** (2018). [On the global “two-sided” characteristic Cauchy problem for linear wave equations on manifolds.](#) *Lett Math Phys*, 108(10)
- Kay, B. S. and **Lupo, U.** (2016)
[Non-existence of isometry-invariant Hadamard states for a Kruskal black hole in a box and for massless fields on 1+1 Minkowski spacetime with a uniformly accelerating mirror](#)
Class. Quantum Grav., 33(215001)
- Wilson, N. R., Pandey, P. A., Beanland, R., Rourke, J. P., **Lupo, U.**, Rowlands, G. and Römer, R. A. (2010)
[On the structure and topography of free-standing chemically modified graphene](#)
New J. Phys., 12(125010)