Umberto Lupo

✉ umberto.lupo@gmail.com — ⌂ ulupo — in in/ulupo — 🐦 @umbislupo

Professional experience

- 7/2020 – present: **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)
  - Supervisor: student projects/internships (6) and master theses (1)
  - Conference organizer, "Biological Evolution Across Scales", Bernoulli Center, EPFL (2023)

- 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 (★773, **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

- **Lupo, U.**, Sgarbossa, D. and Bitbol, A.-F. (2023)
  Pairing interacting protein sequences using masked language modeling
  Proc. Natl. Acad. Sci. U.S.A., in press
  ⓞ github.com/Bitbol-Lab/DiffPALM ★8

- 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 ★15

- 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 ★14

- 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 ★6

- 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 ★37

- 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 ★775
  ○ github.com/giotto-ai/pyflagser ★9

- **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)