

Luna Pianesi

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Work Experience

University of Bielefeld

Assistant lecturer

- Programming in Python, Winter '23, Winter '24
- Graph Neural Networks in Biology (seminar), Summer '24

Bielefeld, DE

Oct. 2023 - current

Education

University of Bielefeld

PhD student in Bioinformatics

Bielefeld, DE

Apr. 2023 - current

University of Cambridge

MS thesis internship

Cambridge, UK

Apr. 2022 - Aug. 2022

University of Trento

MS in Artificial Intelligence Systems

Trento, IT

Sep. 2020 - Mar. 2023

University of Bologna

BS in Genomics

Bologna, IT

Sep. 2017 - Oct. 2020

Research Projects

GNNs and Diffusion Models in a Computational Drug Discovery Pipeline

PhD research project

- Comparison and merging of GNN-based with diffusion-based methods for a drug discovery task
- Pipeline involving ligand generation, docking, activity prediction, pathways analysis and polypharmacy prediction
- Language/framework: **Python, R, PyTorch, PyG, DGL**

University of Bielefeld

Apr. 2023 - current

GNNs and XAI for a New Aurora Kinase Inhibitor

MS thesis research

- Graph neural networks for generation and docking of novel Aurora protein kinase small-molecule inhibitors
- Explainable AI techniques for analysing the docking of generated molecules
- Language/framework: **Python, R, PyTorch, PyG, DGL**

University of Cambridge

Dec. 2021 - Mar. 2023

Explainability of a Pre-Trained GNN for Molecular Property Prediction

MS course project

- Applying Explainable AI techniques for producing explanations of GNN-based model 3D Infomax
- Analysis of generated explanations and biological contextualization
- Language/framework: **Python, PyG, DGL**

University of Trento

Jul. 2022 - Feb. 2023

Investigating SourceSet outside Normality

BS thesis research

- Analysis of Gaussian-graphical-model-based method SourceSet to identify dysregulation in biological network
- Investigation of model behaviour when non-Normal count data is used
- Language/framework: **R**

University of Bologna

Dec. 2019 - Oct. 2020

Technical Skills

Programming	Python, R, Matlab
Programming frameworks	PyTorch, PyTorch Geometric, Deep Graph Library, OpenCV
Professional Softwares	ChimeraX, Chimera
Drawing & Typesetting	L ^A T _E X, Beamer, Microsoft Office
Languages	Italian (Native), English (C2), Mandarin Chinese (B2), German (A2.2), French (learning)

Summer Schools and Workshops

CGSI 2024: Computational Genomics Summer Institute, *summer school*

Los Angeles, California, USA

UCLA

29 Jul. - 2 Aug. 2024

- [\[Website\]](#)

ML4DD 2024: Machine Learning for Drug Discovery, *summer school*

Montreal, Québec, CA

Mila - Quebec AI Institute

12 Jun. - 21 Jun. 2024

- [\[Website\]](#)

A Multidisciplinary Approach to Epistasis Detection, *workshop*

Leiden, NL

Lorentz Center@Oort

17 Jul. - 21 Jul. 2023

- [\[Website\]](#)

Conferences

MoML 2024 Molecular Machine Learning Conference @ *Mila Institute*. Spotlight poster presentation

Reviewer Roles

RECOMB 2025 29th Annual International Conference on Research in Computational Molecular Biology, *subreviewer*

RECOMB 2024 28th Annual International Conference on Research in Computational Molecular Biology, *subreviewer*

ISMB 2024 32nd Conference on Intelligent Systems for Molecular Biology, *subreviewer*

Publications

- [1] Agostinis, F., Chiogna, M., Djordjilovic, V., **Pianesi, L.** and Romualdi, C. “Searching for a source of difference in undirected graphical models for count data - an empirical study ,” *Book of short papers. SIS - Società Italiana di Statistica*, 689-694, 2021. [\[Link\]](#)