Manuel Madeira

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About Me

I am a 4th-year PhD student at EPFL under the supervision of Pascal Frossard and Dorina Thanou. My interests gravitate around generative modelling, graph deep learning and their applications in enabling scientific discoveries. I have proposed novel generative frameworks for graphs and developed methods that incorporate domain knowledge to enhance the controllability and performance of graph generation. Recently, I have also begun exploring vision and language foundational models in the context of digital pathology.

Education

2022 - Present — PhD. in Machine Learning (Expected Graduation: December 2026)
École Polytechnique Fédérale de Lausanne, Switzerland

2018 - 2019 (Fall) — Exchange student in Computer Science
Tsinghua University, China

2018 - 2021 — MSc. in Biomedical Engineering
Instituto Superior Técnico, Portugal
GPA: 19 / 20 (**1st** in class), Thesis: 20/20

2015 - 2018 — BSc. in Biomedical Engineering
Instituto Superior Técnico, Portugal
GPA: 19 / 20 (**1st** in class and **1st** ever to attain such grade)

Research Experience

Jul 2025 - Dec 2025 — **Applied Scientist Intern** at Amazon
Developed a graph-based deep learning framework for predictive modeling in supply chain long-term planning.

Sep 2022 - Present — **Doctoral Assistant** at EPFL
Studied the incorporation of structural constraints into graph discrete diffusion models and developed the first discrete flow matching model for graphs. Employed these methods in real-world applications, including molecular generation and digital pathology.

Sep 2021 - Aug 2022 — **Machine Learning Researcher** at Inductiva Research Labs
Conducted research on deep learning based approaches to solve partial differential equations. Deployed physics-informed neural networks to model heat diffusion and coastal dynamics and analysed their generalization to arbitrary domains.

Mar 2021 - Jun 2021 — **Research Internship** at Institute for Systems and Robotics
Supervisors: Renato Negrinho, João Xavier, and Pedro Aguiar
Researched on L-smoothness exploitation for first-order stochastic optimization methods with theoretical developments on algorithmic analysis.

Sep 2019 - Feb 2020 — **Research Internship** at IST-ID
Transcribed interviews on health technologies assessment in Portugal for the Medi-value Project.

Awards and Honors

2025 — **Top Reviewer**, by NeurIPS 2025
2025 — **Innovation Fellowship Finalist**, by Qualcomm
2022-23 — **EDIC PhD Fellowship**, by EPFL
2016-18 — **1st ranked student in Biomedical Engineering BSc**, by Instituto Superior Técnico
2015-20 — **Diploma of Academic Excellence (Top 10%)**, by Instituto Superior Técnico
2009-15 — **Best student in high school**, by Crédito Agrícola

Publications

[1] A. Carballo-Castro, **MM**, Y. Qin, D. Thanou, and P. Frossard. **Generating Directed Graphs with Dual Attention and Asymmetric Encoding**. In: ArXiv. 2025.

[2] S. Öğüt, C. Vincent-Cuaz, **MM**, et al. **Benchmarking Instance-Level Learnability and Interpretability in Multiple Instance Learning**. In: Under Review. 2025.

[3] B. Chen*, C. Vincent-Cuaz*, L. A. Schoenpflug*, **MM***, et al. **Revisiting Automatic Data Curation for Vision Foundation Models in Digital Pathology**. In: Early Acceptance (Top 9%). MICCAI. 2025.

[4] O. Zaghen, **MM**, L. Toni, and P. Frossard. **Graph Discrete Diffusion: a Spectral Study**. In: *DeLTa and XAI4Science Workshops*. ICLR. 2025.

[5] L. Sbicego, S. Öğüt, **MM**, Y. Qin, D. Thanou, and P. Frossard. **On the Role of Graph Structure in Graph Neural Networks**. In: *ICBINB Workshop*. Selected for PMLR Proceedings. ICLR. 2025.

[6] Y. Qin*, **MM***, D. Thanou, and P. Frossard. **DeFoG: Discrete Flow Matching for Graph Generation**. In: Oral Presentation (Top 1%). ICML. 2024.

[7] **MM**, C. Vignac, D. Thanou, and P. Frossard. **Generative Modelling of Structurally Constrained Graphs**. In: NeurIPS. 2024.

[8] **MM**, D. Thanou, and P. Frossard. **Tertiary Lymphoid Structures Generation through Graph-based Diffusion**. In: *GRAIL Workshop*. MICCAI. 2023.

[9] S. Moalla*, **MM***, L. Riccio*, and J. Lee*. **[Re] Reproducibility Study of Behavior Transformers**. In: *ML Reproducibility Challenge 2022*. Outstanding Paper Award (Honorable Mention). ReScience C. 2023.

[10] **MM**, R. Negrinho, J. Xavier, and P. M. Aguiar. **COCO Denoiser: Using Co-Coercivity for Variance Reduction in Stochastic Convex Optimization**. In: *OPT Workshop*. NeurIPS. 2021.

Talks

ICML 2025, Vancouver, Canada, 2025. *DeFoG: Discrete Flow Matching for Graph Generation.*

AI Alliance: AI in Materials & Chemistry Webinar Series, online. *DeFoG: Discrete Flow Matching for Graph Generation.*

Inductiva Machine Learning for Science & Engineering Summer School, Porto, Portugal, 2025. *An Introduction to Graph Neural Networks.*

BioML Workshop, Lausanne, Switzerland, 2025. *Constrained Graph Generative Models in Science.*

Applied Machine Learning Days, Lausanne, Switzerland, 2025. *Constrained Graph Generative Models in Science.*

DataMakers Fest, Porto, Portugal, 2023. *Generative Models in Science: A Peek into Graph Diffusion Models for Digital Pathology.*

Teaching Experience

Teaching Assistant for:

- Network Machine Learning (Lead TA in 2024/2025)
- Probability and Statistics
- Practice of Object-Oriented Programming
- Analysis I
- Histology

Supervised 4 students.

Software Skills

Languages:	Python, Matlab, Java, Mathematica, R
Frameworks:	PyTorch, Keras, Tensorflow, Pandas, Scikit-learn, NumPy, CVX, CVXPY/CVXOPT, Abaqus
Misc:	Unix, Git, Docker, Kubernetes, SLURM, Run:AI

Extracurricular Activities

2023	Attended Cambridge Ellis Unit Summer School on Probabilistic Machine Learning
2022 - Present	Co-organizer of Deep Learning Sessiong Portugal
2021	Attended Lisbon Machine Learning Summer School
2009-21	Competitive football player (national level)
2015	National finalist in Biology Olympiad

Languages

Portuguese:	Native
English:	C2, TOEFL iBT: 114 / 120
Spanish:	A2
French:	A2
Chinese:	Elementary (Tsinghua course)

Personal Interests

Football, CrossFit, Ski, Reading, Cinema

Community Service

Reviewer for NeurIPS, NPGML workshop (NeurIPS) and ComBayNS workshop (IJCNN)