Niccolò Grillo | ML Researcher/Engineer

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Education

Politecnico di Milano — Milan, ITA

Master of Science, Mathematical Engineering - Statistical Learning, *(110 with honors, GPA: 3.85)* — *Sep. 2023 – Oct. 2025*

- Relevant Subjects: Algorithms, Data Structures, Parallel Computing, Scientific Computing, Stochastic processes, Machine Learning, Deep Learning, Reinforcement Learning, NLP, Real Analysis, Applied Statistics, Optimization Theory.

Politecnico di Milano — Milan, ITA

Pre-Master's Coursework, Mathematical Engineering — *Mar. 2022 – Jul. 2023*

- Relevant Subjects: Numerical Mathematics, PDE theory, Electrical Engineering, Control theory, Complex Analysis.

University of Milano-Bicocca — Milan, ITA

Bachelor of Science, Statistics *(110 with honors)* — *Sep. 2019 – Mar. 2022*

- Final Project: "AutoML techniques of Text Classification for a Sentiment Analysis application.", advisor: Prof. M. Cesarini.

Experience

Axiomatic AI — Sep. 2025 – Present

AI Engineer — *Barcelona, ES*

- Developing physics-grounded AI agents at an MIT-spinout, enabling verifiable automated reasoning for scientific discovery.
- Engineered the agentic backend using LangGraph and FastAPI, implementing retrieval-augmented generation (RAG) pipelines that strictly adhere to physical constraints and simulation parameters.
- Contributed to the core technology stack that secured a 3x increase in valuation, specifically by building the reliability tooling that validates LLM-generated designs against formal scientific proofs.

University of Cambridge — Jan. 2025 – Sept. 2025

Visiting Researcher — *Cambridge, UK*

- Developed HypeR, a novel RL-driven mesh adaptivity method for PDEs, surpassing NeurIPS state-of-the-art error reduction by an order of magnitude.
- Created the first-ever adaptive mesh method simultaneously performing vertex relocation and element refinement via hypergraph representation of the mesh.
- Implemented a multi-agent reinforcement learning policy leveraging geometric deep learning and graph neural networks to jointly optimize mesh geometry and topology.
- Targeting ICLR 2025, under supervision of Prof. Pietro Liò, Prof. Carola-Bibiane Schönlieb, and Prof. Stefania Fresca.

ETH University — Mar. 2024 – Oct. 2024

Research Intern — *Zurich, CH*

- Designed and developed a graph-based multi-agent reinforcement learning framework to solve logic puzzles, achieving state-of-the-art extrapolation beyond training distributions.
- Achieved a 2× speed-up and 6× memory reduction by binding Python implementations to optimized C code, enabling efficient scaling to significantly larger puzzle instances.
- Conducted project within ETH Zurich's DISCO research group under supervision of Prof. Roger Wattenhofer; currently extending work into a benchmark to systematically evaluate and improve reasoning capabilities of large language models (LLMs).

SEC Newgate — Jul. 2021 – Oct. 2021

Data Science Intern — *Milan, ITA*

- Built an AutoML NLP pipeline with LIME-based XAI for emotion detection, improving accuracy and enabling interpretable insights for client reputation management.

Publications

Beyond Interpolation: Extrapolative Reasoning with Reinforcement Learning and Graph Neural Networks

Authors: Niccolò Grillo, Andrea Toccaceli, Benjamin Estermann, Joel Mathys, Stefania Fresca, Roger Wattenhofer.

Published in the AAAI Workshop, january 2025. Extended version in preparation for submission to NeurIPS 2025. — Jan. 2025

Projects

High-Performance Scientific Computing | *C++20, MPI, OpenMP, Pybind11* — Jan. 2024 – Jul. 2024

- Developed a hybrid-parallel Laplace solver (MPI+OpenMP) utilizing custom COO/CSR kernels; achieved near-linear strong scaling on cluster benchmarks.
- Integrated C++ backend with Python via Pybind11, enabling high-level scripting of low-level Robin boundary condition solvers.

Time Series & Vision Competitions (1st Place) | *PyTorch, Transformers* — Sep. 2023 - Jan. 2024

- Secured 1st place (1/300) in time-series forecasting by engineering a hybrid Transformer-LSTM architecture with attention mechanisms to capture long-range dependencies.
- Achieved top 5% in vision task using a ViT (Vision Transformer) fine-tuned with contrastive loss (SimCLR).

Survival Analysis for Neuroendocrine Tumors | *R, Survival Pkg* — Jan. 2023 – Jul. 2023

- Modeled "Time to Progression" for radiotherapy patients using Cox Proportional Hazards and Kaplan-Meier estimators; collaborated with Dr. Fiz (Humanitas Institute).

Achievements

Early Graduation. Successfully completed my bachelor curriculum as the top 1 fastest student out of a cohort of over 150 students, graduating one academic year early.

Invited Talk at Cambridge Foundation AI Series. Presented "Beyond Interpolation" at Cambridge's Foundation AI Seminar on leveraging RL and GNNs for extrapolative reasoning and robust generalization.

Technical Skills

Languages — ML Frameworks: Python, C/C++ (C++20), SQL, R, Bash — PyTorch, TensorFlow, PyG, LangGraph, PydanticAI
Technologies: Git, Docker, Linux, MPI, OpenMP, Pybind11, FastMCP, FastAPI, Docker, GCP