Federico Ottomano

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Summary

Passionate **AI scientist** with a strong background in developing cutting-edge **deep learning models** for the **physical sciences**, with a focus on **solid-state Chemistry**. Currently, my main research interests are **Contrastive Learning**, **Geometric Graph Neural Networks** and **Diffusion Models** for inverse materials design.

Education

2020 - 2024 **PhD candidate** in Computer Science at **University of Liverpool**,
Liverpool, UK.

2017 - 2019 **Master of Science (M.Sc.)** in Pure and Applied Mathematics at **University of Rome "Tor Vergata"**,
Rome, Italy.

2014 - 2017 **Bachelor of Science (B.Sc.)** in Applied Mathematics at **University of Rome "Tor Vergata"**,
Rome, Italy.

2008 - 2013 **High School Diploma** at **Liceo Classico "G.Palmieri"**,
Lecce, Italy.

Projects

Discovery of new transparent conducting materials (TCMs) using Machine Learning.
In partnership with Pilkington (NSG Group) (Ongoing)

Transparent conducting materials (TCMs) represent a widespread class of semiconductors for their combined high electrical conductivity and optical transparency, rendering them versatile for various industrial applications. Employing data-driven methods, we collaborated with fellow experimental chemists to gather and validate material data. This data served as foundation for training state-of-the-art machine learning models to predict optoelectronic properties of materials. Finally, we utilized trained models to conduct a large-scale, high-throughput screening on a purpose-built database of experimentally-reported chemical formulas to accelerate the identification of new TCMs.

Not as simple as we thought: a rigorous examination of data-aggregation in materials informatics.
Digital Discovery Journal link

The utilization of Machine Learning in Materials Science is still severly limited by small and fragmented material datasets. Despite the common belief that more data improves performance, our study on the aggregation of material datasets, including various chemical properties, reveals that simple methods (from concatenation to prioritizing chemical diversity) do not enhance predictive accuracy of machine learning models.

Investigating low-data and extrapolation challenges via contrastive learning of chemical compositions.
Spotlight Talk at NeurIPS Ai4Mat link

Inspired by recent advancements in contrastive learning for handling limited training data and extrapolation challenges in materials informatics, we introduce a stoichiometry-focused supervised contrastive learning framework. This approach is particularly relevant, as crystal structure information is typically unavailable prior to material discovery and synthesis.

Spectral and ergodic properties of completely positive maps and decoherence.
M.Sc. thesis link

My master thesis work investigates spectral and ergodic properties of a special class of maps between C*-algebras in the context of general dynamical systems, to address the phenomenon of quantum decoherence.

Publications

Fidaleo, Francesco et al. (2022). "Spectral and ergodic properties of completely positive maps and decoherence". In: *Linear Algebra and its Applications* 633, pp. 104–126. ISSN: 0024-3795. DOI: https://doi.org/10.1016/j.laa.2021.10.007. URL: https://www.sciencedirect.com/science/article/pii/S0024379521003724.

Ottomano, Federico, Giovanni De Felice, et al. (2023). "Investigating extrapolation and low-data challenges via contrastive learning of chemical compositions". In: *AI for Accelerated Materials Design - NeurIPS 2023 Workshop*. **Spotlight Talk**. URL: https://openreview.net/forum?id=3Huw3pa8TR.

Ottomano, Federico, Giovanni De Felice, et al. (2024). "Not as simple as we thought: a rigorous examination of data aggregation in materials informatics." In: *Digital Discovery*. DOI: DOI:10.1039/D3DD00207A.

Conferences & Workshops

Dec 2023 **37th Conference on Neural Information Processing Systems** (Spotlight Talk at Ai4Mat Workshop),
New Orleans Convention Center, New Orleans, LA, USA.

Oct 2023 **The Mathematical foundations of Artificial Intelligence** (Attendance),
London Mathematical Society, London, UK.

Jul 2023 **Pilkington (NSG) internal workshop** (Talk),
Pilkington Technology Centre, Lathom, UK.

Dec 2022 **36th Conference on Neural Information Processing Systems** (Attendance),
New Orleans Convention Center, New Orleans, LA, USA.

Nov 2022 **Pilkington (NSG) Annual Symposium** (Talk),
Pilkington Technology Centre, Lathom, UK.

Sep 2022 **Leverhulme Centre for Functional Materials Design 2nd Biennial Symposium** (Attendance),
Anfield Stadium, Liverpool, UK.

Jan 2022 **Machine Learning Applications for Chemical Materials Development and Discovery** (Attendance),
University of Liverpool, Liverpool, UK.

Other experience

2023 - Present **Reviewer for 'Computational Materials Science'**
Reviewing submissions for 'Computational Materials Science' Journal.

Skills

Deep Learning: PyTorch, PyTorch Geometric, PyTorch Lightning (*proficient*), Tensorflow, Keras (*basic*).

Data analysis: NumPy, Pandas, Sci-kit learn (*proficient*), Pymatgen (*intermediate*), ASE (*basic*).

Programming languages: Python (*proficient*).

Operating Systems: Linux (*intermediate*), mac OS (*proficient*).

Hobbies

Music:
I have a strong affinity for **jazz**, **gospel**, **R&B**, **neo-soul**, and **funk** music.
I firmly believe in the transformative power of studying music, viewing it as a means to enhance one's expressiveness and to release inner emotions that might be challenging to convey in other ways.

2D/3D animation:
From a young age, I cultivated a genuine passion for animation, encompassing both traditional and modern forms.
As a child, I took it upon myself to explore 3D graphics softwares, embracing my inner nerd. I've consistently viewed this creative process as a means to manifest my dreams into reality. In some free moments, I find myself sketching on paper, weaving impromptu stories, and envisioning nonexistent worlds and people.