Book of Abstract

Machine Learning Methods for Complex and Quantum Systems - ML2025

June 4-6

University of Camerino, Italy

List of presenting Authors:

Adriano Barra, "Sapienza" University of Rome, Italy
Gabriele Belegni, University of Camerino, Italy
Rita Bissoonauth, UNESCO, Addis Ababa, Ethiopia
Luca Brodoloni, Complex Quantum Matter group, University of Camerino, Italy
Simone Cantori, Complex Quantum Matter group, University of Camerino, Italy
Emanuele Costa, University of Barcelona, Spain
Andrea Della Valle, Complex Quantum Matter group, University of Camerino, Italy
Giuseppe A. Falci, University of Catania and INFN, Italy
Claudia Germoni, University of Camerino, Italy
Flavio Gerosa, University of Camerino, Italy
Christopher Gies, University of Oldenburg, Germany
Marco Gori, Siena Artificial Intelligence Lab, University of Siena, Italy
Estelle Maeva Inack, Perimeter Institute for Theoretical Physics, Waterloo, Canada
Alexander Kordyuk, Kyiv Academic University, Ukraine and IFW-Dresden, Germany
Jan A. Krzywda, Leiden University, the Netherlands
Gianluca Lagnese, Jožef Stefan Institute, Ljubljana, Slovenia
Nicola Lo Gullo, University of Calabria, Italy
Alessandro Lovato, Argonne National Laboratory, USA
Marica Magagnini, University of Camerino, Italy
Alessio Mancini, University of Camerino, Italy
Stefano Melacci, Siena Artificial Intelligence Lab, University of Siena, Italy
Leonardo Mogianesi, National Doctorate LESDIT - Universities of Camerino and Modena-Reggio Emilia, Italy
Mateusz Molenda, Institute of Physics, Polish Academy of Sciences, Warszawa, Poland
Rosanna Mosetti, "Sapienza" University of Rome, Italy

Pere Mujal, ICFO - The Institute of Photonic Sciences, Spain
Samuel Partey, Regional Bureau for Science and Culture in Europe - UNESCO
Marcin Płodzień, ICFO - The Institute of Photonic Sciences, Spain
Alfio Quarteroni, Politecnico di Milano, Italy and EPFL, Switzerland
Arnau Rios, University of Barcelona, Spain
Grant Rotskoff, Stanford University, USA
Haichen Wang, Ruhr University Bochum, Germany
Francesco Zamponi, "Sapienza" University of Rome, Italy
Zoltán Zimborás, Algorithmiq Ltd, Finland

Shallow Neural Networks: artificial vs biological and distributed vs selective paradigms

Adriano Barra
Sapienza Università di Roma, Italy

In this talk, by using statistical mechanics of spin glasses as the theoretical leitmotiv, I will show the existence of structural similarities among biologically inspired recurrent neural networks (i.e. the Hopfield model equipped with Hebbian learning and some variations on this theme) and multilayer ones whose learning algorithms are instead statistically driven (as for the restricted Boltzmann machine equipped with contrastive divergence). While the former play as the triumph of the connectionist approach, where distributed processing is massively at work, the latter -in the typical "hot coding vector" largely at use in Machine Learning Communities- naturally recover the so-called "grandmother cell setting" theory of Neuroscience, i.e. the opposite limit, overall blurring the line of separation between these two antithetical learning approaches.

[1] Alemanno, F., Aquaro, M., Kanter, I., Barra, A., & Agliari, E. (2023). Supervised hebbian learning. Europhysics Letters, 141(1), 11001.
[2] Agliari, E., Alessandrelli, A., Barra, A., Centonze, M. S., & Ricci-Tersenghi, F. (2025). Generalized hetero-associative neural networks. J. Stat. Mech. 2025(1), 013302.

Other info:
group webpage: https://www.researchgate.net/lab/Agliari-Barra-Lab-CoScienza-Adriano-Barra
speaker webpage: https://www.adrianobarra.com

Denoising Diffusion Probabilistic Models for DAM Prices Forecasting [POSTER]

Gabriele Belegni, Carlo Lucheroni, Federica Astolfi
University of Camerino, Camerino, Italy

Predicting the outcome of future events is crucial in virtually every aspect of the financial world. In the day ahead electricity market (DAM), big electricity generators and distributors, as well as large consumers, can exploit the knowledge of future prices for better scheduling generation resources, resulting in less expenses and, notably,less pollution. In recent years, many deep learning methods have been designed for forecasting. Among them, a particular class of probabilistic models emerged: diffusion models. In this work we show how diffusion models perform in forecasting DAM prices, highlighting how they represent the state-of-the-art models in this specific task.

Neural quantum Monte Carlo algorithms for quantum simulators

[POSTER]

L.Brodoloni[1,2], J. Vovrosh[3], S. Julià-Farré[3], A. Dauphin[3], S.Pilati[1,2]

[1]*School of Science and Technology, Physics Division, Università di Camerino, 62032 Camerino, Italy*

[2]*INFN, Sezione di Perugia, I-06123 Perugia, Italy*

[3]*PASQAL SAS, 24 rue Emile Baudot - 91120 Palaiseau, Paris, France*

Simulating the low-temperature properties of frustrated quantum spin models is a paradigmatic problem in condensed matter physics. It has recently gained strong interest in the context of quantum-enhanced optimization performed via quantum annealers and quantum simulation performed with neutral atoms or with ion traps. We use a recently-developed self-learning projective quantum Monte Carlo algorithm, which is driven by neural-network states, to simulate disordered quantum Ising models at zero-temperature. Our results show that, if the neural ansatz features sufficiently many hidden neurons, this technique provides unbiased estimates of round-state properties and opens up previously inaccessible regimes. First, we investigate the spin-glass phase of the 2D quantum Edwards-Anderson (EA) model and estimate the quantum critical point in the transverse magnetic field. The results for the replica spin-overlap distribution are consistent with replica symmetry breaking in the spin-glass phase [1]. Finally, we investigate the properties of geometrically frustrated models that describe Rydberg atoms arranged in an amorphous configuration. These models are designed to feature well-controlled local structural properties in the absence of long-range order. The results show that the system undergoes a quantum spin-glass transition, with critical exponents consistent with those of the 2D EA Hamiltonian [2]. These studies are promising for understanding the behavior and benchmarking of modern quantum platforms based on neutral atoms.

[1] Brodoloni, L., and S. Pilati. "Zero-temperature Monte Carlo simulations of two-dimensional quantum spin glasses guided by neural network states." Physical Review E 110.6 (2024): 065305.

[2] Brodoloni, L., et al. "Spin-glass quantum phase transition in amorphous arrays of Rydberg atoms." arXiv preprint arXiv:2505.05117 (2025).

Link to the research group: https://cqm.unicam.it/

Synergy between noisy quantum computers and scalable classical deep learning for quantum error mitigation
[POSTER]

Simone Cantori[1,2], Andrea Mari[1], David Vitali[1,2], Sebastiano Pilati[1,2]

[1]*School of Science and Technology, Physics Division, Università di Camerino, Via Madonna delle Carceri, Camerino (MC), 62032, Italy*

[2]*Sezione di Perugia, INFN, Perugia, 06123, Italy*

Abstract: This study integrates (simulated) noisy data from quantum computers with classical neural networks to enhance quantum error mitigation, enabling accurate predictions for circuits with more qubits than those used for training, outperforming zero-noise extrapolation methods.

We investigate the synergy between noisy quantum computers and scalable classical convolutional neural networks (CNNs) to address the challenge of quantum error mitigation [1]. Our approach combines noisy quantum data $z^{(noisy)}$ with classical circuit descriptors $\boldsymbol{\theta}$ to train CNN models capable of predicting accurate expectation values $m_z = \frac{1}{N}\sum_{n=1}^{N} z_n = \frac{1}{N}\sum_{n=1}^{N} \langle\psi\rangle$ for parameterized quantum circuits with N qubits. This method demonstrates significant improvements over traditional error mitigation techniques such as zero-noise extrapolation (ZNE).

As shown in Fig. 1a, classical-only learning struggles to emulate a specific class of quantum circuits [2]. By contrast, the CNN leverages the additional noisy quantum data to achieve better predictions.

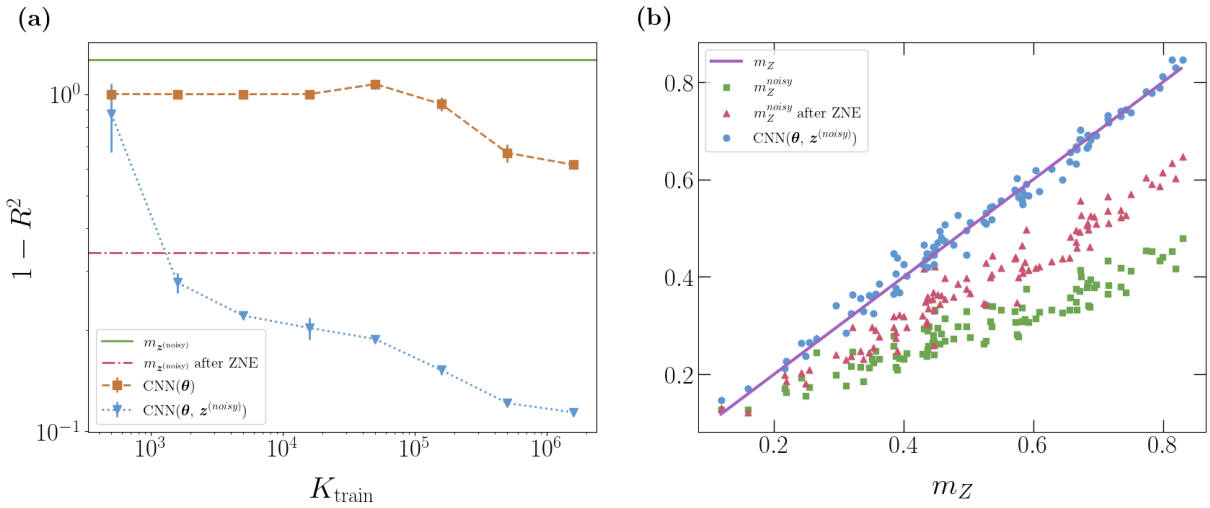


Fig. 1 (a) Prediction error $1 - R^2$ as a function of the number of instances in the training set K_{train}. (b) Scatter plot of predictions versus ground-truth expectation

values m_z for quantum circuits with 16 qubits. The CNN is trained on circuits with less than 10 qubits.

Fig. 1b highlights the strength of our method, showing that CNN predictions not only align closely with ground-truth expectation values but also outperform ZNE-corrected noisy outputs. We utilize a scalable training framework [1-3] where the CNNs are trained on small-scale circuits and successfully generalize to larger circuits.
Additionally, we explore the use of circuit knitting techniques to implement quantum circuits in the neural network training set, enhancing the performance of Variational Quantum Eigensolver algorithms.
These findings demonstrate the potential of combining classical deep learning with noisy quantum computation to enhance the accuracy of quantum circuits [1,4,5], paving the way for more reliable quantum simulations and computations in near-term devices.

References

[1] S. Cantori, A. Mari, D. Vitali, and S. Pilati, "Synergy between noisy quantum computers and scalable classical deep learning for quantum error mitigation", EPJ Quantum Technol. 11, 45 (2024).
[2] S. Cantori, and S. Pilati, "Challenges and opportunities in the supervised learning of quantum circuit outputs", arXiv:2402.04992, (2024)
[3] S. Cantori, D. Vitali, and S.Pilati, "Supervised learning of random quantum circuits via scalable neural networks", Quantum Sci. Technol., 8, 025022, (2023)
[4] Stefan H. Sack, and Daniel J. Egger, "Large-scale quantum approximate optimization on nonplanar graphs with machine learning noise mitigation", Phys. Rev. Research 6, 013223, (2024)
[5] Haoran Liao, Derek S. Wang, Iskandar Sitdikov, Ciro Salcedo, Alireza Seif & Zlatko K. Minev, "Machine learning for practical quantum error mitigation", Nat Mach Intell, 6, 1478–1486, (2024)

Link to the research group: https://cqm.unicam.it/

A Quantum Annealing Protocol to Solve the Nuclear Shell Model

Emanuele Costa, Axel Perez-Obiol, Javier Menendez, Arnau Rios, Artur Garcia-Saez, Bruno Julia-Diaz

University of Barcelona, Spain

The nuclear shell model accurately describes the structure and dynamics of atomic nuclei. However, the exponential scaling of the basis size with the number of degrees of freedom hampers a direct numerical solution for heavy nuclei. In this work, we present a quantum annealing protocol to obtain nuclear ground states. We propose a tailored driver Hamiltonian that preserves a large gap and validate our approach in a dozen nuclei with basis sizes up to 10^5 using classical simulations of the annealing evolution. We explore the relation between the spectral gap and the total time of the annealing protocol, assessing its accuracy by comparing the fidelity and energy relative error to classical benchmarks. While the nuclear Hamiltonian is non-local and thus challenging to implement in current setups, the estimated computational cost of our annealing protocol on quantum circuits is polynomial in the single particle basis size, paving the way to study heavier nuclei.

Machine learning recognition of Volatile Organic Compounds absorption spectra based on experimental and synthetic data

Della Valle, A.[1], D'Arco, A.[2,3], Lupi, S.[3,4], Pilati, S.[5,6], Perali A.[1]
[1]*School of Pharmacy, University of Camerino, Camerino, Italy*
[2]*INFN-LNF, Frascati, Italy*
[3]*Department of Physics, University of Rome 'La Sapienza', Rome, Italy*
[4]*INFN-Sezione di Roma, Rome, Italy*
[5]*School of Science and Technology, University of Camerino, Camerino, Italy*
[6]*INFN-Sezione di Perugia, Perugia, Italy*

Volatile Organic Compounds (VOCs) are characterized by a low boiling point, and they easily evaporate in air. They can be emitted from different sources, both natural and anthropic, contributing to air pollution with dangerous effects on the environment and on human health [1]. Machine learning is increasingly used for the analysis of spectral data [2], suggesting that it might be suitable for the identification of VOCs.

The first part of this work focuses on the realization of a deep learning model for the classification and the quantitative analysis of VOCs' absorption spectra. We generate the training datasets with a multipass gas cell in a Vertex 70v Michelson interferometer, measuring low-concentration VOCs [3].
For each spectrum, the dataset provides the molecular identity, and the concentration of such VOC measured in *ppm*. The dataset is composed of 970 spectra divided in acetone, benzene, ethanol, isopropanol, m-xylene, o-xylene, p-xylene, styrene, and toluene.
The training phase of a deep neural network requires a sufficiently large dataset of examples, which is not always available in this context. For this reason, the second part of this work investigates the creation of synthetic data using a conditional variational autoencoder (cVAE) [4]. The decoder of the cVAE is used to generate synthetic data similar to the experimental spectra. This model extends the generation of new spectra to conditions not present in the original dataset (Fig. 1), e.g., to different concentrations.
This work is divided into three steps:
i) Training of the *master* model on the original experimental dataset to predict molecular identity and concentration;
ii) Training of the cVAE conditioned on the molecular identity and the concentration of the VOC;
iii) Training of the *slave* model on a dataset augmented with synthetic spectra.
The *master* and *slave* models use the same architecture: the model is a deep convolutional neural network, with a sequence of convolutional layers and two heads: a classifier-head recognising the molecular identity, and a multi-regression-head predicting the concentration of the VOC.

In each epoch of the *slave* models' training, the trained conditional decoder is used to generate the synthetic data, with randomly sampled concentrations. These synthetic data are then added to the original training dataset.
The amount of added data is changed to train different *slave* models, and the performance of the model associated with the minimum mean square error is reported in Fig. 2.

The use of cVAE to generate synthetic data not only allows augmentation to train new models but also permits to generate new spectra with concentrations not present in the original training dataset.

References

[1] McDonald, et al. Science, 6377 (2018) 760-764
[2] Mishra, et al. TrAC, 2 (2022) 116804
[3] D'Arco, et al. Sensors, 15 (2022) 5624
[4] Harvey, et al. arXiv:2102.12037 (2022)

Link to the research group: https://cqm.unicam.it/

Figures

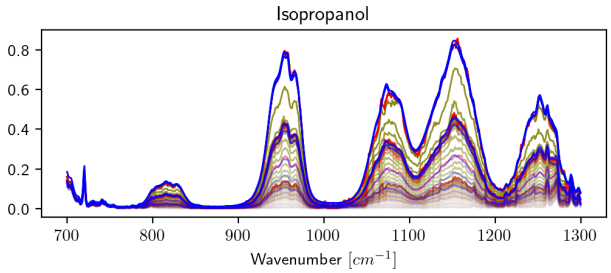


Figure 1. Examples of generated (red, and yellow lines), and original experimental spectra (blue lines) of Isopropanol. Red lines indicate spectra with concentrations available in the dataset, the yellow lines refer to concentrations not present in the dataset.

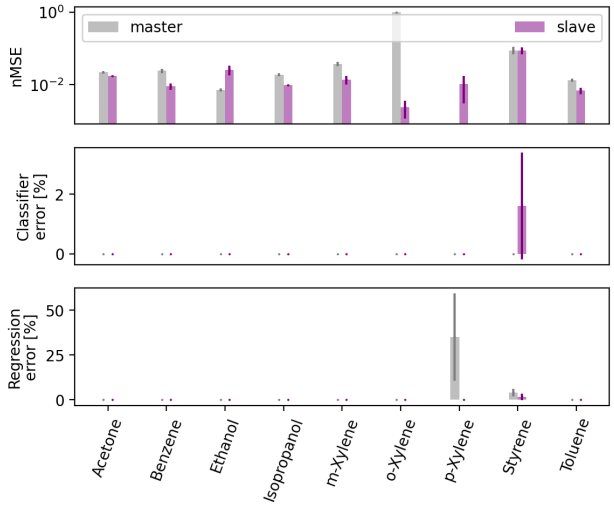


Figure 2. Comparison of performance of master and slave models divided per class on test set.

Graph neural network for social behavioral analysis in rodents [POSTER]

Della Valle, A.[1], Pilati, S.[2,3], Ubaldi, M.[1], Ciccocioppo, R.[1], Perali A.[1]
[1]*School of Pharmacy, University of Camerino, Camerino, Italy*
[2]*School of Science and Technology, University of Camerino, Camerino, Italy*
[3]*INFN-Sezione di Perugia, Perugia, Italy*

Sociality is fundamental in the lives of humans and of many animal species. Social interaction or the lack of it is strongly intertwined with different neuropsychiatric diseases. Social isolation is both cause and effect of many disorders of the central nervous system [1]. The free social interaction test allows a naturalistic and complex analysis of the sociability in rodents [2]. In this behavioural test, two mice are allowed to freely interact in an open field and the amount of time the studied mouse (named "actor") spends interacting with its partner (named "stimulus") is measured. It allows assessing spontaneous behaviours such as grooming, play, aggressive or sexual behaviours, and others. However, while this test permits evaluating different aspects of the sociality, it is quite complex to score. Automatic systems relying on analysis of the distance between animals are usually limited to the detection of simple social behaviours characteristics, such as interaction *vs.* no interaction or active *vs.* passive interaction. On the other hand, the traditional manual scoring allows one to have a finer recognition of the behaviour, but it is prone to human bias, and it requires trained researchers, and it is time-consuming [3]. To overcome these limitations, machine learning (ML) algorithms are increasingly used for social behaviour analysis in rodents. Such interest has increased also thanks to the publication of dataset, including the CalMS21 dataset [4].

In this work, we use graph convolutional neural networks (GCNN) models for the recognition of the mice social behaviours. As network input, we use the coordinates of characteristic keypoints. Training and testing are performed on the CalMS21 dataset, which is composed on the time sequence of 7 keypoints per animal, extracted from top-view camera recording two interacting mice. For each frame, an expert researcher classified one of four possible behaviours (attack, investigation, mount or other) performed by the "actor" mouse.
For our GCNN model, the input data are organized in a fixed shaped graph (see Fig. 1a), with the edges encoding a temporal sequence of the inverse of the distances between the corresponding nodes, and the nodes encoding a categorical tag corresponding to the two animals. This choice allows us to have a representation invariant under geometrical transformations useful for the classification of the behaviours (such as global rotations and translations) and giving more importance to closer nodes. To account for temporal contextuality, the models have access to the coordinates of 29 future and past frames.
The architecture of the GCNN model is sketched in Fig. 1b. It permits mixing the temporal and spatial information. This model is compared with standard convolutional networks relying only the sequences of coordinates or the sequences of the inverse of the distances. The models using the distances of the nodes reach better performance with respect to the coordinates-based models. Moreover, as shown in Table 1, the proposed GCNN model reaches the best performance,

demonstrating the capability of the GCNN to encode the spatiotemporal features useful to recognize the social behaviours in mice.

Table

Model	F1-score$_{social}$	Accuracy
Conv1D on coordinates	71 ± 1	86.4 ± 0.8
Conv1D on distances (inverse)	79.7 ± 0.7	90.2 ± 0.2
GCNN	86.3 ± 0.3	91.6 ± 0.3

Table 1. Comparison of performances for different input data's structure. Data are shown with mean ± standard deviation over 5 runs of training.

Figures

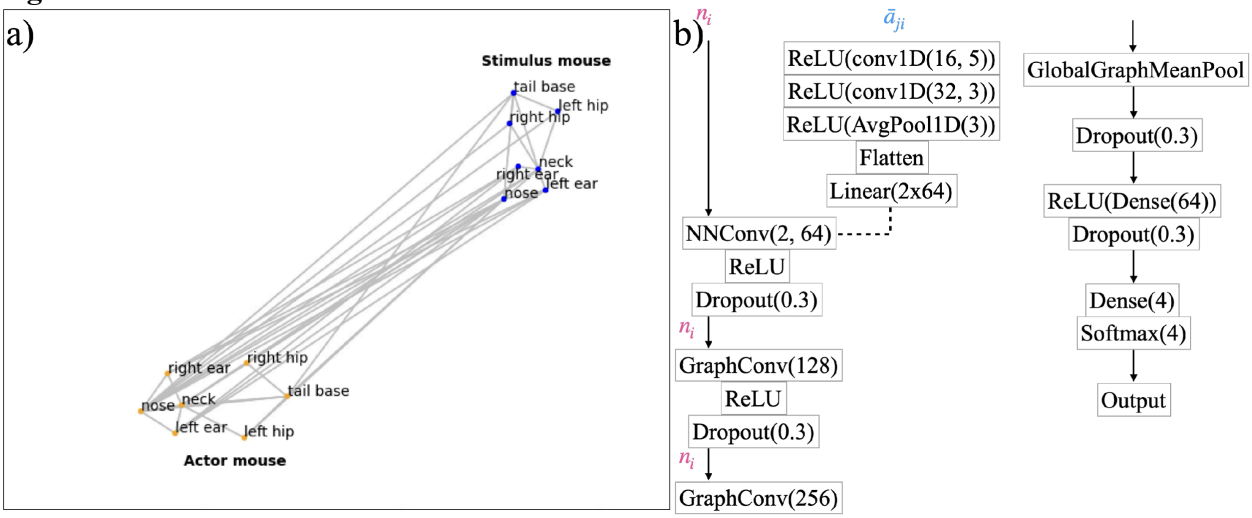


Figure 1. a) Graphical representation of the adopted graph. Most of the connections are based on the facial keypoints, since those animals interact prevalently via the olfactory system. b) Architecture of the graph convolutional neural network.

References

[1] Leong, Victoria et al. "Editorial: Social Interaction in Neuropsychiatry." Frontiers in psychiatry vol. 12 683158. 29 Apr. 2021, doi:10.3389/fpsyt.2021.683158

[2] File, S E, and J R Hyde. "Can social interaction be used to measure anxiety?." British journal of pharmacology vol. 62,1 (1978): 19-24. doi:10.1111/j.1476-5381.1978.tb07001.x

[3] Gulinello, Maria et al. "Rigor and reproducibility in rodent behavioral research." Neurobiology of learning and memory vol. 165 (2019): 106780. doi:10.1016/j.nlm.2018.01.001

[4] Sun, Jennifer J et al. "The Multi-Agent Behavior Dataset: Mouse Dyadic Social Interactions." Advances in neural information processing systemsvol. 2021,DB1 (2021): 1-15.

Link to the research group: https://cqm.unicam.it/

Noise Classification in small Quantum Networks by Supervised Learning: time, space and energy correlation.

Giuseppe A. Falci
University of Catania and INFN - Catania section, Italy

We investigate a machine learning based classification of noise acting on a small quantum network with the aim of detecting spatial or multilevel correlations, and the interplay with Markovianity. We control a three-level system by inducing coherent population transfer exploiting different pulse amplitude combinations as inputs to train a feedforward neural network. We show that supervised learning can classify different types of classical dephasing noise affecting the system. Three non-Markovian (quasi-static correlated, anti-correlated and uncorrelated) and Markovian noises are classified with more than 99% accuracy. On the contrary, correlations of Markovian noise cannot be discriminated with our method. Our approach is robust to statistical measurement errors and retains its effectiveness for physical measurements where only a limited number of samples is available making it very experimental-friendly. Our result paves the way for classifying spatial correlations of noise in quantum architectures [1]. To this end, we propose a design of a sensor consisting in two ultra-strongly coupled qubits driven by a two-tone field. The dynamics is reduced to an effective three-level system in a ladder configuration. We analyze the parameters regime for which it is possible to effectively apply a STIRAP protocol transferring population from the ground state of the two-qubits to the doubly excited state and classify correlations of noise affecting the two qubits [2].

[1] Shreyasi Mukherjee, Dario Penna, Fabio Cirinnà, Mauro Paternostro, Elisabetta Paladino, Giuseppe
A. Falci, Luigi Giannelli, Noise Classification in Three-Level Quantum Networks by Machine Learning,
Machine Learning: Science and Technology 5, 045049 (2024),
https://doi.org/10.1088/2632-2153/ad9193
[2] Dario Fasone, Shreyasi Mukherjee, Dario Penna, Fabio Cirinnà,Mauro Paternostro, Elisabetta
Paladino, Luigi Giannelli and Giuseppe A. Falci,AI-assisted detection of noise correlations by a two-qubit
device, preprint 2025.

Probabilistic Forecasting of Corporate Time Series
[POSTER]

Carlo Lucheroni, Rebecca Pettinari, Beatrice Fusini, Claudia Germoni
University of Camerino, Camerino, Italy

Forecasting future sales values is a fundamental goal for any company, as it helps optimize inventory management and improve the supply chain. The more accurate the forecasts are, the better the resulting decisions can be.
In order to obtain a more nuanced understanding of future outcomes, it is often beneficial to adopt a probabilistic forecasting strategy. For each future time step, probabilistic methods return a range of possible outcomes with corresponding probabilities, rather than a single value (as in point forecast). In addition to classical probabilistic methods, in recent years more robust techniques based on deep learning have been developed for forecasting tasks.
The current work aims to investigate whether these new strategies, which are usually more complex than classical methods, always bring the best results.

Spatio-temporal Graph Neural Networks for DAM prices forecasting

Flavio Gerosa
University of Camerino, Camerino 62032, Italy

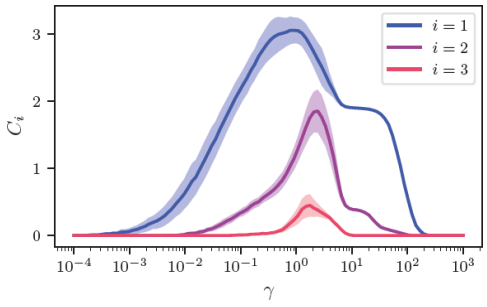
This work investigates the internal mechanisms of spatio-temporal Graph Neural Networks (ST-GNNs) for multivariate time series forecasting. GNNs are neural architectures designed for graph-structured data; ST-GNNs extend these models by capturing both spatial and temporal dependencies. In particular, we model Day-Ahead Market (DAM) electricity prices, structuring each hourly series as a node and inter-hour correlations as edges to forecast values. The models propagate information across the graph and evolve node embeddings over time. Benchmarking against econometric and machine learning models highlights the superior ability of ST-GNNs to uncover latent structures and complex dynamic interactions often missed by traditional approaches.

Open quantum systems as a platform for machine learning

Niclas Götting, Nils-Erik Schütte, Steffen Wilksen, Alexander Steinhoff,
and Christopher Gies
Institute for Physics, Carl von Ossietzky Universität Oldenburg, Oldenburg, Germany

Quantum machine learning (QML) is a vibrant research field with widespread application potential. Importantly, QML can be performed on the noisy intermediate-scale quantum (NISQ) computers that we currently have available. An alternative to gate-based QML approaches lies in using complex physical systems and exploit their inherent dynamics for computing tasks, then termed quantum reservoir computing (QRC) [1,2]. The machine learning paradigm of reservoir computing has proven to be well-suited for various applications such as autonomous learning and time-series prediction. While classically implemented reservoir computers have been researched extensively, their quantum mechanical counterparts are only now coming into the focus of the research community. The promises they bring to the table are, among others, exponential phase-space dimension scaling with system size, and entanglement as a resource without classical analogue.

The presentation gives an introduction to the field and focusses on two aspects: First is the relationship between the reservoir's performance for QML and its *physical* properties in terms of the optical absorption. Connecting both enables us to provide an intuitive explanation of the "sweet-spot" behavior (see the figure) of the QRC performance as a function of dissipation that was reported by several groups.



Short-term memory capacity of degree i in a three-qubit quantum reservoir computer as a function of the dephasing rate γ, exhibiting a sweet-spot behavior for the reservoir's performance. Interestingly, we find a strikingly similar behavior in the optical absorption.

The second aspect addresses, on a more abstract level, measures of expressivity in quantum reservoir computing. In establishing a link between gate-based quantum machine learning and reservoir computing, we show that the role of the reservoir itself is of little impact for its capability to produce non-linear output functions of a given input signal. Moreover, for the currently suggested input-encoding schemes, no exponential advantage of the quantum system can be exploited, posing the general question of quantum advantage in the field of machine learning.

[1] D. Brunner et al., Roadmap on Neuromorphic Photonics, arXiv:2501.07917 (2025)

*[2] P. Mujal et al., Opportunities in Quantum Reservoir Computing and Extreme Learning Machines, Adv. Quant. Technol. **4**, 202100027 (2021)*
*[2] N. Götting et al., Exploring quantum mechanical advantage for reservoir computing, PRA **108**, 052427*
[3] N. Götting et al., Connection between memory performance and optical absorption in quantum reservoir computing, arxiv:2501.15580 (2025)
[4] N.-E. Schütte et al., Expressivity Limits of Quantum Reservoir Computing, arXiv:2501.15528 (2025)

Variational Neural Annealing: Optimization in Physics, Biology, and Finance

Estelle Maeva Inack
Perimeter Institute for Theoretical Physics, Waterloo, Canada

Variational Neural Annealing (VNA) [1] is an innovative optimization framework that emulates classical and quantum annealing processes by integrating variational principles with neural network parameterizations. It effectively utilizes autoregressive models to represent classical and quantum probability distributions during the annealing process, creating a new avenue for exploring complex energy landscapes, such as those encountered in disordered Ising glasses, protein folding, and portfolio optimization.
In this presentation, we will explore the foundational aspects of VNA, starting with its original formulation and extending to its applications across various domains. We will demonstrate, through case studies on prototypical spin glass Hamiltonians, that VNA outperforms traditional simulated classical and quantum annealing methods, particularly in asymptotic limits [1]. Furthermore, we will emphasize VNA's capacity to identify the folded states of lattice protein models [2] and optimize investment portfolios in complex financial environments [3].

[1] "Variational neural annealing", Mohamed Hibat-Allah, Estelle M. Inack, Roeland Wiersema, Roger G. Melko, and Juan Carrasquilla. Nature Machine Intelligence, 3(11):952–961, October 2021
[2] "Lattice Protein Folding with Variational Annealing", Shoummo Ahsan Khandoker, Estelle M. Inack, Mohamed Hibat-Allah, arXiv:2502.20632
[3] "Portfolio Optimization with variational neural annealing", Nishan Ranabhat, Behnam Javanparast, David Goerz, and Estelle M. Inack, manuscript in preparation

Unraveling Electron Interaction Mechanisms in Photoemission Spectra with Machine Learning

Alexander Kordyuk

Kyiv Academic University, Ukraine and IFW-Dresden, Germany

We develop a machine learning-based framework for identifying electron interaction mechanisms in angle-resolved photoemission spectroscopy (ARPES) data. The ML models are trained on synthetic spectra generated using physically motivated parameters, informed by extensive ARPES experimental experience. This approach allows the algorithm to recognize interaction mechanisms responsible for distinct spectral features. We demonstrate the capability of the method to disentangle coherent and incoherent contributions in high-Tc cuprates and try to identify key spectral characteristics responsible for the enhancement of superconducting critical temperature.

Reinforcement Learning for Adaptive Qubit Control

Jan A. Krzywda, and Evert van Nieuwenburg
⟨*aQaL*⟩ *Applied Quantum Algorithms, LIACS, Universiteit Leiden*

Achieving high-fidelity quantum information processing is often hindered by uncontrolled environmental interactions, which induce parameter fluctuations and degrade algorithmic performance. This work explores stabilizing qubit control by exploiting temporal correlations in these fluctuations through advanced feedback-based methods, moving beyond repeated, static estimations of expectation values.

One approach is real-time tracking of Hamiltonian parameters, which originally achieved a three-orders-of-magnitude enhancement in phase gate performance [0]. More recently, in collaboration with an experimental group, we have demonstrated coherent qubit oscillations driven by stochastic noise [1]. We have further improved estimation fidelity and speed through algorithms based on physics-informed models [2], minimal posterior uncertainty [3], and adaptive sampling time and phase control [4]. The algorithms leveraged the sub-ms data processing capabilities of field-programmable gate arrays (FPGAs), which allow for mitigating higher-frequency noise.

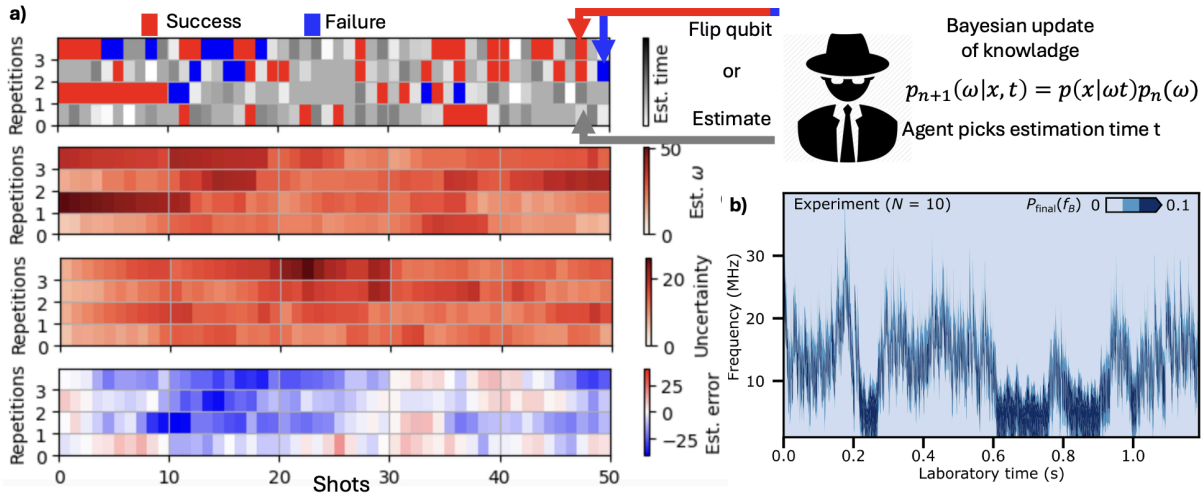


Figure 1 lustration of 4 repetitions of RL scheme, each with 50 shots. For each shot, the agent chooses between the estimation and execution phases, updates its knowledge using Bayesian inference, and selects an estimation strategy. b) Physics-informed estimation of the nuclear field trajectory from [2] (≈ 0.1ms per estimation)

To address faster and more complex environments, we developed a reinforcement learning strategy that optimizes the trade-off between estimation time and algorithm fidelity. By interacting with a simulated environment, the agent learns to exploit temporal noise correlations

through experience, without requiring prior knowledge of the noise model [5]. Analysis of the learned policy reveals adaptive resource allocation between estimation and operation shots, as well as distilled estimation strategies suitable for real-time implementation.

These findings enable FPGA-based implementations of adaptive control algorithms trained on experimental and emulated data, offering a novel active and data-driven paradigm to enhance near-term quantum computing.

[0] M. Shulman, S. Harvey, J. Nichol et al.,Nature Communications 5, 5156 (2014)
*[1] F. Berritta, T. Rasmussen**, J. A. Krzywda**, et al., Nature Communications, 15(1), 1676 (2024)*
*[2] F. Berritta, **J. A. Krzywda** et al., Physical Review Applied, 22(1), 014033. (2024)*
*[3] J. Benestad**, J. A. Krzywda** et al., SciPost Physics, 17(1), 014. (2024)*
*[4] F. Berritta, J. Benestad, L. Pahl, M. Mathews, **J. A. Krzywda** et al. arXiv:2501.05386 (2025)*
*[5**] J. A. Krzywda**, E. van Nieuwenburg, Manuscript in preparation (2025)*

Positive Operator Valued Measures Neural Networks for simulation of light-matter coupled systems

Gianluca Lagnese[1], Darrik Chang[1,2], Markus Schmitt[4], Zala Lenarčič[1]
[1]*Jozef Stefan Institute, SI-1000 Ljubljana, Slovenia*
[2]*ICFO—Institut de Ciències Fotòniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels, Spain*
[3]*ICREA—Institucio Catalana de Recerca i Estudis Avançats, 08015 Barcelona, Spain*
[4]*Forschungszentrum Julich GmbH, Peter Grünberg Institute, Quantum Control (PGI-8), 52425 Julich, Germany*

We employ a recently proposed numerical approach [1] to model open systems dynamics. This methodology is based on the positive operator valued measure (POVM) description of the quantum state: such representation is naturally interpreted as a probability distribution over a complete set of measurements, which can be approximated by a neural network. Then we exploit a time-dependent variational principle (TDVP) to project the dynamics of the evolved state over the neural network manifold. As an example, we target systems made of arrays of atoms trapped in an optical or tweezer lattice with photo-mediated dipole-dipole long-range interaction and correlated dissipation between them. When atoms are placed at distances smaller then the wavelength of light and are prepared in a all-excited state, such a system exhibits a superradiant burst, followed by a non-trivial "subradiant" critical regime with slow power-law relaxation [2, 3]. We explore whether the considered numerical technique has the capacity to described such long-range interacting open systems up to very long times, where the interesting correlated regime appears. A crucial question that we address is the upscaling to larger system sizes, as a potential complementary tool to more standard tensor network techniques, which are not efficient for long-range interacting and two dimensional setups.

[1] M. Reh, M. Schmitt, and M. Garttner, Phys. Rev. Lett. ¨127, 230501 (2021).
[2] L. Henriet, J. S. Douglas, D. E. Chang, and A. Albrecht, Phys. Rev. A 99, 023802 (2019).
[3] S. J. Masson, A. Asenjo-Garcia, Nat Commun 13, 2285 (2022).

Predicting fermionic densities using a Projected Quantum Kernel method

Francesco Perciavalle[1,2], Francesco Plastina[1,2], Michele Pisarra[1,2], Nicola Lo Gullo[1,2]
[1] *Dipartimento di Fisica, Università della Calabria, 87036 Arcavacata di Rende (CS), Italy*
[2] *INFN–Gruppo collegato di Cosenza*

Machine learning is rapidly emerging as a powerful tool in quantum science, while quantum science is also offering new insights and resources for advancing machine learning. On the one hand, machine learning methods have been successfully applied to solving complex quantum physics problems, and on the other hand, the peculiar features of quantum systems have been proposed to improve the performance of classical machine learning algorithms, leading to the emergence of the field of quantum machine learning.
In this talk I present a proposal of a machine learning method to predict the density distribution of one-dimensional fermionic systems. The method we use is a support vector machine (SVM), a supervised learning model whose purpose is to predict the underlying pattern that relates input and output data by mapping the former to an extended space. Specifically, we use a projected quantum kernel (PQK), whose working principle is based on encoding input data into a controllable quantum simulator, identified as a quantum reservoir and experimentally implementable with Rydberg atoms. The input data are given by the features of the external potential to which the fermions are subjected. We compare our results with two well-known classical SVM methods such as the linear kernel and the radial basis function (RBF) kernel. For both quantum problems studied, we find a general common behavior in time of the PQK error that is characterized by a plateau at short times, a sudden drop and then a stabilization. During the stabilization, the PQK outperforms the linear kernel and competes with the RBF kernel.

[1] Francesco Perciavalle, Francesco Plastina, Michele Pisarra, Nicola Lo Gullo,
https://arxiv.org/abs/2504.14002

Variational Learning Quantum Wave Functions

Alessandro Lovato
Argonne National Laboratory, USA

The quantum many-body problem is ubiquitous in physics, with profound implications for condensed matter, quantum chemistry, and nuclear physics. Solving it accurately presents significant challenges due to the exponential growth of the Hilbert space, limiting the applicability of numerically exact techniques to relatively small systems. In this talk, I will discuss how artificial neural networks can be employed to efficiently represent quantum many-body states. I will focus on a variational Monte Carlo method based on neural-network quantum states, which provides a systematically improvable solution to the nuclear Schrödinger equation with a polynomial cost in the number of nucleons. Beyond the nuclear many-body problem, I will also explore applications to condensed-matter systems, such as cold Fermi gases near the unitary limit. Finally, I will offer perspectives on accessing the linear response of confined quantum many-body systems.

Understanding Machine Learning Decisions: Counterfactual Explanations for the k-Nearest Neighborhood Rule

Emilio Carrizosa[1], Renato De Leone[2], Marica Magagnini[2]
[1] Universidad de Sevilla, Sevilla 41012, Spain
[2] Università di Camerino, Camerino 62032, Italy

Machine Learning algorithms usually make decisions without providing any explanations on how they were reached. As a result, such models are not understood and trusted by the users. Moreover, very often, the inherent variability and noise present in real-world scenarios are reflected by data with feature uncertainty, making it a common challenge in machine learning. In sensitive contexts, such as those involving uncertain data, the generation of robust explanations is crucial, they should be able to account for the variability of uncertainty while still offering a degree of freedom.
Counterfactuals are user-friendly explanations that provide valuable information to determine what
should be changed in order to modify the outcome of a black box decision-making model without revealing the underlying algorithmic details [2].
We propose an optimization problem to obtain counterfactual explanations when a k-Nearest Neighborhood classifier is employed in a binary classification. The geometrical framework of the problem supports the quality of the explanations [1].
The approach is extended to handle data with uncertain features that are modeled as convex sets [3]. First, the endogenous solution is introduced. Then, we present a heuristic algorithm based on the Variable Neighborhood Search (VNS) methodology [4]. This heuristic aims to refine an initial feasible solution by constructing counterfactuals that are closer to the input instance, thus improving the solution's proximity.

Keywords: Machine Learning; Mathematical Optimization; Counterfactual Explanations; Uncertain Data; Robust Models.

[1] Magagnini, M., Carrizosa, E. & De Leone, R. "Nearest Neighbors Counterfactuals", in Nicosia, G., Ojha, V., Giesselbach, S., Pardalos, M.P., Umeton, R. (eds) Machine Learning Optimization and Data Science. LOD ACAIN 2024, Series B (Methodological) 58(1), pp. 211–226, 2025.
[2] Guidotti, R., "Counterfactual Explanations and How to find them: literature review and benchmarking", Data Min Knowl Disc, vol. 38, pp. 2770–2824, 2024.
[3] Carrizosa, E., Guerrero, V., & Romero Morales, D., "Visualizing data as objects by dc (difference of convex) optimization", Math. Program, vol. 169, pp. 119–140, 2018.

[4] Carrizosa, E., Dražić, M., Dražić, Z., & Mladenović, N., "Gaussian variable neighborhood search for continuous optimization" Computers & Operations Research, vol. 39, pp. 2206–2213, 2012.

Machine Learning Models for Predicting Multidrug-Resistant Infections and Identifying Features in Retained Introns

Alessio Mancini[1], Emanuela Merelli[2], Marco Piangerelli[2], Sandra Pucciarelli[1] and Leonardo Vito[1,2].

[1]School of Biosciences and Veterinary Medicine, University of Camerino, Italy;
[2]School of Sciences and technology, Computer Science Division, University of Camerino, Italy

Machine Learning methods are increasingly being integrated into medical research, offering significant potential to enhance disease diagnosis and treatment through the effective use of algorithms and tools (1). The availability of extensive high-quality data can improve our understanding of risk factors for various conditions, including cancer, neurological disorders, and healthcare-acquired infections. Our work focuses on applying Machine Learning (ML) models to predict patients' risk of contracting multidrug-resistant urinary tract infections (MDR UTIs) post-hospitalization and to identify nucleotide features responsible for intron retention, providing insights into gene regulation, disease mechanisms, and potential therapeutic targets (1).

For the first study, we utilized DSaaS on a real antibiotic stewardship dataset to predict antibiotic resistance within the Clinical Pathology Operative Unit of the Principe di Piemonte Hospital in Senigallia, Marche, Italy (2). The dataset included information on 1,486 hospitalized patients with nosocomial urinary tract infections (UTIs), using variables such as sex, age, age class, ward, and time period to predict the onset of MDR UTIs. ML methods, including Catboost, Support Vector Machine, and Neural Networks, were employed to build predictive models. Performance metrics such as accuracy (ACC), area under the receiver operating characteristic curve (AUC-ROC), area under the Precision-Recall curve (AUC-PRC), F1 score, sensitivity (SEN), specificity, and Matthews correlation coefficient (MCC) were used for evaluation. Catboost demonstrated the best predictive performance, achieving the highest values across all metrics (MCC 0.909; SEN 0.904; F1 score 0.809; AUC-PRC 0.853; AUC-ROC 0.739; ACC 0.717). The predictive model developed with DSaaS can serve as a valuable support tool for physicians treating hospitalized patients at high risk of acquiring MDR UTIs. These results were obtained using five easily accessible predictors for each patient hospitalization (2). Future enhancements to DSaaS will include unsupervised ML techniques, streaming data analysis, distributed calculation, and big data storage and management, enabling researchers to perform comprehensive data analysis. The DSaaS prototype is available as a demo at the following address: DSaaS Demo.

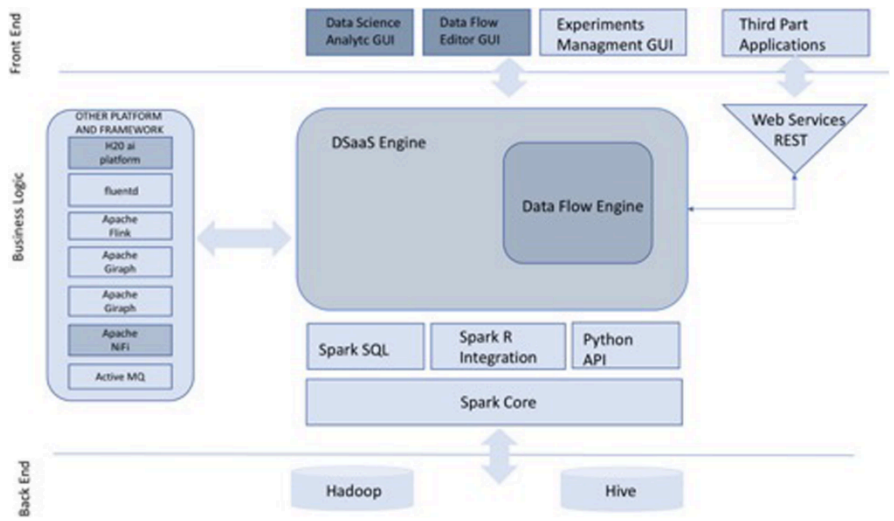


Fig. 1 DSaaS future architecture. In dark gray are shown the operative modules

described in this paper and already operative. In light gray are showed the modules that will be implemented in the future to perform data flow editing, R scripting and a Stewardship UI

For the second study, we analyzed genomic and transcriptomic sequences from the ciliate *Tetrahymena*. *Tetrahymena* exhibits the highest number and percentage of genes with Alternative Splicing (AS) of introns reported in a unicellular eukaryote (3). AS results in the formation of multiple mRNAs from a single gene sequence, which are then translated into corresponding protein isoforms. A specific type of AS is intron retention (IR), where certain introns remain unspliced in the mature mRNA. These retained introns (RIs) may contain premature termination codons, leading to the production of truncated proteins if translated (3). The mechanism determining which introns are retained or removed during splicing remains unknown. We examined various features of intronic sequences, including the absence of repetitive nucleotide motifs (quantified as "entropy"), GC content, and the complexity of secondary structures estimated by the Lempel-Ziv (LZ) measure. Our findings suggest that the key distinguishing features of retained introns (RIs) compared to constitutively spliced introns include a reduced presence of repetitive nucleotide motifs and more compact secondary structures near the 3' splice sites. These features appear to weaken splicing signals, impairing the recognition of intronic sequences and resulting in IR (Fig. 2). Our work provides insights into the regulatory mechanisms underlying intron retention in various organisms and highlights its potential role in modulating phenotypic plasticity. Understanding intron retention patterns in individual patients can offer insights into disease mechanisms and guide the development of personalized treatment strategies.

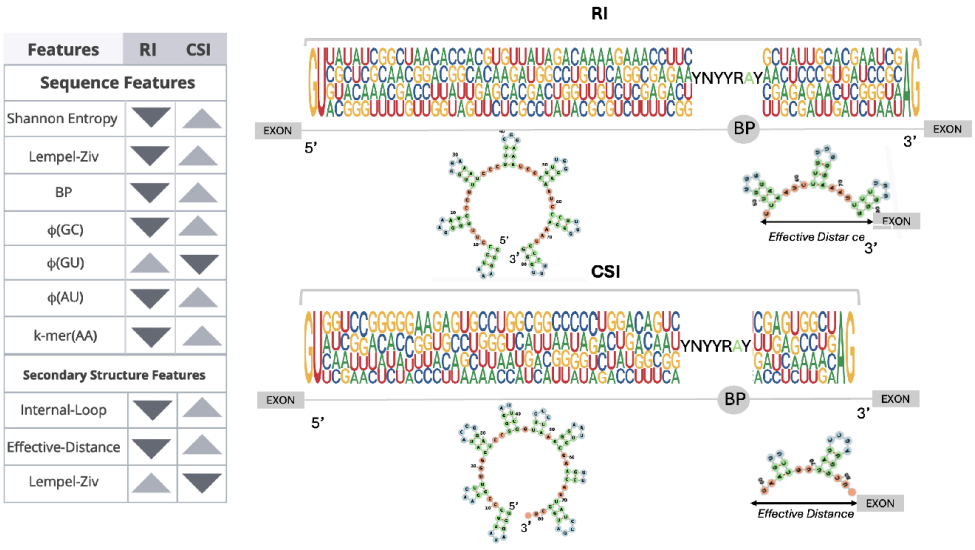


Fig. 2 Differences in features between retained introns (RIs) and constitutively spliced introns (CSIs) are presented. On the left, the features that distinguish RIs from CSIs are listed, with arrows indicating whether the frequency of each feature is higher or lower in the respective intron classes. On the right, a graphical representation illustrates these differences, with GU and AG denoting the highly conserved dinucleotides at the 5' and 3' ends of the introns, respectively. The degenerated YNYYRAY sequence, with the highly conserved A (highlighted in bold), represents the branching motif. The horizontal dotted lines indicate the effective distance between the branching point and the 3' end, i.e. taking into account the RNA secondary structures. The higher entropy in the RI sequences is represented by letters of uniform size,

indicating equal probability for each nucleotide. In contrast, the lower entropy in the CSI sequences is represented by letters of varying sizes, reflecting the differing probabilities of each nucleotide.

In summary, applying ML to predict intron retention and multidrug-resistant infections helps researchers analyze complex data, identify key features, and develop predictive models that provide insights into gene regulation and disease mechanisms. This approach can ultimately contribute to the development of new diagnostic and therapeutic strategies.

References:

1- *Mancini A, Pucciarelli S, Lombardi FE, Barocci S, Pauri P, Lodolini S. Differences between community- and hospital-acquired urinary tract infections in a tertiary care hospital. New Microbiol. 2019;9:43 [1]:[Epub ahead of print]. PMID: 31814033.*
2- *Mancini, A., Vito, L., Marcelli, E. et al. Machine learning models predicting multidrug resistant urinary tract infections using "DsaaS". BMC Bioinformatics **21** (Suppl 10), 347 (2020). https://doi.org/10.1186/s12859-020-03566-7*
3- *Nielsen, H. & Johansen, S. D. Group i introns: Moving in new directions. RNA Biol 6, 375–383, DOI: 10.4161/rna.6.4.9334 (2009).*

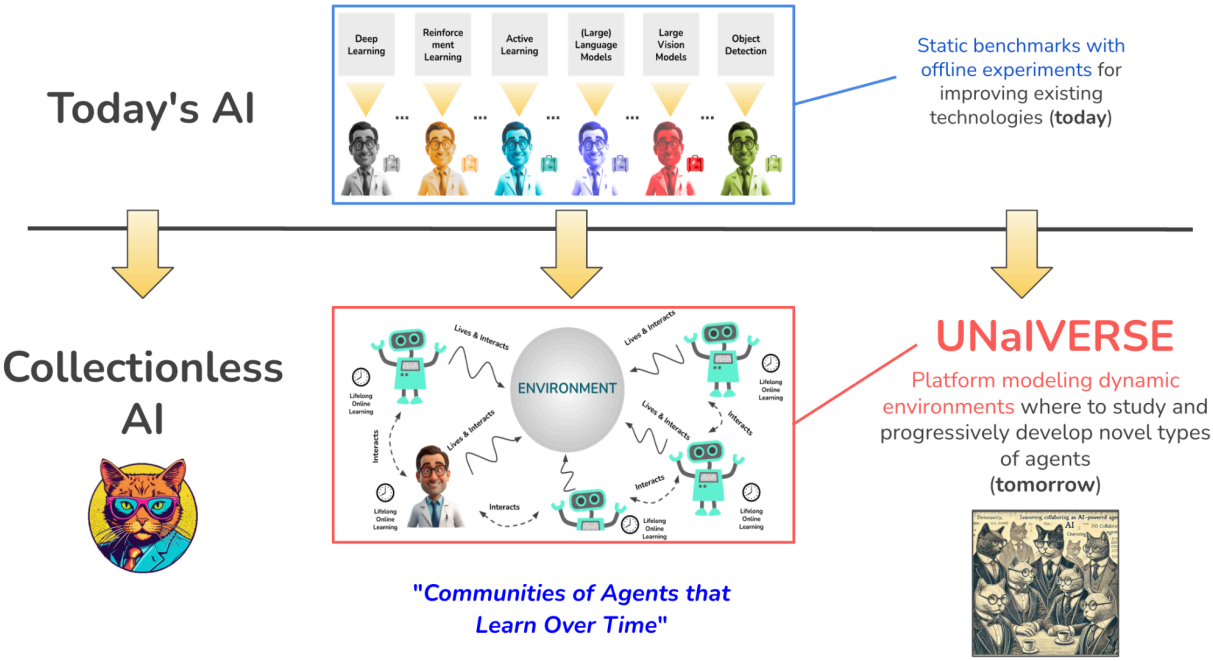
Collectionless AI: The UNaIVERSE Project

Stefano Melacci, *Università degli Studi di Siena*, stefano.melacci@unisi.it
Marco Gori, *Università degli Studi di Siena*, marco.gori@unisi.it

Collectionless Artificial Intelligence (Collectionless AI, Gori and Melacci [2023], https://collectionless.ai) focuses on the perspective in which intelligent agents are developed by learning over time, continuously adapting to the streamed information without storing it, and interacting with the environment, other agents, and humans. This is radically different from the usual procedure of collecting huge datasets and massively learning in an offline manner by stochastic gradient descent or using batches of pre-collected interactions for reinforcement learning. As remarked in [Gori and Melacci, 2023], learning from data collections introduces risks related to data centralization, privacy, energy efficiency, limited customizability, and control. Collectionless AI promotes on-the-edge local computations, where communities of agents learn to interact in an efficient-and-controlled way with each other. This is the context in which the authors of this abstract conceived and introduced the UNaIVERSE project. UNaIVERSE is to Collectionless AI what training and benchmarking based on static datasets are to today's AI. Actually, it is more general than that. UNaIVERSE is a dynamic conceptualization of the notion of learning settings and benchmarks, designed for studying Collectionless AI technologies, but open and fully compatible with other machine learning technologies, allowing them to be studied in a dynamic setting of continuous learning, interaction, progressive development. Classic benchmarking procedures are based on static data collections which are used to train models and static test sets which (hopefully) represent the considered task. UNaIVERSE provides a framework to implement the environment where the agents live, but also how they live, how they can get in touch, and how humans can get in touch with them to see what they are doing, evaluating them by direct interaction. Recall that we (humans/casual users) decide that a Large Language Model works well just by interacting with it, and not by running a benchmark. In a nutshell, static datasets are limited samples of the operating conditions in which the model is expected to work, while UNaIVERSE offers a framework to simulate the environment(s) where agents can develop themselves, being them a simulation of reality or the reality itself. Imagine a world where you can grow your agent, decide who it interacts with, control its exposure, and effectively improve it over time–potentially over a lifetime. UNaIVERSE is such a world. A first prototype of UNaIVERSE, intended to showcase a basic synchronous version of what has been described so far, with agents fully generalizing generative models, classification problems, continual learning, local learning over time, and others, is available at https://github.com/mela64/NARNIAN. This is just an initial implementation to showcase the potentiality of UNaIVERSE (and related research, such as Tiezzi et al. [2024a,b]), intended to be a basis to start building the fundamentals of a framework that we imagine as a

social network of learning agents aggregated in communities and operating in a server-less manner.

Figures



References

- *Marco Gori and Stefano Melacci. Collectionless artificial intelligence, 2023. URL https://arxiv.org/abs/2309.06938. Accepted for publication as a Position Paper at the IEEE International Joint Conference on Neural Networks 2025.*
- *Matteo Tiezzi, Simone Marullo, Federico Becattini, and Stefano Melacci. Continual neural computation. In Joint European Conference on Machine Learning and Knowledge Discovery in Databases, pages 340–356. Springer, 2024a.*
- *Matteo Tiezzi, Michele Casoni, Alessandro Betti, Marco Gori, and Stefano Melacci. State-space modeling in long sequence processing: A survey on recurrence in the transformer era. arXiv preprint arXiv:2406.09062, 2024b.*
- *Stefano Melacci, Alessandro Betti, Michele Casoni, Tommaso Guidi, Matteo Tiezzi, and Marco Gori. A unified framework for neural computation and learning over time, 2024. URL https://arxiv.org/abs/2409.12038*

Links

- *https://collectionless.ai*

MetaHumanTutor: A Realistic AI-Based Virtual Assistant for University Physics Education [POSTER]

Leonardo Mogianesi[1]; Giulia Paludo[2]; Francesco Rasponi[3]; Daniela Amendola[1]; Andrea Perali[1]

[1]University of Camerino, Camerino, Italy
[2]University of Trento, Trento, Italy
[3]University of Napoli, Camerino, Italy

Artificial intelligence (AI) tools have accelerated the evolution of teaching practices in recent years, boosting especially the aspects of interactivity and hands-on activities. This research tries to enhance university-level exercise sessions through a virtual tutor using MetaHuman technology. Within a platform developed with Unreal Engine 5, the AI tutor uses a sequence of technologies to provide a realistic tutoring experience such as NVIDIA ACE plugin for facial animation, ELEVEN Labs for speech synthesis, and GPT-4o for textual interaction. Through the use of Large Language Models (LLMs) the AI tutor is able to both converse with the student and synchronize his facial expressions with the generated words. The aim is to increase the perception and empathy that the student has towards the tutor. Furthermore, this project aims at addressing and promoting the topics of representation and inclusion. The tutor can adopt different gender (male, female, or non-binary). In terms of accessibility for special needs students as well as sensory impairments, the user can interact with the tutor using both written text and their voice and, by activating the OpenDyslexic mode, it is possible to increase readability for dyslexic students. The tutor for the whole duration of the conversation with the student keeps the messages in memory, so that he or she can respond in a personalized manner while remaining coherent with the discussion topic. In this preliminary phase of the project, the presented tool focuses on helping users to understand the fundamentals of Physics such as mechanics, thermodynamics and electromagnetism. Moreover, the AI tutor is designed to convey a sense of empathy during the interaction by accordingly adapting facial expressions and posture coherently with a contextual sentiment analysis. The contribution of this study is about the assessment of effectiveness and usability of the AI tutor as well as overall users' perception, and its impact on the learning experiences. With this purpose, we are conducting a study aimed at evaluating the tool effectiveness in relation to the learning experience via pre-post surveys with a sample of students and experts from University of Camerino's Physics department. The usability assessment is performed by using standardized tools and open-ended questions combined with a thinking-aloud protocol.

Efficient tools for quantum nonlinear sensing with photodetection [POSTER]

Mateusz Molenda[1], Lewis A. Clark[2], Marcin Płodzień[3], Jan Kołodyński[1]
[1]*Institute of Physics, Polish Academy of Sciences, al. Lotników 32/46, 02-668 Warszawa, Poland*
[2]*Department of Optics, Palacky University, 17. listopadu 1192/12, 77146 Olomouc, Czechia*
[3] *ICFO-Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels (Barcelona), Spain*

Machine learning (ML) algorithms have become powerful tools across various scientific domains, yet their application in quantum sciences often suffers from a lack of interpretability. In particular, ML models are frequently treated as black boxes, making it difficult to extract meaningful insights about their learning process and decision-making criteria. To address this challenge, we compare a trained ML model with the Approximate Bayesian Computation (ABC) method for the task of continuous parameter estimation in a nonlinear optomechanical system probed by photodetection. This system consists of an optical cavity strongly coupled to a mechanical mode what precludes the usage of traditional estimation techniques that rely on the computation of the likelihood to observe a particular click trajectory. ML and ABC serve as natural alternatives, yet we demonstrate the former to outperform the latter in both accuracy and efficiency, primarily due to its ability to exploit quantum correlations encoded in the patterns of photodetector clicks. While ABC provides reasonable parameter estimates, it requires significantly longer computational times, making it impractical for real-time applications. In contrast, once trained, the ML model delivers near-instantaneous predictions, making it particularly advantageous for scenarios where rapid inference is essential. Furthermore, our analysis sheds light on how ML models extract key features from quantum measurement data, contributing to a broader understanding of their interpretability in physics-driven problems. This study highlights the potential of ML for accelerating quantum experiments and suggests new avenues for integrating data-driven approaches with traditional physics-based inference methods.

(The work presented here is currently being prepared for publishing.)

[1]. L. A Clark and J. Kolodyński. "Efficient inference of quantum system parameters by Approximate Bayesian Computation". https://arxiv.org/abs/2407.00724
[2]. L. A. Clark, B. Markowicz, and J. Kolodyński. "Exploiting non-linear effects in optomechanical sensors with continuous photon-counting". Quantum 6, 812 (2022).
[3]. M. Aspelmeyer, T. J. Kippenberg, and F. Marquardt. "Cavity optomechanics". Rev. Mod. Phys. 86 (2014).
[4]. S.A. Sisson, Y. Fan, and M. Beaumont. "Handbook of Approximate Bayesian Computation". CRC Press, 2018.

Mid-Infrared Classification for post-consumer plastics combining Infrared spectroscopy and open-source data mining
[POSTER]

Rosanna Mosetti[1,2], Tiziana Mancini[1], Federica Bertelà[1], Salvatore Macis[1], Annalisa D'Arco[1] and Stefano Lupi[1]

[1] *Dept. of Physics, Sapienza University of Rome, P.le A. Moro 5, 00185 Rome, Italy*

[2] *Dept. SBAI, Sapienza University of Rome, Via A. Scarpa 14, 00161 Rome, Italy*

Plastics are essential in everyday life due to their unique chemical and physical properties. However, plastic pollution has become one of the most pressing environmental challenges, driven by the rapid increase in plastic production and consumption, as well as the accumulation of non-degradable post-consumer plastic waste [1-4]. While recycling technologies offer a promising solution for managing this waste, the presence of organic contaminants in recycled resins often hinders their reuse and limits their compliance with quality standards [3,4]. One of the primary obstacles to the widespread adoption of recycled materials in fostering a circular and sustainable economy is the presence of unpleasant odors that frequently characterize the granules at the end of the recycling process. These odors originate from volatile substances that are not entirely removed during recycling. The implementation of innovative selective and/or specific deodorization technologies presents an effective strategy for eliminating such contaminants from the granules. This approach is closely linked to the advancement of plastic classification techniques that can also identify the presence of specific volatile organic compounds (VOCs). The mid-infrared (MIR) region has recently attracted attention due to its inherent advantages over the VIS and Near-IR regions, which are commonly used for optical screening of plastics. The fundamental vibrational modes in this spectral region make MIR frequencies particularly well-suited for high-fidelity machine learning (ML) classification, offering potential solutions for high-throughput classification due to their scalability, accuracy, and capability. Pioneering efforts in high-throughput polymer characterization using MIR spectra are underway, as demonstrated by the works [5-7]. To date, published MIR datasets for preliminary studies do not reflect the molecular heterogeneity of recycled plastics, let alone their complex composition in relation to contaminants. For example, the extensive literature on microplastic databases consists of samples that have been chemically and physically altered by environmental factors such as oxidation and UV irradiation, over which there is no control. Here, we studied various recycled plastics from mechanical extrusion through Attenuated Total Reflectance Infrared (ATR-IR) spectroscopy. An MIR database was generated, curated, and evaluated for real-world post-consumer plastics. Starting from MIR database, we designed and trained ML automatic and rapid recognition method for four plastic classes of interest: high-density polyethylene type B (HDPE-B), high-density polyethylene type P (HDPE-P), low-density polyethylene (LDPE), and polypropylene (PP). We established quantifiable metrics for evaluating the performance. Finally, taking advantage of our extensive research activity in the field of VOCs ultra-sensitive monitoring [8-12], we performed a preliminary identifier and predictive recognition of VOCs

quantities present of the surface of post-consumer plastic granules responsible for the odors. Although this represents a preliminary result, it holds significant industrial relevance, particularly within the context of the circular economy. Specifically, the ability to identify the molecules responsible for the undesirable odors, which concurrently impede the performance of recycled plastics, offers the potential to implement targeted strategies aimed at the removal of these specific molecules.

References:

1. *A. Cabanes, F.J. Valdés, A. Fullana. SM&T, 2020, 25, e00179.*
2. *R. Geyer, J. R. Jambeck and K. L. Law. Sci. Adv., 2017, 3, e1700782.*
3. *M. MacLeod, H. P. H. Arp, M. B. Tekman and A. Jahnke. Science, 2021, 373, 61–65.*
4. *J. Demarteau, A. R. Epstein, P. R. Christensen, M. Abubekerov, H. Wang, S. J. Teat, T. J. Seguin, C. W. Chan, C. D. Scown, T. P. Russell, J. D. Keasling, K. A. Persson and B. A. Helms. Sci. Adv., 2022, 8, eabp8823.*
5. *S. Jiang, Z. Xu, M. Kamran, S. Zinchik, S. Paheding, A. G. McDonald, E. Bar-Ziv and V. M. Zavala. Comput. Chem. Eng., 2021, 155, 107547.*
6. *F. Long, S. Jiang, A. G. Adekunle, V. M Zavala and E. Bar-Ziv. ACS Sustainable Chem. Eng., 2022, 10, 16064–16069.*
7. *N. Stavinski, V Maheshkar, S. Thomas, K. Dantu, L. Velarde. Environ. Sci.: Adv., 2023, 2, 1099.*
8. *V. Galstyan, A. D'Arco, M. Di Fabrizio, N. Poli, S. Lupi, E. Comini. Reviews in Analytical Chemistry 2021, 40 (1), 33-57.*
9. *A. D'Arco, D. Rocco, F. P. Magboo, C. Moffa, G. Della Ventura, A. Marcelli, L. Palumbo, L. Mattiello, S. Lupi, M. Petrarca. Optics Express 2022, 30(11): 19005-19016.*
10. *A. D'Arco, T. Mancini, M.C. Paolozzi, S. Macis, L. Mosesso, A. Marcelli, M. Petrarca, F. Radica, G. Tranfo, S. Lupi, G. Della Ventura. Sensors 2022, 22(15), 5624.*
11. *F. Radica, G. Della Ventura, L. Malfatti, M. Cestelli Guidi, A. D'Arco, A. Grilli, A. Marcelli, P. Innocenzi. Talanta 2021, 233:122510*
12. *T. Mancini, F. Radica, L. Mosesso, M.C. Paolozzi, S. Macis, A. Marcelli, S. Tamascelli, G. Tranfo, G. Della Ventura, S. Lupi, A. D'Arco. JECE, 2025, online.*

Link SapienzaTerahertz group: https://sites.google.com/uniroma1.it/sapienza-terahertz/home

Harnessing quantum back-action for time-series processing

Giacomo Franceschetto,[1] Marcin Płodzień,[1] Maciej Lewenstein,[1,2]
Antonio Acín,[1,2] Pere Mujal [1]
[1]*ICFO - Institut de Ciències Fotòniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels (Barcelona), Spain*
[2]*ICREA - Institució Catalana de Recerca i Estudis Avançats, Passeig de Lluís Companys 23, 08010 Barcelona, Spain*

Quantum measurements affect the state of the observed systems via back-action. While projective measurements extract maximal classical information, they drastically alter the system. In contrast, weak measurements balance information extraction with the degree of disturbance. Considering the prevalent use of projective measurements in quantum computing and communication protocols, the potential benefits of weak measurements in these fields remain largely unexplored. In this work [1], we demonstrate that incorporating weak measurements into a quantum machine-learning protocol known as quantum reservoir computing [2,3] provides advantages in both execution time scaling and overall performance. We analyze different measurement settings by varying the measurement strength across two benchmarking tasks. Our results reveal that carefully optimizing both the reservoir Hamiltonian parameters and the measurement strength can significantly improve the quantum reservoir computing algorithm performance. This work provides a comprehensive and practical recipe to promote the implementation of weak measurement-based protocols in quantum reservoir computing. Moreover, our findings motivate further exploration of experimental protocols that leverage the back-action effects of weak measurements.

[1] G. Franceschetto, M. Płodzień, M. Lewenstein, A. Acín, P. Mujal, arXiv:2411.03979 (2024).

[2] P. Mujal, R. Martínez-Peña, J. Nokkala, J. García-Beni, G. L. Giorgi, M. C. Soriano, and R. Zambrini, Adv. Quantum Technol., 4: 2100027 (2021).

[3] P. Mujal, R. Martínez-Peña, G. L. Giorgi, M. C. Soriano, R. Zambrini, npj Quantum Inf. 9, 16 (2023).

https://www.icfo.eu/research-group/7/quantum-information/home/437/
https://www.icfo.eu/research-group/11/qot/home/437/

Machine learning and quantum frontiers: A multilateral approach to responsible innovation

Samuel Partey
Head of Unit and Regional Advisor for Sciences
UNESCO Regional Bureau for Sceince and Culture in Europe

As machine learning and quantum technologies advance, their implications extend beyond scientific domains into ethics, education, governance, and global cooperation. This talk draws on current initiatives within UNESCO that address the ethical, social, and capacity-building dimensions of emerging technologies. It will explore how machine learning is being integrated into climate science, cultural heritage protection, and education, while highlighting UNESCO's work on the Recommendation on the Ethics of Artificial Intelligence and exploratory dialogues on quantum technologies. The presentation will reflect on how multilateral collaboration, interdisciplinary methods, and inclusive foresight can help ensure that scientific innovation contributes meaningfully to complex global challenges.

Enhancing quantum state tomography via resource-efficient attention-based neural networks

Adriano Macarone Palmieri[1], Guillem Müller-Rigat[1], Anubhav Kumar Srivastava[1], Maciej Lewenstein[1,2], Grzegorz Rajchel-Mieldzioć[1,3], Marcin Płodzień[1]

[1] ICFO - Institut de Ciències Fotòniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels, Barcelona, Spain

[2] ICREA, Pg. Lluis Companys 23, 08010 Barcelona, Spain

[3] NASK National Research Institute, ul. Kolska 12, 01-045 Warszawa, Poland

We propose a method for denoising experimental density matrices that combines standard quantum state tomography with an attention-based neural network architecture [1]. The algorithm learns the noise from the data itself, without *a priori* knowledge of its sources. Firstly, we show how the proposed protocol can improve the averaged fidelity of reconstruction over linear inversion and maximum likelihood estimation in the finite-statistics regime, reducing at least by an order of magnitude the amount of necessary training data. Next, we demonstrate its use for out-of-distribution data in realistic scenarios. In particular, we consider squeezed states of few spins in the presence of depolarizing noise and measurement/calibration errors and certify its metrologically useful entanglement content. The protocol introduced here targets experiments involving few degrees of freedom and afflicted by a significant amount of unspecified noise. These include NISQ devices and platforms such as trapped ions or photonic qudits.

[1] Enhancing quantum state tomography via resource-efficient attention-based neural networks Adriano Macarone Palmieri1, Guillem Müller-Rigat, Anubhav Kumar Srivastava, Maciej Lewenstein, Grzegorz Rajchel-Mieldzioć, and ***Marcin Płodzień,*** *Phys. Rev. Research* ***6****, 033248* ***(2024)***

1. Personal webpage: https://sites.google.com/site/marcinplodzienphysics/home

2. Quantum Optics Theory group at ICFO: https://www.icfo.eu/research-group/11/qot/home/437/

Scientific Machine Learning: Bridging Artificial Intelligence and Fundamental Sciences

Alfio Quarteroni

Professor Emeritus, Politecnico di Milano, Milan, Italy
Ecole Polytechnique Fédérale de Lausanne, Switzerland

While artificial intelligence has achieved remarkable advances in recent years, it still suffers from inaccuracies, uncertainties, and a lack of transparency—often earning the label of a "black box" technology. Scientific machine learning offers a promising solution by integrating data-driven algorithms with digital models rooted in physical principles. This powerful combination fosters a meaningful synergy between artificial intelligence and human expertise, grounded in natural laws and rigorous scientific frameworks. In this presentation, I will illustrate these concepts, through a practical application: the development of a mathematical simulator that accurately replicates cardiac function.

Neural quantum states for one-dimensional & spin many-body systems

Arnau Rios, *Institute of Cosmos Sciences, University of Barcelona, ICCUB*
Javier Rozalén Sarmiento, *Institute of Cosmos Sciences, University of Barcelona, ICCUB*
Alejandro Romero Ros, *Institute of Cosmos Sciences, University of Barcelona, ICCUB*
James Keeble, *University of Bielefeld, Germany*
Mehdi Drissi, *Technical University of Darmstadt, Germany*

In this talk, I will present our efforts in advancing Neural Quantum State (NQS) methods for quantum many-body methods with the ultimate aim to solve nuclear physics systems [1]. First, I will discuss applications in spineless fermionic systems, where the method overperforms CI simulations across a wide range of coupling constants. In particular, our approach can describe behaviours, like bosonization and cristallization, for several particle numbers [2,3]. I will also provide results for self-bound systems, where universality arises for specific values of asymptotic length scales.
Second, I will focus on optimization strategies for NQSs. I will show how a shift from information geometry towards decision geometry allows for the construction of stable and efficient second-order optimization schemes for NQSs [4]. I will also show recent results on the extension of these techniques to spin systems in an effort to generalise the applications of decisional gradient descent methods to a variety of physical systems.

[1] J. W. T. Keeble and A. Rios, Physics Letters B 809, 135743 (2020).
[2] J. W. T. Keeble, M. Drissi, A. Rojo-Francàs, B. Juliá-Díaz, and A. Rios, Phys. Rev. A 108, 063320 (2023).
[3] J. W. Keeble, PhD Thesis (https://doi.org/10.15126/thesis.900505, 2022).
[4] M. Drissi, J. W. T. Keeble, J. Rozalén Sarmiento, and A. Rios, Phil. Trans. R. Soc. A. 382, 20240057 (2024).

Two Approaches to Molecular Representation Learning

Grant M. Rotskoff
Stanford University, USA

Neural networks continue to surprise us with their remarkable capabilities for high-dimensional function approximation. Applications of machine learning now pervade essentially every scientific discipline, but predictive models to describe the optimization dynamics, inference properties, and flexibility of modern neural networks remain limited. In this talk, I will introduce several approaches to both analyzing and building generative models to augment Monte Carlo sampling and sampling high-dimensional distributions. I will focus, in particular, on two applications from chemistry: sampling conformational ensembles of disordered protein domains and molecular optimization. I will also introduce a self-distillation strategy for large scale models that shares conceptually similarities to preference optimization with reinforcement learning, but does not require proximal optimization (PPO) and outperforms direct preference optimization and (DPO).

A non-orthogonal representation of the chemical space

Tiago F. T. Cerqueira[1], Haichen Wang[2], Silvana Botti[2], Miguel A. L. Marques[2]
[1]*CFisUC, Department of Physics, University of Coimbra, Rua Larga, 3004-516 Coimbra, Portugal*
[2]*Research Center Future Energy Materials and Systems of the University Alliance Ruhr and Interdisciplinary Centre for Advanced Materials Simulation, Ruhr University Bochum, Universitätsstraße 150, D-44801 Bochum, Germany*

We present a novel approach to generate a fingerprint for crystalline materials that balances efficiency for machine processing and human interpretability, allowing its application in both machine learning inference and understanding of structure-property relationships. Our proposed material encoding has two components: one representing the crystal structure and the other characterizing the chemical composition that we call Pettifor embedding. For the latter, we construct a non-orthogonal space where each axis represents a chemical element and where the angle between the axes quantifies a measure of the similarity between them. The chemical composition is then defined by the point on the unit sphere in this non-orthogonal space. We show that the Pettifor embeddings systematically outperform other commonly used elemental embeddings in compositional machine learning models. Using the Pettifor embeddings to define a distance metric and applying dimension reduction techniques, we construct a two-dimensional global map of the space of thermodynamically stable crystalline compounds. Despite their simplicity, such maps succeed in providing a physical separation of material classes according to basic physical properties.

Grouplinks:
[1]*https://cfisuc.fis.uc.pt/people.php?oid=127683*
[2]*https://fems.shared-02.uo-cloud.de/research/groups/artificial-intelligence-for-integrated-materials-science*

Neural Network architectures for efficient sampling of statistical physics models

Luca Maria Del Bono,[1,2], Federico Ricci-Tersenghi,[1,2,3] and Francesco Zamponi[1]
[1] *Dipartimento di Fisica, Sapienza Università di Roma, Piazzale Aldo Moro 5, Rome 00185, Italy*
[2]*CNR-Nanotec, Rome unit, Piazzale Aldo Moro 5, Rome 00185, Italy*
[3]*INFN, sezione di Roma1, Piazzale Aldo Moro 5, Rome 00185, Italy*

The task of sampling efficiently the Gibbs-Boltzmann distribution of disordered systems is important both for the theoretical understanding of these models and for the solution of practical optimization problems. Unfortunately, this task is known to be hard, especially for spin glasses at low temperatures. Recently, many attempts have been made to tackle the problem by mixing classical Monte Carlo schemes with newly devised Neural Networks that learn to propose smart moves. In this talk I will review a few physically-interpretable deep architectures, and in particular one whose number of parameters scales linearly with the size of the system and that can be applied to a large variety of topologies. I will show that these architectures can accurately learn the Gibbs-Boltzmann distribution for the two-dimensional and three-dimensional Edwards-Anderson models, and specifically for some of its most difficult instances. I will show that the performance increases with the number of layers, in a way that clearly connects to the correlation length of the system, thus providing a simple and interpretable criterion to choose the optimal depth. Finally, I will discuss the performances of these architectures in proposing smart Monte Carlo moves and compare to state-of-the-art algorithms.

Reference:

Nearest-Neighbours Neural Network architecture for efficient sampling of statistical physics models, L.M.Del Bono, F.Ricci-Tersenghi, F.Zamponi - Machine Learning: Science and Technology 6, 025029 (2025)