Machine Learning in Natural Sciences: from Quantum Physics to Nanoscience and Structural Biology

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## Physical Parametrisations of Mixed Quantum States with Deep Neural Networks

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Being able to efficiently represent mixed quantum states is essential in order to describe the effects of dissipation, such as those arising in Open Quantum Systems, or in order to represent the noisy outcome of a circuit executed on a present-day Quantum Computer.

The challenges in the description of such objects arise from the exponential growth of the Hilbert space and from the need to enforce the positive-definiteness of the resulting matrix.

A compact, physical representation of density matrices in terms of Neural Networks was originally proposed by Torlai and coworkers in 2018, based on the purification of a Restricted Boltzmann Machine, but that approach was limited to shallow networks.

In this talk we will discuss the Gram-Hadamard Density Operator (GHDO), a new **deep** neural-network architecture that can encode positive semi-definite density operators of exponential rank with poly- nomial resources.

We will then show how to embed an autoregressive structure in the GHDO to allow direct sampling of the probability distribution.

Author: VICENTINI, Filippo (EPFL - CQSL)

**Co-authors:** Dr ROSSI, Riccardo (EPFL); CARLEO, Giuseppe (École Polytechnique Fédérale de Lausanne (EPFL))

Presenter: VICENTINI, Filippo (EPFL - CQSL)

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