Variational quantum Monte Carlo with neural network ansatz for open quantum systems

Alexandra Nagy¹, Vincenzo Savona¹

¹ Institute of Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland

The possibility to simulate the properties of many-body open quantum systems with a large number of degrees of freedom is the premise to the solution of several outstanding problems in quantum science and quantum information. The challenge posed by this task lies in the complexity of the density matrix increasing exponentially with the system size. Here, we introduce a variational method to efficiently simulate the non-equilibrium steady state of Markovian open quantum systems based on variational Monte Carlo and on a neural network representation of the density matrix. Thanks to the stochastic reconfiguration scheme, the application of the variational principle is translated into the actual integration of the quantum master equation. We test the effectiveness of the method by modeling the two-dimensional dissipative XYZ and the transverse Ising spin model on a lattice.

In our approach we exploit the representative power of neural networks by developing a comprehensive software adapted for general physical model description and designed to run efficiently on large computational clusters. The algorithm is broken into several independent chains running in parallel using MVAPICH2. Besides the CPU, a GPU accelerated version has also been implemented in order to tackle large system sizes.

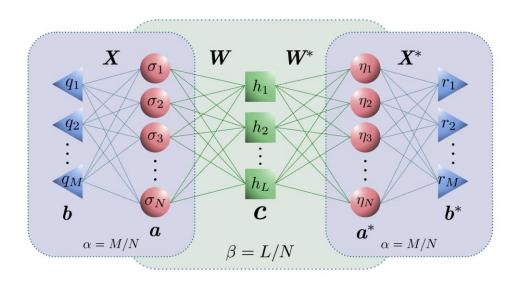


Figure 1. Graphical representation of the neural network ansatz for the density matrix. The input states $|\sigma\rangle$, $|\eta\rangle$ are encoded in the visible layer, represented by circles. The hidden spins in the triangles encode the correlation between the physical spins in each state of the statistical mixture, while the hidden spins in the squares encode the mixture between the states. This structure is easily seen to coincide with a RBM, where the hidden layer is composed by the triangle and square nodes.

Contact address: alexandra.nagy@epfl.ch