Simulating quantum systems with Neural Networks

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The Schrödinger equation is the main pillar of Quantum Mechanics, yet an analytical solution exists solely for some simple cases. As a consequence of this, numerical solutions are in order, and indeed computational approaches tackling this very problem have been around for the last few decades. However, it is widely known that as systems become more complex, even the most powerful supercomputers available fall short.
Motivated by the opportunity to find a solution to this, our work is along a line that is gaining momentum in the Physics community, which is the usage of Machine Learning methods, namely Artificial Neural Networks (ANNs), that are capable of "learning" the wave function of a system without previous exposure to a solution (not to be confused with supervised learning). Our approach is variational: we have an ANN represent the wave function and we train it to minimise the energy expectation, which is an upper bound of the exact ground state energy. This is a well-established method, first published in 2017 [3].
Our contribution is twofold. First, by building a simple ANN we are able to model a nuclear ground state wave function to within 2 keV of the exact energy; this can be seen in Figure 2. Second, we build four different neural networks and we train them to solve the same problem, with the ultimate goal of understanding in a deep level the effect of changes in the network architecture. Whereas this discussion is typically omitted in the literature, we believe that if Machine Learning is to compete against the solid, classical computation methods, a thorough understanding of each element of our model (the Neural Network in this case) is indispensable.

References

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[2] H. Saito, Journal of the Phys. Society of Japan, 87(7) (2017).
[3] G. Carleo and M. Troyer, Science, 355(6325) (2017)

Figures

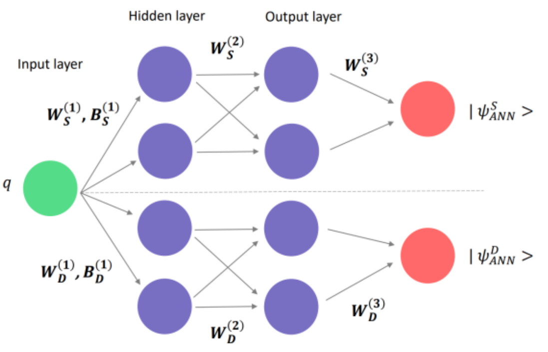

Figure 1: Architecture of a Neural Network used to find the ground state wave function of the deuteron (nuclear bound state).

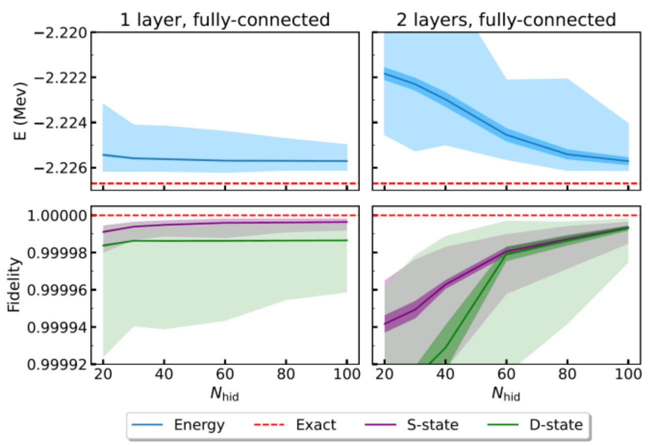

Figure 2: Energy and fidelity (computed with the exact wave function) vs. number of neurons, represented for two distinct models.