Quantum Many-Body problem using Neural Networks

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Problem Statement

The challenge posed by the statistical distribution of spin systems problem in quantum physics originates from the difficulty of describing the non-trivial correlations encoded in the exponential complexity of the wave function of the system. The complexity of a statistical ensemble increases with the increasing number of states in quantum configurational space. A systematic machine learning of the wave function can reduce this complexity to a tractable computational form, for some notable cases of physical interest.

Expected Milestones

- Find the wave function for the system via variational method with variable number of hidden nodes and with a forward feed neural network.
- Use Stochastic Reconfiguration by Metropolis-Hastings algorithm.
- Solve the 1D classical Ising model and then the Heisenberg model.
- Using the above three steps, study the equilibrium spin distribution and also the energy at equilibrium variation on increasing the number of hidden nodes (Verify if it the convergence rate improves).

Dataset

The data sets can be found on Ising_data.

Overview of the Proposed Method

NQS [1] [2]

Consider a quantum system with N discrete-valued degrees of freedom $\mathcal{S} = (\mathcal{S}_1, \mathcal{S}_2 \dots \mathcal{S}_N)$, which may be spins, bosonic occupation numbers, or similar. The many-body wave function is a mapping of the $N-$dimensional set $\mathcal{S}$ to (exponentially many) complex numbers which fully specify the amplitude and the phase of the quantum state. The point of view we take here is to interpret the wave function as a computational black box which, given an input many-body configuration $\mathcal{S}$, returns a phase and an amplitude according to $\Psi(\mathcal{S})$. Our goal is to approximate this computational black box with a neural network, trained to best represent $\Psi(\mathcal{S})$.

References

[1] Giuseppe Carleo, Matthias Troyer: Solving the quantum many-body problem with artificial neural networks Science 10 Feb 2017 : 602-606

[2] Stephen R: ClarkUnifying Neural-network Quantum States and Correlator Product States via Tensor Networks arXiv:1606.02318v1 2017