Abstract

Obtaining an accurate ground state wave function is one of the great challenges in the quantum many-body problem. We propose a new class of wave functions, neural network backflow (NNB). The backflow approach, pioneered originally by Feynman, adds correlation to a mean-field ground state by transforming the single-particle orbitals in a configuration-dependent way. NNB uses a feed-forward neural network to find the optimal transformation. NNB directly dresses a mean-field state, can be systematically improved and directly alters the sign structure of the wave-function. It generalizes the standard backflow which we show how to explicitly represent as a NNB. We benchmark the NNB on a Hubbard model at intermediate doping finding that it significantly decreases the relative error, restores the symmetry of both observables and single-particle orbitals, and decreases the total double-occupancy. Finally, we illustrate interesting patterns in the weights and bias of the optimized neural network.

Introduction

Two approaches for wave function:

Approach I: wave function ansatz parameterized with tuning parameter $D$ to cover the whole Hilbert space, but can be expensive.
- Multi-determinant
- Tensor network states
- Neural Network states

Approach II: mean field solution with physics understanding, but could be challenging to improve.
- Slater-Determinant
- BDG wave function

Approach II is systematically improved.
- Multi-determinant
- Tensor network states
- Neural Network states

Neural Network Backflow (NNB)

Q: Is it possible to take advantages of both Approach I and Approach II to construct a quantum many-body wave function?

A: Yes. We prove that the standard backflow can be represented through a three-layer artificial neural network. NNB naturally generalizes the backflow transformation.

\[
\phi_{k\sigma}^B(r_i; \mathbf{r}) = \phi_{k\sigma}(r_i, \mathbf{r}) + a_{k\sigma}^N(r_i, \mathbf{r})
\]

For each spin orbital, there is a NNB
- Input: system configuration
- Output: configuration dependent correction to single particle orbital
- Hidden: Fully Dense + ReLU

Q: Is it possible to realize the standard backflow with machine learning?

A: Yes. NNB starts with the mean-field solution physics, can directly change the sign structure, and can be systematically improved.

Results

We benchmark the quality of our NNB on a 4 x 4 square Hubbard model in the non-trivial regime with $U=8$ and filling=0.875.

\[
H = -t \sum_{\langle i,j \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) + \sum_i U n_{i\uparrow} n_{i\downarrow}
\]

Energy decreases as hidden neuron increases.

Conclusions

- NNB achieves good performance for Hubbard model at nontrivial filling.
- NNB could be generalized to frustrated spin systems as well as the continuum. In the latter case, the input could be represented as a lexicographically ordered set of particle locations.
- NNB provides a new approach toward combining machine learning methodology with dressed mean-field variational wave-functions, which allows us to take simultaneous advantage of their respective strengths.

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References