Backflow Transformations via Neural Network for Quantum Many-Body Wave-Functions

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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[1], 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[2] 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[3-6]

Approach II: mean field solution with physics understanding, but could be challenging to improve.

- Slater-Determinant

$$\psi_{SD}(\boldsymbol{r}) = \det[M^{SD,\uparrow}]\det[M^{SD,\downarrow}]$$
$$M^{SD,\sigma}_{ik} = \phi_{k\sigma}(r_{i\sigma})$$

- BDG wave function

$$\psi_{BDG}(\boldsymbol{r}) = \det[\Phi]$$
$$\Phi_{ij} = \sum_{k,l=1}^{N} \phi_{k\uparrow}(r_{i,\uparrow})\, S_{kl}\, \phi_{l\downarrow}(r_{j,\downarrow})$$

- Standard backflow[2] on lattice to improve mean field

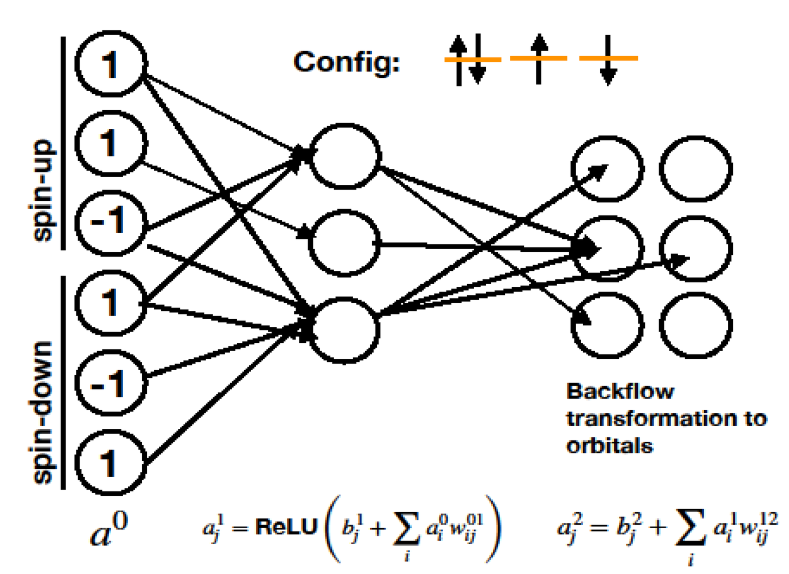
$$\phi^b_{k\sigma}(r_{i,\sigma};\boldsymbol{r}) = \phi_{k\sigma} + \sum_j \eta_{ij,\sigma}\phi_{k\sigma}(r_{j,\sigma})$$
$$\eta_{ij,\sigma} = tD_iH_j\theta_{|i-j|,\sigma}$$

with $D_i = n_{i,\uparrow}n_{i,\downarrow}$, $H_i = (1-n_{i,\uparrow})(1-n_{i,\downarrow})$. $\theta_{1,\sigma}$ and $\theta_{2,\sigma}$ are the only non-zero variational parameters.

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?

$$\phi^b_{k\sigma}(r_{i,\sigma};\boldsymbol{r}) = \phi_{k\sigma}(r_{i,\sigma}) + a^{NN}_{ki,\sigma}(\boldsymbol{r})$$



For each spin orbital, there is a NNB

- Input: system configuration
- Output: configuration dependent correction to single particle orbital
- Hidden: Fully Dense+ReLU

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

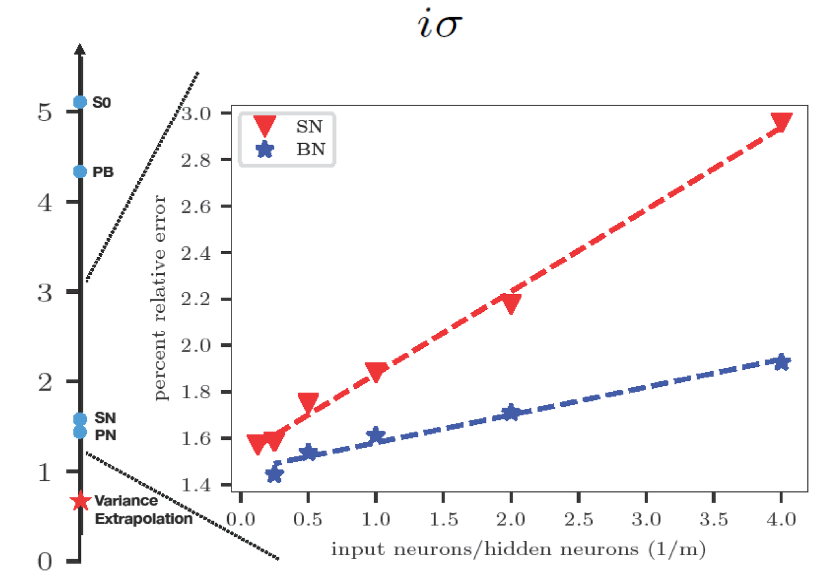
Q: Is it possible to realize the standard backflow with machine learning?

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

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.

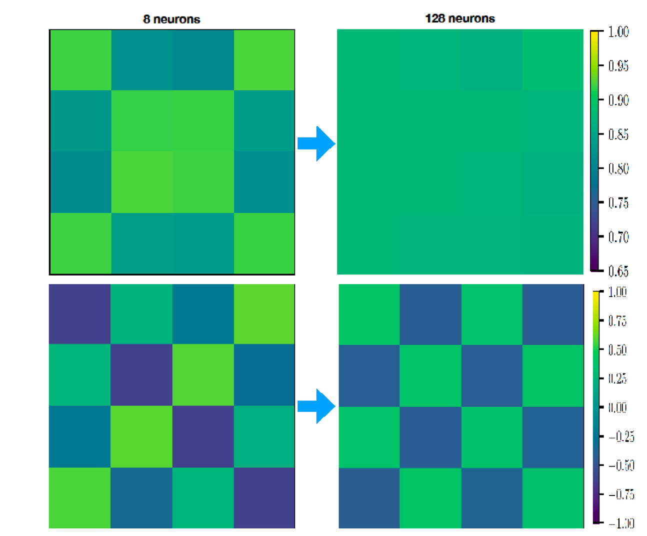
$$H = -t\sum_{i\sigma}(c^\dagger_{i\sigma}c_{i+1\sigma} + h.c.) + \sum_i U n_{i\uparrow}n_{i\downarrow}$$



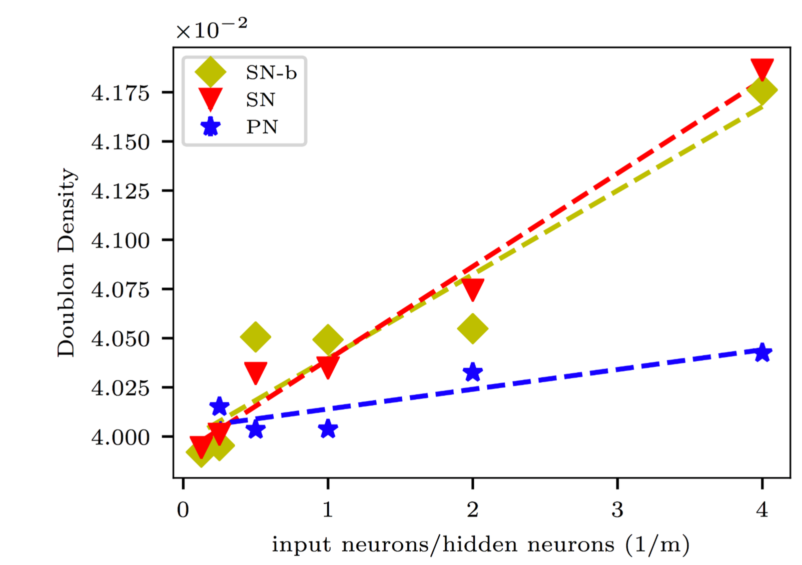
→ Slater-Determinant + NNB

→ BDG + NNB

Energy decreases as hidden neuron increases.

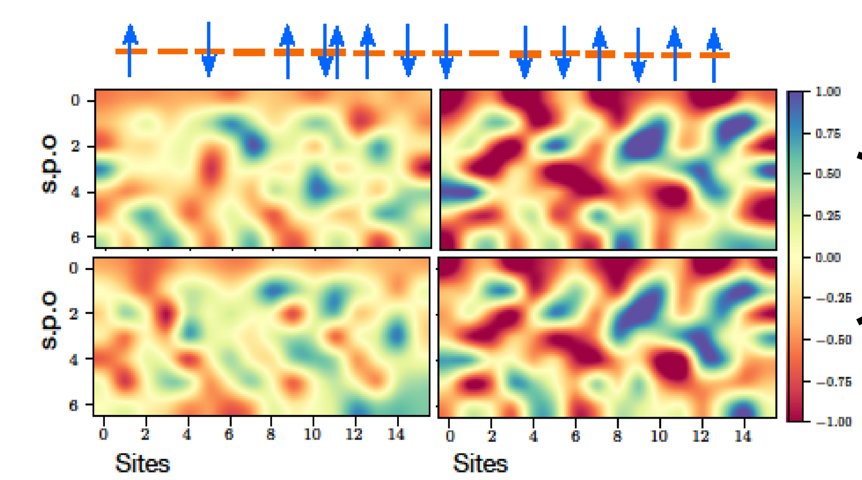


As hidden neuron increases, spin and charge density become more symmetric.



As hidden neuron increases, doublon density decreases.

Q: Could we understand what the neural network learns?



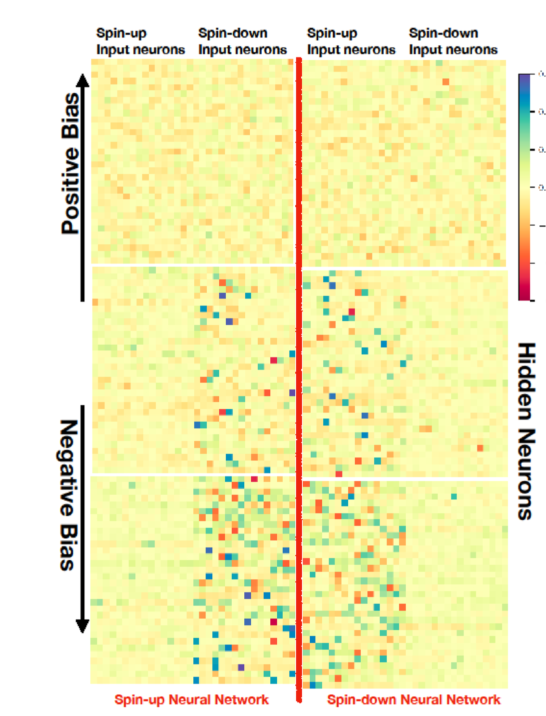
Slater-Determinant Slater-Determinant+NNB

Spin-up orbitals

Spin-down orbitals

NNB roughly restores the symmetry and alters the sign structure.

Spin-up Spin-down



For weights between input layer and hidden layer:

- Spin-up network has large weights connected to spin-down configuration; vice versa.
- Larger weights in negative bias and smaller weights in positive bias.

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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