Artificial Neural Networks as Variational Ansatz

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Neural networks in spin systems

Heisenberg spin $\frac{1}{2}$ model

$$\hat{H} = J \sum_{\langle ij \rangle} \hat{S}_i \hat{S}_j$$

1. Exponential size $\mathcal{H}$
2. Sign problem

Desired ansatz features:
1. Compact representation
2. Fast evaluation
3. Optimization

RBM (NQS)

$$\psi(\sigma) = e^{a_i \sigma_i} \prod_j \cosh(W_{ij} \sigma_i + b_j)$$

Carleo and Troyer, Science (2017)
Carleo, Nomura, Imada (2018)
Cai and Liu, PRB (2018)
Melko group
Feedforward neural networks

Properties of Neural Nets:
1. Universal function approximator
2. Circuit equivalent
Formally includes MPS, PEPS

Questions:
1. Are feedforward nets give practical representations?
2. How fast does the accuracy improve?

Cybenko (1989)
Supervised learning

Setup:
- Input data - basis configurations
- Target values - ED vector $\psi_0$
- Loss - $L_2(\psi - \psi_0)$

Evaluation: How fast does the accuracy improve?
- $\Delta = 1 - \langle \psi | \psi_0 \rangle$
Preliminary results

Neural networks for spin systems
Feedforward neural networks
Supervised learning

Preliminary results

- Kagome, 18 sites
- Kagome, 24 sites
- Square, 24 sites
- Square, 30 sites
Depth and system size dependence scenarios

1. Benefit of depth $> 1$
2. How does the slope depend on $N$?
3. Polynomial representation?

![Graph showing system size vs. number of parameters](image-url)
Summary:

- Numerical evidence of compact representation
- Exponential scaling of accuracy with network size

Next steps:

- VMC optimization
- System size dependence
- Iterative Lanczos step