Artificial Neural Networks as Variational Ansatz

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Neural networks in spin systems

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

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

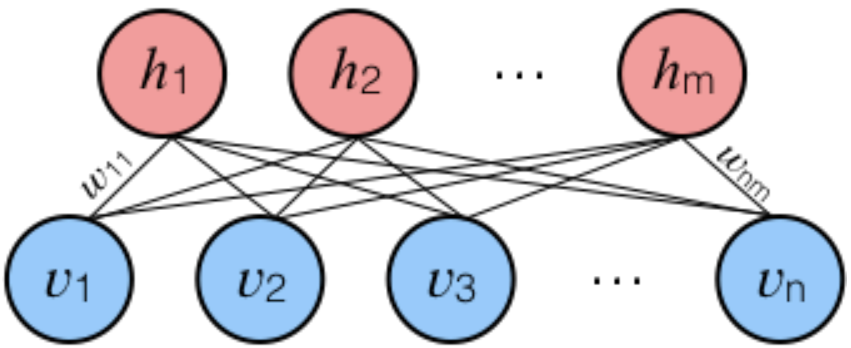
1. Exponential size $\mathcal{H}$
2. Sign problem

Desired ansatz features:

1. Compact representation
2. Fast evaluation
3. Optimization

RBM (NQS)

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



1. Carleo and Troyer, Science (2017)
2. Carleo, Nomura, Imada (2018)
3. Gao and Duan, Nature Comm. (2018)
4. Cai and Liu, PRB (2018)

5. Melko group

Feedforward neural networks

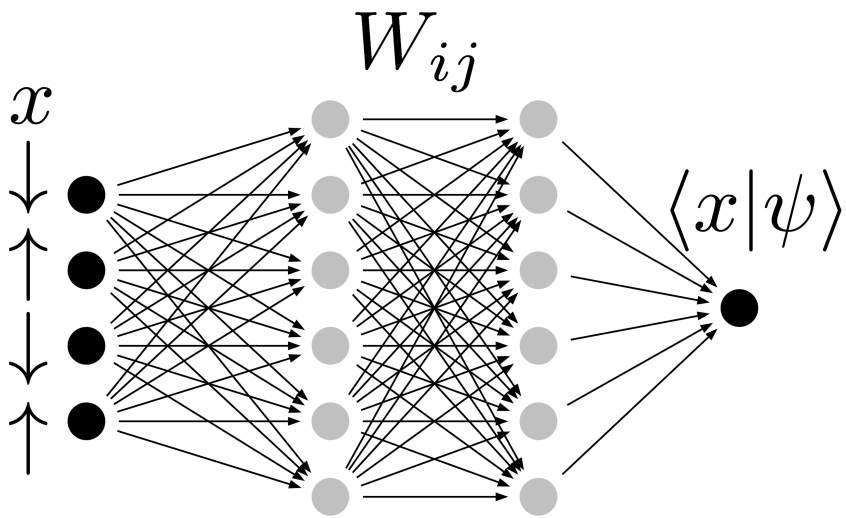
Properties of Neural Nets:

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?



universal function approximator

1. Cybenko (1989)

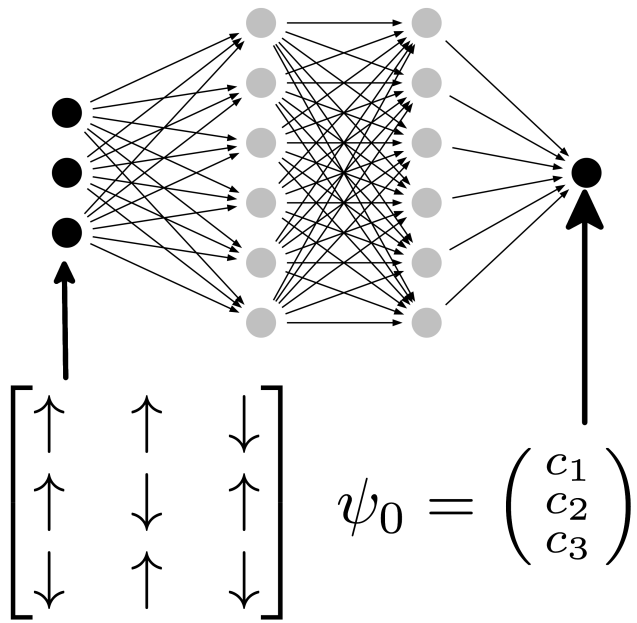
Supervised learning

Setup:

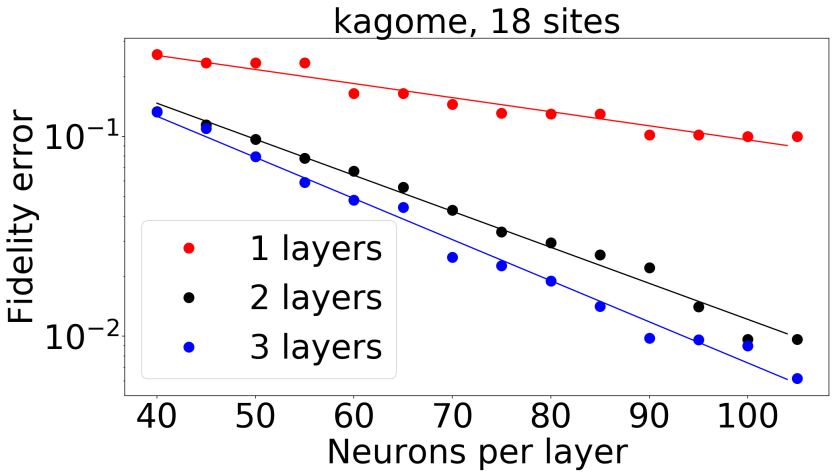
- Input data - basis configurations
- Target values - ED vector ψ_0
- Loss - $L_2(\psi - \psi_0)$

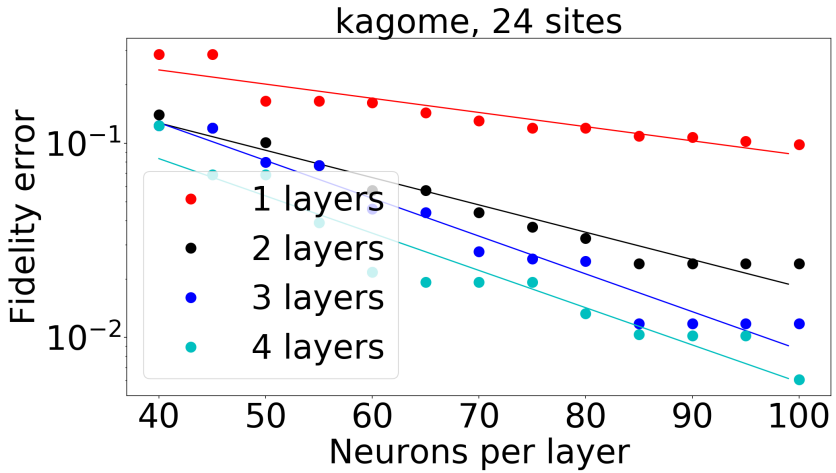
Evaluation: How fast does the accuracy improve?

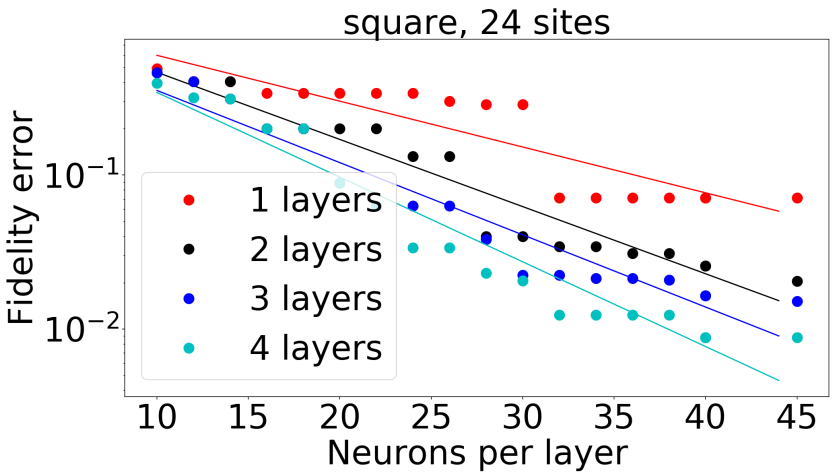
- $\Delta = 1 - \langle \psi | \psi_0 \rangle$

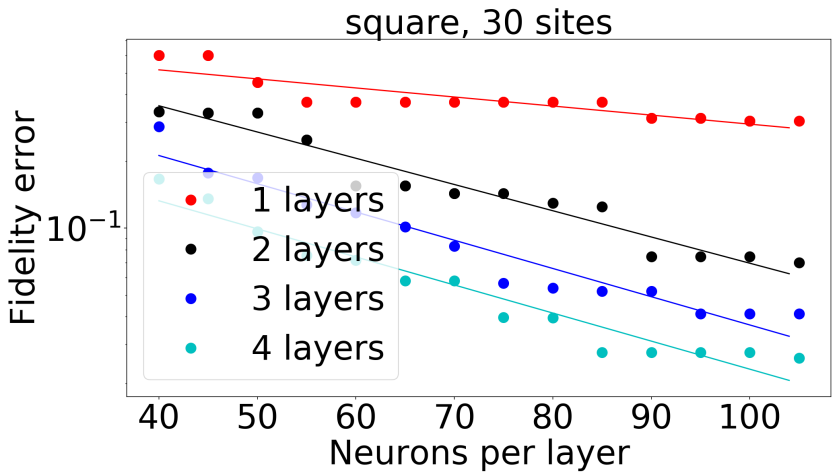


Preliminary results



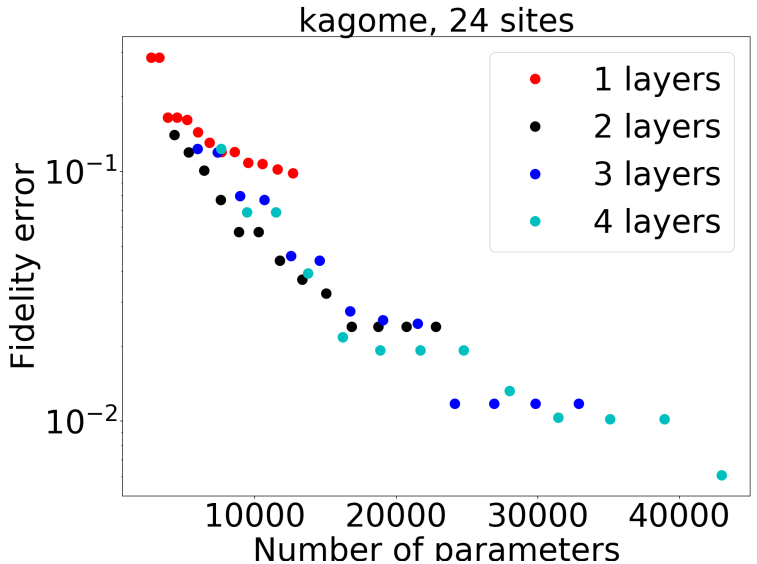


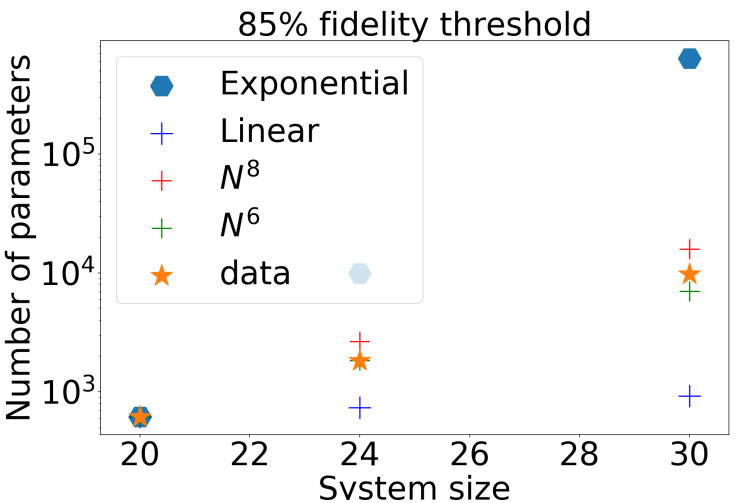




Depth and system size dependence scenarios

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

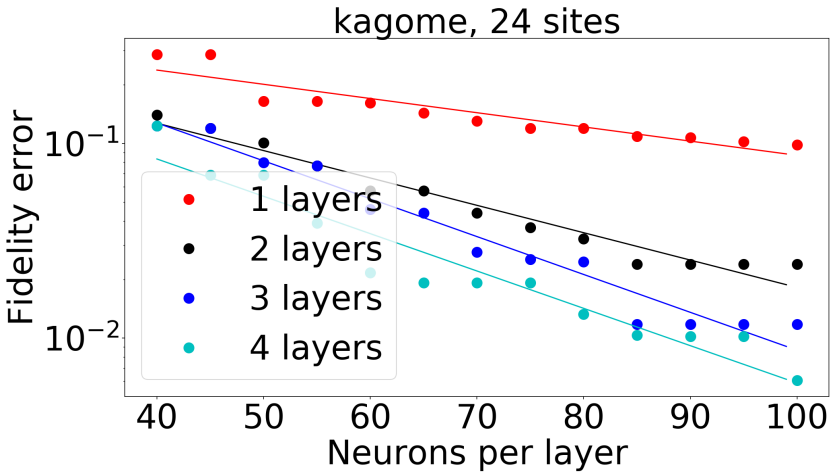




Summary and further steps

Summary:

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



Next steps:

- VMC optimization
- System size dependence
- Iterative Lanczos step