Neural Network Quantum States

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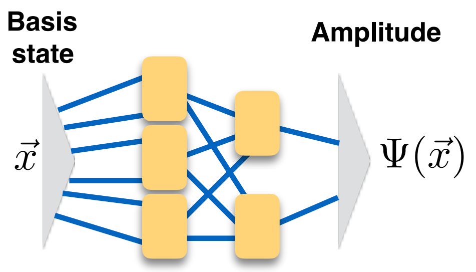
Neural Network Quantum States

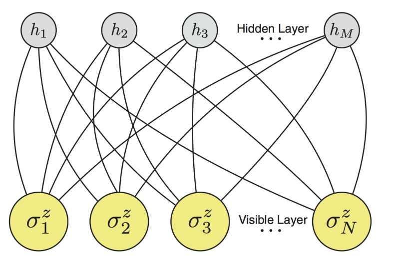
Goal: Represent quantum states with neural networks (NQS).

Examples:



$\Psi(\vec{x}) = \exp(\boldsymbol{W}_n\, g(\cdots\, g(\boldsymbol{W}_1\vec{x}))))$

$g(x) = \tanh(x)$



$E(\boldsymbol{\sigma}, \boldsymbol{h}) = -\sum_{ij} h_i W_{ij} \sigma_j$

$\Psi(\boldsymbol{\sigma}) \equiv \sum_h P(\boldsymbol{\sigma}, \boldsymbol{h}) = \sum_h e^{E(\boldsymbol{\sigma},\boldsymbol{h})}$

Motivation:

1) Able to capture long range correlations
2) Take advantage of modern ML methods
3) Fast Computation with GPUs

see: **SoftwareX 10, 100311 (2019)**

Variational Monte Carlo

Goal: Given a variational wavefunction $\Psi(\vec{x}|\{\alpha\})$ which depends on parameters α, we want to find the optimal parameters which minimises the energy $\langle \hat{H}\rangle$ of a given Hamiltonian $\hat{H}$.

Monte Carlo Method:

Expectation values can be estimated

$$\langle \hat{H}\rangle = \sum_{\vec{x}} \left(\sum_{\vec{x}'} H_{\vec{x}\vec{x}'} \frac{\Psi^*(\vec{x}')}{\Psi^*(\vec{x})} \right) \frac{|\Psi(\vec{x})|^2}{\sum_{\vec{x}} |\Psi(\vec{x})|^2}$$

$$\approx \left\langle \sum_{\vec{x}'} H_{\vec{x}\vec{x}'} \frac{\Psi^*(\vec{x}')}{\Psi^*(\vec{x})} \right\rangle_M$$

Monte Carlo average over a sample M from the distribution $|\Psi(\vec{x})|^2$

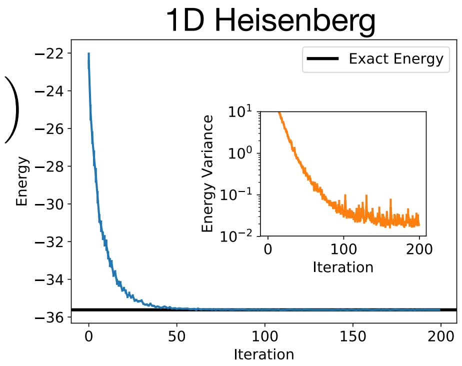
Estimate the gradients

$$\frac{\partial \langle \hat{H}\rangle}{\partial \alpha} = 2\mathrm{Re}\left(\langle \mathcal{O}^\dagger \hat{H}\rangle - \langle \mathcal{O}^\dagger\rangle\langle \hat{H}\rangle \right)$$

$$\mathcal{O}(\vec{x}) = \frac{\partial}{\partial \alpha} \log(\Psi(\vec{x}))$$

Update parameters

$$\alpha \rightarrow \alpha - \eta \frac{\partial \langle \hat{H}\rangle}{\partial \alpha}$$



see: **SoftwareX 10, 100311 (2019)**

Condensed Matter Applications

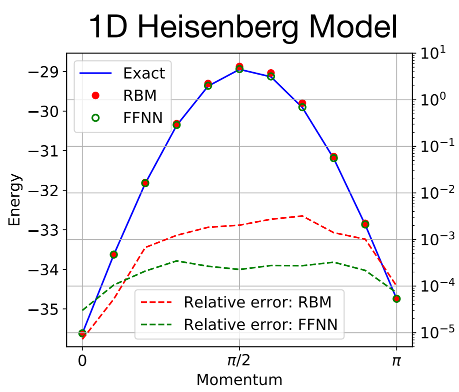
Abelian Spatial Symmetries

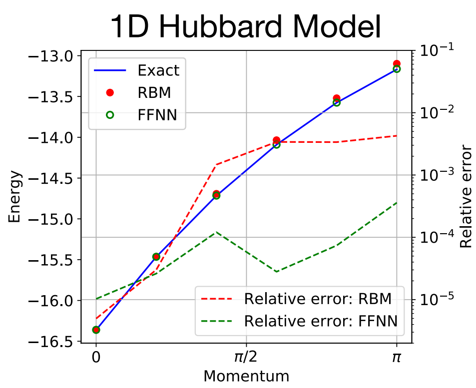
Goal: Given an abelian spatial symmetry group G with generators $\{\hat{T}_1, \hat{T}_2, \ldots\}$. We want the state to satisfy: $\Psi(\hat{T}_i\vec{x}) = \omega_i \Psi(\vec{x})$

Method:

1) The symmetry group G divides the group into equivalence classes: $[\vec{x}] = \{g\vec{x} : \forall g \in G\}$
2) Pick a representative for each class: $\vec{x}_{\text{canonical}} \in [\vec{x}]$
3) Define the wavefunction $\Psi(\vec{x}) = (\omega_i)^{r_i}\Psi(\vec{x}_{\text{canonical}})$

Results: Applying the method for 1D translational symmetry.





see: **Physical Review Letters 121, 167204 (2018)**

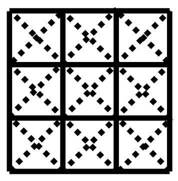
Frustrated Magnetism

Goal: Apply the methodology to a frustrated magnetic model. (Not sign-problem free.)

Model:

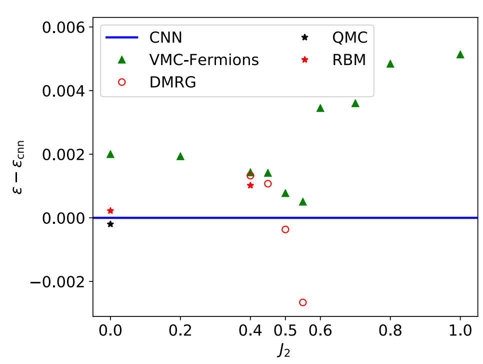
Spin-1/2 Heisenberg model on square lattice with nearest and next-nearest neighbour interactions.

$$\hat{H} = J_1 \sum_{\langle ij\rangle} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j + J_2 \sum_{\langle\langle ij\rangle\rangle} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j$$

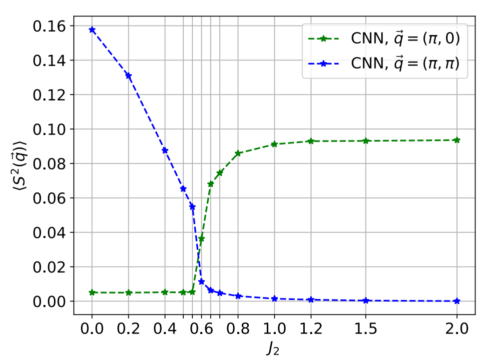


Results: 10 by 10 Square Lattice

Comparing with other Methods



Spin-Spin Structure Factor: $S^2(\vec{q}) \propto \sum \langle \hat{\boldsymbol{S}}_i \hat{\boldsymbol{S}}_j\rangle e^{i\vec{q}\cdot(\vec{r}_i - \vec{r}_j)}$



see: **Physical Review B 100 (12), 125124**