The Use of Restricted Boltzmann Machines for Modeling a Many-body Quantum System

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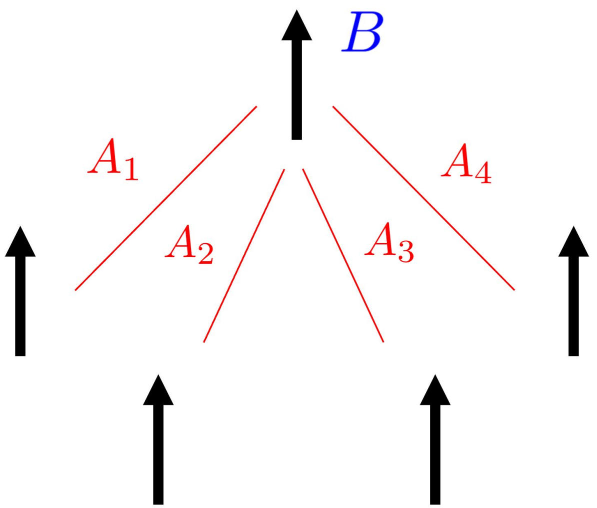
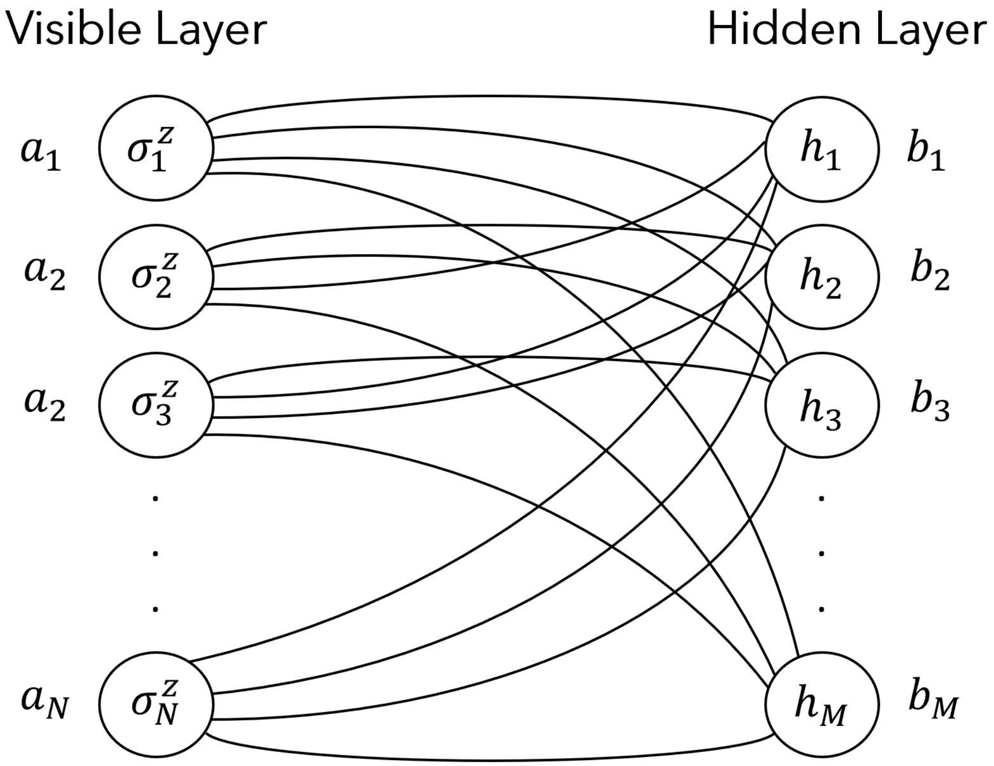
Restricted Boltzmann Machine

$$H = BS_0^z + \sum_{k=1}^{N-1} A_k \mathbf{S}_0 \cdot \mathbf{S}_k$$





Model Parameters:

a_j (N elements)

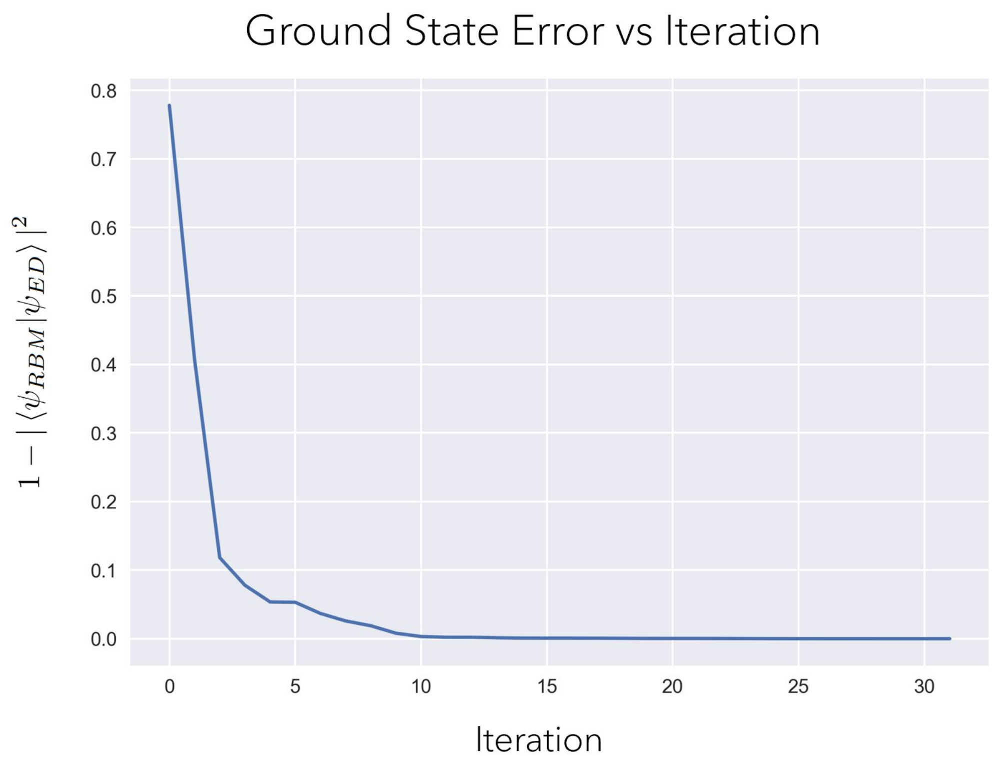
b_i (M elements)

W_{ij} (N×M elements)

$$\Psi(S; \mathbf{a}, \mathbf{b}, \mathbf{W}) = \sum_{\{h_i\}} e^{\sum_j a_j \sigma_j^z + \sum_i b_i h_i + \sum_{ij} W_{ij} h_i \sigma_j^z}$$

Ground State Determination

$$E(\mathbf{a}, \mathbf{b}, \mathbf{W}) = \frac{\langle \psi_{RBM} | H | \psi_{RBM} \rangle}{\langle \psi_{RBM} | \psi_{RBM} \rangle}$$



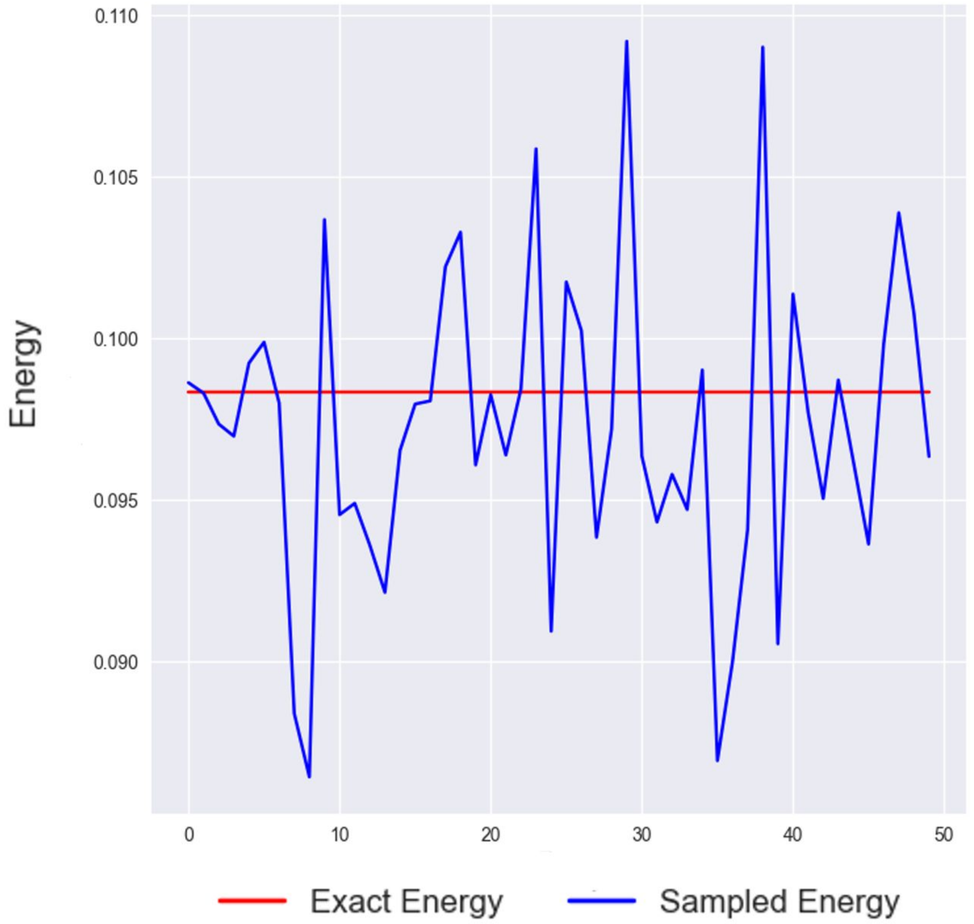
- The variational energy is minimal when ψ_{RBM} accurately models the ground state
- Learning is achieved through this minimization
- RBM is sufficiently expressive to model the ground state

Network Training

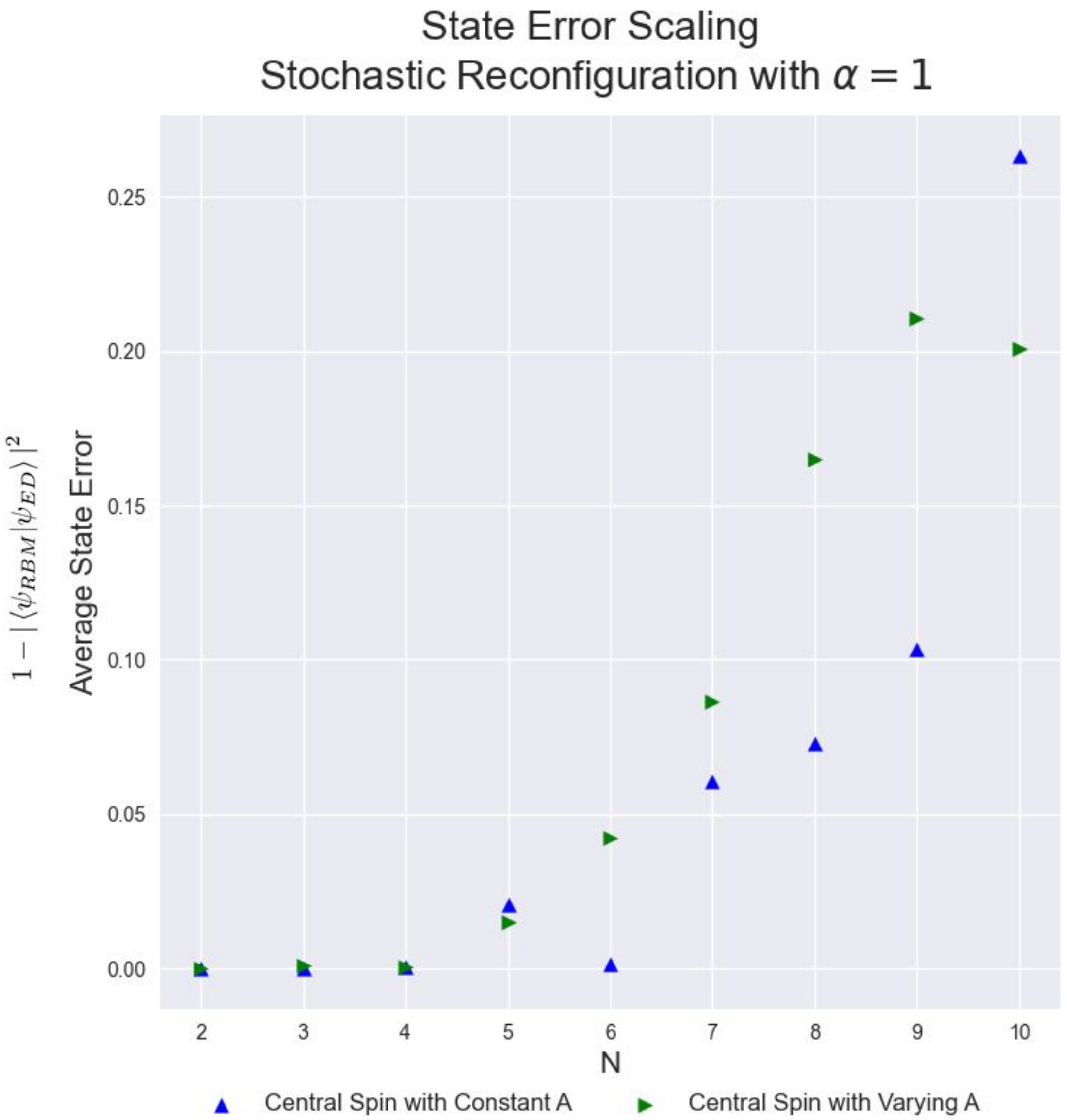
- Stochastic Reconfiguration [1]
- Monte Carlo Sampling [1]

$$
\begin{aligned}
\langle \hat{H} \rangle &= \frac{\sum_{\sigma,\sigma'} \Psi^*(\boldsymbol{\sigma}) \langle \boldsymbol{\sigma} | \hat{H} | \boldsymbol{\sigma}' \rangle \Psi(\boldsymbol{\sigma}')}{\sum_{\sigma} |\Psi(\boldsymbol{\sigma})|^2} \\
&= \sum_{\boldsymbol{\sigma}} \left(\sum_{\boldsymbol{\sigma}'} \langle \boldsymbol{\sigma} | \hat{H} | \boldsymbol{\sigma}' \rangle \frac{\Psi(\boldsymbol{\sigma}')}{\Psi(\boldsymbol{\sigma})} \right) \frac{|\Psi(\boldsymbol{\sigma})|^2}{\sum_{\sigma'} |\Psi(\boldsymbol{\sigma}')|^2} \\
&\approx \left\langle \sum_{\boldsymbol{\sigma}'} \langle \boldsymbol{\sigma} | \hat{H} | \boldsymbol{\sigma}' \rangle \frac{\Psi(\boldsymbol{\sigma}')}{\Psi(\boldsymbol{\sigma})} \right\rangle_{\boldsymbol{\sigma}}
\end{aligned}
$$

Monte Carlo Energy Sampling



Hamiltonian Comparison



$$H = BS_0^z + \sum_{k=1}^{N-1} A_k \mathbf{S}_0 \cdot \mathbf{S}_k$$

- Constant coupling

$$A_k = 1 \ \forall k, \ B = 1$$

- Varying coupling

$$A_k = \frac{A}{N_0} e^{\frac{-k}{N_0}}$$

$$A = \frac{N}{2}, \ B = \frac{N}{2}, \ N_0 = \frac{N}{2}$$

References

1. G. Carleo and M. Troyer, Solving the quantum many-body problem with artificial neural networks, Science 355, 602 (2017)