Restricted Boltzmann machines as variational wave functions

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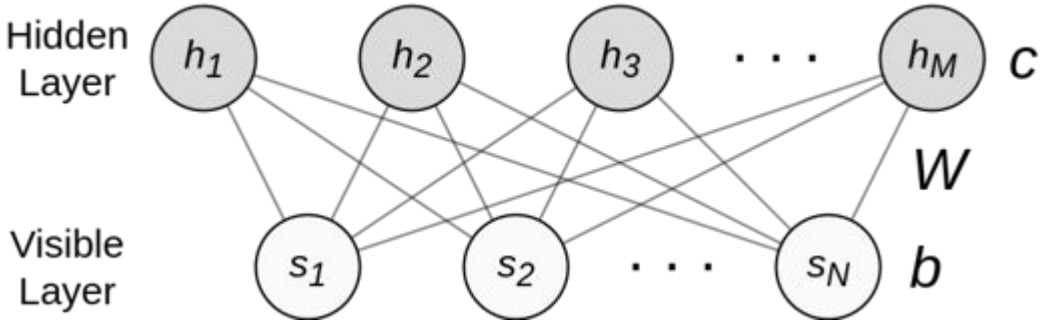
RBMs



$$E(s,h) = -b^T s - c^T h - h^T W s$$

$$\Psi(s) = \sum_{\{h\}} e^{-E(s,h)} = e^{b^T s} \prod_{i=1}^{M} 2\cosh(c_i + W_{i.} s)$$

Variational Monte Carlo

Stochastic Reconfiguration

$$\omega_{t+1} = \omega_t - \alpha S^{-1} F$$

$$S_{kk'} = \langle O_k^* O_{k'} \rangle - \langle O_k^* \rangle \langle O_{k'} \rangle$$

$$F_k = \langle E_L O_k^* \rangle - \langle E_L \rangle \langle O_k^* \rangle$$

$$E_L(s) = \frac{H\Psi_\omega(s)}{\Psi_\omega(s)} \quad O_k(s) = \partial_{\omega_k} \log \Psi_\omega(s)$$

RBM-like wave function

$$\theta_i(s) = c_i + W_i.s$$

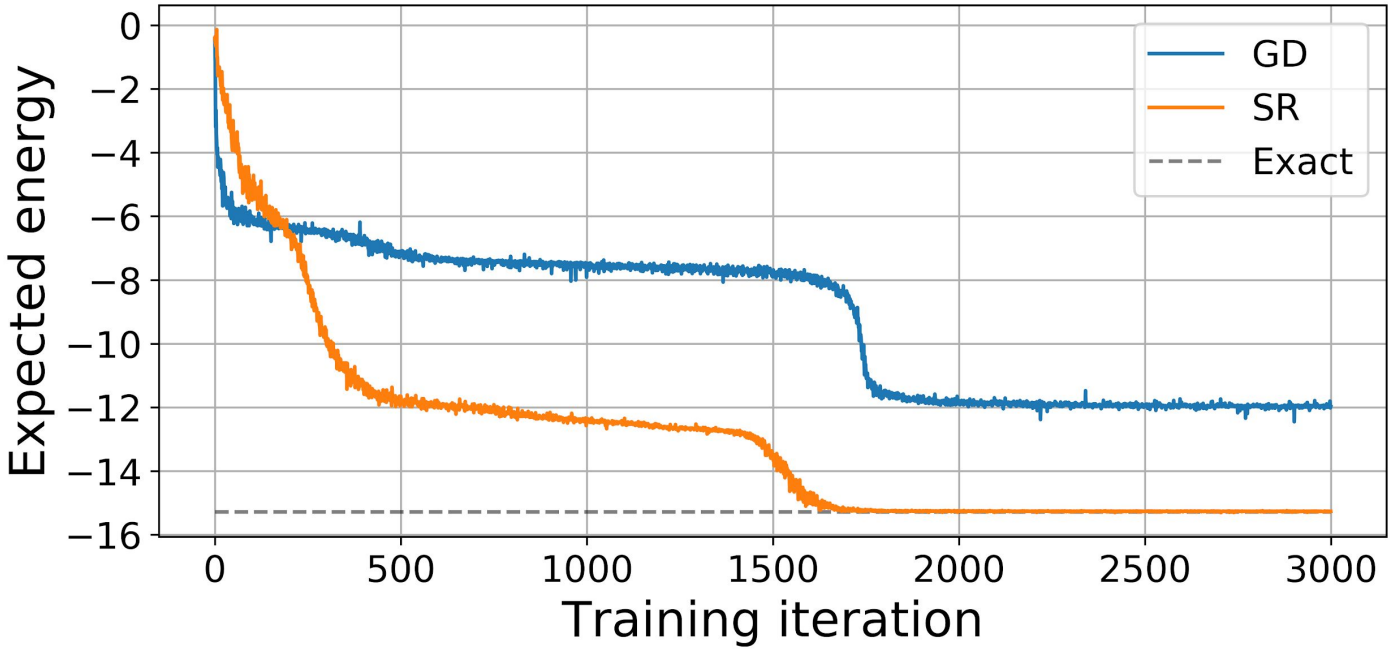
$$O_{b_j}(s) = s_j$$

$$O_{c_i}(s) = \tanh\left[\theta_i(s)\right]$$

$$O_{W_{ij}}(s) = s_j \tanh\left[\theta_i(s)\right]$$

Results

Importance of natural gradient



Results

Importance of uncorrelated samples