FYS4411 - Project 2
The restricted Boltzmannn machine applied to the quantum many body problem

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Abstract

NICE ABSTRACT

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A Finding the derivatives

In this section, we derive the expressions for the various derivatives stated in section **SECTION**. We begin with the local energy.

A.1 The local energy

The local energy is given by:

$$E_L = \frac{1}{\Psi}\hat{H}\Psi = \sum_{i=1}^{N}\left(-\frac{1}{2\Psi}\nabla_i^2\Psi + \frac{1}{2}\omega^2 r_i^2\right) + \sum_{i<j}\frac{1}{r_{ij}} \tag{1}$$

Thus, we must compute:

$$\frac{1}{\Psi}\nabla_i^2\Psi \tag{2}$$

This may be rewritten as:

$$\frac{1}{\Psi}\nabla\left(\Psi\frac{1}{\Psi}\nabla\Psi\right) = \left(\frac{1}{\Psi}\nabla\Psi\right)^2 + \nabla\left(\frac{1}{\Psi}\nabla\Psi\right) = \left[\nabla\log\Psi\right]^2 + \nabla^2\log\Psi \tag{3}$$

The logarithm of our trial wavefunction is given by:

$$\log\Psi = -\log Z - \sum_{i=1}^{M}\left(\frac{(X_i - a_i)^2}{2\sigma^2}\right) + \sum_{j=1}^{N}\log\left(1 + \exp\left(b_j + \sum_{i=1}^{M}\frac{X_i w_{ij}}{\sigma^2}\right)\right) \tag{4}$$

The derivative with respect to one coordinate is now given by:

$$\begin{aligned}\frac{\partial\log\Psi}{\partial X_k} &= \frac{(a_k - X_k)}{\sigma^2} + \sum_{j=1}^{N}\frac{w_{kj}\exp\left(b_j + \sum_{i=1}^{M}\frac{X_i w_{ij}}{\sigma^2}\right)}{\sigma^2\left(1 + \exp\left(b_j + \sum_{i=1}^{M}\frac{X_i w_{ij}}{\sigma^2}\right)\right)} \\ &= \frac{a_k - X_k}{\sigma^2} + \sum_{j=1}^{N}\frac{w_{kj}}{\sigma^2\left(1 + \exp\left(-b_j - \sum_{i=1}^{M}\frac{X_i w_{ij}}{\sigma^2}\right)\right)}\end{aligned} \tag{5}$$

Whereas the second derivative is:

$$\frac{\partial^2\log\Psi}{\partial X_k^2} = -\frac{1}{\sigma^2} + \sum_{j=1}^{N}\frac{w_{kj}^2\exp\left(-b_j - \sum_{i=1}^{M}\frac{X_i w_{ij}}{\sigma^2}\right)}{\sigma^4\left(1 + \exp\left(-b_j - \sum_{i=1}^{M}\frac{X_i w_{ij}}{\sigma^2}\right)\right)^2} \tag{6}$$

The local energy can now be found by using equation 3, and inserting equation 5 and equation 6.

A.2 The derivatives with respect to the parameters

For our optimization method, we require:

$$\frac{1}{\Psi}\frac{\partial\Psi}{\partial\alpha_k} = \frac{\partial}{\partial\alpha_k}\log\Psi \tag{7}$$

Where α_k is any of the variational parameters a, b or w. These derivatives are given by:

$$\frac{\partial\log\Psi}{\partial a_k} = \frac{a_k - X_k}{\sigma^2} \tag{8}$$

$$\frac{\partial \log \Psi}{\partial b_k} = \frac{\exp\left(b_k + \sum_{i=1}^{M} \frac{X_i w_{ik}}{\sigma^2}\right)}{1 + \exp\left(b_k + \sum_{i=1}^{M} \frac{X_i w_{ik}}{\sigma^2}\right)} = \frac{1}{1 + \exp\left(-b_k - \sum_{i=1}^{M} \frac{X_i w_{ik}}{\sigma^2}\right)} \tag{9}$$

Finally, the derivative with respect to the weights, w_{kl} is given by:

$$\frac{\partial \log \Psi}{\partial w_{kl}} = \frac{X_k \exp\left(b_l + \sum_{i=1}^{M} \frac{X_i w_{il}}{\sigma^2}\right)}{\sigma^2 \left(1 + \exp\left(b_l + \sum_{i=1}^{M} \frac{X_i w_{il}}{\sigma^2}\right)\right)} = \frac{X_k}{\sigma^2 \left(1 + \exp\left(-b_l - \sum_{i=1}^{M} \frac{X_i w_{il}}{\sigma^2}\right)\right)} \tag{10}$$