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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COOL INTRO

2 Theoretical model

Our system of N electrons confined in an isotropic harmonic oscillator potential is described by the Hamiltonian:

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

Where this is in natural units, i.e. $\hbar = c = e = m_e = 1$. Here ω is the frequency of the oscillator trap and $1/r_{ij}$ is the distance between particle i and j. The first term describes the interaction of the electrons with the potential, and we refer to it as the noninteracting part. The second term describes the Coloumb interaction between the electrons, and we refer to it as the interacting part.

We now wish to find the energy, E of our system by solving the time-independent Schrödinger equation:

$$H\Psi = E\Psi \tag{2}$$

We are chiefly interested in finding a bound on the ground-state energy of our system. We achieve such an upper bound by invoking the variational principle, as formulated in **GRIFFITHS**, which states that:

$$E_0 \leq \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \tag{3}$$

Where E_0 is the ground-state energy and Ψ_T is any (not necessarily normalized) wavefunction. Our approach is therefore to choose a trial wavefunction, Ψ_T, and the compute $E' = \langle \Psi_T | H | \Psi_T \rangle$ by using a variational Monte Carlo approach. The variational method then guarantees that our approximation to the energy, E' will be larger than the ground state energy E_0.

2.1 Neural-network quantum states

We follow the approach outlined by **REFERENCE** to determine our trial wavefunction. They choose to interpret the problem of solving equation 2 as a multi-dimensional minimization and feature extraction problem. We therefore employ a neural network to find the optimal wavefunction.

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MUCHO METHOD

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EXCELLENT DISCUSSION

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6.1 Outlook

MAGNIFICIENT OUTLOOK

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Appendices

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:

$$E_L = \frac{1}{\Psi}\hat{H}\Psi = \sum_{i=1}^{N}\left(-\frac{1}{2\Psi}\nabla_i^2\Psi + \frac{1}{2}\omega^2 r_i^2\right) + \sum_{i<j}\frac{1}{r_{ij}} \tag{4}$$

Thus, we must compute:

$$\frac{1}{\Psi}\nabla_i^2\Psi \tag{5}$$

This may be rewritten as:

$$\frac{1}{\Psi}\nabla\left(\Psi\frac{1}{\Psi}\nabla\Psi\right) = \left(\frac{1}{\Psi}\nabla\Psi\right)^2 + \nabla\left(\frac{1}{\Psi}\nabla\Psi\right) = [\nabla\log\Psi]^2 + \nabla^2\log\Psi \tag{6}$$

The logarithm of our trial wavefunction is given by:

$$\log\Psi = -\log Z - \sum_{i=1}^{M}\left(\frac{(X_i - a_i)^2}{2\sigma^2}\right) + \sum_{j=1}^{N}\log\left(1 + \exp\left(b_j + \sum_{i=1}^{M}\frac{X_i w_{ij}}{\sigma^2}\right)\right) \tag{7}$$

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

$$\begin{aligned}
\frac{\partial\log\Psi}{\partial X_k} &= \frac{(a_k - X_k)}{\sigma^2} + \sum_{j=1}^{N}\frac{w_{kj}\exp\left(b_j + \sum_{i=1}^{M}\frac{X_i w_{ij}}{\sigma^2}\right)}{\sigma^2\left(1 + \exp\left(b_j + \sum_{i=1}^{M}\frac{X_i w_{ij}}{\sigma^2}\right)\right)} \\
&= \frac{a_k - X_k}{\sigma^2} + \sum_{j=1}^{N}\frac{w_{kj}}{\sigma^2\left(1 + \exp\left(-b_j - \sum_{i=1}^{M}\frac{X_i w_{ij}}{\sigma^2}\right)\right)}
\end{aligned} \tag{8}$$

Whereas the second derivative is:

$$\frac{\partial^2\log\Psi}{\partial X_k^2} = -\frac{1}{\sigma^2} + \sum_{j=1}^{N}\frac{w_{kj}^2\exp\left(-b_j - \sum_{i=1}^{M}\frac{X_i w_{ij}}{\sigma^2}\right)}{\sigma^4\left(1 + \exp\left(-b_j - \sum_{i=1}^{M}\frac{X_i w_{ij}}{\sigma^2}\right)\right)^2} \tag{9}$$

The local energy can now be found by using equation 6, and inserting equation 8 and equation 9.

A.2   The derivatives with respect to the parameters

For our optimization method, we require:

$$\frac{1}{\Psi}\frac{\partial\Psi}{\partial\alpha_k} = \frac{\partial}{\partial\alpha_k}\log\Psi \tag{10}$$

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

$$\frac{\partial\log\Psi}{\partial a_k} = \frac{X_k - a_k}{\sigma^2} \tag{11}$$

$$\frac{\partial \log \Psi}{\partial b_k} = \frac{\exp\left(b_k + \sum_{i=1}^{M} \frac{X_i w_{ik}}{\sigma^2}\right)}{1 + \exp\left(b_k + \sum_{i=1}^{M} \frac{X_i w_{ik}}{\sigma^2}\right)} = \frac{1}{1 + \exp\left(-b_k - \sum_{i=1}^{M} \frac{X_i w_{ik}}{\sigma^2}\right)} \tag{12}$$

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

$$\frac{\partial \log \Psi}{\partial w_{kl}} = \frac{X_k \exp\left(b_l + \sum_{i=1}^{M} \frac{X_i w_{il}}{\sigma^2}\right)}{\sigma^2 \left(1 + \exp\left(b_l + \sum_{i=1}^{M} \frac{X_i w_{il}}{\sigma^2}\right)\right)} = \frac{X_k}{\sigma^2 \left(1 + \exp\left(-b_l - \sum_{i=1}^{M} \frac{X_i w_{il}}{\sigma^2}\right)\right)} \tag{13}$$

A.3   The derivatives with Gibbs sampling

In Gibbs sampling, we represent the wavefunction as $\Psi = \sqrt{F_{rbm}}$, instead of $\Psi = F_{rbm}$. Note, however, that we only ever differentiate the logarithm of the wavefunction. As $\log \sqrt{\Psi} = \frac{1}{2} \log \Psi$, however, this is only a marginal change. Specifically:

$$E_L = [\nabla \log \sqrt{\Psi}]^2 + \nabla^2 \log \sqrt{\Psi} = \frac{1}{4}[\nabla \log \Psi]^2 + \frac{1}{2}\nabla^2 \log \Psi \tag{14}$$

$$\frac{\partial}{\partial \alpha_k} \log \sqrt{\Psi} = \frac{1}{2}\frac{\partial}{\partial \alpha_k} \Psi \tag{15}$$

$$\frac{\partial}{\partial b_k} \log \sqrt{\Psi} = \frac{1}{2}\frac{\partial}{\partial b_k} \log \Psi \tag{16}$$

$$\frac{\partial}{\partial w_{kl}} \log \sqrt{\Psi} = \frac{1}{2}\frac{\partial}{\partial w_{kl}} \log \Psi \tag{17}$$

Where the derivatives on the right-hand side are given in the previous section.

B   Deriving the spin of the ground state wavefunction

The Pauli exclusion principle