

FYS4411 - Project 2

The restricted Boltzmann machine applied to the quantum many body problem

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Abstract

NICE ABSTRACT

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1 Introduction

COOL INTRO

2 Theoretical model

MUCH THEORY

3 Methods

MUCHO METHOD

4 Results

GROUNDBREAKING RESULTS

5 Discussion

EXCELLENT DISCUSSION

6 Conclusion

BRILLIANT CONCLUSION

6.1 Outlook

MAGNIFICENT OUTLOOK

References

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:

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

Thus, we must compute:

$$\frac{1}{\Psi} \nabla_i^2 \Psi \quad (2)$$

This may be rewritten as:

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

The logarithm of our trial wavefunction is given by:

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

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

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

Whereas the second derivative is:

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

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:

$$\frac{1}{\Psi} \frac{\partial \Psi}{\partial \alpha_k} = \frac{\partial}{\partial \alpha_k} \log \Psi \quad (7)$$

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

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

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

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

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

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:

$$E_L = [\nabla \log \sqrt{\Psi}]^2 + \nabla^2 \log \sqrt{\Psi} = \frac{1}{4} [\nabla \log \Psi]^2 + \frac{1}{2} \nabla^2 \log \Psi \quad (11)$$

$$\frac{\partial}{\partial \alpha_k} \log \sqrt{\Psi} = \frac{1}{2} \frac{\partial}{\partial \alpha_k} \log \Psi \quad (12)$$

$$\frac{\partial}{\partial b_k} \log \sqrt{\Psi} = \frac{1}{2} \frac{\partial}{\partial b_k} \log \Psi \quad (13)$$

$$\frac{\partial}{\partial w_{kl}} \log \sqrt{\Psi} = \frac{1}{2} \frac{\partial}{\partial w_{kl}} \log \Psi \quad (14)$$

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