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

Daniel Heinesen[1], Gunnar Lange[2] & Aram Salihi[2]
[1]Department of Theoretical Astrophysics, University of Oslo, N-0316 Oslo, Norway
[2]Department of Physics, University of Oslo, N-0316 Oslo, Norway

May 24, 2018

Abstract

NICE ABSTRACT! Also check out our GitHub[1]

[1]`https://github.com/dulte/FYS4411/tree/master/Project2`

Contents

1 Introduction

The interest in applying machine learning methods to quantum mechanical system has experienced a veritable surge in recent years, and many different methods and applications are currently being explored (see e.g. [Broecker et al., 2017] or [Botu and Ramprasad, 2015]). A particularly interesting application of machine-learning to the quantum many-body system is presented by [Carleo and Troyer, 2017]. They interpret the quantum many-body wavefunction as a system of exponential complexity, where we are interested in extracting some features, such as the energy. When viewed from this perspective, machine learning algorithms and neural networks are a natural way to attack the problem, as these are methods designed for extracting features from highly complex systems. They present a method which they title neural-network quantum states, where they use restricted Boltzmann machines to represent the wavefunction.

We apply their method to a system of fermions in an isotropic harmonic oscillator trap with Coloumb repulsion. This system has the advantage of being well-studied, as both analytic ([Taut, 1994]) and numeric ([Pedersen Lohne et al., 2011]) results are available for selected system configurations. This enables us to benchmark our results, and compare the performance of neural-network quantum states to other algorithms.

We focus on the ground state of our system, and therefore only investigate the case of 1 and 2 electrons, in 1, 2 and 3 dimensions. We use restricted Boltzmann machines to attain the form of our wavefunction, and the use Variational Monte Carlo (VMC) methods to establish an upper bound on the ground state energy. The weights and biases in our neural network are minimized using a stochastic gradient approach with a fixed learning rate. We compare three different sampling methods in our VMC calculations - Metropolis sampling, importance sampling and Gibbs sampling. For each of these methods, we investigate how our system behaves as we vary the parameters associated with the system. We also include an analysis of the errors involved, using the blocking method.

2 Theory

2.1 The Hamiltonian

We consider a D-dimensional system of P electrons confined in an isotropic harmonic oscillator trap. Working in natural units ($\hbar = c = e = m_e = 1$), the Hamiltonian of such a system is given by:

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

Here ω is the frequency of the oscillator trap, r_i is the D-dimensional position vector of electron i and $1/r_{ij}$ is the distance between electron 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:

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

Where Ψ is the wavefunction of the system.

2.2 Analytic solution

We are chiefly interested in the ground-state energy of our system, as this is the state that the system will fall into if left unperturbed by e.g. thermal excitation. If we ignore the interacting

part, then we have an analytic solution to the ground-state wavefunction for two electrons, which according to [Griffiths, 2004] is given by:

$$\psi(r_1, ..., r_P) = C \exp\left(-\frac{\omega}{2}\sum_{i=1}^{P} r_i^2\right) \tag{3}$$

Where C is a normalization constant. Furthermore, the ground-state energy (in natural units) of such a system is given by:

$$\frac{E}{\omega} = P\frac{D}{2} \tag{4}$$

Note, however, that all of the above expressions are only valid up to $P = 2$, as we are dealing with spin-1/2 fermions, to which the Pauli exclusion principle applies. Therefore, we can only have two particles in the ground-state, and these particles must have opposite spin. More precisely, they must be in the singlet state (total spin 0) in the noninteracting case, as discussed in appendix B. In what follows, we therefore restrict ourselves to $P \in \{1, 2\}$.

We also have analytic results for some special cases in the interacting case. In particular, according to [Taut, 1994] and [Pedersen Lohne et al., 2011], the energy is 3 (in natural units) for 2 particles in the 2-dimensional case with $\omega = 1$.

2.3 The variational principle

In the general case, where analytic solutions are not available, it is desirable to use a numeric method to find the ground state energy, or at least an upper bound on the ground state energy. We achieve such an upper bound by invoking the variational principle, as formulated in [Griffiths, 2004], which states that:

$$E_0 \leq \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \tag{5}$$

Where E_0 is the ground-state energy and Ψ_T is any (not necessarily normalized) trial wavefunction for our system. We therefore choose a class of trial wavefunctions, Ψ_T, and then compute $E' = \langle \Psi_T | H | \Psi_T \rangle$ by using a 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. We then adjust our trial wavefunction within our class of wavefunctions, to give the lowest possible energy, hoping to attain a decent estimate for the actual ground-state energy of our system.

2.4 Neural-network quantum states and Restricted Boltzmann Machines

To actually determine our class of trial wavefunction, we follow the approach outlined by [Carleo and Troyer, 2017]. They choose to interpret the problem of solving equation 2 as a multi-dimensional minimization and feature extraction problem. As neural networks were designed to tackle exactly this class of problem, we choose to employ a neural network to find our trial wavefunction.

We follow the approach advocated by [Carleo and Troyer, 2017] and choose a restricted Boltzmann machine (RBM) as the basis for our neural network. Restricted Boltzmann Machines (RBM) are described in great detail in the literature, see e.g. [Hinton, 2010]. We therefore provide only a rough outline on how to apply them. We begin by setting up a vector of M visible nodes, $\mathbf{X}$, which corresponds to the position states of our system (with one state per particle, P and dimension, D, i.e. $M = PD$), and a vector of N hidden nodes, $\mathbf{H}$ which correspond to some feature of our system that we wish to use to predict our wavefunction. Each of these nodes have a bias associated with them, which determine their relative importance. Additionally, there are also weights associated with connections between the hidden nodes and the visible nodes, but there are no connections between nodes in the same layer (hence *restricted* Boltzmann machine). The RBM method then

consists of modelling the probability distribution for our system, given some visible nodes $\mathbf{X}$ and some hidden nodes $\mathbf{H}$, by a Boltzmann distribution function of the form:

$$F_{rbm}(\mathbf{X}, \mathbf{H}) = \frac{1}{Z} \exp\left(-\frac{1}{T_0} E(\mathbf{X}, \mathbf{H})\right) \tag{6}$$

Where Z is a normalization constant and T_0 is some reference temperature (set to 1 in what follows). The energy, $E(\boldsymbol{X}, \boldsymbol{H})$ relates the weights and biases to the probability distribution. In the standard RBM formulation, both $\boldsymbol{X}$ and $\boldsymbol{H}$ are binary variables. We choose the hidden nodes $\boldsymbol{H}$ to be binary, $h_i \in \{0, 1\}$. The visible nodes, $\boldsymbol{X}$, however, represent the position of the electrons in our system, and must therefore be modelled as a continuous function. We therefore use an extension of standard RBM known as Gaussian-Bernoulli Deep Boltzmann Machine's (GDBM), as described by [Wang et al., 2014]. They implement the energy as:

$$E(\mathbf{X}, \mathbf{H}) = \sum_{i=1}^{M} \frac{(X_i - a_i)^2}{2\sigma^2} - \sum_{j=1}^{N} b_j H_j - \sum_{i=1}^{N} \sum_{j=1}^{M} \frac{X_i w_{ij} H_j}{\sigma^2} \tag{7}$$

Where a_i is the bias associated with the visible node X_i, b_i is the bias associated with the hidden node H_i and w_{ij} is the weight associated with the coupling between X_i and H_j. As discussed in [Wang et al., 2014], this makes the marginal distribution of the h_i Bernoulli distribution, whereas the marginal distribution of X_i form a normal distribution with variance σ^2.

As our wavefunction is a function of the position coordinates only, we choose to interpret the marginal distribution of the visible nodes as our wavefunction. This marginal distribution is given by:

$$F_{rbm}(\mathbf{X}) = \sum_{h_i \in \mathbf{H}} F_{rbm}(\mathbf{X}, \mathbf{H}) \tag{8}$$

Which gives, after some algebra done in [Hjorth-Jensen, 2018], our class of trial wavefunctions as:

$$\Psi_T(\mathbf{X}) = F_{rbm}(\mathbf{X}) = \frac{1}{Z} \exp\left(-\sum_{i=1}^{M} \frac{(X_i - a_i)^2}{2\sigma^2}\right) \prod_{j=1}^{N} \left(1 + \exp\left(b_j + \sum_{i=1}^{M} \frac{X_i w_{ij}}{\sigma^2}\right)\right) \tag{9}$$

This trial wavefunction, given biases and weights a, b, w, is then plugged into equation 5 to find an upper bound on the ground-state energy of our system. We seek to optimize this wavefunction with respect to a, b and w. **TALK ABOUT IF THIS CAN BE EXACT FOR NONINTERACTING**

2.5 Variational Monte Carlo methods

Having established our trial wavefunction, it remains to use the variational principle to estimate the ground state energy. We use a Monte Carlo approach to estimate the inner product given in equation 5. A more detailed description of this may be found in [Hjorth-Jensen, 2015], and we therefore only sketch a procedure. We begin by considering the probability distribution associated with our trial wavefunction, given by:

$$P(\mathbf{X}) = \frac{|\Psi_T|^2}{\int d\mathbf{X} |\Psi_T|^2} \tag{10}$$

Where the normalization integral is to be carried out over all particles and dimension (i.e. over M variables). If we now define the local energy (by solving equation 2 for E) as:

$$E_L(\mathbf{X}) = \frac{1}{\Psi_T} H \Psi_T \tag{11}$$

Then the expectation value of the Hamiltonian (which gives the energy) is given by:

$$E_0 \leq E[H] = \int d\mathbf{X} P(\mathbf{X}) E_L(\mathbf{X}) \approx \frac{1}{K} \sum_{i=1}^{K} E_{L,i} \tag{12}$$

Thus, we can get an approximation to the ground state energy by averaging the local energy for various system configurations. This method is, however, contingent upon our ability to efficiently compute the local energy and sample the position space.

2.6 The local energy

The local energy is defined in equation 11, with the Hamiltonian given in equation 1. Note that the most complicated part of this expression is the second derivative of the wavefunction. We derive an analytic expression for this is in appendix A.1. The local energy is then given by:

$$\begin{aligned} \frac{1}{\Psi_T} H\Psi_T = &-\frac{1}{2} \sum_{k=1}^{M} \left[\frac{a_k - X_k}{\sigma^2} + \sum_{j=1}^{N} \frac{w_{kj}}{\sigma^2 \left(1 + \exp\left(-b_j - \sum_{i=1}^{M} \frac{X_i w_{ij}}{\sigma^2}\right)\right)} \right]^2 \\ &+ \frac{M}{2\sigma^2} - \frac{1}{2} \sum_{k=1}^{M} \sum_{j=1}^{N} \frac{w_{kj}^2 \exp\left(-b_j - \sum_{i=1}^{M} \frac{X_i w_{ij}}{\sigma^2}\right)}{\sigma^4 \left(1 + \exp\left(-b_j - \sum_{i=1}^{M} \frac{X_i w_{ij}}{\sigma^2}\right)\right)^2} + \frac{1}{2} \sum_{i=1}^{M} \omega^2 X_i^2 + \sum_{i=1}^{P} \sum_{j=1}^{i} \frac{1}{r_{ij}} \end{aligned} \tag{13}$$

2.7 Sampling the position space

To make sense of equation 12, we must sample our position space, to get a good estimate for the local energy of the system. We employ three different sampling techniques.

2.7.1 The Metropolis algorithm

The Metropolis algorithm is described in further detail in [Hjorth-Jensen, 2015]. We begin by noting that the wavefunction gives the probability of finding the particle at a point in position space. We will therefore get the most reliable estimates for our local energy if we sample where the wavefunction (and thus the probability distribution) is large, and we avoid wasting CPU cycles. The Metropolis algorithm is one way to achieve this. This is achieved by proposing to move a single particle according to:

$$\boldsymbol{r}_{\mathrm{i,new}} = \boldsymbol{r}_{\mathrm{i}} + \boldsymbol{\xi} dx \tag{14}$$

Where $\boldsymbol{r}_{\mathrm{i}}$ is the position of particle i, dx is a chosen step size and $\boldsymbol{\xi}$ is a D-dimensional vector of random numbers, whose distribution we discuss in section 3.3. To find out whether we should sample local energy at this new position, we compute the ratio:

$$\Theta = \frac{P(\boldsymbol{X}_{\mathrm{new}})}{P(\boldsymbol{X})} = \frac{|\Psi(\boldsymbol{X}_{\mathrm{new}})|^2}{|\Psi(\boldsymbol{X})|^2} \tag{15}$$

Where $\boldsymbol{X}_{\mathrm{new}}$ is the position of the particles after updating the position of particle i according to 14. Note that this ratio determines if the particle is more likely to be found at the position $\boldsymbol{X}_{\mathrm{new}}$ than at position $\boldsymbol{X}$. The move is only accepted if $\Theta \geq \theta$, where $\theta \in [0, 1]$ is a uniformly distributed random variable. Thus, if the probability of finding the particle at $\mathbf{X}_{\mathrm{new}}$ is larger than the probability of finding the particle at $\mathbf{X}$, then we accept the move. If not, then the larger the energy difference the less probable it is that the move is accepted. As such, we should eventually end up moving fairly close to the most likely position, without getting stuck in it.

2.7.2 The Metropolis-Hasting alogrithm/importance sampling

We compare the Metropolis algorithm to an alternative, known as importance sampling. This is described in further detail in [Hjorth-Jensen, 2015]. Note that the Metropolis sampling described in the previous section picks positions at random, and as such does not have a preference for proposing steps that move the system to a region of high probability density (given by $|\Psi|^2$). As such, some CPU cycles will be wasted on positions that have a very small probability of occurring. Importance sampling seeks to alleviate this problem by introducing a quantum force, which "pushes" the system in the direction of high probability. This changes the way a new step is proposed, as discussed in section 3.3. This force is, on particle i given by:

$$F_i(\boldsymbol{X}) = \frac{2}{\Psi_T}\nabla_i \Psi_T = 2\nabla_i \log \Psi_T \tag{16}$$

We compute this in appendix A.1 and show that this force is given by:

$$F_i(\boldsymbol{X}) = 2\sum_{k=1}^{D}\left(\frac{a_k - X_k}{\sigma^2} + \sum_{j=1}^{N}\frac{w_{kj}}{\sigma^2\left(1+\exp\left(-b_j - \sum_{i=1}^{M}\frac{X_i w_{ij}}{\sigma^2}\right)\right)}\right) \tag{17}$$

The analysis in [Hjorth-Jensen, 2015] shows that the correct way to include this in our algorithm is by multiplying the transition probability w defined in equation 15 by a Green's function given by:

$$G(\mathbf{X}, \mathbf{X}') = \frac{1}{(4\mathcal{D}\Delta t)^{3/2}}\sum_{i=1}^{M}\exp\left(-\frac{(X_i - X_i' - \mathcal{D}\Delta t F_i(\mathbf{X}'))^2}{4\mathcal{D}\Delta t}\right) \tag{18}$$

Where $\mathcal{D}$ is a diffusion parameter, which in our case equals $1/2$. The modified transition probability is given by:

$$w_{\text{importance}} = \frac{|\Psi(\boldsymbol{X}_{\text{new}})|^2}{|\Psi(\boldsymbol{X})|^2}\frac{G(\boldsymbol{X}, \boldsymbol{X}_{\text{new}})}{G(\boldsymbol{X}_{new}, \boldsymbol{X})} \tag{19}$$

This transition probability is implemented exactly as in the previous section.

2.7.3 Gibbs Sampling

Gibbs sampling is an alternative to Metropolis/Metropolis-Hastings algorithm, which is described in greater detail in [Wang et al., 2014]. Here we have a more direct connection between the probability distribution of the neural network and the wavefunction. In order to establish a direct physical connection to the probability distribution of the RBM, we now model our wavefunction as:

$$\Psi_{T,\text{Gibbs}} = \sqrt{F_{rbm}(\boldsymbol{X})} \tag{20}$$

Where Ψ_T is given in equation 9. Note that, as the wavefunction is real-valued, this implies $|\Psi_{T,\text{Gibbs}}(\boldsymbol{X})|^2 = F_{rbm}(\boldsymbol{X})$, i.e. the marginal distribution directly models the position probability distribution.

We are also interested in the conditional distribution of the hidden nodes. This gives, after a few lines of Algebra done in [Hjorth-Jensen, 2018]:

$$\begin{aligned} P(H_j = 1|\boldsymbol{X}) &= \frac{1}{1+\exp\left(-b_j - \frac{1}{\sigma^2}\sum_{i=1}^{M}X_i w_{ij}\right)} \\ P(H_j = 0|\boldsymbol{X}) &= \frac{1}{1+\exp\left(b_j + \frac{1}{\sigma^2}\sum_{i=1}^{M}X_i w_{ij}\right)} \end{aligned} \tag{21}$$

We now initialize the weights, biases and position $\boldsymbol{X}$, as discussed in section 3.2. We can then compute the marginal distributions for $\boldsymbol{X}$ given in equation 21. We then draw a uniform random

number $\theta \in [0,1]$ for each H_i, and update H_i according to equation 21. Then the positions are updated according to their conditional distribution, which is, as shown in [Hjorth-Jensen, 2018] **WRITE MORE HERE**

$$X_i \sim \mathcal{N}\left(\sum_{j=1}^{N} w_{ij} H_j, \sigma^2\right) \tag{22}$$

We then compute the local energy using this $\boldsymbol{X}$. Note that we here cannot use equation 11, as this is only valid for $\Psi_T = F_{rbm}(\boldsymbol{X})$. However, the new expression for local energy only differs by some numerical factors to the previous expression, as discussed in appendix A.3.

2.8 Optimizing our wavefunction in parameter space

For our neural network to be successful, we must be able to minimize the energy of our wavefunction. This is done by varying the parameters a_i, b_i and w_{ij}, and computing the local energy. The variational method then guarantees that the lowest energy we find will be larger than the ground state energy. We employ a stochastic gradient method to find the minimum in our parameter space. Defining a vector of all parameters, $\boldsymbol{\theta}$, we iterate this vector according to:

$$\boldsymbol{\theta}^{i+1} = \boldsymbol{\theta}^i + \gamma \frac{\partial \overline{E}_L}{\partial \boldsymbol{\theta}^i}(\boldsymbol{\theta}^i) \tag{23}$$

Where $\overline{E}_L$ is the energy computed by means of the variational Monte Carlo method (given by equation 12) and γ is the step size, which we vary. The derivative is with respect to all parameters. It is shown in [Heinesen et al., 2018] that the derivative of this expectation value of the energy is given by:

$$\frac{\partial \overline{E}_L}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}) = 2\left(\left\langle \frac{1}{\Psi_T}\frac{\partial \Psi_T}{\partial \boldsymbol{\theta}}\overline{E}_L(\boldsymbol{\theta})\right\rangle - \left\langle \frac{1}{\Psi_T}\frac{\partial \Psi_T}{\partial \boldsymbol{\theta}}\right\rangle \langle \overline{E}_L(\boldsymbol{\theta})\rangle\right) \tag{24}$$

We must therefore compute the derivative of our trial wavefunction, given in equation 9, with respect to all of our variational parameters. This is done in detail in appendix A.2 for Metropolis/importance sampling and in appendix A.3 for Gibbs sampling. We iterate this method until the absolute value of our gradient, $\frac{\partial \overline{E}_L}{\partial \boldsymbol{\theta}}$ is small enough **DANIEL ADD STUFF**.

3 Methods

3.1 An overview of the structure of our program

Our entire program may be found on our GitHub[2]. It is an extension of the program presented in [Heinesen et al., 2018]. The program consists of 3 main classes:

`main.cpp` The main class first reads in the parameter files. It then sets up the initial guess for the weights of the neural networks and runs the stochastic descent method. Finally, it runs the full simulation with the optimized weights.

`simulation.cpp` This class contains the minimization method itself, and also runs the main Monte Carlo loop.

`system.cpp` The system class contains all the functions for the wavefunction, the different sampling methods, and the acceptance checks. It also contains the function for computing the local energy and the derivatives of the wavefunction as a function of the various parameters.

In addition, we implement various auxiliary classes, that read in parameters, dump variables to file and do statistical analysis. These are described in greater detail on our repository.

[2] `https://github.com/dulte/FYS4411/tree/master/Project2`

3.2 Initializing our system

3.2.1 Initializing the position

To initialize our system, we must distribute our particles. How we distribute the particles, however, depends on the sampling method employed. When using the Metropolis algorithm or Gibbs sampling, we distribute our particles according to:

$$\boldsymbol{r}_i = \boldsymbol{\xi} \tag{25}$$

Where $\boldsymbol{\xi}$ is a vector of D number, normally distributed with $\xi \sim 0.5\mathcal{N}(0,1)$ as we find that this gives a good spread.

When using importance sampling, however, we must distribute our particles slightly differently, as discussed in [Hjorth-Jensen, 2015]. In this case, the initial distribution of particles is given by:

$$\boldsymbol{r}_i = \boldsymbol{\xi'}\sqrt{dx} \tag{26}$$

Where $\boldsymbol{\xi'}$ is a vector of D number distributed as $\mathcal{N}(0,1)$ and dx is a step size which we tune, as described further in section 3.6.

3.2.2 Initializing the parameters

We wish to minimize our wavefunction as a function of the biases a, b and the weights w. This is done by iterating equation 23. However, we require an initial guess for the vector of parameters, $\boldsymbol{\theta}^0$. We choose this initial guess to be uniformly distributed in $[0, 0.01]$.

3.2.3 Initializing the simulation

To initialize the simulation, we set the parameters in the parameter file found on our GitHub[1]. This gives the option to set a number of parameters of the system. Specifically, the parameter file allows the following parameters to be set at runtime:

- The number of Monte Carlo cycles
- The number of particles, P
- The number of hidden nodes, N
- The number of dimensions, D
- The oscillator frequency ω
- The spread in the visible nodes, σ
- The diffusion parameter D (setting this to 0 deactivates importance sampling)
- The step size, dx
- The learning rate, γ
- Whether or not the system is interacting
- Whether the energy should be computed numerically or analytically
- Whether or not to use Gibbs sampling

3.3 Proposing a new position

As discussed in section 2, both the Metropolis algorithm and the Metropolis-Hasting algorithm rely on proposing a new position of the system. The general form for this updating was given in equation 14. We now discuss how this is concretely implemented for the different sampling method.

For straightforward Metropolis sampling, there is no bias in selecting this position. We therefore simply define the new position by:

$$\boldsymbol{r}_{\text{i,new}} = \boldsymbol{r}_i + \boldsymbol{\xi} dx \tag{27}$$

Where $\boldsymbol{\xi}$ consists of D numbers, uniformly distributed in $[-1, 1]$ and dx is a step size.

For importance sampling, we add a bias in selecting the new position. This bias is introduced by including the quantum force, presented in equation 17. The details of how to implement this bias are presented in [Hjorth-Jensen, 2015]. This gives that the new step should be selected according to:

$$\boldsymbol{r}_{\text{i,new}} = \boldsymbol{r}_i + \boldsymbol{\xi'}\sqrt{dx} + \mathcal{D}\boldsymbol{F}_i dx \tag{28}$$

Where $\boldsymbol{F}_i$ is the quantum force on particle i, $\mathcal{D}$ is the diffusion parameter (equal to $1/2$) and $\boldsymbol{\xi'} \sim \mathcal{N}(0, 1)$. Note that dx may in general not be the same as above, and we investigate which dx gives the best values for each case separately, as discussed in section 3.6.

3.4 Implementing the optimization of the biases and the weights

To find the best trial wavefunction, we run the optimization algorithm given in equation 23 until the absolute value of the gradient is less than some ϵ, or we have surpassed 100 iterations. We use 100 times fewer Monte Carlo cycles to compute the local energy in the optimization loop than in the actual simulation used to determine the energy.

3.5 The errors in our energy

We wish to provide error bounds on the energies that we find. Note that the local energies constitute a highly correlated system, as the state of the system in the current Monte Carlo step differs only by the position of a single particle from the state in the previous Monte Carlo step. The variance of the energy is therefore not a good indicator of the error in our system. Instead, we use a technique known as blocking. This is described in further detail in [Jonsson, 2018] and we follow the same procedure as outline in [Heinesen et al., 2018].

Blocking works by averaging successive observations of the local energy. Such a pairwise operation preserves the variance of the data, but reduces the covariance of the data. We keep doing this until the covariance is small enough, as described in detail in [Jonsson, 2018]. To ensure that we can this as frequently as possible, we let our number of Monte Carlo cycles be a power of 2.

3.6 Tuning the parameters

We note that our results are contingent upon a number of parameters, in addition to the biases and weights that our minimization algorithm tunes. Specifically, we must choose the learning rate, γ, the step size dx, the number of hidden nodes N, the spread in the visible nodes, σ and the number of Monte Carlo cycles.

We tune each of these parameters in turn, hoping to get close to a global optimum in parameter space without having to do a complete stochastic descent. Note that the step size γ and the number of hidden nodes N are intimately related, as γ determines the rate of convergence whereas N determines the dimensionality of the convergence problem. We therefore choose to tune these parameters simultaneously, as they strongly influence one another.

3.6.1 Tuning the step size, dx

The step size dx determines how well we are able to sample the position space, as it describes how far our proposed next position should be from the previous position. To find the best possible step size dx, we investigate the behavior of the energy for different dx, and look at the acceptance rate. For this analysis, we fix some values of σ, γ and N that give acceptable values. We then choose a dx that gives a good estimate of the energy, whilst having neither an extremely high nor an extremely high acceptance rate.

We first do this for the simplest possibles system (1 particle in 1 dimension), checking both the brute-force Metropolis sampling and importance sampling (note that Gibbs sampling does not use a dx). For brute-force sampling, we accept a lower acceptance rate than for importance sampling, as importance sampling should lead to a higher acceptance rate.

We also do the same analysis for 2 particles in 2 dimensions, including interaction, as we have analytic answers for this system available in [Taut, 1994].

3.6.2 Tuning the spread in the visible nodes, σ

We vary σ, using the dx found above and acceptable values of γ and N and look at what energy we are able to attain. We do this only with Gibbs sampling, as this is where σ is most relevant. We then use this σ in the other cases as well. We do this separately for the simplest system (1 dimension, 1 particle) and for the interacting system (2 dimensions, 2 particles and interaction). We then use this σ in all subsequent runs.

3.6.3 Tuning the learning rate, γ and the number of hidden nodes, N

We choose to tune the learning rate γ and number of hidden nodes N simultaneously, as explained above. We choose the values for dx and σ found previously, and look at the absolute value of the gradient as a function of the iterations of the minimization iterations. (1 particle and 1 dimension). We then choose the combination of parameters that gives the lowest gradient over multiple iterations. We again do this separately for Metropolis sampling, importance sampling and Gibbs sampling, and separately for the simplest system (1 particle 1 dimension) and the interacting system (2 particles, 2 dimensions with interaction).

3.6.4 Choosing the number of Monte Carlo steps

Note that the numbers of Monte Carlo steps required will depend on the method used to sample the space, as e.g. importance sampling will accept more steps and therefore require fewer cycles. As we are limited to 2 particles, however, we can afford to use a fairly large number of Monte Carlo cycles. We therefore choose to use enough Monte Carlo steps to ensure convergence in the uncertainty in the energy, and use the same number of Monte Carlo cycles independent of the sampling method.

3.7 Benchmarking our results

Having chosen the parameters of our system, we can now benchmark our results. We look at the ground state energy for 1 and 2 particles, in 1,2 and 3 dimensions, both with and without interaction. Note that we have analytic results for the noninteracting case, given by equation 4, and that we have analytic results in the interacting case with 2 dimension.

Note, that the variational principle only guarantees that we attain an upper bound on the ground state energy. As such, we can only check that our result is larger than or equal to the analytic result.

4 Results

4.1 Tuning our neural network quantum state in the simplest system

We begin by tuning the parameters of our NQS in the simplest possible case (1 dimension with 1 particle).

4.1.1 Tuning dx

We show the energy and acceptance rate using brute-force Metropolis sampling for various step sizes in figure 1 below: As explained in section **SECTION**, we end up choosing $dx = 1$. We show the equivalent plot with importance sampling in figure 2 In the case of importance sampling, we choose $dx = 0.1$ as explained in **SECTION**.

4.1.2 Tuning σ

We vary σ, using Gibbs sampling. This is shown in figure 3. As explained in section **SECTION**, we choose $\sigma = 0.7$ in this case.

4.1.3 Tuning N and γ

As discussed in section **SECTION**, we tune the learning rate, γ and the number of hidden nodes, N together. This gives the plot shown in figure 4 for the standard Metropolis algorithm. As explained in section **SECTION**, we here choose **FINISH**. The equivalent plot for importance sampling is shown in figure 5 Here, we chose **FINISH**. Finally, the same plot for Gibbs sampling is shown in figure 6

4.2 Tuning our neural network quantum state in the interacting system

We perform the same analysis as in the previous section also in the interacting system with 2 particles in 2 dimension.

4.2.1 Tuning dx

We show the results of tuning the step size in the interacting case in figure 7 below: As explained in section **SECTION**, we choose $dx = 1$ in this case. We show the equivalent plot with importance sampling in figure 8 As explained in section **SECTION**, we choose $dx = 0.1$ in this case.

4.2.2 Tuning σ

As in the previous section, we also vary σ in the interacting system, using Gibbs sampling. This is shown in figure 9. As explained in section **SECTION**, we choose $\sigma = 0.82$ in this case.

5 Discussion

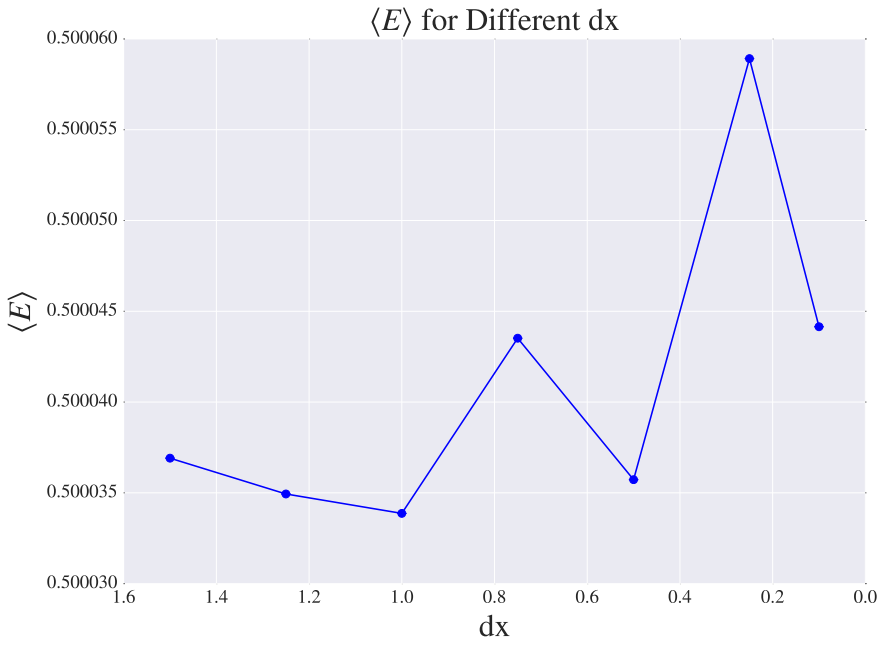
EXCELLENT DISCUSSION

6 Conclusion

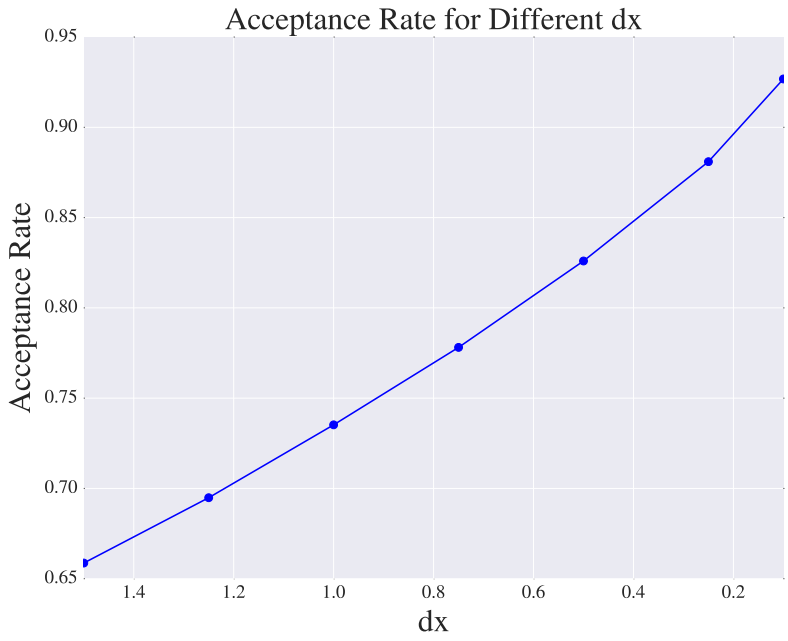
BRILLIANT CONCLUSION

6.1 Outlook

MAGNIFICIENT OUTLOOK



(a) Mean energy

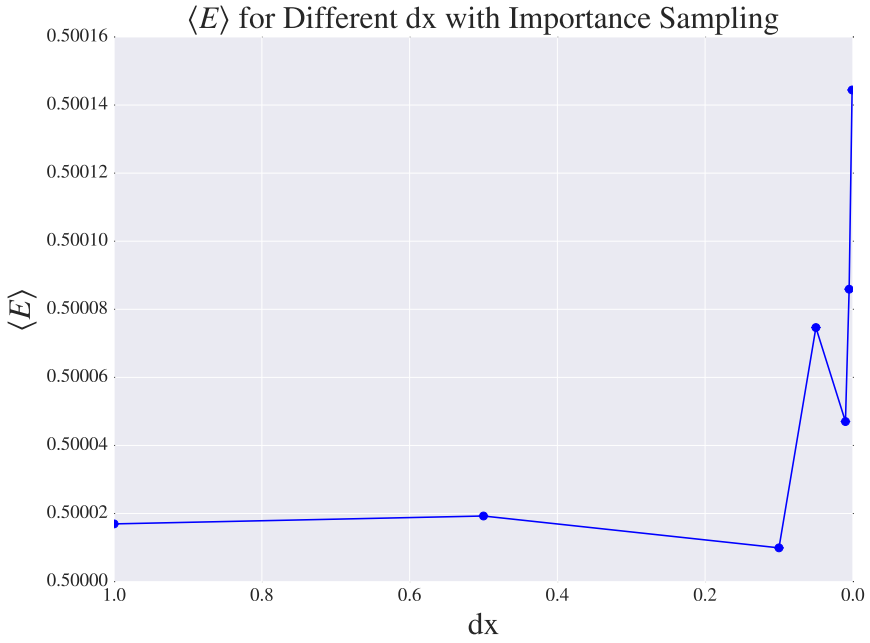


(b) Acceptance rate

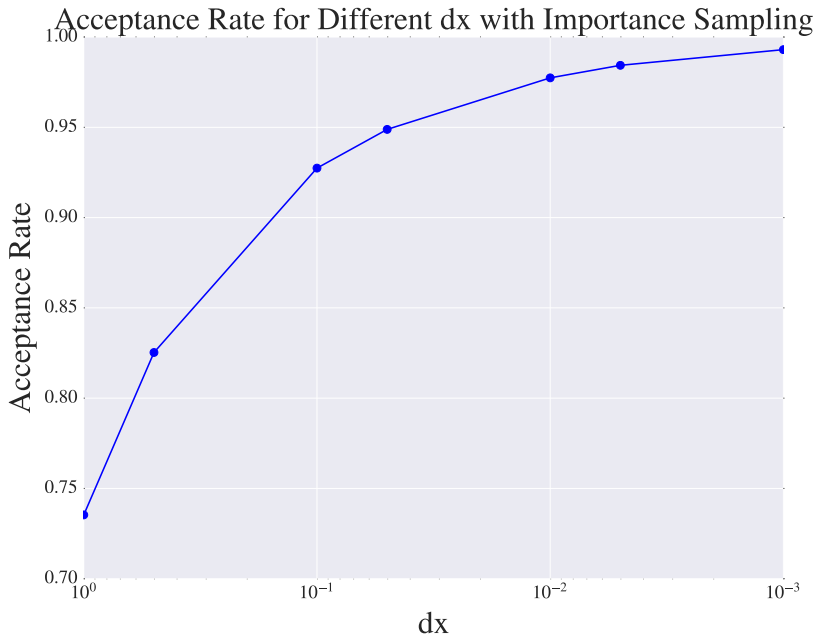
Figure 1: Plot of the mean energy and corresponding acceptance rate for various values of dx, using 1 particle in 1 dimension and 2^{20} Monte Carlo steps **CHECK THIS**. This was produced using brute-force Metropolis sampling with $N = 2$, $\gamma = 0.3$ and $\sigma = 1$.

References

[Botu and Ramprasad, 2015] Botu, V. and Ramprasad, R. (2015). Adaptive machine learning framework to accelerate ab initio molecular dynamics. *International Journal of Quantum Chem-*



(a) Mean energy



(b) Acceptance rate

Figure 2: Same as figure 1, but using importance sampling

istry, 115(16):1074–1083.

[Broecker et al., 2017] Broecker, P., Carrasquilla, J., Melko, R. G., and Trebst, S. (2017). Machine learning quantum phases of matter beyond the fermion sign problem. *Scientific Reports*, 7(1):8823.

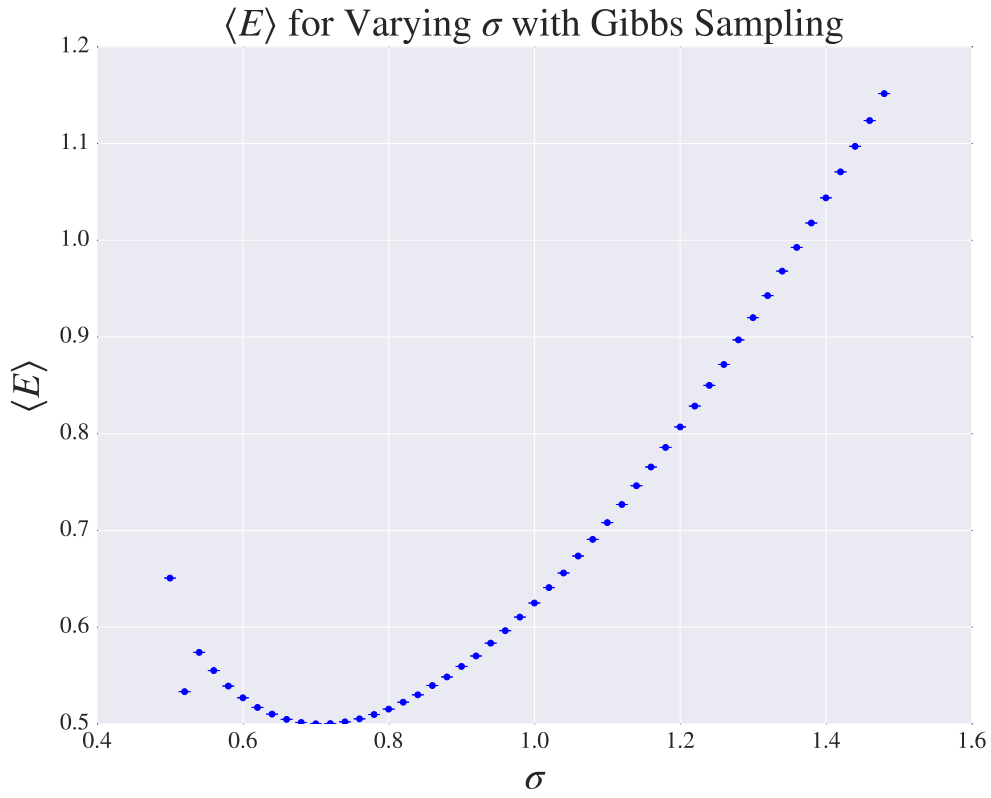


Figure 3: Mean energy for various values of σ for a system of 1 particle in 1 dimension, using Gibbs sampling and 2^{10} Monte Carlo steps. This is with $N = 2$ and $\gamma = 0.3$

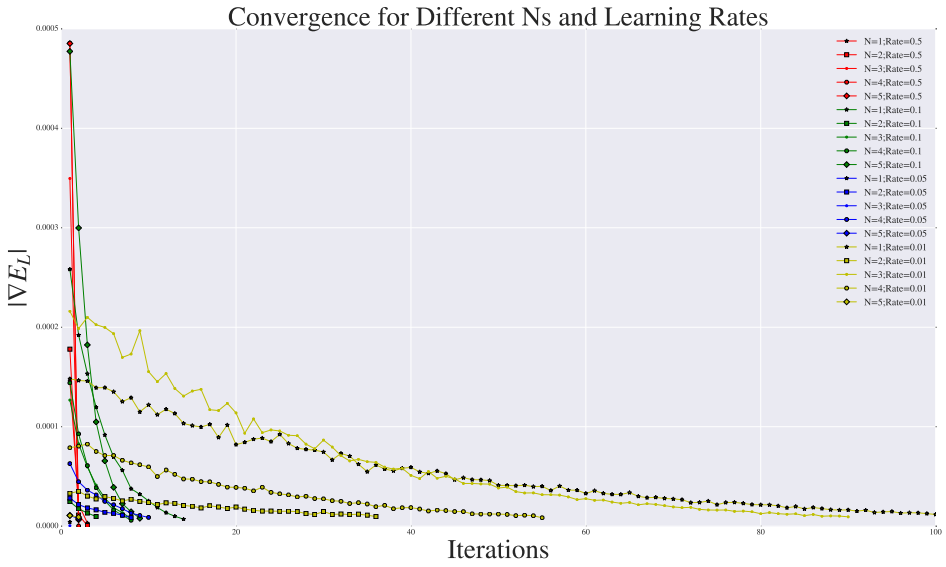


Figure 4: Plot of the absolute value of the gradient as a function of iterations for various values of N and γ. This was performed using brute-force Metropolis sampling, using 1 particle in 1 dimension and 2^{20} Monte Carlo cycles. We used $dx = 1$, $\sigma = 0.7$.

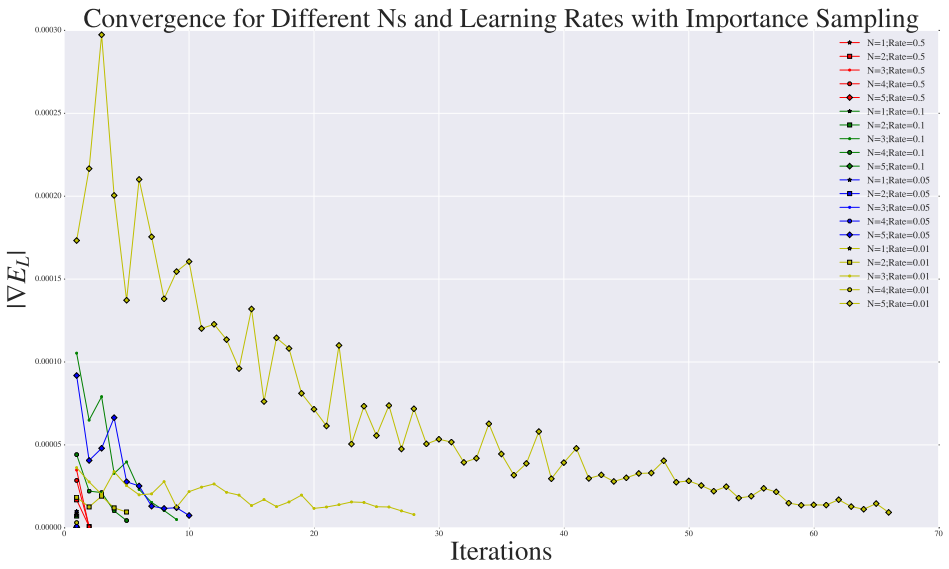


Figure 5: Same as figure 4, but using importance sampling, and therefore $dx = 0.1$

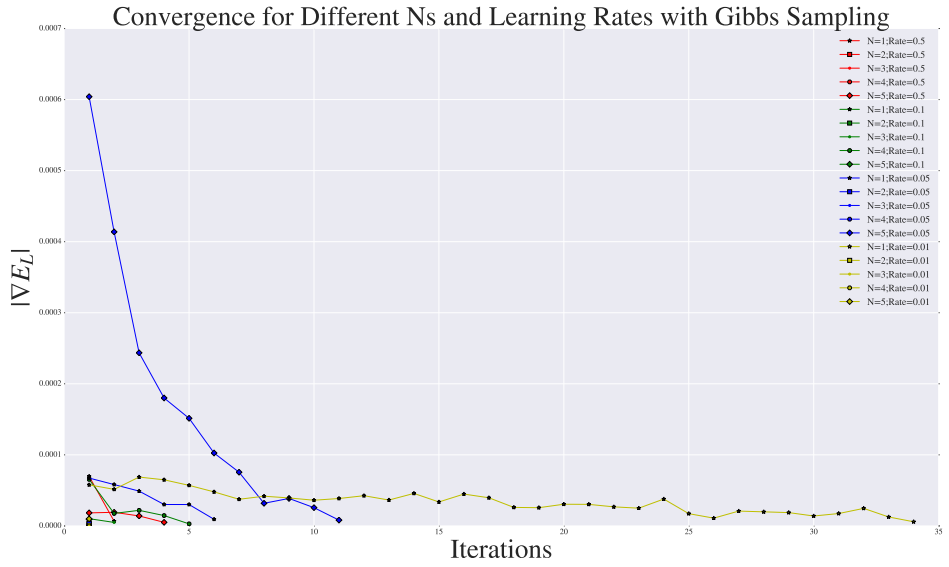
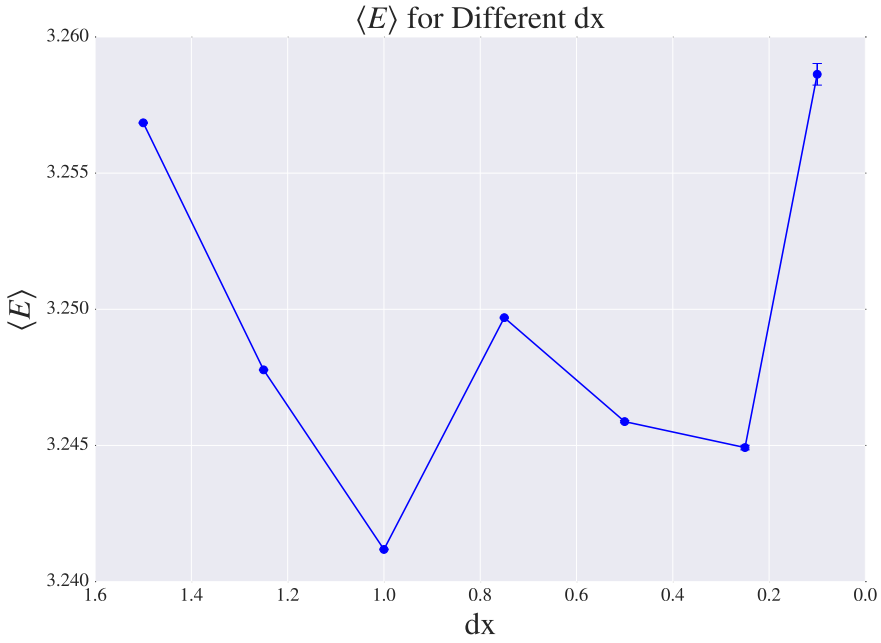
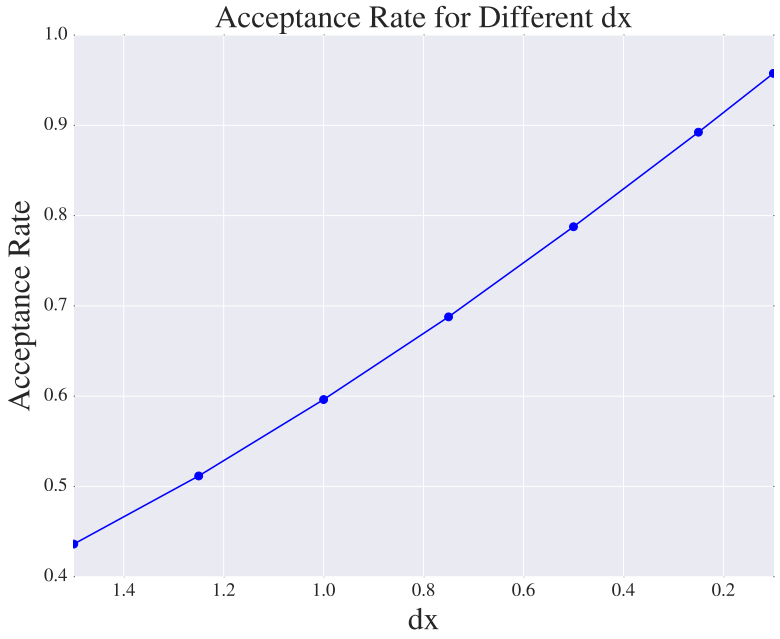


Figure 6: Same as figure 4 but using Gibbs sampling



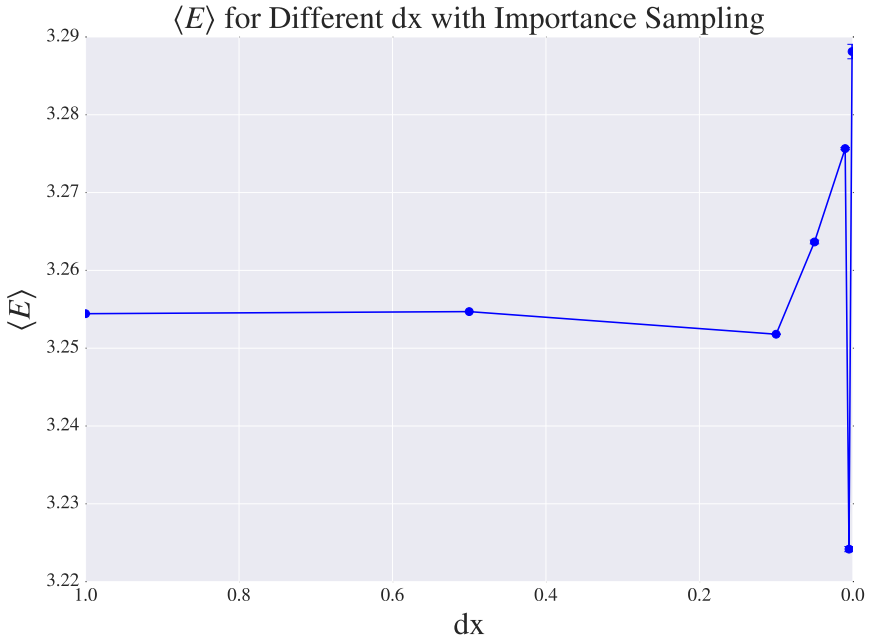
(a) Mean of the energy



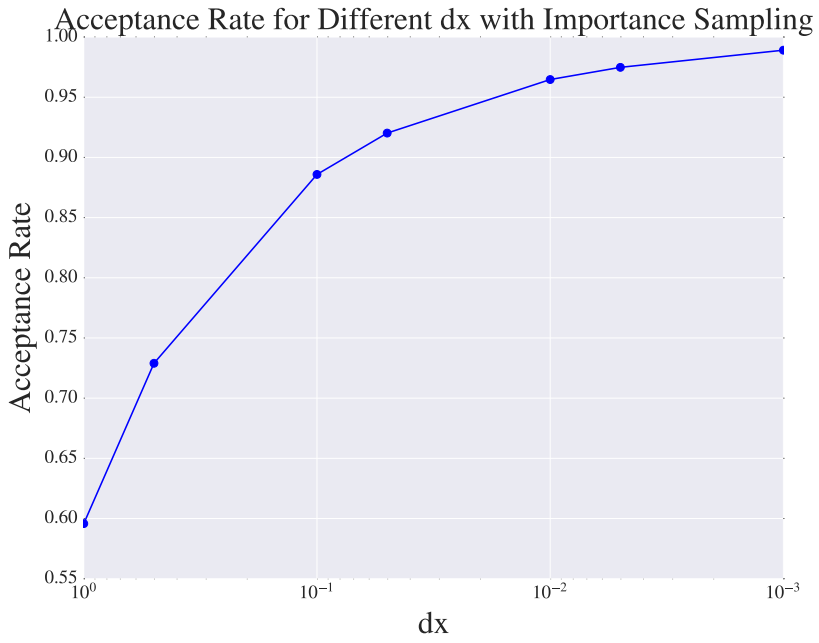
(b) Acceptance ratio

Figure 7: Plot of the mean energy and corresponding acceptance rate for various values of dx using 2 particles in 2 dimensions and 2^{20} Monte Carlo steps. This was produced using brute-force Metropolis sampling with $N = 2, \gamma = 0.3$ and $\sigma = 1$

[Carleo and Troyer, 2017] Carleo, G. and Troyer, M. (2017). Solving the quantum many-body problem with artificial neural networks. *Science*, 355(6325):602–606.



(a) Mean of the energy



(b) Acceptance ratio

Figure 8: Same as figure 7 but with importance sampling

[Griffiths, 2004] Griffiths, D. (2004). *Introduction to Quantum Mechanics*. 2 edition.

[Heinesen et al., 2018] Heinesen, D., Lange, G., and Salihi, A. (2018). FYS4411 - Project 1 Variational Monte Carlo.

[Hinton, 2010] Hinton, G. (2010). A Practical Guide to Training Restricted Boltzmann Machines.

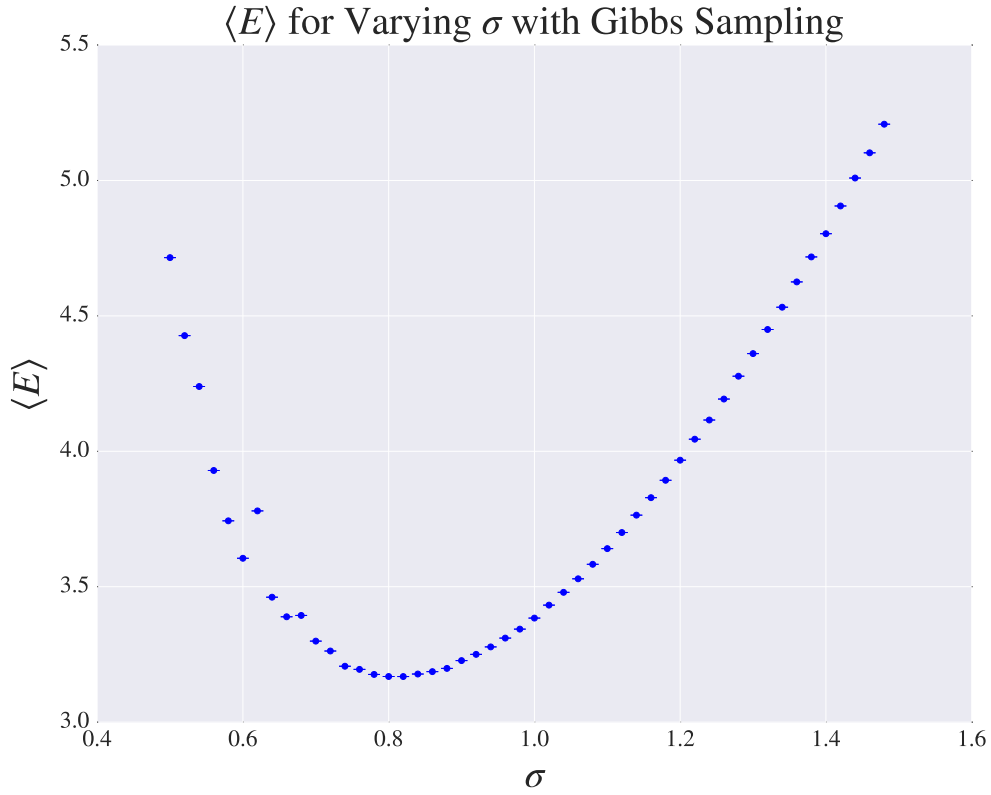


Figure 9: Mean energy as a function of σ for an interacting system with 2 electrons in 2 dimensions, using 2^{20} Monte Carlo steps. This is with $N = 2$ and $\gamma = 0.05$ **CHECK THIS**

Technical report, University of Toronto, Toronto.

[Hjorth-Jensen, 2015] Hjorth-Jensen, M. (2015). *Computational Physics*. Oslo.

[Hjorth-Jensen, 2018] Hjorth-Jensen, M. (2018). Project 2, The restricted Boltzmannn machine applied to the quantum many body problem.

[Jonsson, 2018] Jonsson, M. (2018). *LECTURE NOTES FOR BLOCKING METHOD*.

[Pedersen Lohne et al., 2011] Pedersen Lohne, M., Hagen, G., Hjorth-Jensen, M., Kvaal, S., and Pederiva, F. (2011). Ab initio computation of the energies of circular quantum dots. *Phys. Rev. B*, 84(11):115302.

[Taut, 1994] Taut, M. (1994). Two electrons in a homogeneous magnetic field: particular analytical solutions. *Journal of Physics A: Mathematical and General*, 27(3):1045.

[Wang et al., 2014] Wang, N., Melchior, J., and Wiskott, L. (2014). Gaussian-binary Restricted Boltzmann Machines on Modeling Natural Image Statistics.

Appendices

A Finding the derivatives

In this section, we derive the expressions for the various derivatives needed in section 2. We begin with the local energy.

A.1 The local energy

The local energy is given by:

$$E_L = \frac{1}{\Psi_T}\hat{H}\Psi_T = \sum_{i=1}^{N}\left(-\frac{1}{2\Psi_T}\nabla_i^2\Psi_T + \frac{1}{2}\omega^2 r_i^2\right) + \sum_{i<j}\frac{1}{r_{ij}} \tag{29}$$

Thus, we must compute:

$$\frac{1}{\Psi_T}\nabla_i^2\Psi_T \tag{30}$$

This may be rewritten as:

$$\frac{1}{\Psi_T}\nabla\left(\Psi_T\frac{1}{\Psi_T}\nabla\Psi_T\right) = \left(\frac{1}{\Psi_T}\nabla\Psi_T\right)^2 + \nabla\left(\frac{1}{\Psi_T}\nabla\Psi_T\right) = \left[\nabla\log\Psi_T\right]^2 + \nabla^2\log\Psi_T \tag{31}$$

The logarithm of our trial wavefunction is given by:

$$\log\Psi_T = -\log Z - \sum_{i=1}^{M}\left(\frac{(X_i - a_i)^2}{2\sigma^2}\right) + \sum_{j=1}^{N}\log\left(1 + \exp\left(b_j + \sum_{i=1}^{M}\frac{X_i w_{ij}}{\sigma^2}\right)\right) \tag{32}$$

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

$$\begin{aligned}\frac{\partial\log\Psi_T}{\partial X_k} &= \frac{(a_k - X_k)}{\sigma^2} + \sum_{j=1}^{N}\frac{w_{kj}\exp\left(b_j + \sum_{i=1}^{M}\frac{X_i w_{ij}}{\sigma^2}\right)}{\sigma^2\left(1 + \exp\left(b_j + \sum_{i=1}^{M}\frac{X_i w_{ij}}{\sigma^2}\right)\right)} \\ &= \frac{a_k - X_k}{\sigma^2} + \sum_{j=1}^{N}\frac{w_{kj}}{\sigma^2\left(1 + \exp\left(-b_j - \sum_{i=1}^{M}\frac{X_i w_{ij}}{\sigma^2}\right)\right)}\end{aligned} \tag{33}$$

Whereas the second derivative is:

$$\frac{\partial^2\log\Psi_T}{\partial X_k^2} = -\frac{1}{\sigma^2} + \sum_{j=1}^{N}\frac{w_{kj}^2\exp\left(-b_j - \sum_{i=1}^{M}\frac{X_i w_{ij}}{\sigma^2}\right)}{\sigma^4\left(1 + \exp\left(-b_j - \sum_{i=1}^{M}\frac{X_i w_{ij}}{\sigma^2}\right)\right)^2} \tag{34}$$

The local energy can now be found by using equation 31, and inserting equation 33 and equation 34. Inserting this into equation 29 gives the expression for the local energy stated in the main text.

A.2 The derivatives with respect to the parameters

For our optimization method, we require:

$$\frac{1}{\Psi_T}\frac{\partial\Psi_T}{\partial\alpha_k} = \frac{\partial}{\partial\alpha_k}\log\Psi_T \tag{35}$$

Where α_k is any of the biases a, b or the weights w of the restricted Boltzmann machine. These derivatives are given by:

$$\frac{\partial \log \Psi_T}{\partial a_k} = \frac{X_k - a_k}{\sigma^2} \tag{36}$$

$$\frac{\partial \log \Psi_T}{\partial b_k} = \frac{\exp\left(b_k + \sum_{i=1}^{M} \frac{X_i w_{ik}}{\sigma^2}\right)}{1 + \exp\left(b_k + \sum_{i=1}^{M} \frac{X_i w_{ik}}{\sigma^2}\right)} = \frac{1}{1 + \exp\left(-b_k - \sum_{i=1}^{M} \frac{X_i w_{ik}}{\sigma^2}\right)} \tag{37}$$

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

$$\frac{\partial \log \Psi_T}{\partial w_{kl}} = \frac{X_k \exp\left(b_l + \sum_{i=1}^{M} \frac{X_i w_{il}}{\sigma^2}\right)}{\sigma^2\left(1 + \exp\left(b_l + \sum_{i=1}^{M} \frac{X_i w_{il}}{\sigma^2}\right)\right)} = \frac{X_k}{\sigma^2\left(1 + \exp\left(-b_l - \sum_{i=1}^{M} \frac{X_i w_{il}}{\sigma^2}\right)\right)} \tag{38}$$

A.3 The derivatives with Gibbs sampling

In Gibbs sampling, we represent the wavefunction as $\Psi_{T,\text{Gibbs}} = \sqrt{F_{rbm}(\boldsymbol{X})}$, instead of $\Psi_T = F_{rbm}(\boldsymbol{X})$. Note, however, that we only ever differentiate the logarithm of the wavefunction. As $\log\sqrt{\Psi_T} = \frac{1}{2}\log\Psi_T$, this gives only a marginal change. Specifically:

$$E_L = [\nabla \log\sqrt{\Psi_T}]^2 + \nabla^2 \log\sqrt{\Psi_T} = \frac{1}{4}[\nabla \log\Psi_T]^2 + \frac{1}{2}\nabla^2 \log\Psi_T \tag{39}$$

$$\frac{\partial}{\partial a_k}\log\sqrt{\Psi_T} = \frac{1}{2}\frac{\partial}{\partial a_k}\log\Psi_T \tag{40}$$

$$\frac{\partial}{\partial b_k}\log\sqrt{\Psi_T} = \frac{1}{2}\frac{\partial}{\partial b_k}\log\Psi_T \tag{41}$$

$$\frac{\partial}{\partial w_{kl}}\log\sqrt{\Psi_T} = \frac{1}{2}\frac{\partial}{\partial w_{kl}}\log\Psi_T \tag{42}$$

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

B Deriving the spin of the ground state wavefunction

In this section we derive the spin of the exact two-particle ground state wavefunction in the non-interacting case.

Consider the unperturbed wavefunction for the ground state of the two electron system, given by:

$$\psi(\boldsymbol{r}_1, \boldsymbol{r}_2) = C\exp\left(-\omega\left(r_1^2 + r_2^2\right)/2\right) \tag{43}$$

Since this wavefunction is symmetric under permutation of coordinate, the Pauli exclusion principle states that the spin wavefunction must be antisymmetric function in to achieve a wavefunction that is totally antisymmetric under permutation of coordinates. This wave function must then be the singlet, and will look like:

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle - |\downarrow\rangle\right) \tag{44}$$

This has spin 0, as can be seen by applying the spin operator $\boldsymbol{S}^2$ to this state:

$$\boldsymbol{S}^2|\psi\rangle = \frac{1}{\sqrt{2}}\left(\underbrace{\boldsymbol{S}^2|\uparrow\rangle}_{=\frac{3}{4}\hbar^2} - \underbrace{\boldsymbol{S}^2|\downarrow\rangle}_{=\frac{3}{4}\hbar^2}\right) = 0 \tag{45}$$