FYS4411 - Project 1
Variational Monte Carlo

Daniel Heinesen, Gunnar Lange & Aram Salihi

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Abstract

Abstract awesomeness

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3.1 Minimizing computation in the non-interacting case

For the non-interacting case ($a = 0$), certain shortcuts are possible, to save FLOPS.

3.1.1 Computing the numerical energy

From the Schrödinger equation:

$$\hat{H}\Psi_T = \left(-\frac{1}{2}\nabla^2 + V\right)\Psi_T = E\Psi_T \tag{1}$$

The kinetic energy is, numerically, given by (in dimensionless form):

$$T = -\frac{1}{2}\nabla^2\Psi_T \tag{2}$$

This gives, for particle i and component j:

$$T_{ij} \approx \frac{\Psi_T(\boldsymbol{r_1}, ..., \boldsymbol{r_{i,j}} + h, ..., \boldsymbol{r_n}) - 2\Psi_T(\boldsymbol{r}) + \Psi_T(\boldsymbol{r_1}, ..., \boldsymbol{r_{i,j}} - h, ..., \boldsymbol{r_n})}{h^2} \tag{3}$$

Which gives, for the simplest trialfunction ($a = 0$):

$$T_{ij} = -\frac{1}{2}\Psi_T \left(\frac{\exp\left(-\alpha_j (x_j + h)^2\right)}{\exp\left(-\alpha_j x_j^2\right)} - 2 + \frac{\exp\left(-\alpha_j (x_j - h)^2\right)}{\exp\left(-\alpha_j x_j^2\right)} \right) \frac{1}{h^2} = -\frac{1}{2h^2}\Psi_T \left(\exp\left(-2\alpha_j x_j h - \alpha_j h^2\right) + \exp\left(2\alpha_j x_j h - \alpha_j h^2\right)\right. \tag{4}$$

4 Results and discussion

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5.1 Conclusion

5.2 Outlook

Appendices

A Finding the drift force

We wish to compute:

$$\vec{F} = 2\frac{1}{\psi_T}\nabla\psi_T \tag{5}$$

B Finding the analytic expression for the local energy

We wish to find:

$$E_L = \frac{1}{\Psi_T}\nabla^2\Psi_T \tag{6}$$

Where Ψ_T is given by:

$$\exp\left[-\alpha \sum_i^n \left(x_i^2 + y_i^2 + z_i^2\right)\right] \prod_{i<j} f(a, |\mathbf{r}_i - \mathbf{r}_j|) \tag{7}$$

Look first at $a = 0$. In this case, this reduces to the harmonic oscillator potential. The local energy is then:

$$\exp\left[\alpha \sum_i^n \left(x_i^2 + y_i^2 + z_i^2\right)\right] \left(-\frac{\hbar^2}{2m_i}\nabla_i^2 + V\right) \exp\left[-\alpha \sum_i^n \left(x_i^2 + y_i^2 + z_i^2\right)\right] \tag{8}$$

In the simple harmonic oscillator case, this gives:

$$E_L(\mathbf{r}, \alpha) = -\frac{\hbar^2}{2m}\sum_{i=1}^n 2\alpha\left(2\alpha(x_i^2 + y_i^2 + z_i^2) - 3\right) + \frac{1}{2}m\omega_{ho}^2 \sum_{i=1}^n (x_i^2 + y_i^2 + z_i^2) \tag{9}$$

FIX FOR ONE/N PARTICLES AND LOWER DIMENSION Similarly for the drift force:

$$F = \frac{2\nabla\Psi_T}{\Psi_T} \tag{10}$$

$$F = -2\alpha\sum_{i=1}^n (x_i + y_i + z_i) \tag{11}$$

Now for the ugly part:
For one particle, ∇_k:

$$\nabla_k \Psi_T = \nabla_k \left(\Psi_T(\mathbf{r}) = \nabla_k \prod_{i=1}^{n} \phi(\mathbf{r}_i) \exp\left(\sum_{i<j} u(r_{ij}) \right) \right) \tag{12}$$

Now apply the product rule. For the first term, all terms are unchanged except where $i = k$, giving the first term as:

$$\nabla_k \phi(\mathbf{r}_k) \left[\prod_{i \neq k} \phi(\mathbf{r}_i) \right] \exp\left(\sum_{i<j} u(r_{ij}) \right) \tag{13}$$

The second term is trickier. We can rewrite it as follows:

$$\prod_i \phi(\mathbf{r}_i) \nabla_k \left[\exp\left(\sum_{i<j} u(r_{ij}) \right) \right] = \prod_i \phi(\mathbf{r}_i) \nabla_k \left[\exp\left(\sum_{j=1}^{n} \sum_{i=1}^{j-1} u(r_{ij}) \right) \right] \tag{14}$$

This is calculated by using the chain-rule. To evaluate the innerfunction, we must look at $1 \leq j \leq k$, $j = k$ and $j \geq k$. Begining with $1 \leq j \leq k$, the first sum is from 1 up the kth particle, meaning all terms differentiated before k vanishes and we are left with $u(r_{ik})$, thus leaving with us with:

$$\prod_i \phi(\mathbf{r}_i) \nabla_k \left[\exp\left(\sum_{j=1}^{k} \sum_{i=1}^{k-1} u(r_{ij}) \right) \right] = \prod_i \phi(\mathbf{r}_i) \exp\left\{ \left(\sum_{i<j} u(r_{ij}) \right) \right\} \left[\sum_{i=1}^{k-1} \nabla_k u(r_{ik}) \right] \tag{15}$$

For $j = k$, we see that the first sum goes from and end up at kth particle, meaning this sum vanishes, secondly, the second sum is evaluated at $1 \leq i \leq k-1$, leaving with constants up to $k-1$, thus this term becomes 0.

$$\prod_i \phi(\mathbf{r}_i) \nabla_k \left[\exp\left(\sum_{j=1}^{n} \sum_{i=1}^{j-1} u(r_{ij}) \right) \right] = 0 \tag{16}$$

For $j > k$,the first sum goes from $k+1 \leq j \leq n$ and the second $1 \leq i \leq k$. The second sum vanishes, because all constants are differentiated away except the last term $i = k$. This leaves us with:

$$\prod_i \phi(\mathbf{r}_i) \nabla_k \left[\exp\left(\sum_{j=k+1}^{n} \sum_{i=1}^{k} u(r_{ij}) \right) \right] = \prod_i \phi(\mathbf{r}_i) \exp\left\{ \left(\sum_{i<j} u(r_{ij}) \right) \right\} \left[\sum_{j=k+1}^{n} \nabla_k u(r_{kj}) \right] \tag{17}$$

We can now write the second term as 14):

$$\prod_i \phi(\mathbf{r}_i) \exp\left\{ \left(\sum_{i<j} u(r_{ij}) \right) \right\} \left[\sum_{j=k+1}^{n} \nabla_k u(r_{kj}) + \left[\sum_{i=1}^{k-1} \nabla_k u(r_{ik}) \right] \right] \tag{18}$$

This can be rewritten to:

$$\prod_i \phi(\mathbf{r}_i) \exp\left\{ \left(\sum_{i<j} u(r_{ij}) \right) \right\} \left[\sum_{j \neq k} \nabla_k u(r_{kj}) \right] \tag{19}$$

FORKLAR denne delen litt. Thus the first derivative of the trial wavefunction can be written as:

$$\nabla_k \Psi_T = \nabla_k \phi(\mathbf{r}_k) \left[\prod_{i \neq k} \phi(\mathbf{r}_i) \right] \exp\left(\sum_{i<j} u(r_{ij}) \right) + \prod_i \phi(\mathbf{r}_i) \exp\left\{ \left(\sum_{i<j} u(r_{ij}) \right) \right\} \left[\sum_{j \neq k} \nabla_k u(r_{kj}) \right] \tag{20}$$

Lastly we will calculate the second derivative of the trial function, where we use the product rule and the chain rule. We will then obtain the following:

$$\nabla_k^2 \Psi_T = \underbrace{\nabla_k^2 \phi(\mathbf{r}_k) \left[\prod_{i\neq k} \phi(\mathbf{r}_i)\right] \exp\left(\sum_{i<j} u(r_{ij})\right)}_{\mathrm{I}} +$$

$$\underbrace{2\left(\nabla_k \phi(\mathbf{r}_k) \left[\prod_{i\neq k} \phi(\mathbf{r}_i)\right] \exp\left\{\left(\sum_{i<j} u(r_{ij})\right)\right\} \left[\sum_{j\neq k} \nabla_k u(r_{kj})\right]\right)}_{\mathrm{II}} +$$

$$\underbrace{\prod_i \phi(\mathbf{r}_i) \exp\left\{\left(\sum_{i<j} u(r_{ij})\right)\right\} \left[\sum_{j\neq k} \nabla_k u(r_{kj})\right]^2}_{\mathrm{III}} +$$

$$\underbrace{\prod_i \phi(\mathbf{r}_i) \exp\left\{\left(\sum_{i<j} u(r_{ij})\right)\right\} \left[\sum_{j\neq k} \nabla_k \nabla_k u(r_{kj})\right]}_{\mathrm{IV}}$$

Where the derivatives of the different parts are obtained from previous. We will now divide the second derivative by the trial wavefunction, and obtain:

$$\frac{1}{\Psi_T}\nabla_k^2 \Psi_T = \underbrace{\frac{\nabla_k^2 \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_{\phi(\mathbf{r}_k)})}}_{\mathrm{I}} + \underbrace{2\frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} \sum_{j\neq k} \nabla_k u(r_{kj})}_{\mathrm{II}} + \underbrace{\left(\sum_{j\neq k} \nabla_k u(r_{kj})\right)^2}_{\mathrm{III}} + \underbrace{\left[\sum_{j\neq k} \nabla_k \nabla_k u(r_{kj})\right]}_{\mathrm{IV}} \quad (21)$$

We will now carry out the differentiation in term (II), (III) and (IV). Begining with the (II), by using the chain rule we can rewrite (II) as:

$$2\frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} \sum_{j\neq k} \frac{\partial u(r_{kj})}{\partial r_{kj}} \frac{\partial r_{kj}}{\partial \mathbf{r}_k} = 2\frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} \left(\sum_{j\neq k} \frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} u'(r_{kj})\right)$$

Where we have used $\nabla_k r_{kj} = (\mathbf{r}_k - \mathbf{r}_j)/r_{kj}$. Looking at (III), we can write out the square into two factors. The second paranthese the summation index is replaced by a dummy index i. Thus will look as:

$$\left(\sum_{j\neq k} \nabla_k u(r_{kj})\right)^2 = \left(\sum_{j\neq k} \nabla_k u(r_{kj})\right)\left(\sum_{i\neq k} \nabla_k u(r_{ki})\right) \quad (22)$$

From (II) we found the derivative of this function. Thus this can be expressed as (combining also the double sum):

$$\left(\sum_{j\neq k} \nabla_k u(r_{kj})\right)^2 = \sum_{i,j\neq k} \left(\frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}}\right)\left(\frac{\mathbf{r}_k - \mathbf{r}_i}{r_{ki}}\right) u'(r_{kj})u'(r_{ki}) \quad (23)$$

The last part (IV), we must use the chain rule and product rule together. We will obtain the following term:

$$\sum_{j\neq k} \nabla_k \nabla_k u(r_{kj}) = \sum_{j\neq k} \nabla_k \left(\left(\frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}}\right)^2 u''(r_{kj}) + u'(r_{kj}) \nabla_k \left(\frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}}\right)\right) \quad (24)$$

Note that this is a unit vector squared:

$$\left(\frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}}\right)^2 = 1 \tag{25}$$

and the last part is found by using the qoutient rule. This is the divergence to the vectors, since we are evaluating for specific particle k, and gradient to scalar (we must look for all combination of k particle):

$$\nabla_k \left(\frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}}\right) = \frac{r_{kj}\left(\nabla_k \cdot \mathbf{r}_k - \nabla_k \cdot \mathbf{r}_j\right) - (\mathbf{r}_k - \mathbf{r}_j)\nabla_k r_{kj}}{r_{kj}^2} \tag{26}$$

This simply becomes:

$$\nabla_k \left(\frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}}\right) = \frac{3r_{kj}^2 - \mathbf{r}_k^2 + 2(\mathbf{r}_k \cdot \mathbf{r}_j) - \mathbf{r}_j^2}{r_{kj}^3} \tag{27}$$

Note that $r_{kj} - \mathbf{r}_k^2 + 2(\mathbf{r}_k \cdot \mathbf{r}_j) - \mathbf{r}_j^2 = 0$, this leaves us with:

$$\nabla_k \left(\frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}}\right) = \frac{2}{r_{kj}} \tag{28}$$

Thus expression (IV) can be expressed as:

$$\sum_{j\neq k} \nabla_k \nabla_k u(r_{kj}) = \sum_{j\neq k} \nabla_k \left(u''(r_{kj}) + \frac{2}{r_{kj}} u'(r_{kj})\right) \tag{29}$$

Combining (I), (II), (III) and (IV), we we will get that the second derivative of the trial function is:

$$\begin{aligned}\frac{1}{\Psi_t}\nabla_k^2 \Psi_T = \frac{\nabla_k^2 \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_{\phi(\mathbf{r}_k)})} + 2\frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)}\left(\sum_{j\neq k} \frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} u'(r_{kj})\right) + \\ \sum_{i,j\neq k}\left(\frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}}\right)\left(\frac{\mathbf{r}_k - \mathbf{r}_i}{r_{ki}}\right) u'(r_{kj}) u'(r_{ki}) + \sum_{j\neq k} \nabla_k \left(u''(r_{kj}) + \frac{2}{r_{kj}} u'(r_{kj})\right)\end{aligned} \tag{30}$$