FYS4411 Project 1

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1a

In this exercise I will use Monte Carlo integration to compute the expectation value for the energy.

$$\langle E \rangle = \frac{\int d\mathbf{r_1} d\mathbf{r_2} \psi_T^*(r_1, r_2) \hat{H} \psi_T(r_1, r_2)}{\int d\mathbf{r_1} d\mathbf{r_2} \psi_T^*(r_1, r_2) \psi_T(r_1, r_2)}$$

I need a wavefunction for this, so first I choose the ground state wavefunction solution the hydrogen atom, $e^{-\alpha r}$, for both the particles. This gives the total wavefunction

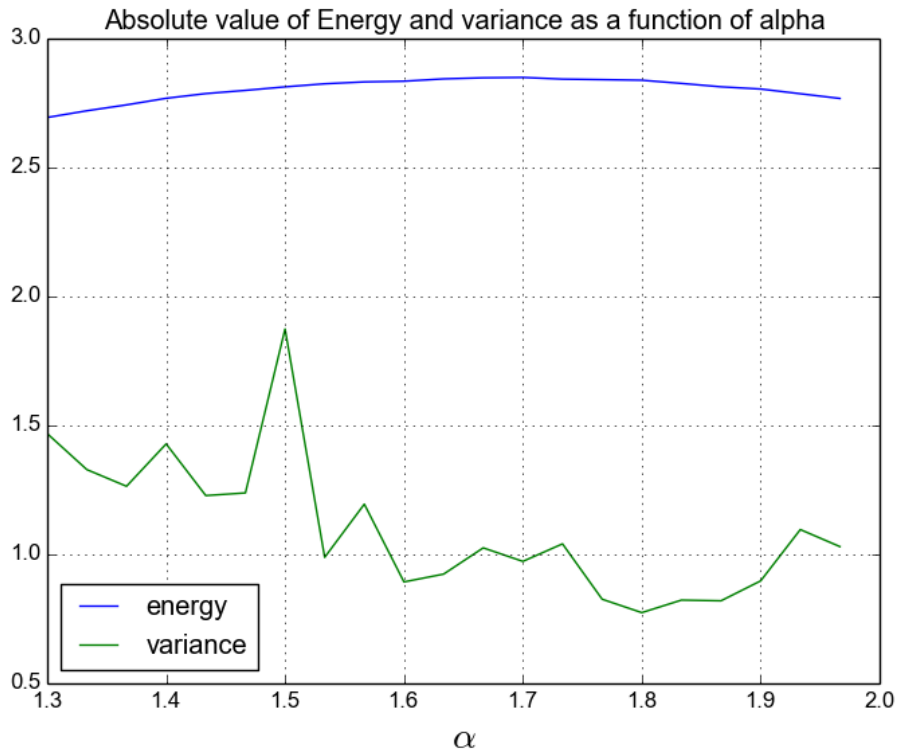
$$\Psi_T(r_1, r_2) = e^{-\alpha(r_1 + r_2)}$$

This is not the correct wavefunction, but it can give a decent first evaluation.

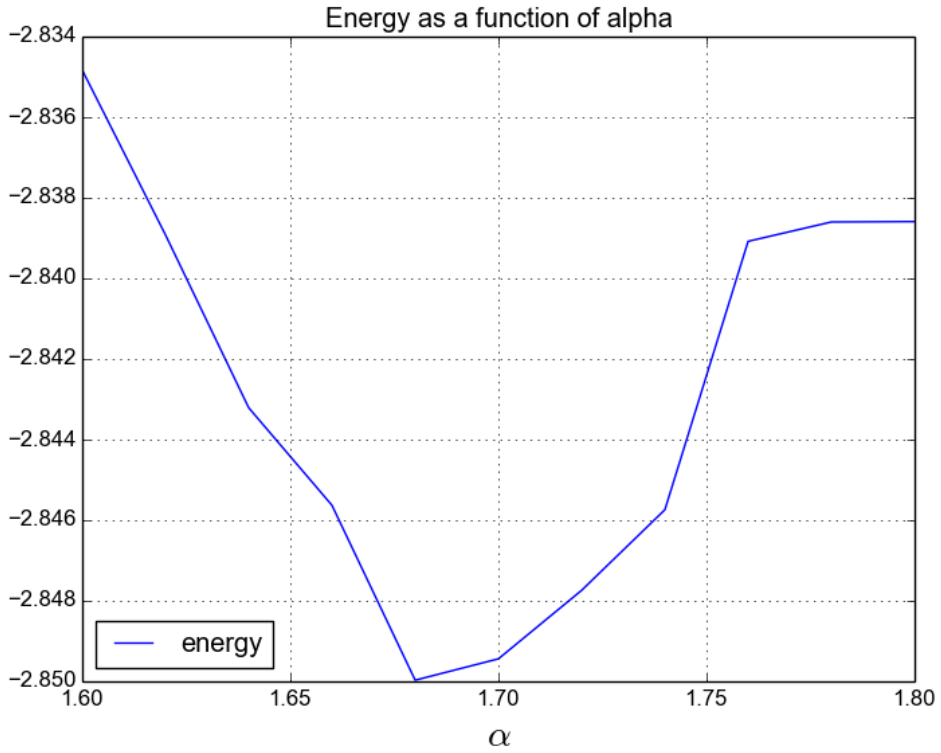
In the Metropolis algorithm, I will check wether a move given by, $\mathbf{R}' = \mathbf{R} + \delta \cdot r$, will be accepted. r is a random number in $[0, 1]$. The acceptance criteria is given by

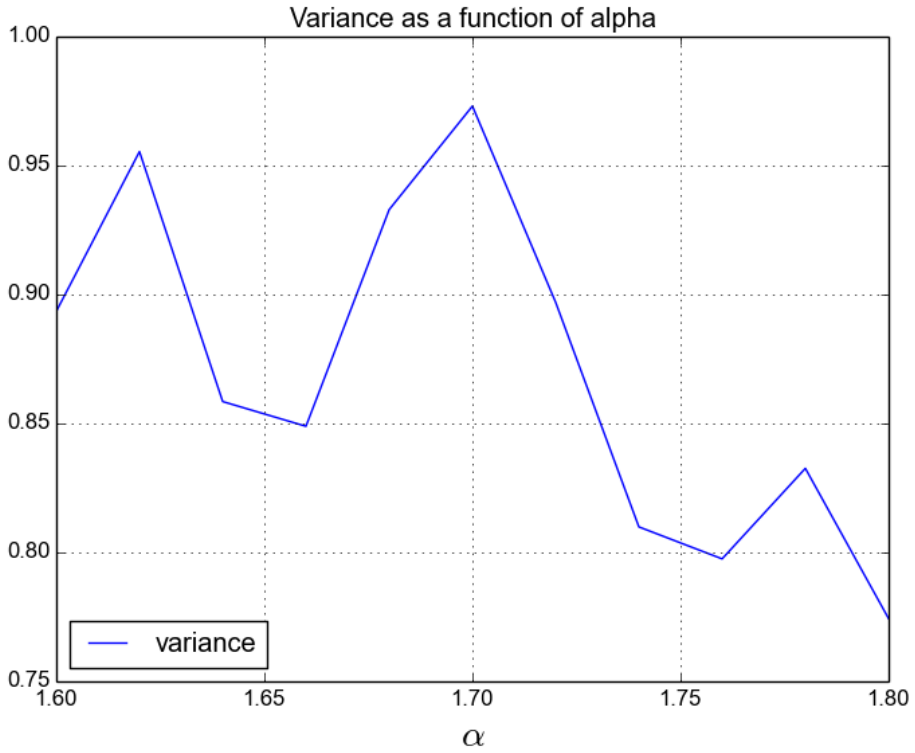
$$\frac{P(\mathbf{R}')}{P(\mathbf{R})} = \frac{\int d\mathbf{R}' \psi_T^*(\mathbf{R}') \psi_T(\mathbf{R}')}{\int d\mathbf{R} \psi_T^*(\mathbf{R}) \psi_T(\mathbf{R})} \geq r$$

Because of the variational principle, the trial energy will always be higher than the true energy. Therefore we can adjust α and the steplength δ until we get the lowest possible energy. The best steplength δ is a steplength that will accept around 50% of the proposed steps. Using an algorithm that loops over different steplengths, I adjust α and plot the energy and variance as a function of α. I start the steplength at $\delta = 1.2$ and increase it by $0.5 * r$, $r \in [0, 1]$ for each step. Testing if the number of accepted steps are within $[0.49, 0.51]$ I either accept the step length or increase it.



By looking closer at the energy and variance around $\alpha = 1.68$, we see that we get an energy of $\langle E \rangle = -2.84997$, with a variance of $\sigma^2 = 0.932912$. This is pretty close to the real value of $E_{exact} = -2.903$. We see however that the variance is smaller for $\alpha = 1.8$, 1.9 and 1.6.



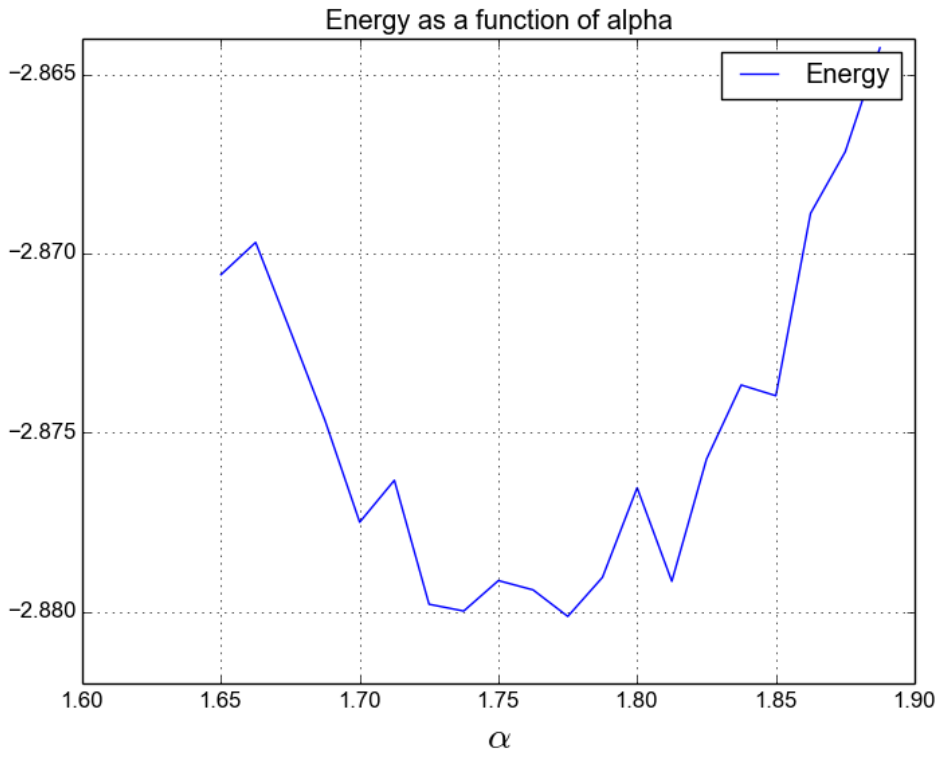


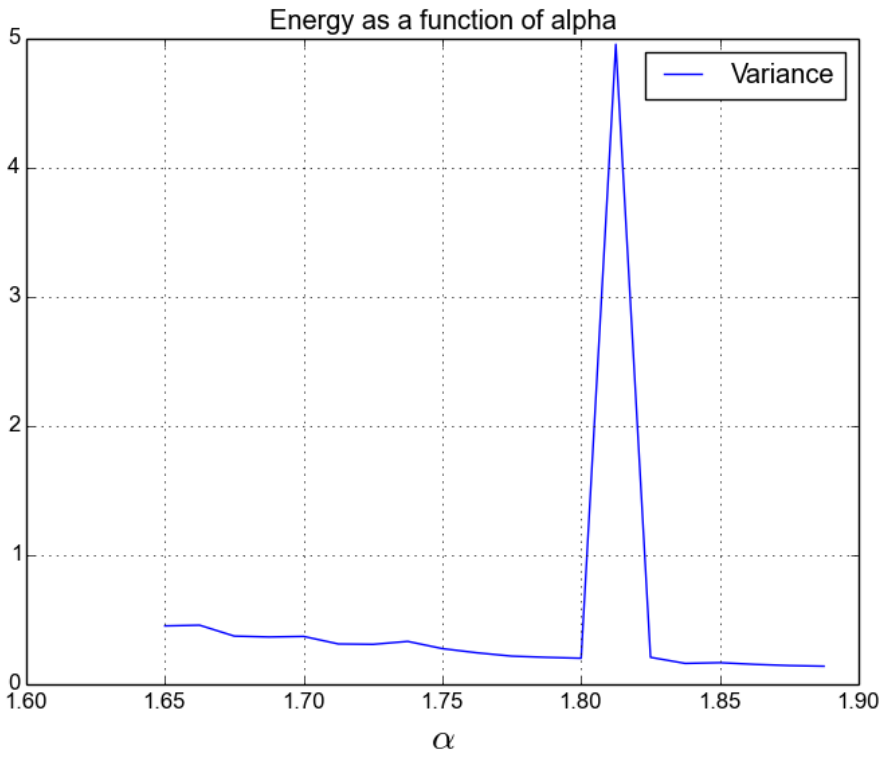
We can get a better result by improving our test function, Ψ_T. We can introduce a

Jastrow factor. Here $r_{12} = |r_1 - r_2|$.

$$\Psi_T(r_1, r_2) = e^{-\alpha(r_1+r_2)} e^{\frac{r_{12}}{2(1+\beta r_{12})}}$$

Setting $\beta = 1.0$, we see that we can achieve a better energy, namely $\langle E \rangle = -2.88013$.





b

$$\Psi_T = e^{-\alpha(r_1+r_2)}$$
$$E_L = \frac{1}{\Psi_T}\hat{H}\Psi_T$$
$$\hat{H} = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}}$$
$$\nabla_1^2\Psi_T = \frac{1}{r_1^2}\frac{\partial}{\partial r_1}\left(r_1^2\frac{\partial\Psi_T}{\partial r_1}\right) = -\frac{2}{r_1}\alpha\Psi_T + \alpha^2\Psi_T$$

Combining these calculations, we get the expression for the local energy.

$$E_L = (\alpha - 2)\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{1}{r_{12}} - \alpha^2$$

Now finding the closed-form expression for E_L for the second wavefunction.

$$\Psi_T = e^{-\alpha(r_1+r_2)}e^{\frac{r_{12}}{2(1+\beta r_{12})}}$$

First looking at

$$\nabla_1^2\Psi_T = \frac{1}{r_1^2}\frac{\partial}{\partial r_1}\left(r_1^2\frac{\partial\Psi_T}{\partial r_1}\right)$$

$$\frac{\partial\Psi_T}{\partial r_1}$$