

FYS4411 Project 1

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March 12, 2015

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

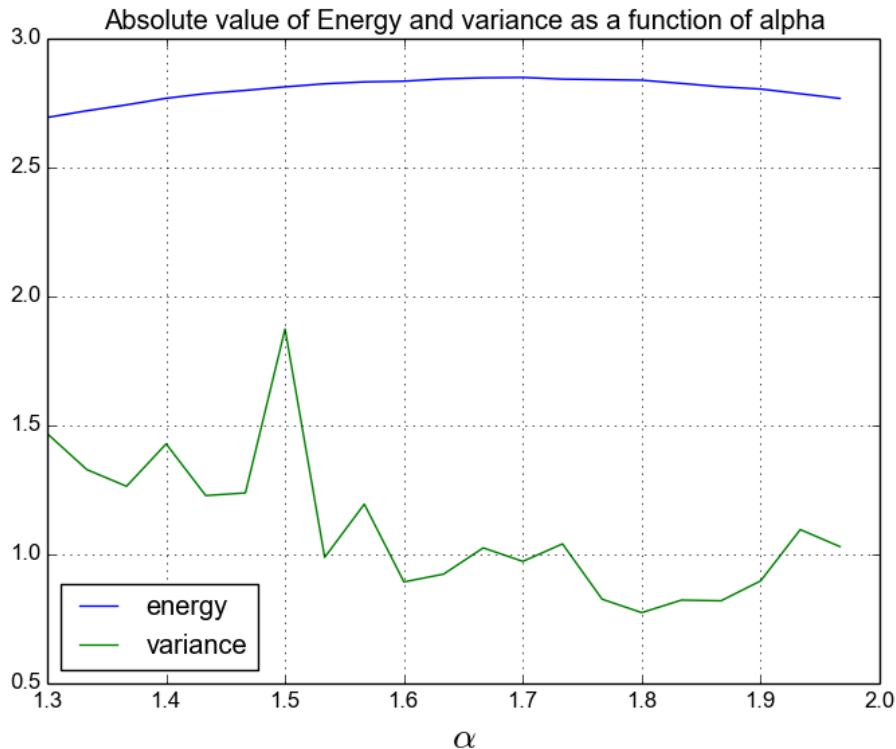
$$\Psi_T(r_1, r_2) = e^{-\alpha(r_1+r_2)}$$

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

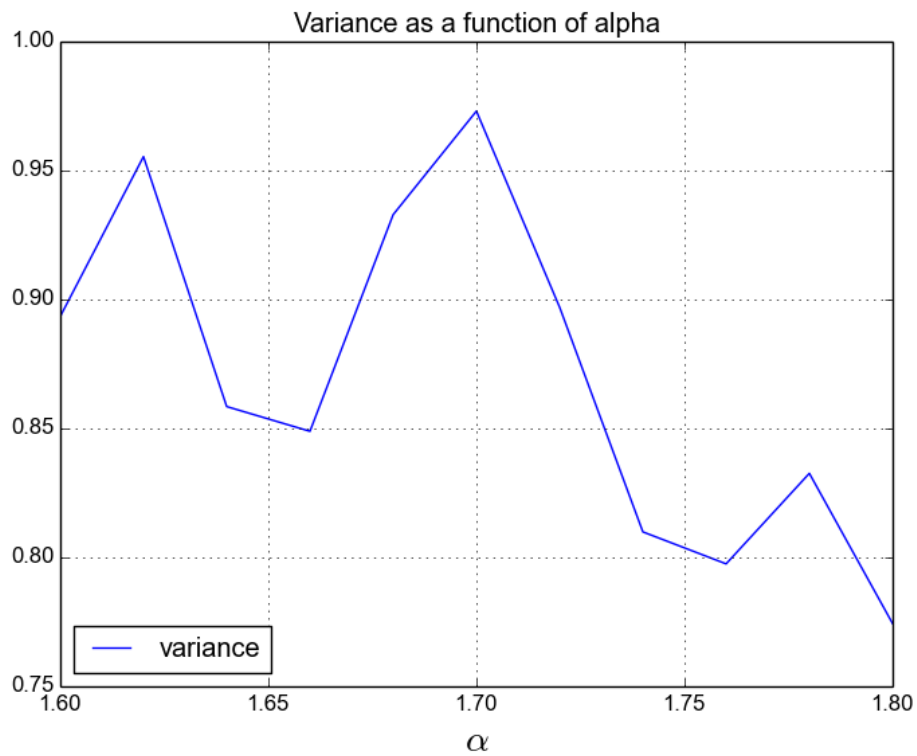
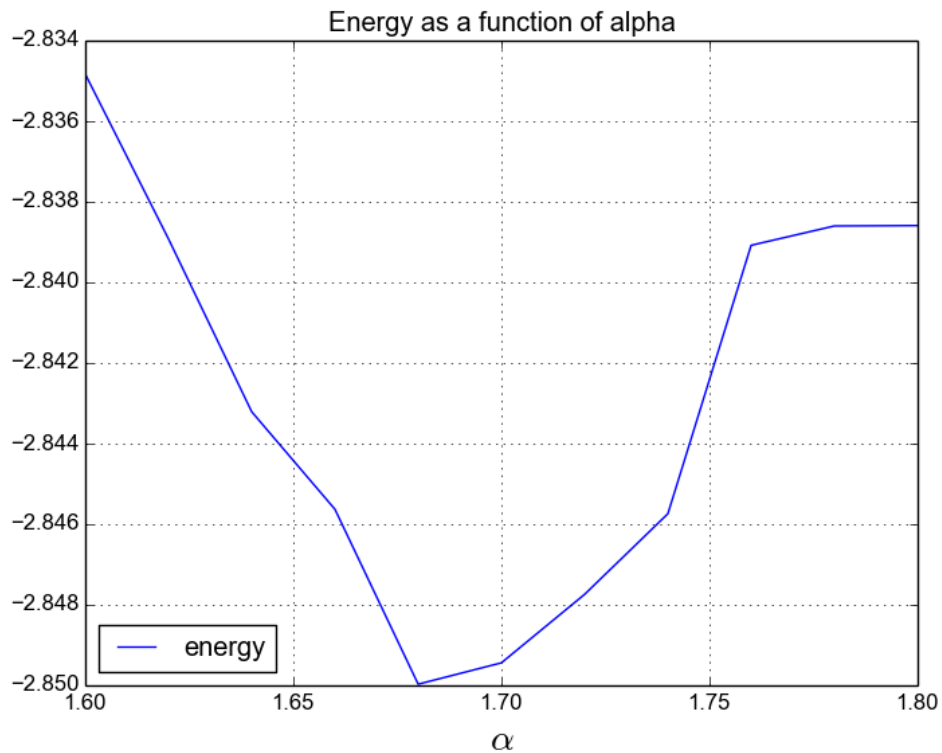
In the Metropolis algorithm, I will check whether a move given by, $\mathbf{R}' = \mathbf{R} + \delta \cdot \mathbf{r}$, will be accepted. r is a random number in $[0, 1]$. The acceptance criteria is given by

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

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.

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