Computational Physics II 5640, Spring 2017

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1 Variational Quantum Monte Carlo.

Here we solve for the ground state of the 1D Harmonic Oscillator solution of the Schrodinger Wave Equation:

$$-\frac{1}{2}\frac{d^2\psi(x)}{dx^2} + \frac{x^2}{2}\psi(x) = E\psi(x). \tag{1}$$

To this end we begin with a trial wave function

$$\psi_\alpha(x) \propto e^{-\alpha x^2}, \tag{2}$$

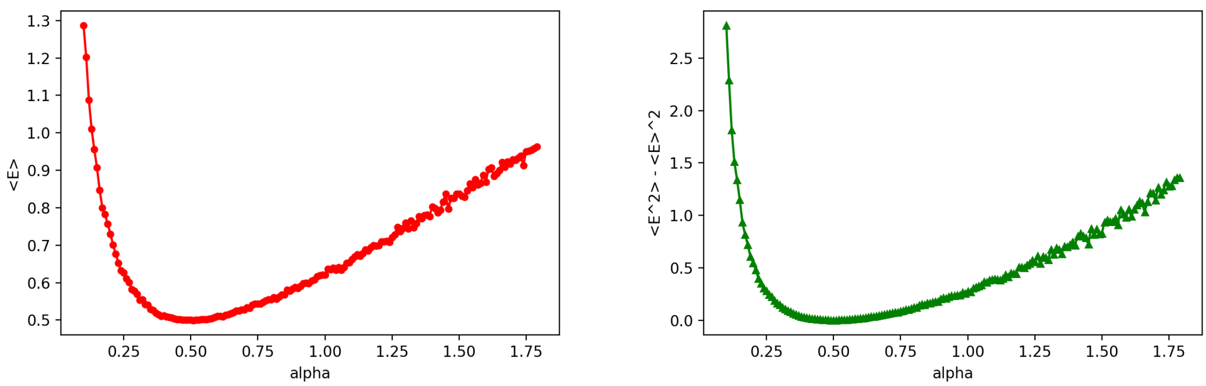
where α is the variational parameter, and we push towards a minimum in α of the expectation value of the local energy, $\langle E \rangle$. We produce an equation for $\langle E \rangle$, by plugging our trial wave function into equation 1:

$$\begin{aligned} \frac{d^2}{dx^2} &\Rightarrow \frac{d}{dx} - 2\alpha x \exp(-\alpha x^2), \\ &= 4\alpha^2 x^2 \exp(-\alpha x^2) - 2\alpha \exp(-\alpha x^2), \\ &= 2\alpha(1 - 2\alpha x^2)\psi_\alpha(x), \\ &\Rightarrow E = 0.5x^2 + \alpha(1 - 2\alpha x^2), \end{aligned} \tag{3}$$

therefore,

$$E_L(x) = \alpha + x^2(0.5 - 2\alpha^2). \tag{4}$$

We use a Markov-chain Monte Carlo in order to produce Monte Carlo averages for $\langle E_L \rangle$ and the variance, $\langle E_L^2 \rangle - \langle E_L \rangle^2$ systematically over a range of α, and plot them in figure 1.



(a) (b)

Figure 1: Expectation values from our Random Walk simulations.

We find our minimum at $\alpha = 0.5$, the value from the exact ground state solution.

Next we want to know the number of iterations it takes to find our ground state. We begin by computing the gradient of $\langle E_L \rangle$,

$$\frac{d\langle E_L \rangle}{d\alpha} = 2\left(\left\langle E_L \frac{d\ln\psi}{d\alpha}\right\rangle - E_L \left\langle \frac{d\ln\psi}{d\alpha}\right\rangle\right) = 2\left(\left\langle E_L x^2 \right\rangle - E_L \left\langle x^2 \right\rangle\right). \tag{5}$$

With an arbitrary initial value of α we use the damped steepest decent method to find the optimum α. The results can be found in figure 2, where we find that the solution is found in very few iterations.

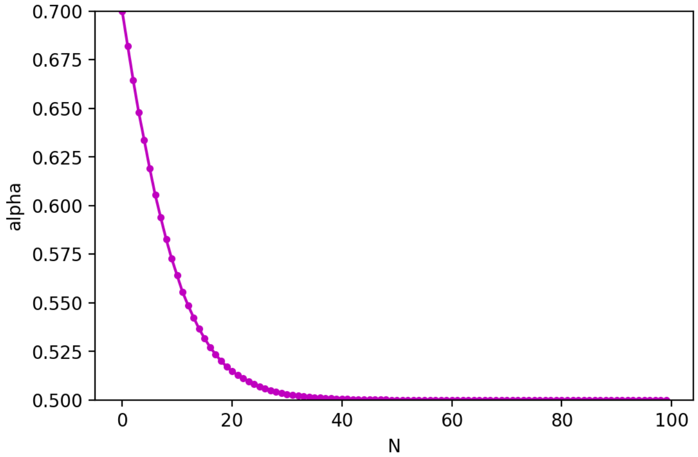


Figure 2: α as function of iteration. $\alpha_0 = 0.7$, and $\gamma = 0.05$

2 Diffusion Quantum Monte Carlo

We implement the DMC method to study the single-particle Schrodinger Wave Equation in 3D:

$$i\frac{\partial \Phi}{\partial t} = -\frac{1}{2}\nabla^2\Phi + V(\vec{r})\Phi, \tag{6}$$

where we insist that $\hbar = m = 1$. This leads to a Green's function of the form,

$$W(\vec{r}')G_{\text{diff}}(\vec{r}', \vec{r}; \Delta\tau) = \exp(\Delta\tau(E_T - V(\vec{r}'))) \times \frac{1}{\sqrt{2\pi\Delta\tau}} \exp\left(-\frac{|\vec{r}' - \vec{r}|^2}{2\Delta\tau}\right). \tag{7}$$

We perform the DMC by creating m_0 random vector walkers, and repeating for each of our set of random walkers the steps:

1. $\vec{r}_{\text{new}} = \vec{r}_{\text{now}} + \sqrt{\Delta\tau}(\xi_1, \xi_2, \xi_3)$, where ξ_i is a Gaussian random variable with zero mean and unit variance.
2. Find $W(\vec{r}_{\text{new}})$. Let $s = [W]$, and if $(W - [W]) > \text{rand}[0, 1]$, then $s = s + 1$.
3. If $s = 0$, then remove this walker. Else create $s - 1$ copies of the walker and append them to the end.

After which we update reference energy, $E_T = E_T + \alpha \ln(M_T/M)$, where M is the current number of walkers, M_T is the target number, and α is a small number.

Figures 3 and 4 present our results for a DMC simulation of the 3D harmonic oscillator with potential, $V(\vec{r}) = \frac{|\vec{r}|^2}{2}$, with ground state:

$$E_0 = 1.5, \quad \Phi_0(\vec{r}) = \frac{e^{-|\vec{r}|^2/2}}{(2\pi)^{3/2}}. \tag{8}$$

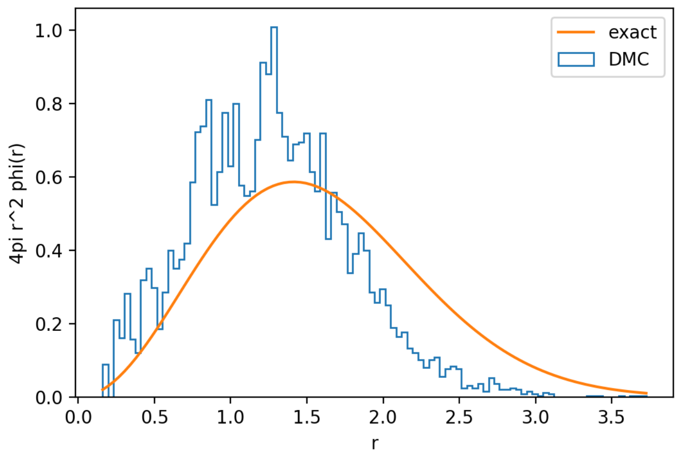


Figure 3: Comparing DMC with exact solution, $4\pi r^2 \Phi_0(r)$. DMC represents a histogram of the final state's $|r_i| = \sqrt{x_i^2 + y_i^2 + z_i^2}$.

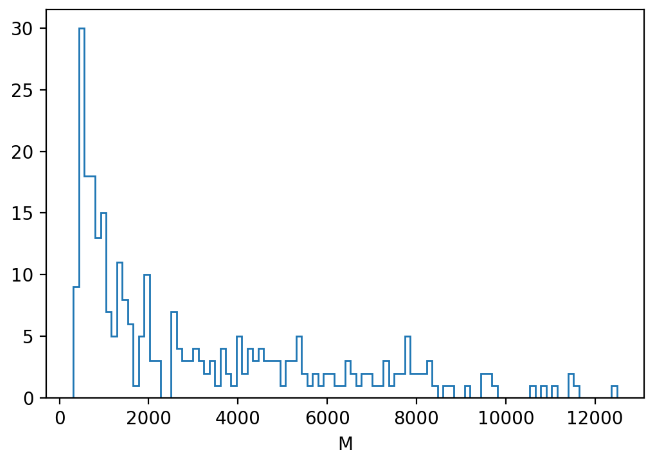


Figure 4: Histogram of M for all iterations

As you can see from figure 3 our solution is not exact, but without knowing M_T, or α, or having any idea how long to run for it becomes difficult to get an exact fit. But we do find our $\langle E_T \rangle \approx 1.45$, wich is in close agreement to our expected value of 1.5.