PHYS 5640 - Project 5

Steven Stetzler

1 Variational Quantum Monte Carlo

We seek to solve the Schroedinger equation for a 1D harmonic oscillator using numerical techniques. The Schroedinger equation for this system is

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

In order to solve Eq. 1 numerically, we will consider a trial wave function $\psi_\alpha(x)$ which is parameterized by the parameter α. Here, we will use the trial wave function $\psi_\alpha(x) \propto \exp\left(-\alpha x^2\right)$. The word "variational" within the name of this method refers to how we vary the parameter α in order to find the wave function with the lowest energy. The value of α where the energy E is minimized is the best approximation for the ground state wave function that our trial wave function can provide. First, we will define the "local energy" of the trial wave function, which can be found by plugging $\psi_\alpha(x)/Z$ (with $Z = \int_{-\infty}^{\infty}|\psi_\alpha(x)|^2dx$) into Eq. 1.

$$-\frac{1}{2}\frac{d^2\frac{\psi_\alpha(x)}{Z}}{dx^2} + \frac{x^2}{2}\frac{\psi_\alpha(x)}{Z} = E\frac{\psi_\alpha(x)}{Z}$$

$$-\frac{1}{2}\frac{d^2\exp(-\alpha x^2)}{dx^2} + \frac{x^2}{2}\exp(-\alpha x^2) = E\exp(-\alpha x^2)$$

$$-\frac{1}{2}(4\alpha^2x^2 - 2\alpha)\exp(-\alpha x^2) + \frac{x^2}{2}\exp(-\alpha x^2) = E\exp(-\alpha x^2)$$

$$-\frac{1}{2}(x^2 - 2) + \frac{x^2}{2} = E$$

$$\boxed{\rightarrow E_L(x) = \alpha + x^2\left(\frac{1}{2} - 2\alpha^2\right)}$$

The value of E for a trial wave function $\psi_\alpha(x)$ can be found by using a Markov Chain Monte Carlo (MCMC) technique to sample the probability distribution provided by the trial wave function, given by

$$\mathbf{Pr}(x) = \left|\frac{\psi_\alpha(x)}{\int_{-\infty}^{\infty}|\psi_\alpha(x)|^2}\right|^2 = \frac{|\psi_\alpha(x)|^2}{|\int_{-\infty}^{\infty}|\psi_\alpha(x)|^2dx|^2}$$

MCMC techniques allow one to randomly walk through a parameter space according to some probability distribution. The distribution of locations of the walker will provide a sampling from $\mathbf{Pr}(x)$. Computing observables (e.g. the local energy E_L) after each step the walker takes will provide a distribution over the observable. Luckily, since MCMC technique rely on ratios of probabilities, then we don't actually need to compute the normalization $Z = \int_{-\infty}^{\infty}|\psi_\alpha(x)|^2dx$ in the probability distribution above. Within the MCMC code I wrote, at each iteration of the walk a new state x' is chosen uniformly from a small range around the current state x. The walker accepts its new position with probability

$$\mathbf{P}_{accept} = \frac{|\psi_\alpha(x')|^2}{|\psi_\alpha(x)|^2} = \frac{\exp\left(-2\alpha x'^2\right)}{\exp\left(-2\alpha x^2\right)} = \exp\left(-2\alpha\left(x'^2 - x^2\right)\right)$$

I simulated $N_{walkers} = 2,000$ walkers walking through the parameter space of the trial wave function for $N = 10,000$ steps, computing the observable E_L and E_L^2 at every step. I computed the average value of E_L

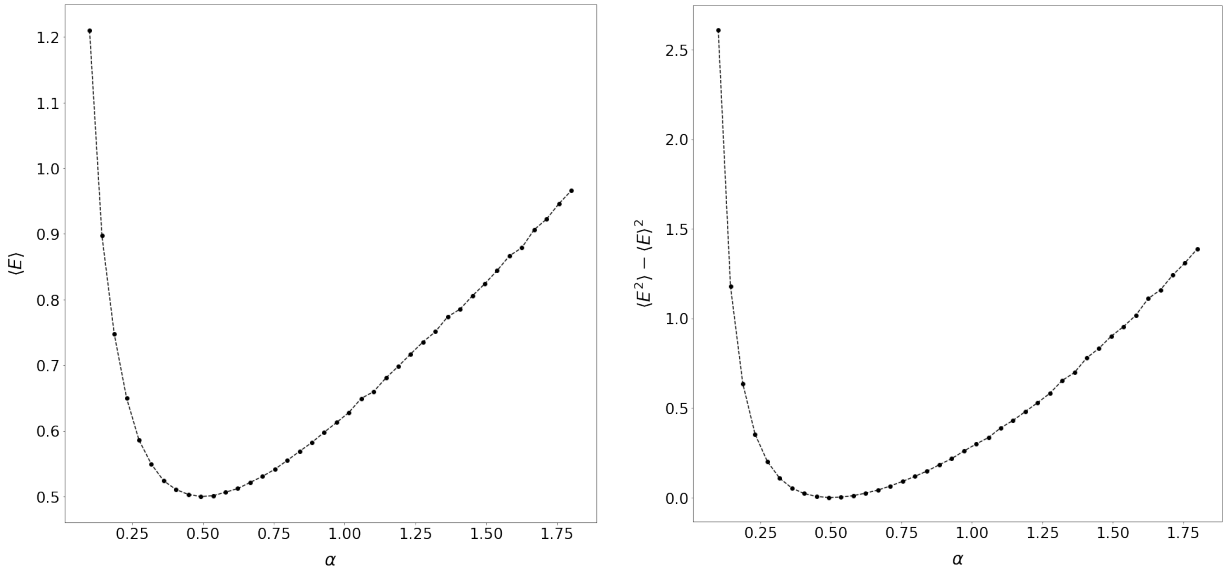

Figure 1: The average energy (left) and the standard deviation of the energy (right) of the trial wave function $\psi_\alpha(x)$ as a function of the variational parameter α.

and E_L^2 at the end of the set of walks. I repeated this for several values of α so that we can explore how the choice of α affects both the average energy $\langle E_L \rangle$ and the standard deviation of the energy $\langle E_L^2 \rangle - \langle E_L \rangle^2$. Figure 1 shows the average energy and the standard deviation of the energy of the trial wave function as a function of the parameter α.

Since we know that a best value of α exists that minimizes the energy of the trial wave function, we can try to use minimization methods to find this α. One minimization method to consider is the method of steepest descent in which the value of a parameter of a function is updated according to the gradient of that function with respect to that parameter. This update rule allows to compute the path to the minimum of the function with respect to the parameter (given by the direction of the gradient of the function with respect to the parameter). In other words, after we have an idea of what the local energy E_L is during our walk through the parameter space, we can update our value of α with the following rule:

$$\alpha^{(n+1)} = \alpha^{(n)} - \gamma \frac{d\langle E_L \rangle}{d\alpha}. \tag{2}$$

The damping factor γ is used to slow the update of α upon each iteration of the parameter, so as not to continually overshoot the final step to the α which minimizes $\langle E_L \rangle$. Now, we must compute the derivative $\frac{d\langle E_L \rangle}{d\alpha}$. We can find this by first writing $\langle E_L \rangle$ as[1]

$$\langle E_L \rangle = \frac{\int \psi_\alpha(x) \hat{\mathcal{H}} \psi_\alpha(x) dx}{\int |\psi_\alpha(x)|^2 dx}.$$

[1] within this equation, we drop the complex conjugate since we know that $\psi_\alpha(x)$ is a real function.

Thus taking the derivative with respect to α we obtain

$$\begin{aligned}
\frac{d\langle E_L\rangle}{d\alpha} &= \frac{\int|\psi_\alpha(x)|^2dx\frac{d}{d\alpha}\int\psi_\alpha(x)\hat{\mathcal{H}}\psi_\alpha(x)dx - \int\psi_\alpha(x)\hat{\mathcal{H}}\psi_\alpha(x)dx\frac{d}{d\alpha}\int|\psi_\alpha(x)|^2dx}{\left(\int|\psi_\alpha(x)|^2dx\right)^2} \\
&= \frac{\int|\psi_\alpha(x)|^2dx2\int\frac{d\psi_\alpha(x)}{d\alpha}\hat{\mathcal{H}}\psi_\alpha(x)dx - \int\psi_\alpha(x)\hat{\mathcal{H}}\psi_\alpha(x)dx2\int\psi_\alpha(x)\frac{d\psi_\alpha(x)}{d\alpha}dx}{\left(\int|\psi_\alpha(x)|^2dx\right)^2} \\
&= 2\left(\frac{\int\frac{d\psi_\alpha(x)}{d\alpha}\hat{\mathcal{H}}\psi_\alpha(x)dx}{\int|\psi_\alpha(x)|^2dx} - \frac{\int\psi_\alpha(x)\hat{\mathcal{H}}\psi_\alpha(x)dx}{\int|\psi_\alpha(x)|^2dx}\frac{\int\psi_\alpha(x)\frac{d\psi_\alpha(x)}{d\alpha}dx}{\int|\psi_\alpha(x)|^2dx}\right) \\
&= 2\left(\frac{\int\psi_\alpha(x)\frac{\frac{d\psi_\alpha(x)}{d\alpha}}{\psi_\alpha(x)}\frac{\hat{\mathcal{H}}\psi_\alpha(x)}{\psi_\alpha(x)}\psi_\alpha(x)dx}{\int|\psi_\alpha(x)|^2dx} - \frac{\int\psi_\alpha(x)\frac{\hat{\mathcal{H}}\psi_\alpha(x)}{\psi_\alpha(x)}\psi_\alpha(x)dx}{\int|\psi_\alpha(x)|^2dx}\frac{\int\psi_\alpha(x)\frac{\frac{d\psi_\alpha(x)}{d\alpha}}{\psi_\alpha(x)}\psi_\alpha(x)dx}{\int|\psi_\alpha(x)|^2dx}\right)
\end{aligned}$$

If we notice that

$$\frac{d\ln\psi_\alpha(x)}{d\alpha} = \frac{1}{\psi_\alpha(x)}\frac{d\psi_\alpha(x)}{d\alpha}$$

then we can rewrite the previous equation as

$$\frac{d\langle E_L\rangle}{d\alpha} = 2\left(\frac{\int\psi_\alpha(x)\frac{d\ln\psi_\alpha(x)}{d\alpha}\frac{\hat{\mathcal{H}}\psi_\alpha(x)}{\psi_\alpha(x)}\psi_\alpha(x)dx}{\int|\psi_\alpha(x)|^2dx} - \frac{\int\psi_\alpha(x)\frac{\hat{\mathcal{H}}\psi_\alpha(x)}{\psi_\alpha(x)}\psi_\alpha(x)dx}{\int|\psi_\alpha(x)|^2dx}\frac{\int\psi_\alpha(x)\frac{d\ln\psi_\alpha(x)}{d\alpha}\psi_\alpha(x)dx}{\int|\psi_\alpha(x)|^2dx}\right)$$

and if we use the definitions $E_L = \frac{\hat{\mathcal{H}}\psi_\alpha(x)}{\psi_\alpha(x)}$, we can rewrite the above as

$$\frac{d\langle E_L\rangle}{d\alpha} = 2\left(\frac{\int\psi_\alpha(x)\frac{d\ln\psi_\alpha(x)}{d\alpha}E_L\psi_\alpha(x)dx}{\int|\psi_\alpha(x)|^2dx} - \frac{\int\psi_\alpha(x)E_L\psi_\alpha(x)dx}{\int|\psi_\alpha(x)|^2dx}\frac{\int\psi_\alpha(x)\frac{d\ln\psi_\alpha(x)}{d\alpha}\psi_\alpha(x)dx}{\int|\psi_\alpha(x)|^2dx}\right)$$

Finally, replacing each term with the expectation values that these terms represent we obtain

$$\boxed{\frac{d\langle E_L\rangle}{d\alpha} = 2\left(\langle E_L\frac{d\ln\psi_\alpha(x)}{d\alpha}\rangle - \langle E_L\rangle\langle\frac{d\ln\psi_\alpha(x)}{d\alpha}\rangle\right).}$$

Expressing $\frac{d\ln\psi_\alpha(x)}{d\alpha}$ as

$$\frac{d\ln\psi_\alpha(x)}{d\alpha} = \frac{d}{d\alpha}\left(-\alpha x^2 - \ln(Z)\right) = -x^2$$

then we can compute $\frac{d\langle E_L\rangle}{d\alpha}$ as

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

Providing a closed form for $\frac{d\langle E_L\rangle}{d\alpha}$ allows us to update α according to Eq. 2 after some number of iterations of the MCMC using the values of the observable E_L and the position of the walker x.

Figure 2 shows the value of α after several iterations of the update rule (Eq. 2) with a damping factor of $\gamma = 0.05$ starting at $\alpha = 0.7$. Each Monte Carlo average $\langle ...\rangle$ is computed using an arrangement of $N_{walkers} = 1,000$ walkers walking for $N = 10,000$ iterations. Once this walk terminates and the Monte Carlo average is computed, a new value of α is proposed using Eq. 2 and the walk is restarted with the new trial wave function. This process is repeated 100 times, converging on the value of α which minimizes the energy of $\psi_\alpha(x)$.

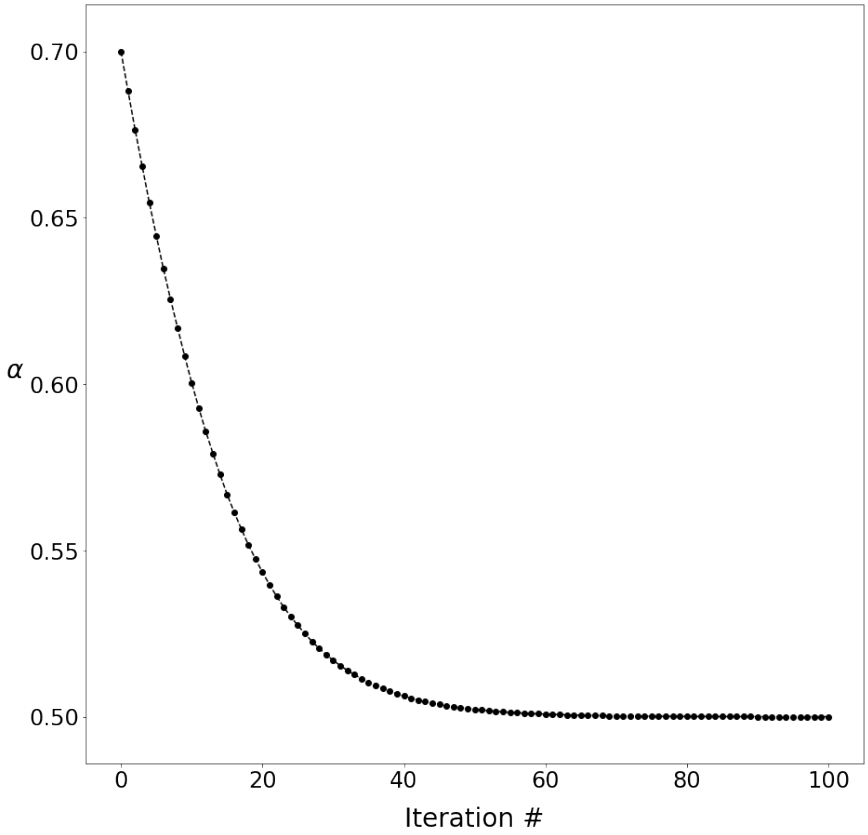

Figure 2: The variational parameter α after several iterations of applying the update rule Eq. 2.

2 Diffusion Quantum Monte Carlo

We will use Diffusion Monte Carlo (DMC) to study the single particle Schroedinger equation in three dimensions:

$$i\frac{\partial \Phi}{\partial t} = -\frac{1}{2}\nabla^2\Phi + V(\mathbf{r})\Phi \tag{3}$$

Diffusion Monte Carlo works by converting the Schroedinger equation into the imaginary time Schroedinger equation and then evolving trial states with a trial energy E_T in accordance with this imaginary time equation. The imaginary time Schroedinger equation takes the form

$$-\frac{\partial \psi(\mathbf{r},\tau)}{\partial \tau} = -\frac{1}{2}\nabla^2\psi(\mathbf{r},\tau) + (V(\mathbf{r}) - E_T)\,\psi(\mathbf{r},\tau).$$

Diffusion Monte Carlo gets its name from the fact that the above equation resembles the diffusion equation where $\psi(\mathbf{r})$ can be interpreted as the "density" of diffusion particles and the term $V(\mathbf{r}) - E_T$ describes an increase or decrease in the density of particles according to the potential $V(\mathbf{r})$. The long-time limit ($\tau \to \infty$) of evolving this equation is the ground state $\phi_0(\mathbf{r})$ with $E_T = E_0$. In simulation, the imaginary time axis is discretized into sub-intervals of length $\Delta\tau$ and solving the imaginary time Schroedinger equation is converted into solving a tractable integral which utilizes the Green's function

$$G(\mathbf{r}', \mathbf{r}; \Delta\tau) = e^{\Delta\tau\left(E_T - V(\mathbf{r}')\right)}\frac{1}{\sqrt{2\pi\tau}}e^{-\frac{|\mathbf{r}'-\mathbf{r}|^2}{2\Delta\tau}}$$

During the simulation, a set of walkers is initialized to random positions $\mathbf{r}_i$. For each of them, a new position $\mathbf{r}_i'$ is proposed from each walker's surrounding neighborhood. All moves are accepted; however, some walkers are either killed, cloned, or left alone, with the probability for each event determined using the Green's function above. Walkers are killed or cloned in accordance with the potential $V(\mathbf{r})$ so that there are few walkers where $V(\mathbf{r})$ is large and there are many walkers where $V(\mathbf{r})$ is small, which properly maps out the shape of $\psi(\mathbf{r})$.

I implemented the DMC scheme to sample the ground state wave function of the 3D harmonic oscillator which has a potential $V(\mathbf{r}) = \frac{|r|^2}{2}$. This system has a ground state energy of

$$E_0 = \frac{3}{2}, \qquad \phi_0(\mathbf{r}) = \frac{e^{-|\mathbf{r}|^2/2}}{(2\pi)^{3/2}}. \tag{4}$$

I initialized the simulation to have 10^5 walkers randomly placed within the unit ball ($|\mathbf{r}| < 1$), set a target energy of $E_T = 1$, discretized the imaginary time space using $\Delta\tau = 0.01$, and set the target number of walkers to be $M_T = 10^5$. I terminated the simulation after 500 clone / kill cycles. At the end, I histogrammed the position of the walkers, which provides a sampling for the distribution $4\pi|\mathbf{r}|^2\phi(\mathbf{r})$ ($\phi_0(\mathbf{r})$ integrated over the angles ϕ and θ). Figure 3 shows the histogram of the walkers along with a plot of the analytic result (Eq. 4).

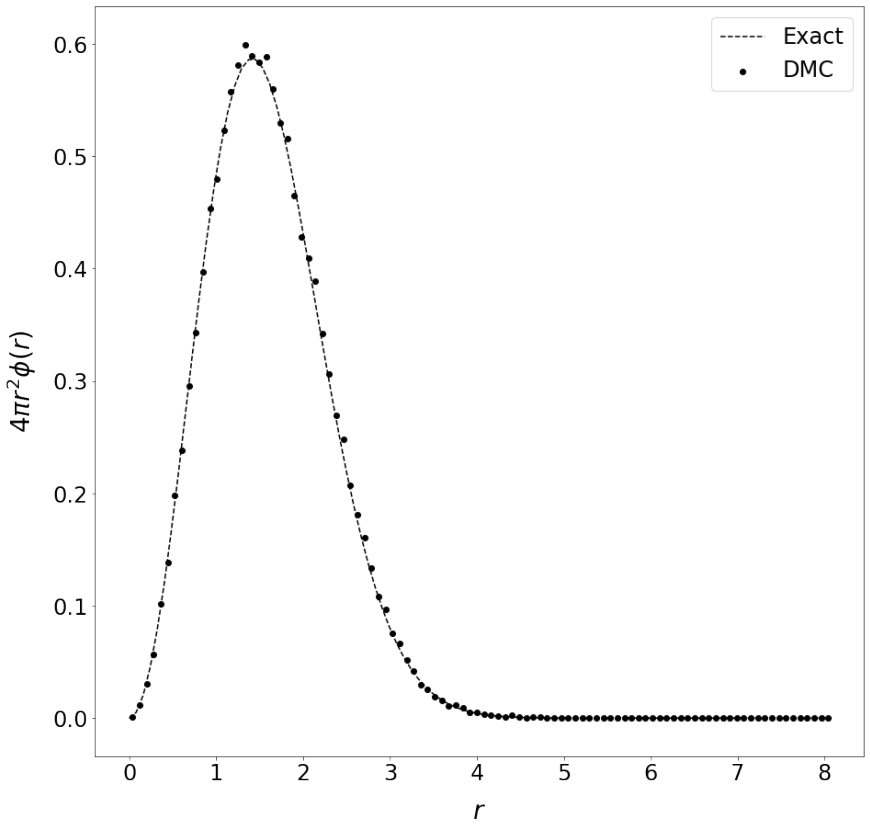

Figure 3: The results of the DMC simulation with $M_T = 10^5$ and $\Delta\tau = 0.01$ after 500 clone / kill cycles. The dashed line represents the analytic ground state (Eq. 4).