Variational Monte Carlo for the Quantum Harmonic Oscillator

Rama Khalil

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Contents

1 Introduction

In this assignment, we use the Metropolis Monte Carlo (MC) algorithm to simulate a system of two interacting electrons confined in a two-dimensional harmonic oscillator potential. The goal is to find the ground state energy of the system using Variational Monte Carlo.

2 Theory

2.1 One-electron system

To make things simpler, we start with a single particle in a one-dimensional harmonic oscillator, described by the dimensionless Hamiltonian:

$$H = -\frac{1}{2}\frac{d^2}{dz^2} + \frac{z^2}{2} \tag{1}$$

The trial wave function is taken as a Gaussian:

$$\Psi(z) = e^{-\alpha z^2} \tag{2}$$

Using this, the local energy can be evaluated analytically:

$$E_L(z) = \alpha + z^2\left(\frac{1}{2} - 2\alpha^2\right) \tag{3}$$

This serves as a reference for verifying the implementation of the variational Monte Carlo method, as by setting $\alpha = 1/2$, we get the exact analytical solution for the Ground state:

$$E_0 = \alpha = \frac{1}{2} \tag{4}$$

2.2 Two-electrons system

Moving on to the two-electron system, now the particles are confined in a two-dimensional harmonic oscillator potential.
In dimensionless units, and taking into account the Coulomb repulsion, the Hamiltonian of the system reads:

$$H = \sum_{i=1}^{2}\left(-\frac{1}{2}\nabla_i^2 + \frac{1}{2}r_i^2\right) + \frac{\lambda}{r_{12}} \tag{5}$$

where $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ is the inter-electron distance.
We let our trial wave function now be a product of a Gaussian function with a Jastrow factor:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \exp\left(-\frac{1}{2}(r_1^2 + r_2^2)\right) \cdot \exp\left(\frac{\lambda r_{12}}{1 + \alpha r_{12}}\right) \tag{6}$$

The corresponding expression for the local energy is:

$$E_L = \frac{1}{2}\left[r_1^2 + r_2^2 - 4 + \frac{4\lambda}{(1 + \alpha r_{12})^2 r_{12}} - \frac{2\lambda(x_1 - x_2)^2}{r_{12}^3(1 + \alpha r_{12})^3} - \frac{2\lambda(y_1 - y_2)^2}{r_{12}^3(1 + \alpha r_{12})^3}\right] + \frac{\lambda}{r_{12}} \tag{7}$$

This system is not exactly solvable, but for $\lambda = 1$, the known ground state energy is $E = 3$. The goal of the VMC procedure is to approximate this energy by minimizing with respect to the variational parameter α.

3 Numerical Method

3.1 MC-Algorithm

The Variational MC method relies on the generation of a Markov chain of configurations where the probability that a particle is at a specific point in space is proportional to the square of the wavefunction, $|\Psi(x_1, x_2, \ldots)|^2$.
The algorithm is fully described below:

1. The particle is initialized with a random position.

2. A new trial position for one particle is chosen by displacing it randomly:

$$x_i^{\text{new}} = x_i + \delta, \quad \delta \in [-h, h]$$

3. The acceptance probability is calculated as:

$$p = \frac{|\Psi(\ldots, x_i^{\text{new}}, \ldots)|^2}{|\Psi(\ldots, x_i^{\text{old}}, \ldots)|^2}$$

4. Accept the new position with probability p:

   - If $p \geq 1$, accept.
   - If $p < 1$, accept with probability p.

5. Repeat steps 2–4 for all particles many times to generate statistically representative samples.

6. At each accepted step, evaluate the local energy:

$$E_L(\vec{x}) = \frac{H\Psi(\vec{x})}{\Psi(\vec{x})}$$

7. Accumulate the average energy $\langle E_L \rangle$ and its variance:

$$\text{Var}(E_L) = \langle E_L^2 \rangle - \langle E_L \rangle^2$$

3.2 Golden Section Search

The Golden search algorithm is a method that efficiently locates the minimum of a function in a specified interval $[a, b]$ without requiring derivatives. The algorithm proceeds by repeatedly evaluating the function at two intermediate points c and d inside the interval, given by:

$$c = b - \frac{b-a}{\phi}, \quad d = a + \frac{b-a}{\phi} \tag{8}$$

where $\phi = \frac{1+\sqrt{5}}{2}$ is the Golden ration.

The function value at those intermediate points is then compared at each step, and the interval is updated by discarding the half that does not contain the minimum.
In our case, we wish to minimize the local energy, which is computed using MC algorithm and local energy evaluations for each α. The search continues until the width of the interval falls below a given tolerance.

3.3 Limitations of the Model

Although the Variational Monte Carlo method provides good results for approximating the ground state energy, we still used some simplifications and approximations, which can be grouped into two categories:

3.3.1 Physical limitations

Simplified trial wavefunction The results are highly dependent on the choice of the trial wave function. For the 1D harmonic oscillator, the trial wavefunction $\Psi(z) = e^{-\alpha z^2}$ corresponds to the exact analytical solution when $\alpha = 0.5$. However, for the 2D two-electron system with Coulomb interaction, the chosen trial wavefunction is an approximation.

3.3.2 Numerical limitations

Resolution VS Computational costs   The Metropolis algorithm performs a local random walk in configuration space, with the convergence rate being dependent on the step size h, where too small h leads to poor exploration, while too large h results in lower acceptance rates.
Hence, one has to find an optimal value of h where both the acceptance and convergence rates are considered good enough for the results to be acceptable.

Finite sampling   Since only a finite number of samples are drawn from the configuration space, the results may not fully capture the behavior of the system. And since the variational parameter α is optimized numerically, it may not converge exactly to the true minimum.

4 Results

4.1 One-electron system

Figure 1 shows both the local energies and corresponding variance as functions of the variational parameter α.
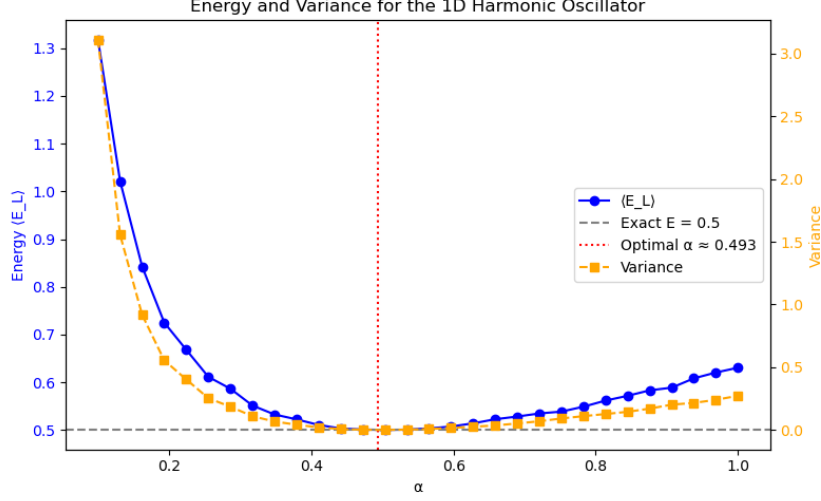

Figure 1: Energy and Variance for different alphas.

We can observe that VMC gave the expected results, the energy indeed reaches a minimum near:

$$\alpha \approx 0.493 \tag{9}$$

This agrees with the theoretical value of $\alpha = 0.5$, the variance at this point also reaches its minimum, indicating that the trial wavefunction at this point represents an eigenstate of the system.
Figure 2 is a plot of the histogram over the sampled positions obtained from the Metropolis algorithm along with the probability density of the trial wave function:
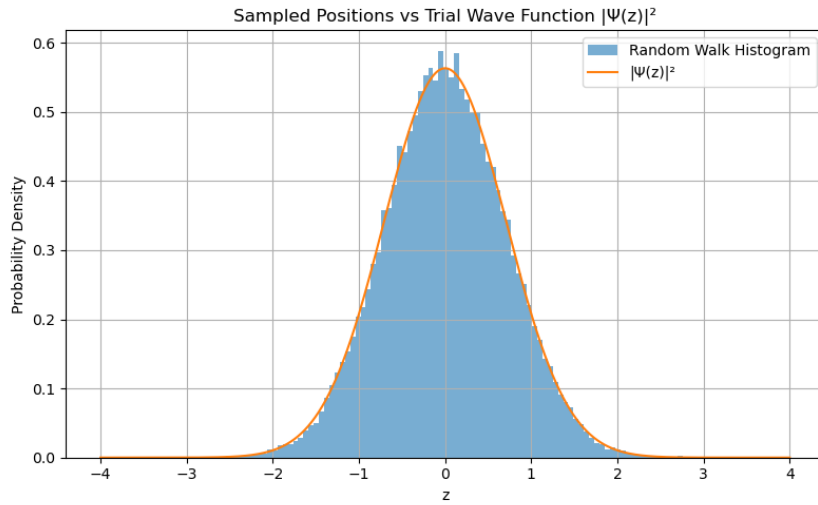

Figure 2: Random walk VS probability density function.

The agreement between the two curves confirms that the random walk correctly samples the space defined by our trial wave function.

4.2 Two-electron system

Figure 3 shows the results for the two-dimensional harmonic oscillator when $\lambda = 1$. We can clearly observe a minimum around $\alpha = 0.345$, which corresponds to the optimal value that best captures the correlation between the electrons introduced by the Jastrow factor.
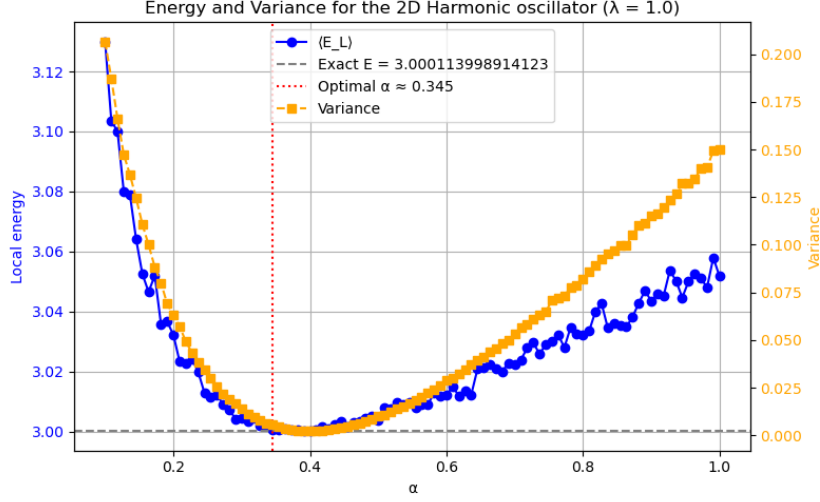

Figure 3: Energy and Variance for $\lambda = 1$.

The obtained result shows excellent agreement with the literature value of

$$E = 3\hbar\omega = 3 \tag{10}$$

confirming the precision of our implementation.

Figure 4 shows the energy and corresponding variance for the two-dimensional harmonic oscillator with a strong Coulomb repulsion, $\lambda = 8$:
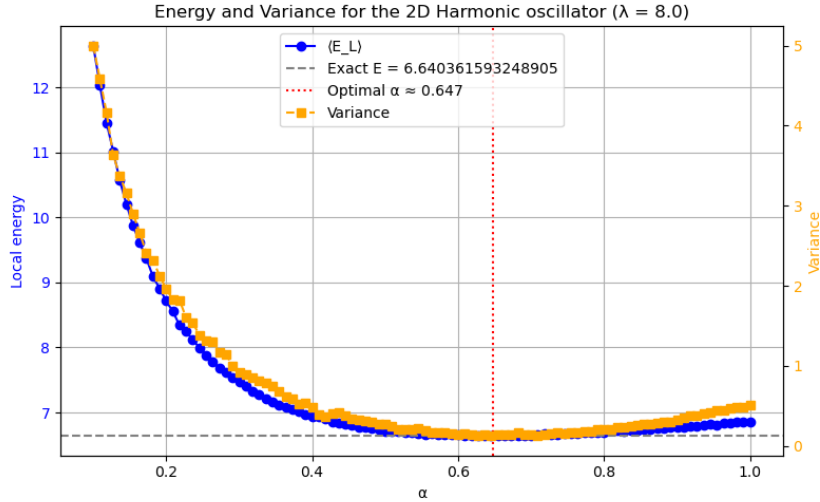

Figure 4: Energy and Variance for $\lambda = 8$.

The lowest energy obtained is in close agreement with the exact result $E \approx 6.64$. The variance also shows a minimum at approximately the same α, indicating that the Jastrow factor in our trial wave functions can still effectively capture correlation effects even at high interaction strength.

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5   Discussion

After confirming the results for a one-electron system, the VMC was successfully applied to a two-electron system in a 2D harmonic oscillator, where for $\lambda = 0$, the two electrons are non-interacting, and the expected energy $E = 2$ was accurately computed. As λ increased, a clear minimum appeared as a function of the variational parameter α, capturing the electron-electron correlation.

The overall results confirm that our VMC method accurately captures the physical behavior of the system across different regimes of interaction.