Quantum Monte Carlo

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Abstract

(To be completed)

1 Introduction

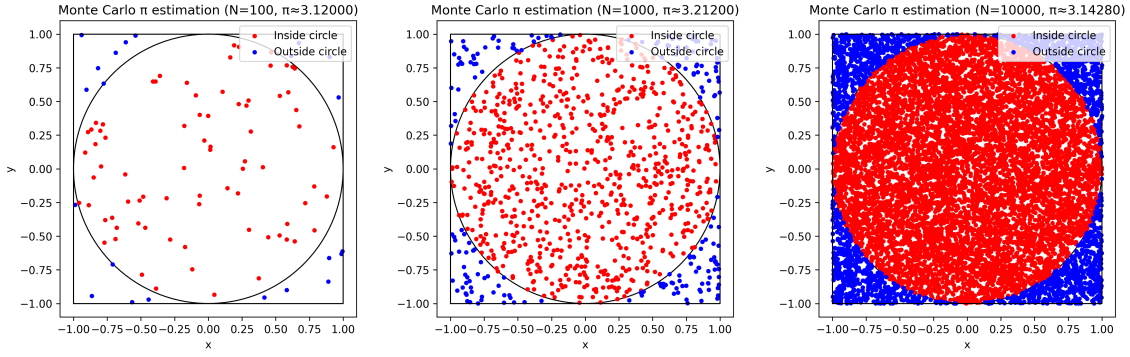
(To be completed)

2 Monte Carlo Method

Monte Carlo method is a class of classical computational algorithm which aims to find a numerical value of interest through iterative random sampling according to a probability distribution. Such method is often applied when analytical solutions are too complex to solve. A simple case in which Monte Carlo method can be used is to approximate the value of π with only the knowledge of how to calculate the area of a circle. The process is outlined as such [KW08]:

1. Consider a square with edge length of 2, and centered at $(0, 0)$.
2. Then, draw the inscribed circle of such a square which has radius 1, also centered at $(0, 0)$.
3. **Uniformly at random** select a point within the square.
4. Calculate the ratio of the number of points within the circle and the total number of points sampled. This should approximate $\frac{\pi}{4}$.
5. Repeat Step 3 and 4 until a certain threshold. Calculate the approximated value of π by multiplying the ratio stated in Step 4 by 4.

By applying this process, we can obtain the following result (link to code, see A.1):



The key idea from this demonstration is that random sampling can be used to evaluate a definite integral [KW08]:

$$I = \int_0^1 \int_0^{\sqrt{1-x^2}} \mathrm{d}y\mathrm{d}x$$

From the above demonstration, it is observed that the main goal of Monte Carlo method is to solve a certain mathematical problem with the core process to be iterated random sampling, where each additional iteration gives more accurate results.

3 Variational Monte Carlo

In quantum many-body problems, investigating the ground-state energy of the many-body system is essential, as the system's ground state captures its equilibrium properties [FMNR01]. However, as the number of interacting particles in a given system scale, analytically solving the Schrödinger's equation of the entire system while incorporating the interaction of particles within becomes intractable. In this case, the Variational Monte Carlo (abbreviated as VMC) method provides a practical approximation to the ground state energy.

3.1 Main Process of VMC

To begin with, consider the following relevant physical definitions.

Definition 3.1. *Consider a general quantum system, denoted mathematically as a Hilbert space $\mathcal{H}$, with N particles. Each particle i has 3-dimensional position vector $\mathbf{r}_i$. Define a $3N$-dimensional vector $\mathbf{R} = (\mathbf{r}_1, \ldots, \mathbf{r}_N)$. A general quantum state $|\Psi\rangle$ in this system can be denoted as:*

$$|\Psi\rangle = \int \Psi(\mathbf{R}) \, |\mathbf{R}\rangle \, \mathrm{d}\mathbf{R} \tag{1}$$

where $\Psi(\mathbf{R})$ is the position-space wavefunction, which satisfies the following properties:

1. $|\Psi(\mathbf{R})|^2 \geq 0$
2. $\int \Psi^*(\mathbf{R})\Psi(\mathbf{R})\mathrm{d}\mathbf{R} = 1$

Definition 3.2. *An **observable** $\mathcal{O}$ is a Hermitian operator, where measuring $\mathcal{O}$ mathematically amounts to doing a projective measurement with respect to the orthonormal basis of eigenvectors of $\mathcal{O}$.*

Definition 3.3. *Given an observable $\mathcal{O}$ and a quantum state $|\Psi\rangle$, the **expected value** of this observable with respect to this state is*

$$\langle \mathcal{O} \rangle = \langle \Psi | \mathcal{O} | \Psi \rangle \tag{2}$$

*and the **variance** of the above observable and the above state is:*

$$(\Delta \mathcal{O})^2 = \left\langle \mathcal{O}^2 \right\rangle - (\langle \mathcal{O} \rangle)^2 \tag{3}$$

To characterize the time evolution of the quantum state, the observable $\hat{H}$ is introduced to give the following.

Definition 3.4. *The **time-dependent Schrödinger's equation** of a given quantum state* $|\Psi\rangle$ *that is dependent on time* t *is*

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle \tag{4}$$

where i *is the imaginary unit,* $\hbar$ *is Planck's constant,* $\hat{H}$ *is the Hamiltonian operator for the quantum state* $|\Psi\rangle$*.*

In the context of VMC, the quantity of interest is the ground state energy. After the system reaches this equilibrium, the Hamiltonian can be considered to be time-independent. Thus, from 3.4

Definition 3.5. *If the Hamiltonian* $\hat{H}$ *is time-independent, it induces the **time-independent Schrödinger's equation** for* $|\Psi\rangle$ *to be:*

$$\hat{H}|\Psi\rangle = E|\Psi\rangle \tag{5}$$

From Eq. (2) and Eq. (5), it follows that

$$\left\langle \hat{H} \right\rangle = E \tag{6}$$

which indicates that, for an eigenstate $|\Psi\rangle$ of the Hamiltonian $\hat{H}$, the expected value of $\hat{H}$ is the eigenvalue of $|\Psi\rangle$, which physically represents the energy of the system when it is in the state of $|\Psi\rangle$.
If the ground state wavefunction is denoted to be $\Psi_0(\mathbf{R})$, it follows from Eq. (6), the ground state energy E_0 is:

$$\begin{aligned} E_0 &= \langle\Psi_0|\hat{H}|\Psi_0\rangle \\ &= \int \Psi_0^*(\mathbf{R})\hat{H}\Psi_0(\mathbf{R})\mathrm{d}\mathbf{R} \end{aligned}$$

To approximate this energy, a trial wavefunction Ψ_T is first selected, satisfying certain conditions [FMNR01]:

1. Ψ_T and $\boldsymbol{\nabla}\Psi_T$ must be continuous wherever the potential is finite.
2. The integrals $\int \Psi_T^*\Psi_T$, $\int \Psi_T^*\hat{H}\Psi_T$, and $\int \Psi_T^*\hat{H}^2\Psi_T$ all must exist

With this trial wavefunction, the expected value of the Hamiltonian is calculated to be [FMNR01] [Aci97] [KW08]:

$$E_V = \frac{\int \Psi_T^*(\mathbf{R})\hat{H}\Psi_T(\mathbf{R})\mathrm{d}\mathbf{R}}{\int |\Psi_T(\mathbf{R})|^2\mathrm{d}\mathbf{R}} \geq E_0 \tag{7}$$

To use VMC, sampling needs to be conducted according to a certain probability distribution. The trial energy E_V can be considered as an expected value of all local energies E_{loc}. From Eq. (5), energy of the system in state $|\Psi\rangle$ can also be calculated as:

$$E = \frac{\hat{H}|\Psi\rangle}{|\Psi\rangle}$$

Therefore, each local energy sampled from $\mathbf{R}$ is evaluated to be [KW08]:

$$E_{\mathrm{loc}}(\mathbf{R}) = \frac{\hat{H}\Psi_T(\mathbf{R})}{\Psi_T(\mathbf{R})} \tag{8}$$

This gives the probability density for sampling to naturally be [KW08]:

$$f(\mathbf{R}) = \frac{|\Psi_T(\mathbf{R})|^2}{\int |\Psi_T(\mathbf{R})|^2 \mathrm{d}\mathbf{R}} \tag{9}$$

From Eq. (8) and Eq. (9), Eq. (7) becomes:

$$E_V = \int f(\mathbf{R}) E_{\mathrm{loc}}(\mathbf{R}) \mathrm{d}\mathbf{R} \tag{10}$$

which can be approximated by [FMNR01][Aci97]:

$$E_V \approx \frac{1}{M} \sum_{m=1}^{M} E_{\mathrm{loc}}(\mathbf{R}_m) \tag{11}$$

The essential steps of VMC have been established, showing how the ground-state energy can be estimated through Monte Carlo sampling. However, in this process, two key challenges remain: the choice and optimization of the trial wavefunction and the sampling of the configuration $\mathbf{R}$. These two aspects will be discussed in the following sections.

3.2 Selection and Optimization of the Trial Wavefunction

3.3 Sampling Method

In the previous section, it is discussed how a trial wavefunction can be selected and optimized. Yet, it is still unclear how a configuration $\mathbf{R}$ is sampled such that it satisfies the probability density in Eq. (9).

Naïvely, one should sample according to this probability density function. However, it should be noted that the integral present in the denominator of Eq. (9) becomes computationally implausible to calculate or normalize when the dimension of $\mathbf{R}$ scales, because as stated before, configuration $\mathbf{R}$ is a $3N$-dimensional vector. Furthermore, uniformly sampling in a $3N$-dimensional space suffers from the "curse of dimensionality" where if only a given number of data points are being sampled, the samples would be so sparse that they cannot represent the population well [MRR+53]. Furthermore, depending on the form of the selected trial wavefunction, the wavefunction can take different shapes and correlations which further complicates a naïve sampling method.

Hence, Metropolis et al. developed an algorithm that accepts or rejects a configuration starting from an initial configuration using only probability ratios [MRR+53]. This algorithm ensures that the final list of accepted configurations follows the same distribution as the probability density distribution [MRR+53].

Analogous to the paper in which Metropolis et al. demonstrated how they sampled according to the Boltzmann distribution, the following steps is taken to sample the selected trial wavefunction [MRR+53]:

1. Place the N particles in any configuration, and denote it as $\mathbf{R}_1$. Calculate $|\Psi_T(\mathbf{R}_1)|^2$.
2. Since the initial configuration is a vector that contains the Cartesian positions of N particles, it is possible to select one particle, say particle i, who has the initial position of (x_i, y_i, z_i), and displace particle within a small cube, say with an edge length of ε. Mathematically, this displacement is denoted as:

$$x_i \mapsto x_i + \varepsilon\delta_x, y_i \mapsto y_i + \varepsilon\delta_y, z_i \mapsto z_i + \varepsilon\delta_z$$

where $\delta_x, \delta_y, \delta_z \in [-1, 1]$. Denote the new configuration as $\mathbf{R}_2$. Calculate $|\Psi_T(\mathbf{R}_2)|^2$.
3. Calculate the ratio between the amplitude probabilities of the two configurations:

$$p := \frac{|\Psi_T(\mathbf{R}_2)|^2}{|\Psi_T(\mathbf{R}_1)|^2}$$

4. If $p \geq 1$, confirm moving the particle to the new position. If $p < 1$, move the particle to the new position with probability p. Mathematically, move the particle to the new position with probability

$$P = \min(1, p)$$

5. If the new configuration is accepted, repeat step 2 to 4 which generates another configuration and determine whether to accept or reject it based on the latest accepted configuration. If the new configuration is rejected, start from the latest accepted configuration, and repeat step 2 to 4.
6. This above process returns a list of M configurations $\mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{R}_M$.

This algorithm developed by Metropolis et al. prevents one from needing to sample configurations that grows exponentially large as the dimension scales, and efficiently generates a set of configurations who satisfy the probability distribution from the trial wavefunction.
From the list of M configurations, it is then possible to calculate the local energy for each configuration following Eq. (8), and compute the variational approximation of the ground-state energy using Eq. (11).

4 Diffusion Monte Carlo

5 Path Integral Monte Carlo

Acknowledgments

If you have discussions with your classmates about your chosen topic, you can thank them here.

Appendix

A Monte Carlo Method

A.1 Using Monte Carlo Method to Find π

The link to the Jupyter Notebook that demonstrates this process can be accessed here on GitHub.

References

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