Quantum Monte Carlo

Hannah Baek, Tobias Tian
University of British Columbia
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Abstract

(To be completed)

Next Steps and Updated Timeline

We highlighted in our proposal that this paper will explore the background of three variants of QMC: PIMC, DMC, and VMC. After generally reading about each of the three variants, we have decided to put our main focus on VMC, where we give explanations as detailed as possible. This is also the one on which we choose to give a code demonstration. Therefore, for the next steps, there are three main goals. The first one is to continue to refine the explanation of VMC at each critical step. The second one is to complete writing the code demonstration for VMC. The last one is to explain DMC and PIMC in a less detailed but still complete way. To summarize, what further needs to be done is:

1. Refine the VMC process to explain the two remaining challenges.
2. Complete writing the code demonstration for VMC.
3. Explain theoretically what DMC does and how it contrasts with VMC, we will focus on [Tro11] [FMNR01] [KW08].
4. Explore PIMC and briefly touch on the Fermion sign problem, here we will focus on [Tro11] [TW05].

Our updated timeline:
Nov. 12 - Nov. 16: Complete writing about VMC process. Explain as detailed as possible on how trial wavefunction are chosen and optimized, and how sampling is conducted.
Nov. 17 - Nov. 23: Complete writing about both DMC and PIMC. Highlight on the comparison between VMC and DMC, and highlight the sign problem in PIMC.
Nov. 24 - Nov. 30: Complete the code demonstration for VMC.
Dec. 1 - Dec. 7: Finalize and refine the paper by systematically going through it checking for inconsistencies and errors.

1 Introduction

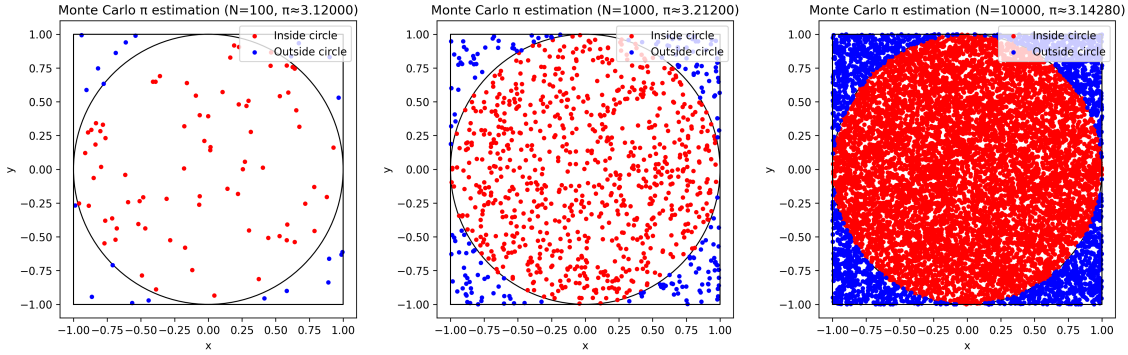
(To be completed)

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:



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

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.

References

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