Monte Carlo Importance Sampling in Variational Techniques

Solving for Ground State Energy in One Dimensional Quantum Harmonic Oscillator

Deependra Singh
2011058

I Introduction

Monte Carlo techniques are an effective tool at approximating the solutions for problems where the exact solution is difficult to find or is non-existent. Such problems includes finding the exact solutions for the Schrondinger's equation of different system, which only exists for certain idealized systems, like square wells, free particle, harmonic oscillator, etc. One of the most importanct questions for such microscopic idealized systems is finding the ground energy states and the corresponding ground state energy.

The go to method in quantum mechanics when the exact ground state energy solutions are not available is the variational method. Its computational equivalent is the Variational Monte Carlo technique (VMS) which is an application of Monte Carlo integration using Importance Sampling and Sampling techniques like Metropolis-Hastings algorithm, etc. The VMC techniques can also be extended to the evaluation of higher dimensional integratals involving ground state energy for many particle systems, and is more efficient and simpler than analytic methods. In this project, we have demonstrated the application of Monte Importance Sampling by using VMC technique in solving for ground state energy of a one dimensional quantum harmonic oscillator.

II Monte Carlo Importance Sampling

Monte Carlo Importance Sampling, unlike what its name suggests, is not a sampling algorithm but a variance-reduction technique used in Monte Carlo intergration. Instead of drawing samples from a uniform distribution as in standard or crude-Monte Carlo integration, in importance sampling we choose a different distribution to sample our points to generate more **important points**.

II.I Why is it needed?

Suppose the integral to be evaluated is:

$$I = \int_a^b f(x)\, dx$$

Following crude-Monte Carlo Method, we draw the N samples x_i from a uniform distribution between $[a, b]$ and following the principle of large numbers, the estimator for the integral is given by:[1]

$$\mathbb{E}(x_i)_{(crude)} = \frac{(b-a)}{N} \sum_{i=1}^{N} f(x_i)$$

The variance and error are given by:

$$\sigma^2_{(crude)} = \frac{(b-a)}{N} \sum_{i=1}^{N} f^2(x_i) - \left(\frac{(b-a)}{N} \sum_{i=1}^{N} f(x_i) \right)^2$$

$$\sigma_{I(crude)} = \frac{\sigma_{(crude)}}{\sqrt{N}}$$

From the equation of error, we see that the two ways to reduce this error is by increasing the number of trials or reducing the variance. Since the former would lead to an increase in the computation time, reducing the variance is a better alternative. The larger statistical error in drawing samples from a uniform distribution is due to the fact that a large portion of samples is drawn from points which do not have a significant contributions to the integral. If instead we sample from a distribution where the points having more contribution to the integral (important points) are selected at greater frequency compared to others, the variance will be drastically reduced. This is the idea behind of Importance sampling, that is to concentrate the sample where the integrand is larger.

II.II How does it work?

Suppose there is a random variable x defined by the probability distribution function (PDF) $p(x)$ defined on $[a, b]$, such that the expectation value of another function $f(x)$ is given by:

$$\langle f(x) \rangle = \int_a^b p(x) f(x)\, dx$$

For N random samples x_i drawn from $p(x)$, the estimator for the integral is given as:

$$\mathbb{E}(x_i) = \frac{1}{N} \sum_{i=1}^{N} p(x_i) f(x_i)$$

Now instead of sampling from $p(x)$, we choose a proxy distribution $q(x)$ defined on the same range $[a, b]$. Then the integral can be written as:

$$\langle f(x) \rangle = \int_a^b \left(\frac{p(x) f(x)}{q(x)} \right) q(x)\, dx$$

Let N random samples X_i be drawn from the distribution $q(x)$, then the integral becomes:

$$\mathbb{E}(X_i) = \frac{1}{N}\sum_{i=1}^{N}\frac{p(X_i)f(X_i)}{q(X_i)}$$

The choice of $q(x)$ decides the amount of variance reduction induced in the estimation. It may be possible to find an importance distribution that allows the simulation to converge the fastest, but often times, we a close estimation is good enough.[2]

Requirements for importance distribution $q(x)$

- $q(x)$ should be chosen such that it is higher for higher values of the integrand $|p(x)f(x)|$ or carries almost the same shape as the integrand

  $$\frac{p(x)f(x)}{q(x)} \approx constant$$

  Looking at the second condition, the best choice for $q(x)$ would be $p(x)$, yielding result

  $$\mathbb{E}(X_i) = \frac{1}{N}\sum_{i=1}^{N} f(X_i)$$

  However, this would be problematic if $p(x)$ is difficult to sample from, which leads to our second requirement.

- $q(x)$ should be easy to sample from.

II.III Example Problem

[1] Let the integral to be evaluated be:

$$I = \int_0^{\pi}\frac{1}{x^2+\cos^2 x}\,dx$$

Now, using Monte Carlo Importance sampling, let the normalized sampling distribution (PDF) be:

$$g(x) = \frac{\beta e^{-\beta x}}{1-e^{-\pi\beta}}$$

such that $g \geq 0\ \forall\ x \in [a,b]$, and where β is the parameter to be adjusted for minimum variance. $g(x)$ is chosen because graphically it has an almost similar shape to $f(x)$ for $\beta \in [0.5, 1.5]$, as shown in the figure below.

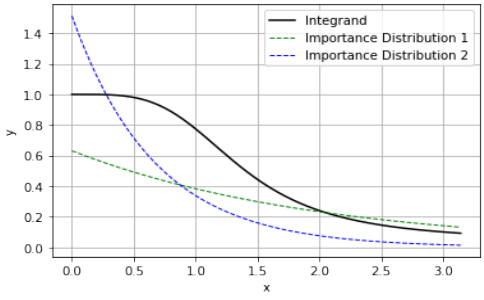

Figure 1

The estimator for N samples X_i generated from $g(x)$ using Inverse Transform Sampling Method[3] is given as:

$$\mathbb{E}(X_i) = \frac{1}{N}\sum_{i=1}^{N}\frac{f(X_i)}{g(X_i)}$$

On plotting a graph between the variance σ^2 for different parameter values β chosen at 1000 samples, we get the following result. As shown the minimum variance is achieved when the parameter $\beta = 0.8$.

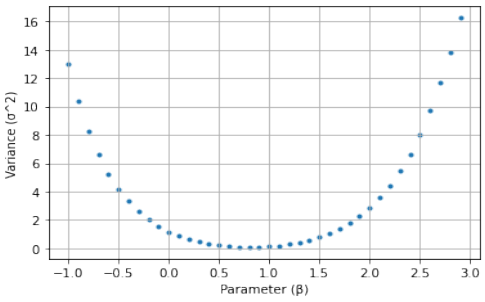

Figure 2: σ^2 *vs* β **for Importance Sampling**

Using this value as the parameter, we plot the following the graphs comparing the solutions and variances between crude-Monte Carlo Integration and Monte Carlo Importance Sampling.

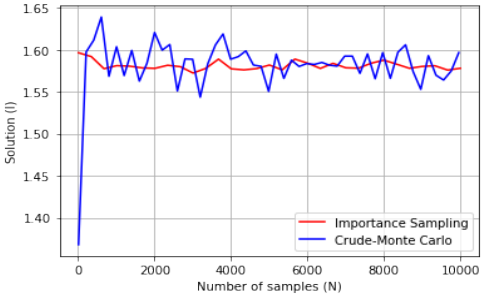

Figure 3: I *vs* N **comparison for Standard Monte Carlo and Importance Sampling integration**

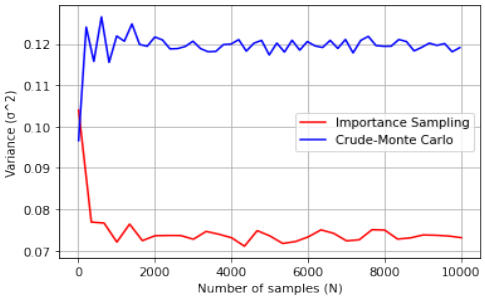

Figure 4: σ^2 *vs* N **comparison for Standard Monte Carlo and Importance Sampling integration**

We observe that Importance Sampling method converges the solution quicker compared to the standard crude method, with much lower variances, thereby proving the effectiveness of Importance Sampling.

III Application in Variational Monte Carlo (VMC) Techniques

[1] VMC is the computational variant of Variational Method in Quantum Mechanics that can be used for solving for ground state energies of quantum mechanical systems. We start by choosing a trial wave function Ψ_T with an adjustable parameter, whose form is chosen based on importance sampling to imitate the exact ground state wave function. For the appropriate optimatization of the parameter, the solution for the ground state energy would approximate to the exact solution E_0. If the trial wave function Ψ_T is identical with the exact ground state wave function, an exact estimate of the ground state energy is obtained. Thus, the variance should approach zero as our trial function approach the exact ground state.

Following variational method in quantum mechanics, for Hamiltonian $\hat{H}$ of a system, the expection value for the energy is given by:

$$\langle H \rangle = E_T = \frac{\int \Psi_T^* \hat{H} \Psi_T \, dR}{\int \Psi_T^* \Psi_T \, dR} \geq E_0$$

$$E_T = \int \rho(R) E_L(R) dR$$

where E_L is the local energy function and $\rho(R)$ is the probabability density function defined as:

$$\rho(R) = \frac{\Psi_T^2}{\int \Psi_T^2 \, dR}$$

$$E_L(R) = \frac{\hat{H}\Psi_T}{\Psi_T}$$

By sampling N samples R_i from the importance distribution $\rho(R)$, the estimator for the integral comes down to:

$$E_T = \frac{1}{N} \sum_{i=0}^{N} E_L(R_i)$$

III.I Ground State Energy of One Dimensional Harmonic Oscillator

The Hamiltonian for a one dimensional harmonic oscillator is given by:

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d}{dx^2} - \frac{m\omega^2 x^2}{2}$$

We will solve the problem in units of $\hbar\omega$ and $m = 1$, therefore the Hamiltonian becomes:

$$\hat{H} = -\frac{1}{2} \frac{d}{dx^2} - \frac{x^2}{2}$$

Let the trial wave function be $\Psi_T = e^{-\beta x}$, the corresponding pdf and local energy function is given by:

$$\rho(x) = Ae^{-2\beta x}$$

$$E_L(x) = \beta + (0.5 - 2\beta^2)x^2$$

where A is the normalization factor which will can be calculated by solving the integral $\int \Psi_T^2 \, dR$ using importance distribution Ψ_T for $x \in [-3, 3]$. The integration has been done in the range $[-3, 3]$ because the values beyond that range are very small and do not contribute much to the integratal.

For the ground state energy, we will use the pdf as the importance distribution for sampling. The sampling method used is Metropolis algorithm[4] and the distribution of samples is shown in the histogram below.

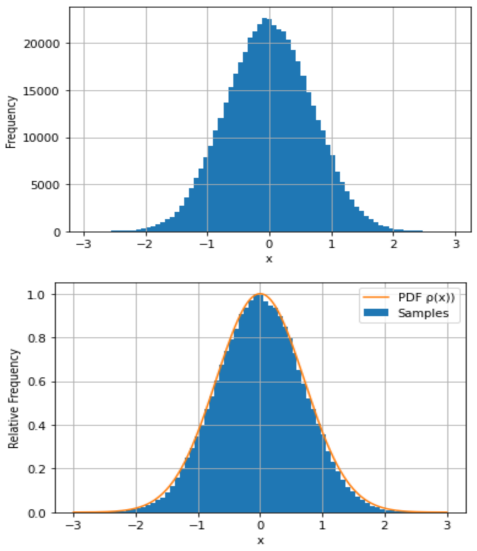

Figure 5: **Sampling using Metropolis algorithm: a)Plot of samples in x with their frequency of occurence, b)Plot of samples in x with their relative frequency compared to the maximally occuring sample**

The plots showing the variation of the solution and the variance with the parameter are shown below. As seen from the figures, the lowest value of variance (= 0) occurs for $\beta =$ 0.5 and at the same value the solution converges to exact solution of the ground state energy ($= 0.5\hbar\omega$). Hence our trial wave function is close to the actual ground state.

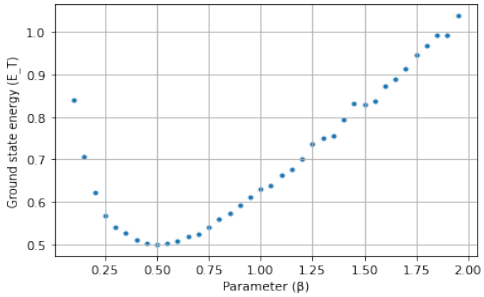

Figure 6: E_T *vs* β

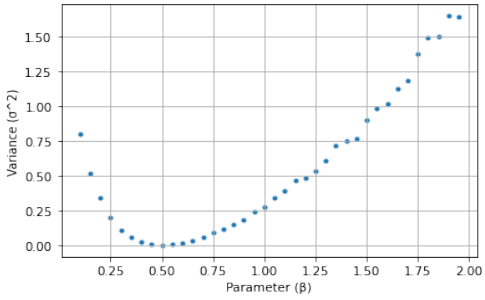

Figure 7: σ^2 *vs* β

IV Conclusion

Advantages of Importance Sampling

- It is unbiased just like the standard case.
- When it is inefficient to sample from the integrand or pdf: By choosing an appropriate importance distribution following the requirements from section 1, the variance of the integral can be improved. The variance $\mathbb{V}(X)$ for a sampling distribution $q(x)$ is given as:

$$\mathbb{V}_q(X) \;=\; \frac{1}{N}\mathbb{V}_q\left(\frac{p(X)f(X)}{q(X)}\right)$$

- When it is not possible to sample from the given integrand or pdf: We can choose an importance distribution of a similar shape, sampling from which is easier compared to the functions previously given.
- When the sampling distribution is unnormalized: For a given unnormalized pdf $\widetilde{p}(x)$, for finding the expectation value of a function $f(x)$, we can choose another unnormalized importance distribution $\widetilde{q}(x)$, such that the estimator tallies to:

$$\mathbb{E}(x_i) = \frac{1}{N^2}\sum_{i=1}^{N}\frac{\widetilde{p}(x_i)}{\widetilde{q}(x_i)}\sum_{i=1}^{N}\frac{\widetilde{p}(x_i)f(x_i)}{\widetilde{q}(x_i)}$$

  [2] where the ratio of the normalization factor is given by the first summation on the right, hence we can determine it using the unnormalized importance distribution itself.

Disadvantages of Importance Sampling

- The main drawback of importance sampling is the variance itself. Since the sampling is unbiased, a few bad samples with large weights can drastically throw off the estimator. Hence, usually a biased estimator is preferred.
- The tail ends of a distribution can add to the trouble. While $q(x)$ might be roughly the same shape as $f(x)$, serious difficulties arise if $q(x)$ gets small much faster than $f(x)$ out in the tails. These usually improbable samples may be orders of magnitude larger than the typical values $\frac{f(x)}{q(x)}$ and can affect the Monte Carlo estimator drastically.[5]

References

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[2] Eric C. Anderson. Lecture notes for stat 578c statistical genetics. `https://ib.berkeley.edu/labs/slatkin/eriq/classes/guest_lect/mc_lecture_notes.pdf`, October 1999.

[3] Mengsey Loi. Monte carlo integration and sampling methods. `https://towardsdatascience.com/monte-carlo-\integration-and-sampling-methods-25d5af53e1`.

[4] Jake. Bayesian statistics: Metropolis-hastings from scratch in python. `https://towardsdatascience.com/bayesian-statistics-metropolis-\hastings-from-scratch-in-python-c3b10cc4382d`.

[5] Importance sampling and monte carlo simulations. `https://acme.byu.edu/0000017a-1bb8-db63-\a97e-7bfa0bea0000vol1lab16montecarlo2-pdf`.