Solving Quantum Systems Numerically

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***Abstract*—This report discuses and implements the extended trapezoidal, extended Simpson and Monte Carlo numerical methods as integration techniques to determine the probability of finding a particle inside a 1D and 3D quantum mechanical system. This report discusses the validation's performed on the implementation of these methods and evaluates the performances of each method in terms of time complexity and efficiency, the report also analyses the use of sampling methods in the Monte Carlo method. The probability of finding a particle in a 1D ground state using trapezoidal rule is 0.4976 , using the Simpson rule is 0.4976 and with the Monte Carlo is 0.4976. The probability of finding a a particle in the 3D ground state using trapezoidal is 0.12255, using the Simpson rule is 0.12232 and with the Monte Carlo 0.12319. The probability of finding a particle in the 3D first excited state using trapezoidal is 0.11740, using the Simpson is 0.11715 and with the Monte Carlo method is 0.11814. The report also shows that the Monte Carlo is more efficient than the Newton-Cotes methods when evaluating higher dimension integrands, and utilising sampling techniques in the Monte Carlo method results in greatly reduced computational time and sample evaluations.**

I. Introduction

QUANTUM mechanical systems evolve continuously and determinstlticly when unobserved, described by the Schrödinger equation. Measuring the position of a particle at a particular time for a wave function $\psi(x,t)$ requires the probability of finding that particle, calculated by integrating $|\psi(x)|^2$ between two positions x_1 and x_2. The aim of this report is to use numerical methods to determine this probability for 1D and 3D quantum-mechanical systems that cannot be solved analytically. This report utilises two main integration techniques; Newton-cotes formulas of which this report focuses on the extended trapezoidal and Simpson rule, which are based on evaluating the the integrand at equally spaced points[1]. The Monte Carlo method, which utilises repeated random sampling to obtain numerical results making use of the law of large numbers to solve systems of many degrees of freedom and as such are useful to solve n-dimensional equations. The report also looks at various sampling techniques that the Monte Carlo method may use to improve efficiency. This report evaluates the above statement and methods, discussing their effectiveness and their computational performance. The report also discusses the validations and tests performed on the methods, ensuring correct implementation.

II. Theory

A. 1D Quantum-Mechanical System

A 1D quantum system with the wavefunction;

$$\psi_0(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} \exp^{\frac{-m\omega x^2}{2\hbar}}, \tag{1}$$

this is the ground state for a particle in a simple harmonic oscillator potential.$\psi_0(x)$ is the wavefunction, m is the mass of the particle and ω is the natural angular frequency of the oscillator. The probability of finding a particle between x_1 and x_2 is;

$$P = \int_{x_1}^{x_2} |\psi(x)|^2 dx, \tag{2}$$

where P is the probability. Thus the probability of finding a particle described by the wavefunction in equation (1) is;

$$P = \int_0^{2\sqrt{\frac{\hbar}{mw}}} \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{2}} \exp^{\frac{-m\omega x^2}{\hbar}} dx, \tag{3}$$

the limits are $x_1 = 0$ and $x_2 = 2\sqrt{\frac{\hbar}{mw}}$. To utilise sensible units when integrating the system and to improve debugging, I performed equation nondimensionalisation to assist in understanding the dynamics of the system . The scaled dimensionless position variable is $x' = x\sqrt{\frac{\hbar}{mw}}$, which when appplied to equation (3) results in the following;

$$P = \int_0^2 \left(\frac{1}{\sqrt{\pi}}\right) \exp^{-x'^2} dx', \tag{4}$$

B. 3D Quantum-Mechanical Ground State System

The 3D quantum-mechanical ground state wavefunction is;

$$\Psi_0(x,y,z) = \psi_0(x)\psi_0(y)\psi_0(z), \tag{5}$$

where $\Psi_0(x,y,z)$ is the overall ground state and $\psi_0(x), \psi_0(y), \psi_0(z)$ are given by equation (1) for their respective coordinate axis. Utilising equation (2) and the nondimensionalisation process described for equation (4) the probability of finding a particle is;

$$P = \iiint_V \left(\frac{1}{\pi}\right)^{\frac{3}{2}} \exp^{-(x'^2+y'^2+z'^2)} dx'dy'dz', \tag{6}$$

integrating from 0 to 2 in all three dimensions.

C. 3D Quantum-Mechanical First Excited State System

The 3D first excited state wavefunction is given by;

$$\Psi_1(x,y,z) = \frac{1}{\sqrt{2}}[\psi_1(x)\psi_0(y) + i\psi_0(x)\psi_1(y)]\psi_0(z), \tag{7}$$

where $\Psi_1(x,y,z)$ is the 3D wavefunction for the first excited state with one unit of orbital angular momentum. $\psi_0(x)$, $\psi_0(y), \psi_0(z)$, are described above and $\psi_1(x)$ is described as ;

$$\psi_1(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} \sqrt{\frac{2m\omega}{\hbar}} x \exp^{\frac{-m\omega x^2}{2\hbar}}, \tag{8}$$

where $\psi_1(x)$ is equivalent to $\psi_1(y)$, Applying the nondimensionalisation method discussed above, the probability of finding a particle is;

$$P = \iiint_V \left(\frac{1}{\pi}\right)^{\frac{3}{2}} (x^2 + y^2) \exp^{-(x'^2+y'^2+z'^2)} dx'dy'dz', \tag{9}$$

integrating from 0 to 2 in all three dimensions. Equations (4), (6) and (9) are all evaluated using the Monte Carlo and Newton-Cotes methods.

III. Newton-Cotes Method

A. Extended Trapezoidal Rule

The extended trapezoidal rule is a quadrature method that is part of the Newton-Cotes formulas. This method evaluates an integrand by interpolating between two points linearly and estimates the integral between them .The following is the equation for extended trapezoidal rule;

$$\int_{x_0}^{x_{n-1}} f(x)dx = h[\frac{1}{2}f(x_0)+f(x_1)+...+f(x_{n-2})+f(x_{n-1})] \tag{10}$$

where h is the step size for N samples taken between two points. The implementation is described in [3] and was adjusted using vectorisation to improve efficiency. The following equation describes the sampling method used,

$$I_{j+1} = \frac{1}{2}I_j + \frac{1}{2}h_j \sum_{i=1}^{2^{j-1}} f(x_0 + \frac{2i-1}{2}h_j) \tag{11}$$

where I_j is the integral evaluated in the previous iteration, h is the step size and I_{j+1} is the integral being evaluated.

B. Simpson Rule

The Simpson rule builds on the trapezoidal rule by taking a third point, which now approximates the tops of the sub-integrals as quadratic curves instead of straight lines. The Simpson equation is;

$$\int_{x_i}^{x_{i+2}} f(x)dx = h[\frac{1}{3}f(x_i) + \frac{4}{3}f(x_{i+1}) + \frac{1}{3}f(x_{i+2})] \tag{12}$$

which is then extended in a similar manner as equation (10) to obtain the extended Simpson Rule.The Simpson rule is implemented as described by [3] and is determined by using the trapezoidal rule as shown below;

$$S_j = \frac{4}{3}I_{j+1} - \frac{1}{3}I_j \tag{13}$$

where s_j is Simpson integral, $\frac{4}{3}I_{j+1}$ is the current trapezoidal integral, $\frac{1}{3}I_j$ is the previous trapezoidal integral, and makes use of vectorisation. Two integration functions are coded which implement the theory above and utilises the relative accuracy criterion for convergence discussed in [3]. The functions return the integral and the number of function evaluations required.

C. 3D Newton-Cotes

The newton-cotes methods to evaluate three dimensional integrals utilises the same successive sampling techniques discussed above. In three dimensions a triple nested loop is made, which iterates through every combination of x,y and z coordinate value. The combination of all these points are then evaluated and summed, the method then follows the same procedure discussed for the 1D case. One function has been made for each method and has the same functionality as their 1D counterparts

IV. Monte Carlo Method

A. Flat Sampling

The Monte Carlo method utilises the idea of random sampling to evaluate an integrand. The equation is;

$$I = \frac{V}{N}\sum_{i=1}^{N} f(x_i) \tag{14}$$

where I is the estimation of the integral, N is the number of random samples, V is the volume , f is the integrand and x_i is a random sample generated using a uniform distribution.The error in the estimate is;

$$error = \frac{V}{\sqrt{N}}\sigma_{f_i} \tag{15}$$

where σ_{f_i} is the standard deviation of the samples, discussed in [4]. The implementation follows [4] closely, however vectorisation is used, which disregards the need for loops and simplifies the implementation in n-dimensions. To improve the efficiency of the algorithm, I sample 100000 points, evaluate this and add this to a running total of the integrand which takes the average over the new total number of samples. This allows the method to reach an arbitrary higher degree of accuracy given enough time without causing memory issues.

B. Importance Sampling

Monte Carlo utilises importance sampling , which biases the random samples to regions where the integrand has more weight. The implementation is in [4]. To utilise the method discussed in [4] a probability distribution function (PDF) is required for the quantum system and the random samples need to be biased, I utilise the transformation method , discussed in [4].

$$P(k) = ak + b \tag{16}$$

where P(x) is the sampling PDF that is normalised and to ensure P(k) does not go to zero, a = -0.625 and b = 1.3125. k is the deviate which has been distributed according to equation (16) by applying the transformation method to a uniform distribution, the equation below maps a uniform distributed value x to the new deviate;

$$k = -\frac{b}{a} - \sqrt{\frac{2xa + b^2}{a^2}} \tag{17}$$

where x is a uniform distributed value. The method follows the implementation described above introducing the necessary steps described in [4] to account for the new PDF and random

variable. The Monte Carlo keeps improving its accuracy until he convergence criterion $error/integral$ (the relative error) is lower than the relative accuracy supplied. The method returns the integral, number of evaluations required, the relative error and the distribution of the samples.

C. Monte Carlo 3D

The Monte Carlo method important method when evaluating 3D functions due to its scalability when compared to the Newton-Cotes methods. In 3D, N random samples are taken in all three dimensions separately using vectorisation, and set's of (x,y,z) are produced N times, which are then evaluated. The method then follows the same implementation as described above for the 1D case. The sampling is done in each dimension separately and and then combined, The method returns the integral, number of evaluations required, the relative error.

V. Validation

Validation tests and analysis the implementation of the numerical methods and provides a foundation from which the aims of the report can addressed.

A. Sampling Validation

The following figure illustrate the correct implementation of the uniform(flat) sampling method used in the Monte Carlo method,

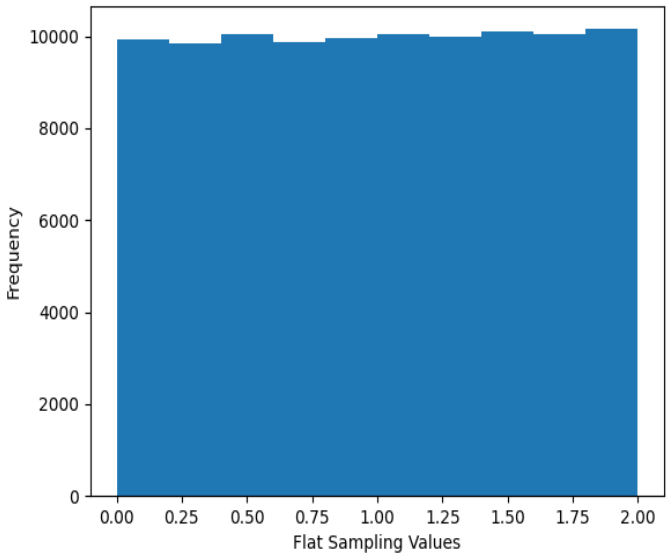

Fig. 1. The figure illustrates the flat sampling method to generate random variables for the Monte Carlo method, the x axis is the value of the random variable sampled using a uniform distribution, y axis represents the frequency of the value.

Figure (1) shows that the implementation is correct as a uniform distribution is used to generate values between 0 and 2 which is then evaluated by the integrands. Figure (2) shows the importance sampling distribution of the random variables generated using equation (17). The figure shows that the implementation is correct as it follows the equation (16) when generating values between 0 and 2 for the quantum system.

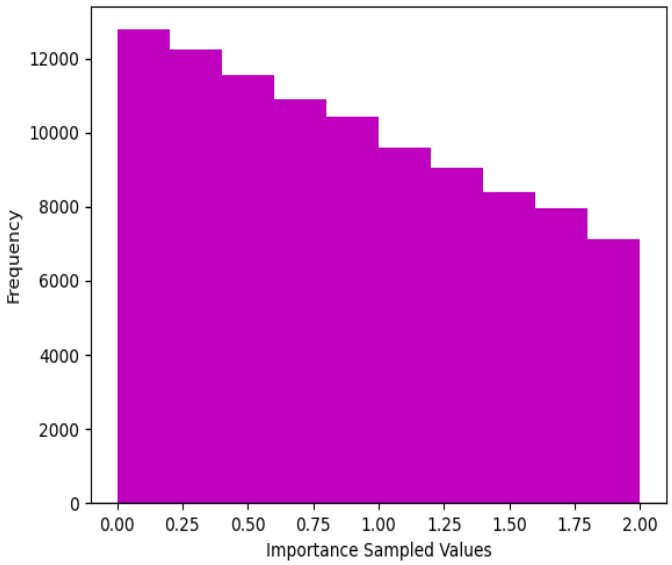

Fig. 2. The figure illustrates the importance sampling method used to generate biased random variables for the Monte Carlo method, the x axis is the value of the biased sampled generated using distribution in equation (17), y axis represents the frequency of the value.

B. Validation Test 1

Test 1 is;

$$y = 12x^3 - 9x^2 + 2, \tag{18}$$

the 1D equation has an analytical solution and when integrated between $x_1 = 1$ $x_1 = 6$ has a value of 3250. Utilising the 1D Monte Carlo method, the evaluation is 3249.5753 with a relative error of 0.001, requiring 17020000 samples. Utilising the 1D trapezoidal method , the evaluation is 3250.5951 for a relative accuracy of 0.001, requiring 65 function evaluations. The Simpson method obtains 3250.0 for the same relative accuracy, requiring 5 function evaluations.

C. Validation Test 2

Test 2 is:

$$y = \cos(x), \tag{19}$$

the 1D equation has an analytical solution, and when integrated between $x_0 = 0$ $x_1 = \frac{\pi}{2}$ has a solution of 1. The PDF for the quantum system and equation (19) can be used here as they have similar distributions. Using the Monte Carlo With flat sampling, the evaluation is 1.0000107 ,requiring 56020000 samples. With importance sampling, the value is 1.0001211, requiring 17720000 samples both with a relative error of 0.0001. Using the trapezoidal method, the value obtained was 0.999999987 , requiring 4097 function evaluations. Using the Simpson rule, the value is 1.000000002, requiring 65 evaluations, both methods are for a relative accuracy of 0.0000001.

D. Validation Test 3

Test 3 is;

$$f(x, y, z) = x^2 + y^2 + z^2, \tag{20}$$

the 3D equation has an analytical solution and when integrated between 0 and 1 for all coordinates has a solution of 1. Using the 3D Monte Carlo method with no sampling, gives a solution of 0.9999552 with a relative error of 0.0001, requiring 26720000 samples. Using the 3D trapezoidal rule, the solution is 1.00195, requiring 4913 evaluations. Using the Simpson rule, the result is 1.0, requiring 125 evaluations, both methods are for a relative accuracy of 0.01

E. Validation Test 4

Test 4 is;

$$f(x, y, z) = 6xyz, \tag{21}$$

the 3D equation has an analytical solution, and when integrated between x_1, y_1, z_1 = [0,-1,3] and x_2, y_2, z_2 = [1,2,1] has a solution of -18. The 3D Monte Carlo method results in -17.991 with a relative error of 0.01, requiring 1420000 samples . The 3D trapezoidal method results in -16.5 for a relative accuracy of 0.1, requiring 35937 function evaluations, due to the time complexity running at higher accuracy's would take significantly more time. The Simpson method returns -17.875 for an accuracy of 0.01, requiring 16974593 evaluations, higher accuracy's follow the same problem seen in the trapezoidal method.

VI. Result

A. 1D Quantum System

Utilising the 1D trapezoidal integration function on equation (4) , the probability of finding a particle between $x_1 = 0$ and $x_2 = 2$ is 0.49766107995074826 for a relative accuracy of 0.000001, requiring 513 evaluations. Using the 1D Simpson rule, the resulting probability is 0.49766113031942394 for the same relative accuracy, requiring 65 evaluations. The Simpson rule reaches the convergence criterion with fewer evaluations because the method cancels out the h^3 and h^4 error terms from the trapezoidal method, reducing the error in the method. The following is a plot of the 1D quantum system, with the importance sampling PDF used as part of the Monte Carlo method;

Figure 3 shows the 1D quantum ground state squared and the PDF used in importance sampling. The figure demonstrates that the PDF is a reasonably good approximation to the function, which should bias the random points in favour of the ground state and reduce the number of samples required to converge. For a relative error of 0.0001 the Monte Carlo method produces 0.4976723437860402 for flat sampling, requiring 161120000 samples, with importance sampling the value obtained was 0.4976354841884228, requiring 34220000 samples. As discussed the sampling method reduces the number of samples required to converge. The following shows a plot of the square root of the number of samples as a function of the relative error;

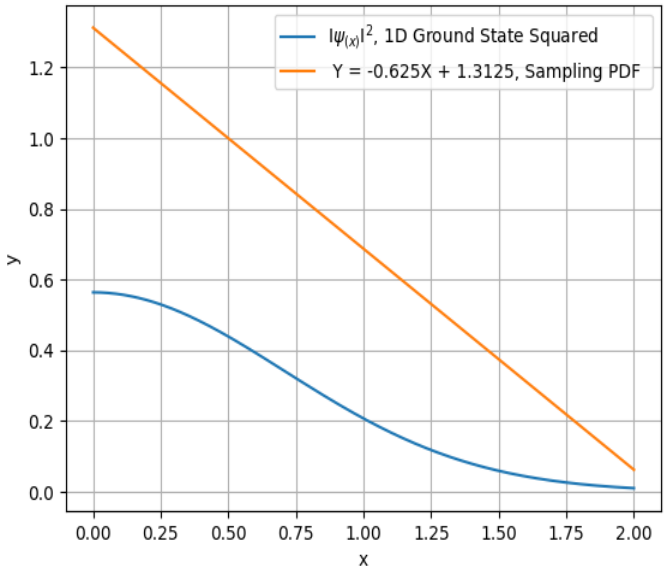

Fig. 3. The figure shows the plot the 1D quantum probability distribution, the plot also shows the PDF used in importance sampling of the quantum system. The x axis shows the position between the limits, and the the y axis is the corresponding value when evaluated using the respective functions.

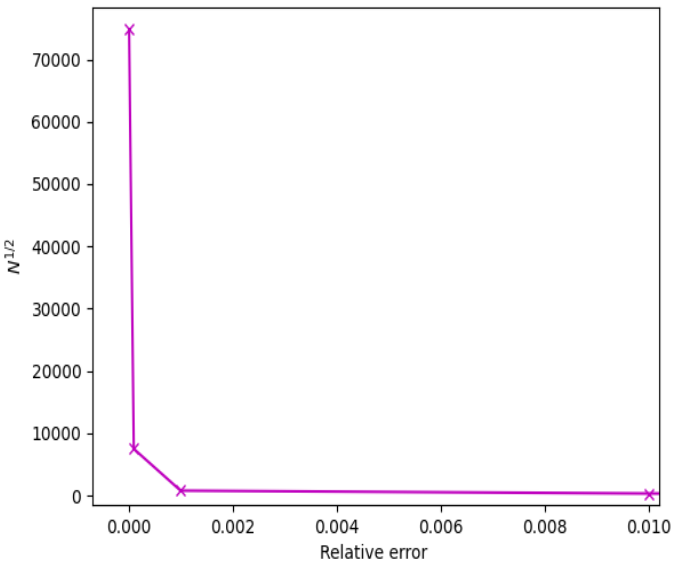

Fig. 4. The figure shows how the square root of samples required to find the probability for the 1D quantum ground state changes depending on the relative error, which determines the convergence criterion for the method.

the figure shows that the relative error is proportional to $\frac{1}{\sqrt{N}}$, and as the relative error decreases the number of samples required to evaluate the integral increases. The implementation of this specific convergence criterion meant that after evaluating for an error of 1×10^{-5}, the time taken to evaluate 1×10^{-6} increased exponentially due to the relation just discussed. The algorithm would find achieving an error of 1×10^{-6} difficult due to the time complexity. The estimated number of samples required is 6×10^{11} , calculated using the above relation.

B. 3D Ground State Quantum System

Integrating equation (6) using the trapezoidal method results in a probability of 0.12255149119840822,requiring 274625 function evaluations and using the Simpson rule produces 0.12232061368701695, requiring 35937 evaluations both utilising a relative accuracy of 0.01. Due to three dimensions the time complexity in both algorithms increase exponentially, hence smaller accuracy's are limited . The following shows the plot of the 3D ground state squared;

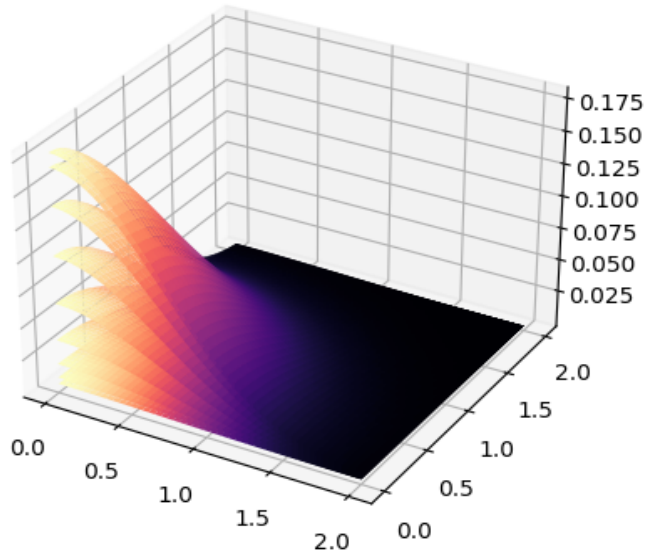

Fig. 5. The figure is a 3D plot of the 3D ground state squared, where each layer is a constant z value between the limits 0 and 2, while the x and y values are variables. BY plotting multiple different z values 3D plot of the function needed to integrate over is made.

The figure shows that importance sampling can be used in each dimension individually as they follow the same distribution ass the PDF. Using the Monte Carlo method with no sampling, the evaluation is 0.12319913230436916, requiring 52220000 samples for a relative accuracy of 0.001. Using importance sampling, the evaluation is 0.12364893821943718, requiring 820000 samples for the same relative accuracy. Comparing the three dimension methods, it is evident that the Monte Carlo method is more computational efficient and the time complexity is reduced when evaluating functions of higher dimensions.The probability of finding a particle in the 3D ground state is just the cube of the probability of the ground state in 1D, this is due to the 1D function being repeated in x,y and z axis and also because the volume is cubed.

C. 3D First State Quantum System

Using equation (9) with the 3D trapezoidal method, results in a probability of 0.11740235696921497, requiring 16974593 function evaluations for a relative accuracy of 0.01 The Simpson rule results in 0.11715851883708302, requiring 2146689 function evaluations for the same relative accuracy. The Monte Carlo with flat sampling results in 0.11814468606787538, requiring 50320000 samples for a relative error of 0.001. Using sampling in the Monte Carlo method, the integral is 0.1181563929455191 and the number of samples required is 820000 for the same relative error.

VII. Conclusion

The aim of this project was to use the Newton-Cotes and the Monte Carlo numerical methods to integrate and determine the probability of finding a particle inside a 1D and 3D quantum-mechanical system that does not have an analytical solution. The project also aimed to determine the advantages and disadvantages of using these methods in regards's to computational efficiency and time complexity. The probability of findings a particle in the 1D ground state between $x_1 = 0$ and $x_2 = 2$ was 0.497 (3 d.p) , the probability of finding the particle in the 3D ground state between $x_1, y_1, z_1 = 0$ and $x_2, y_2, z_2 = 2$ is 0.123 (3 d.p) and the probability of finding a particle in the 3D first excited state between $x_1, y_1, z_1 = 0$ and $x_2, y_2, z_2 = 2$ is 0.118 (3.d.p). These values were reproduced between the two primary methods and the implementation of these methods were also validated. The report also showed that the Monte Carlo method was more efficient in terms of time complexity and implementation when the integrand is greater than one dimension and the use of sampling techniques greatly reduces the number of samples required to achieve a given relative error. To further investigate the properties of the Monte Carlo method the metropolis algorithm could be implemented so that adaptive importance sampling could be used, which would improve sampling efficiency.

References

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