Variational Monte Carlo Technique

Ground State Energies of Quantum Mechanical Systems

Sukanta Deb

In this article, I discuss the use of the Variational Monte Carlo technique in the determination of ground state energies of quantum harmonic oscillators in one and three dimensions. In order to provide a better understanding of this technique, a pre-requisite concept of Monte Carlo integration is also discussed along with numerical examples. The technique can be easily extended to study the ground state energies of hydrogen atom, particle in a box, helium atom and other complex microscopic systems involving N particles in d-dimensions.

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1. Introduction

There exist many problems in science and engineering whose exact solution either does not exist or is difficult to find. For the solutions of those problems, one has to resort to approximate methods. In the context of quantum mechanics, the exact solutions of the Schrödinger's equation exist only for a few idealized systems. There are varieties of systems for which the Schrödinger's equation either cannot be solved exactly or it involves very lengthy and cumbersome calculations [1]. For example, solving the Schrödinger equation to study the properties of a system with hundreds or thousands of particles often turns out to be impractical [2].

One of the most important tasks in quantum mechanics is the determination of the ground state energies of the microscopic systems. In this article, I show how the Variational Monte Carlo (hereafter, VMC) method can be used to determine the ground state energy of a

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quantum mechanical system. This method can be extended to study much more complex many-body quantum mechanical systems involving higher dimensions. The VMC technique [3] provides a simple, robust and efficient way to solve the ground state energy of a quantum many-particle system. Since the method is relatively insensitive to the size of the system, it can be applied to large systems where some other methods are computationally not feasible [2].

The VMC method uses the Metropolis *et al.* [4] algorithm combined with the Monte Carlo integration using importance sampling [5] and the variational principle in quantum mechanics [1] in order to determine the ground state energy of the system. Determination of the ground state energies of a many-particle system in d-dimensions involves $(d \times N)$-dimensional integral. Evaluation of these higher dimensional integrals using analytical methods becomes very difficult and practically impossible. This is where the VMC technique comes to the rescue and proves to be very powerful and efficient.

In the study of the quantum mechanical system of liquid He^4, the MC method was first utilized by McMillan [6]. The system was studied using a variational wave function and the MC method using the Metropolis algorithm. Liquid He^4 is a system of bosons with a symmetric wave function. It was not until 1977 that the VMC method was used by Ceperley *et al.* [7] to study a fermionic system whose wave functions are antisymmetric. Since then, VMC methods have been applied to a wide variety of problems. They have been used to study the ground state properties of many different systems – atoms, molecules and solids [3, 8, 9].

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Before I discuss the technique and its far-reaching implications, I would like to introduce to the readers in short about the MC methods – its history, origin and some of the important terms associated with the VMC technique

with detailed illustrations. In Section 2, the history and the origin of the MC techniques are discussed. Section 3 deals with the evaluation of integrations using crude and importance-sampling MC methods. In Section 4, the generation of samples according to a given probability distribution are discussed using the Metropolis algorithm. Section 5 deals with the description of the VMC technique. In Section 6, applications of the VMC in the determination of ground state energies of quantum harmonic oscillators in one and three dimensions are discussed. Finally, in Section 7, summary and discussions are presented.

2. History and Origin of Monte Carlo Methods

The term 'Monte Carlo' has been named after the famous Mediterranean casino town in Monaco. The Monte Carlo (MC) method refers to a class of statistical methods which use random numbers (probabilistic method) similar to those in a casino game of chance, to solve a real and physical (nonprobabilistic) problem [5]. Since the method uses random numbers, it is therefore stochastic in nature and has associated statistical properties. With the advent of modern computers, the random sampling required in most analyses can easily be obtained in a more robust, faster and efficient way. Some of the methods of generating random numbers from a given probability distribution are discussed in Appendix A. MC methods are widely used in many areas of science and engineering and are particularly useful for solving complicated higher-dimensional integrals and in the study of N-body systems. In quantum mechanics, the MC methods are used to simulate many-particle systems using random numbers.

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The earliest documented use of random sampling to find the solution of an integral is that of the French naturalist Comte de Buffon (1777). He showed that the probability that a needle of length l thrown randomly onto a grid of

parallel lines with distance $d \geq l$ apart intersects a line is $\frac{2l}{\pi d}$. This is known as the Buffon's needle problem [5].

In the 1930s, Enrico Fermi made use of the MC techniques in studying the behaviour of the newly discovered neutron [5]. Sampling experiments were carried out in order to see how neutral particles are expected to interact with the condensed matter. This led to substantial insight and helped in the understanding of the analytical theory of neutron diffusion and transport. Major advances of the MC techniques were made during World War II by scientists such as John Von Neumann, Enrico Fermi, S M Ulam and Nicholas Metropolis working on the development of nuclear weapons in Los Alamos National Laboratory, USA [10, 11].

3. Monte Carlo Integration Using Importance Sampling

Suppose we want to evaluate the integral

$$I = \int_a^b f(x)\mathrm{d}x,$$

where $f(x)$ is a smooth function defined on the interval $[a, b]$. In the 'crude'-MC method, the integral is approximated as [5]

$$I_{(\mathrm{crude})} = \int_a^b f(x)\mathrm{d}x \approx \frac{(b-a)}{N}\sum_{i=1}^{N} f(x_i),$$

where x_i's are uniformly distributed random numbers between a and b. The variance in f is given by

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

The error in the integration is given by

$$\sigma_{\mathrm{I(crude)}} = \sqrt{\frac{\sigma^2_{(\mathrm{crude})}}{N}} = \frac{\sigma_{(\mathrm{crude})}}{\sqrt{N}}.$$

Hence, in the 'crude'-MC method, the error estimate is proportional to the variance and inversely proportional to the square root of the number of trials. Hence, there are only two ways of reducing the error. Firstly, either by increasing the number of trials, or, secondly, by reducing the variance. The later choice is much more suitable as it requires lesser computational time [12].

In the case of 'crude'-MC integration, it samples the function homogeneously, i.e., it samples with the uniform distribution. Therefore, if the significant contributions to the integral come from a small region within the integration volume, there will be only a few samples there which can lead to large statistical errors, even though the number of trials are increased. The result of the MC integration can be greatly improved using the idea of importance sampling. In this, sampling points are chosen from a distribution which concentrates the points where the function to be integrated happens to be larger [12].

Let $g(x)$ be a PDF defined on $[a, b]$ that has nearly the same shape as that of $f(x)$ in the sense that

$$\frac{f(x)}{g(x)} \approx \text{constant}$$

with the property

$$\int_a^b g(x)\mathrm{d}x = 1 \quad \text{and} \quad g(x) > 0, \quad \forall x \in [a, b]\,.$$

Therefore, we write

$$I = \int_a^b f(x)\mathrm{d}x = \int_a^b \left[\frac{f(x)}{g(x)}\right] g(x)\mathrm{d}x\,.$$

The integral can now be calculated with the random numbers generated from the distribution $g(x)$ (also called weight function) and evaluating $\frac{f(x_i)}{g(x_i)}$ at these points.

That is

$$\left\langle \frac{f(x)}{g(x)} \right\rangle = \frac{1}{N} \sum_{i=1}^{N} \frac{f(x_i)}{g(x_i)},$$

where N is the number of MC steps and $x_i's$ are the random numbers distributed as $g(x)$. Another way to deal with this integral is to define

$$\mathrm{d}G(x) = g(x)\mathrm{d}x,$$

where

$$G(x) = \int_a^x g(x)\mathrm{d}x$$

is the integral of $g(x)$. Now we make a change of variables using

$$r = G(x),$$

where r is a sequence of random numbers uniformly distributed in $[0, 1]$, i.e., $0 \leq r \leq 1$. Therefore,

$$I = \int_a^b \left[\frac{f(x)}{g(x)}\right] \mathrm{d}G(x) = \int_0^1 \frac{f(G^{-1}(r))}{g(G^{-1}(r))}\mathrm{d}r \approx \frac{1}{N} \sum_{i=1}^{N} \frac{f(G^{-1}(r_i))}{g(G^{-1}(r_i))},$$

where r_i are the random numbers uniformly distributed in $[0, 1]$. It should be noted that the form of $g(x)$ should be so chosen that it minimizes the variance of the integrand $\frac{f(x)}{g(x)}$. A proper choice of $g(x)$ would make the integrand $\frac{f(x)}{g(x)}$ nearly flat and hence the variance will be reduced to a great extent. The variance is calculated from

$$\sigma^2_{(\mathrm{imp})} = \frac{1}{N} \sum_{i=1}^{N} \tilde{f}(x_i)^2 - \left(\frac{1}{N} \sum_{i=1}^{N} \tilde{f}(x_i) \right)^2,$$

where $\tilde{f}(x_i) = \frac{f(x_i)}{g(x_i)}$ and the error of integration is given by

$$\sigma_{\mathrm{I(imp)}} = \sqrt{\frac{\sigma^2_{(\mathrm{imp})}}{N}}.$$

Illustrations of evaluating MC integrations using the 'crude'-MC and 'importance sampling'-MC are given with the following examples.

Let us evaluate the integral

$$I = \int_0^{\pi} \frac{1.0}{x^2 + \cos^2(x)} \mathrm{d}x \,.$$

Using the 'crude'-MC technique

$$I_{(\mathrm{crude})} = \int_a^b f(x)\mathrm{d}x \approx \frac{(b-a)}{N} \sum_{i=1}^{N} f(r_i),$$

where $a = 0$, $b = \pi$, $r_i \in [0, 1]$, $\forall i = 1, \ldots, N$ and

$$f(x) = \frac{1.0}{x^2 + \cos^2(x)}.$$

The value of the integral is found to be $I_{(\mathrm{crude})} = 1.5952 \pm 0.0126$ with a variance of ${\sigma^2}_{(\mathrm{crude})} = 1.3511$. Here, N is taken to be $10,000$.

Let us now evaluate the above integral using the 'importance sampling'-MC. Let us choose the importance function to be of the form

$$g(x) = A \exp(-\lambda x),$$

where $g(x) \geq 0$, A is the normalization constant and λ is the parameter to be determined for the variance to be minimized. Normalization condition

$$\int_0^{\pi} g(x)\mathrm{d}x = 1$$

yields

$$A = \frac{\lambda}{1 - \exp(-\pi\lambda)}.$$

Now, using the condition

$$G(x) = r, \quad 0 \leq r \leq 1,$$

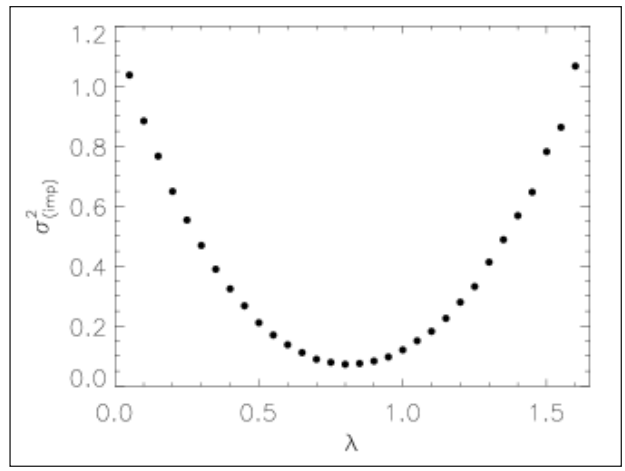

Figure 1. Plot of $\sigma^2_{(imp)}$ versus λ-values. Minimum value of $\sigma^2_{(imp)}$ occurs at $\lambda = 0.80$. This value of λ is chosen in the importance function $g(x) = A\exp(-\lambda x)$ for evaluating the integral.

we get

$$G^{-1}(r) = -\frac{1}{\lambda}\ln\left[\frac{1-\exp(-\pi\lambda)}{\lambda}\right].$$

With $N = 10,000$, the value of

$$\frac{1}{N}\sum_{i=1}^{N}\frac{f(G^{-1}(r_i))}{g(G^{-1}(r_i))}$$

is calculated for different values of $\lambda \in [0.05, 1.60]$ in steps of 0.05 and the variance $\sigma^2_{(\mathrm{imp})}$ is obtained. *Figure* 1 shows the plot of $\sigma^2_{(\mathrm{imp})}$ versus λ-values. From the figure, it can be seen that $\sigma^2_{(\mathrm{imp})}$ has the minimum value of 0.0729 at $\lambda = 0.80$. The value of the integral corresponding to this value of λ and $\sigma^2_{(\mathrm{imp})}$ is found to be

$$I_{(\mathrm{imp})} = 1.5810 \pm 0.0027.$$

Therefore, variance is reduced by a factor of ~ 20 using the 'importance sampling'-MC technique as compared to the variance using the 'crude'-MC technique.

Let us now consider the evaluation of the integral

$$\int_0^\infty \frac{1}{1+(x-1)^2}\exp(-x)\mathrm{d}x$$

using the MC method. Again, let us choose the importance function to be of the form

$$g(x) = A\exp(-\lambda x),$$

where $g(x) \geq 0$, A is the normalization constant and λ is the parameter to be determined for the variance to be minimized. Normalization condition

$$\int_0^\infty g(x)\mathrm{d}x = 1$$

yields

$$g(x) = \lambda\exp(-\lambda x).$$

Now using the condition

$$G(x) = r, \quad 0 \leq r \leq 1,$$

we get

$$G^{-1}(r) = -\frac{1}{\lambda}\ln r.$$

With $N = 10,000$, the value of

$$\frac{1}{N}\sum_{i=1}^{N}\frac{f(G^{-1}(r_i))}{g(G^{-1}(r_i))}$$

is calculated for different values of $\lambda \in [0.05, 2.50]$ in steps of 0.05 and the variance $\sigma^2_{(\mathrm{imp})}$ is obtained. *Figure* 2 shows the plot of $\sigma^2_{(\mathrm{imp})}$ versus λ-values. From the figure, it can be seen that $\sigma^2_{(\mathrm{imp})}$ has the minimum value of 0.0471 at $\lambda = 1.15$. The value of the integral corresponding to this value of λ and $\sigma^2_{(\mathrm{imp})}$ is found to be

$$I_{(\mathrm{imp})} = 0.6967 \pm 0.0022.$$

The evaluation of the integral using the 'crude'-MC becomes cumbersome using uniform sampling when the range of integration $(b-a)$ is ∞. So a cut-off such as $(b-a) = L >> 1$ should be used. One has to choose L

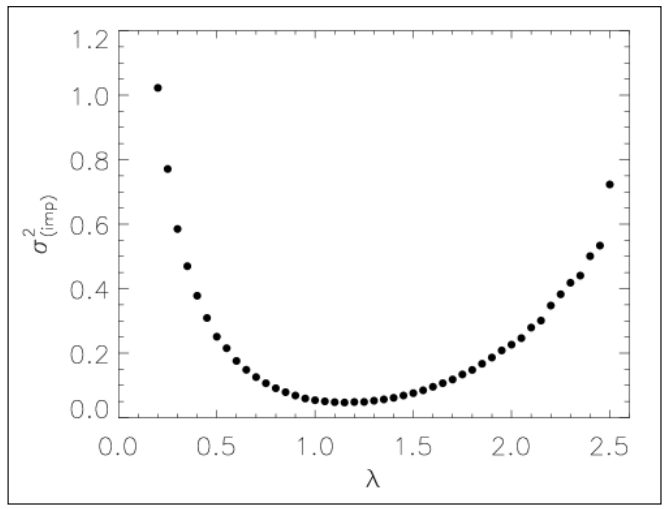

Figure 2. Plot of $\sigma^2_{(imp)}$ versus λ-values. Minimum value of $\sigma^2_{(imp)}$ occurs at $\lambda = 1.15$. This value of λ is chosen in the importance function $g(x) = A\exp(-\lambda x)$ for evaluating the integral $\int_0^\infty \frac{1}{1+(x-1)^2}\exp(-x)\mathrm{d}x$.

carefully so that it is neither very large nor very small. However, the determination of optimal value of cut-off L is a formidable task. There exists no such clear-cut rule to calculate the value of this cut-off. In the case of the integral considered here, if we set $L = 10$, then $I_{(\mathrm{crude})} = 0.7017 \pm 0.0047$ with a variance of $\sigma^2_{(\mathrm{crude})} = 0.2251$ for $N = 10,000$. On the other hand, if $L = 100$ and $N = 10,000$, then $I_{(\mathrm{crude})} = 0.7191 \pm 0.0049$ with a variance of $\sigma^2{}_{(\mathrm{crude})} = 0.2355$. In both the cases, we can see that the variance is larger than that determined using the 'importance sampling'-MC technique. Also, there is no definite rule for determining the cut-off in the 'crude'-MC when the range of integration becomes ∞. This limits the accuracy of the value of the integral determined using this method. In contrast, the importance sampling-MC does not require such cut-off values.

4. Metropolis Algorithm

Methods such as importance sampling can be efficient in generating random numbers from weight functions which are simple and are restricted to one dimension. However, the generation of random numbers from a complicated weight function in many dimensions turns out to be difficult or sometimes impossible using the importance sampling, as the form of the weight function is

difficult to discern from the problems involved [13]. Apart from that, the weight function $g(x)$ should be integrable and the integral of it (i.e., $G(x)$) should be invertible which is sometimes difficult to obtain analytically, and numerically it often turns out to be clumsy or inaccurate [14].

The algorithm of Metropolis *et al.* [4] is one of the most simple, efficient and robust ways for generating random numbers according to a specified probability distribution of any arbitrary form. The advantage of this algorithm lies in the fact that through the use of random numbers, it provides an elegant and efficient way toward answers to problems that are complicated to solve analytically. The algorithm has been listed as one of the top 10 algorithms of the 20th century [15,16].

Suppose we want to generate a set of points $x_i, i = 1, \ldots, n$, distributed according to a PDF $f(x)$ in one dimension. The Metropolis algorithm generates a sequence of points $x_i, i = 1, \ldots, n$, as those visited successively by a random walker moving through the configuration space. The longer the walk, the closer it approximates the desired distribution. This random number sequence is generated as follows [13]:

- Choose a starting point x_0.
- Choose a fixed maximum step-size h.
- Generate the next point x_1.
- Suppose that the walker is at a point x_i.
- Choose a new configuration x_{trial} randomly and uniformly in the interval $[x_i - h/2, x_i + h/2]$.
- Calculate the ratio

$$r = \frac{f(x_{\text{trial}})}{f(x_i)}.$$

The Metropolis algorithm generates a sequence of points x_i, $i = 1, \ldots, n$, as those visited successively by a random walker moving through the configuration space.

There are two important issues in applying the Metropolis algorithm. Firstly, where to start the random walk, i.e., what to choose for the initial point x_0. Secondly, how to choose the step-size h.

- If $r \geq 1$, the trial step is accepted, i.e., $x_{i+1} = x_{\text{trial}}$.
- If $r < 1$, the trial step is accepted with probability r. Choose a random number $\eta \in [0, 1]$ and the next configuration is generated according to

$$x_{i+1} = x_{\text{trial}}, \quad \text{if } \eta < r,$$
$$= x_i, \quad \text{if } \eta \geq r.$$

There are two important issues in applying the Metropolis algorithm. Firstly, where to start the random walk, i.e., what to choose for the initial point x_0. Secondly, how to choose the step-size h. Pertaining to the first issue of the choice of x_0, an approximate starting point is a probable one where the distribution function $f(x)$ is large. However, in the case of a multi-dimensional problem if the maximum is not known, then the random walker must be allowed to 'thermalize' before the actual sampling begins. That is, to remove any dependence on the starting point, the algorithm is run for some large number of steps which are then discarded [12,13].

On the other hand, if the trial steps are to be taken within the neighbourhood of x_i, the step-size h should be chosen carefully. Let us suppose that x_i is at a maximum of f, the most likely place for it to be. If h is large, then $f(x_{\text{trial}}) << f(x_i)$ and most trial steps will be rejected. On the other hand, if h is chosen to be very small, most trial steps will be accepted. But the random walker will never move very far, and so also lead to a poor sampling of the distribution. A good rule of thumb is that the size of the trial step h be chosen so that [13]

$$\text{Acceptance ratio} = \frac{\text{No. of steps accepted}}{\text{Total number of trial steps}} \sim 0.5\,.$$

Now, let us apply the Metropolis algorithm in sampling from the distribution $f(x) = \exp[-0.5x^2]$. *Figure* 3

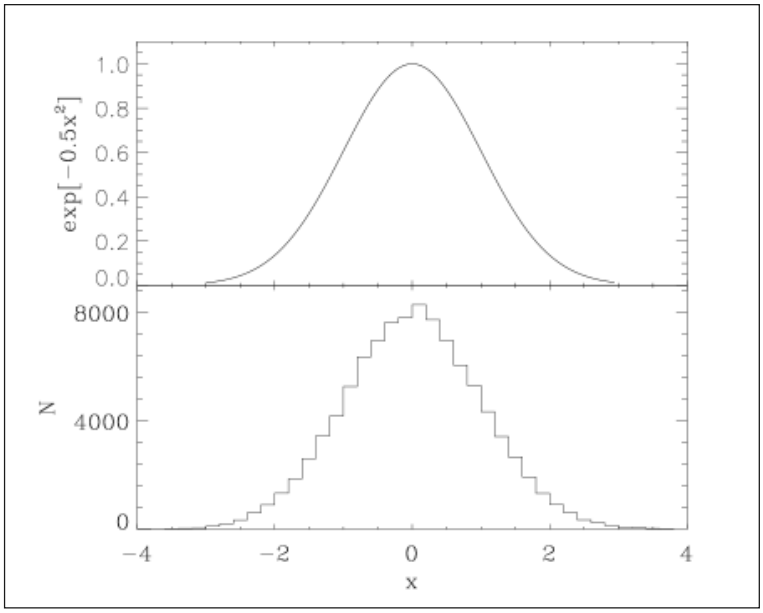

Figure 3. The upper panel shows the plot of the function $f(x) = \exp(-0.5x^2)$ as a function of x. The lower panel shows the histogram plot for the generation of the random variable x having PDF $f(x)$ using the Metropolis algorithm.

shows the histogram plot for the generation of the random variable having the PDF$f(x)$ using the Metropolis algorithm with the number of MC steps equal to $10,0000$ and step-size set equal to 3 such that the acceptance ratio is equal to $0.4930(\sim 0.5)$.

We apply the Metropolis algorithm in the evaluation of the 1-d integral

$$\int_0^1 x\sqrt{1-x^2}\mathrm{d}x.$$

Let us choose the importance function to be of the form $g(x) = A\left[\exp(x^2) - 1.0\right]$. Normalization condition

$$\int_0^1 g(x)\mathrm{d}x = 1$$

gives $A = 2.1615$. Hence the normalized importance function is

$$g(x) = 2.1615\left[\exp(x^2) - 1\right].$$

Therefore

$$\int_0^1 f(x)\mathrm{d}x = \int_0^1 \left[\frac{f(x)}{g(x)}\right] g(x)\mathrm{d}x = \frac{1}{N}\sum_{i=1}^{N}\frac{f(x_i)}{g(x_i)},$$

where x_i's are sampled from the distribution $g(x)$ using the Metropolis algorithm. For $N = 10,000$ and $h = 0.42$, the value of the integral is found to be $I_{(\mathrm{mp})} = 0.3334 \pm 0.0002$, with $\sigma^2_{(\mathrm{mp})} = 0.0030$. This value is comparable to the actual value of 0.3333.

5. Variational Monte Carlo (VMC) Technique

In the VMC method, the variational principle of quantum mechanics is used to approximate the ground state energy of a microscopic system. The method employs a set of adjustable parameters to yield a trial wave function Ψ_{T}, whose form is chosen following a prior analysis of the physical system being investigated. The trial wave function Ψ_{T} when best optimized, approximates the exact wave function. If the trial wave function Ψ_{T} is identical with the exact ground state wave function, then the VMC method gives the exact estimate of the ground state energy.

The behaviour of a quantum mechanical many-particle system is described by the Schrödinger's equation [1, 5]:

$$\hat{H}\Psi(\mathbf{R}) = E\Psi(\mathbf{R})\,. \tag{1}$$

$\hat{H}$ is the Hamiltonian of the system given by

$$\hat{H} = \sum_{i=1}^{N}\left[-\frac{\hbar^2}{2m}\nabla_i^2 + U_{\mathrm{ext}}(r_i)\right] + \sum_{i<j} V_{ij},$$

where $-\frac{\hbar^2}{2m}\nabla_i^2$ is the kinetic energy, $U_{\mathrm{ext}}(r_i)$ is the external potential of the ith particle, V_{ij} is the interaction potential between the ith and jth particles, and ∇_i^2 is the Laplacian of the ith particle.

The variational theorem of quantum mechanics states that the expectation value of the Hamiltonian $\hat{H}$ evaluated with any trial wave function Ψ_{T} is an upper bound on the ground state energy $E_{\min}$ [1]:

$$\left\langle \hat{H} \right\rangle = E_{\mathrm{T}} = \frac{\int \Psi_{\mathrm{T}}(\mathbf{R})^{\star} \hat{H} \Psi_{\mathrm{T}}(\mathbf{R}) \mathbf{dR}}{\int \Psi_{\mathrm{T}}(\mathbf{R})^{\star} \Psi_{\mathrm{T}}(\mathbf{R}) \mathbf{dR}} \geq E_{\min}\,.$$

In order to evaluate this integral with MC methods via the Metropolis algorithm using importance sampling, it is written in terms of a probability density function $\rho(\mathbf{R})$, and a local energy E_{L} [3]:

$$E_{\mathrm{T}} = \int \rho(\mathbf{R}) E_{\mathrm{L}}(\mathbf{R}) \mathrm{d}\mathbf{R}, \qquad (2)$$

where

$$\rho(\mathbf{R}) = \frac{\Psi_{\mathrm{T}}^2}{\int \Psi_{\mathrm{T}}^2 \mathrm{d}\mathbf{R}}$$

and

$$E_{\mathrm{L}} = \frac{\hat{H}\Psi_{\mathrm{T}}}{\Psi_{\mathrm{T}}}\,.$$

The local energy is a function which depends on the positions of the particles and is a constant if Ψ_{T} is an exact eigenfunction of the Hamiltonian. The more closely Ψ_{T} approaches the exact eigenfunction, the less strongly E_{L} will vary with R. This means that the variance should approach zero as our trial wave function approaches the exact ground state.

In the evaluation of the ground state energy, the variational wave function is generally chosen to be real and non-zero almost everywhere in the region of integration. We want to solve the integral in (2) with importance sampling MC integration using Metropolis algorithm. The energy approximation as given in (2) becomes

$$E_{\mathrm{T}} = \int \rho(\mathbf{R}) E_{\mathrm{L}}(\mathbf{R}) \mathrm{d}\mathbf{R} \approx \frac{1}{M} \sum_{i=1}^{M} E_{\mathrm{L}}(R_i), \qquad (3)$$

where R_i are sampled from the probability density $\rho(\mathbf{R})$.

6. Application of VMC to Quantum Harmonic Oscillators

In this section, the applications of the VMC technique in the determination of ground state energies of quantum harmonic oscillators in one and three dimensions are discussed.

6.1 *Harmonic Oscillator in One Dimension*

We know that the Hamiltonian ($\hat{H}$) of a one-dimensional harmonic oscillator is given by

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}kx^2\,,$$

where m is the mass of the particle and $k = m\omega^2$ is a spring constant, with ω denoting the angular frequency of oscillation. The first term represents the kinetic energy operator for a particle of mass m and the second term represents the potential energy operator for a particle in a potential well.

If the energy is measured in units of $\hbar\omega$ and distance in units of $\sqrt{\frac{\hbar}{m\omega}}$, then the solution of the Schrödinger equation

$$\hat{H}\Psi = E\Psi$$

yields the well-known ground state energy $E_0 = \frac{1}{2} = 0.5$ (in units of $\hbar\omega$) in case of one dimension.

In terms of the units considered, the hamiltonian becomes

$$\hat{H} = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}x^2\,.$$

Let us consider the trial wave function to be of the form $\Psi_{\mathrm{T}} = \exp(-\beta x^2)$, where β is the parameter to be

determined from the VMC. The above form of the wave function is chosen following the physical requirement

$$\Psi_{\mathrm{T}} \to 0 \qquad \text{as} \qquad x \to \pm\infty\,.$$

Therefore, the local energy

$$E_{\mathrm{L}} = \frac{\hat{H}\psi(x)}{\psi(x)}$$

becomes

$$E_{\mathrm{L}} = \beta + (0.5 - 2.0\beta^2)x^2$$

so that the ground state energy can be evaluated from the integral

$$E_{\mathrm{T}} = \int E_{\mathrm{L}}\rho(x)\mathrm{d}x\,.$$

To get the minimum value of this integral, β is varied in the range $0.1 - 2.0$ in steps of 0.05. The value of E_{T} and the variance calculated are plotted as a function of β in *Figure* 4. The plot of the harmonic oscillator wave function is shown in *Figure* 5. The solid line shows the actual wave function while the data points marked by plus-sign are that obtained from the VMC.

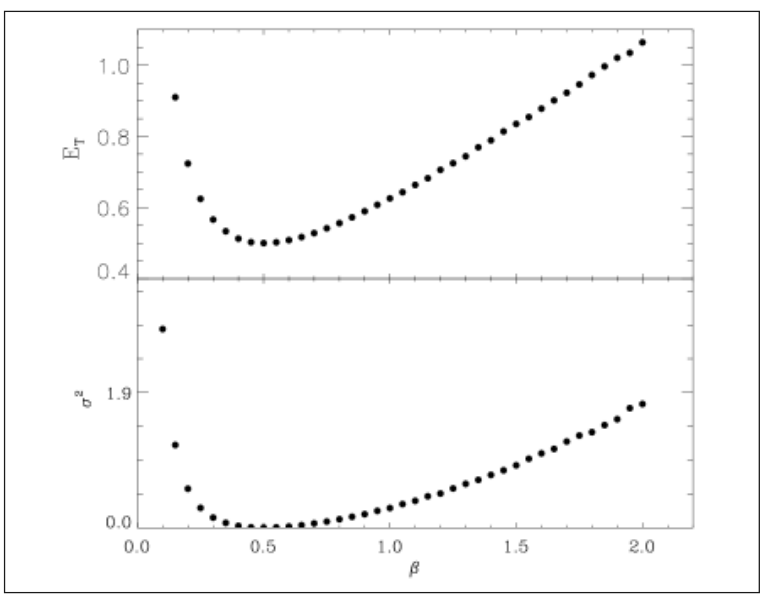

Figure 4. The upper panel shows the plot of energy for various values of the trial parameter β in the range 0.1–2.0 in steps of 0.05. The lower panel shows the plot of the variance for the same values of β.

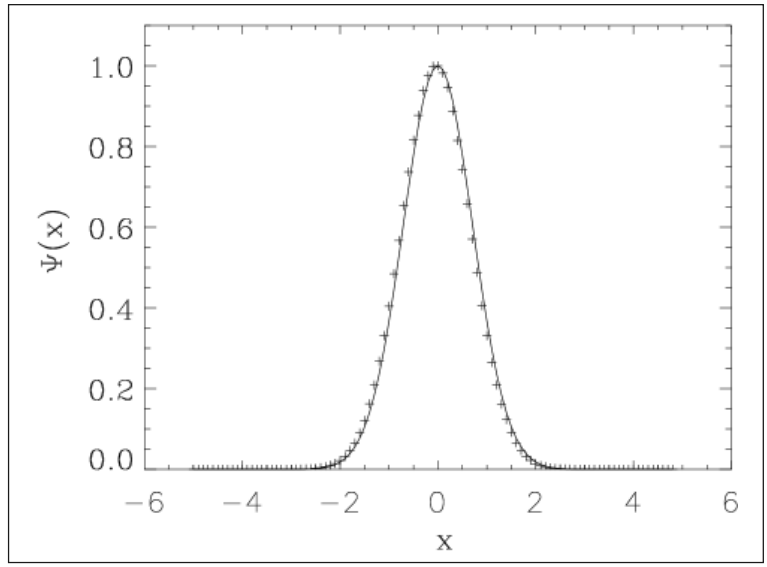

Figure 5. Plot of the wave function $\Psi(x)$ as a function of x. The solid line shows the actual wave function while the data points marked by plus-sign are those obtained from the VMC.

Now, I consider the various cases of addition of quartic (x^4) and sextic (x^6) term in the Hamiltonian

$$\hat{H} = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\,.$$

The change in the ground state energies and the variances obtained for these different cases are listed in *Table* 1. We can see that the variance σ^2 is 0 for $\beta = 0.500$ in the case $V(x) = \frac{1}{2}x^2$. This is because the trial wave function $\Psi_{\mathrm{T}}(x) = \exp(-0.5x^2)$ is the exact wave function in this case. However, in the other cases, we can easily see that the variance (σ^2) is not 0, but still the minimum. This is because the trial wave functions are not exact and hence the variance (σ^2) departs from zero in other cases.

Table 1. Energies and variances for different forms of harmonic oscillator potentials.

Potential $[V(x)]$	β	Energy $[E_{\mathrm{T}}]$	Variance $[\sigma^2]$
$\frac{1}{2}x^2$	0.500	0.500	0.000
$\frac{1}{4}x^4$	0.550	0.430	0.061
$\frac{1}{2}x^2 + \frac{1}{4}x^4$	0.750	0.625	0.020
$\frac{1}{2}x^2 + \frac{1}{4}x^6$	0.800	0.671	0.364

6.2 *Harmonic Oscillator in Three Dimensions*

The Hamiltonian in three dimensions is given by

$$\hat{H} = -\frac{1}{2}\nabla^2 + \frac{1}{2}r^2\,,$$

where ∇^2 is the Laplacian operator. In spherical polar co-ordinates, it is given by (for a spherically symmetric wave function having no angular dependence)

$$\nabla^2 = \frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}}{\mathrm{d}r}.$$

Let the trial wave function be of the form

$$\Psi_{\mathrm{T}}(r) = \exp(-\beta r^2)\,.$$

The local energy E_{L} is found to be

$$E_{\mathrm{L}} = \frac{\hat{H}\Psi_{\mathrm{T}}(r)}{\Psi_{\mathrm{T}}(r)} = 3\beta + (0.5 - 2\beta^2)r^2.$$

The values of E_{T} and variances (σ^2) are calculated for various values of β in the range $[0.1, 0.2]$ in steps of 0.05. The minimum value $E_{\mathrm{min}}^{(\mathrm{VMC})} = 1.5$ and variance $\sigma^2_{\mathrm{min}} = 0$ is found for $\beta = 0.5$. In this case, the ground state energy obtained from the VMC method is exactly the same as that known to be obtained from the Schrödinger method. This implies that the form of the trial wave function corresponds to the exact ground state wave function for the system.

7. Summary and Discussion

In this article, I have discussed about the practical implementation of the VMC technique in the determination of the ground state energies of quantum harmonic oscillators in one and three dimensions. An incisive description of the paraphernalia required for understanding the VMC technique is also presented. The results

obtained using the VMC technique are found to be in excellent agreement with those known to be determined from the Schrödinger method. The advantage of this method lies in the fact that irrespective of the analytical complexity of the problem involved, it stumbles towards an approximation of the result of the problem in higher dimensions. The capability and robustness of the VMC technique in dealing with the analytic complexity and many-particle systems in higher dimensions is one of its most important advantages. The accuracy of the VMC technique depends heavily on the form of the trial wave function chosen for the quantum mechanical system under consideration. The chosen trial wave function should satisfy all the necessary boundary conditions of the physical system under study so as to get a precise and accurate value of the ground state energy.

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Appendix A. Generation of Random Numbers

The kernel of the MC technique is the generation of random numbers. Random numbers are characterised by the fact that the value of a number cannot be predicted from the previous numbers. Therefore, if a sequence of random numbers is constructed, the probability density function (PDF) for a new number is independent of all the numbers generated so far. Random numbers for use in calculations are very hard to obtain, although they may occur in certain experiments. For example, random numbers occur in experiments such as the radioactive decay of a nucleus, cosmic ray hits in a detector or the generation of noise in electronic circuits. However, the numbers generated from these experiments may not be useful as they may lack necessary uniformity as required for MC calculations [1].

MC calculations are made more effective and robust using random numbers generated from computer algorithms. Those random numbers are called pseudo-random numbers. One important property of the pseudo-random numbers is that their distribution can be made uniform within a prescribed range. In the generation of the pseudo-random numbers from computer algorithms, the next numbers are generated from the previous ones by a mathematical formula. Fortunately, these pseudo-random numbers have the required properties of randomness which make them suitable for MC simulations [1]. Although the random numbers generated from the computer are nearly random in nature, there exists always a correlation between the numbers after a long cycle, i.e., there is a period before the same set of random numbers is generated. The computer algorithms are usually based on a random seed that starts the sequence of numbers. That is, if we construct a sequence two times with the same initial seed, the same numbers are produced [1].

1. The Transformation Method

Given a sequence $r_1, r_2 \ldots, r_n$ uniformly distributed in $[0, 1]$, the next step is to determine a sequence $x_1, x_2 \ldots, x_n$ distributed according to the desired PDF $f(x)$. Therefore, the task is to find a function $x(r)$ that is distributed according to a specified PDF $f(x)$, given that r is distributed according to a uniform distribution between 0 and 1 [2].

The probability to obtain a value of r in the interval $[r, r + \mathrm{d}r]$ is $g(r)\mathrm{d}r$. This must be equal to the probability to obtain a value of x in the interval $[x(r), x(r) + \mathrm{d}x(r)]$, which is $f(x)\mathrm{d}x$. This means that the probability that r is less than some value r' is equal to the probability that x is less than $x(r')$ [2], i.e.,

$$\begin{aligned} P(r \leq r') &= P(x \leq x(r')) \\ \Rightarrow G(r) &= F(x(r)), \end{aligned}$$

where F and G are the cumulative distribution functions corresponding to the PDFs f and g, respectively.

We know that the cumulative distribution function for the uniform PDF is

$$G(r) = r, \qquad r \in [0, 1]\,.$$

Therefore,

$$F[x(r)] = \int_{-\infty}^{x(r)} f(x')\mathrm{d}x' = \int_{-\infty}^{r} g(r')\mathrm{d}r' = r\,.$$

This shows that the CDF $F(x)$ treated as a random variable is uniformly distributed between 0 and 1. Solution for $x(r)$ may be obtained from the above equation depending on the $f(x)$ given.

1.1 *Uniform Distribution*

The uniform distribution [2] for the continuous variable $x(-\infty < x < \infty)$ is defined by

$$\begin{aligned} f(x;a,b) &= \frac{1}{b-a}, && a \le x \le b\,, \\ &= 0, && \text{otherwise.} \end{aligned}$$

That is, x is likely to be found anywhere between a and b. The CDF $F(x)$ is related to the PDF $f(x)$ by

$$F(x) = \int_{-\infty}^{x} f(x')\mathrm{d}x'\,.$$

Suppose we want ot generate a random variable according to the uniform PDF $f(x)$ defined above. The CDF $F(x)$ is given by

$$\begin{aligned} F(x) &= \int_{-\infty}^{x} f(x';a,b)\mathrm{d}x' \\ \Rightarrow F(x) &= \int_{-\infty}^{x} \frac{1}{b-a}\mathrm{d}x' \\ \Rightarrow F(x) &= \frac{x-a}{b-a}, \quad a \le x \le b\,. \end{aligned}$$

Now, to solve for $x(r)$, let us set

$$F(x) = r, \quad r \in [0,1]\,.$$

Therefore,

$$\frac{x-a}{b-a} = r \Rightarrow x = a + (b-a) * r \Rightarrow x(r) = a + (b-a) * r\,.$$

Hence, the variable $x(r)$ is distributed according to the PDF $f(x)$ given above. From this, we see that the uniform random numbers are important as they can be used to generate arbitrary PDFs by means of transformation from a uniform distribution [2].

1.2 *Exponential Distribution*

The exponential PDF [2] for the continuous variable $x(0 \le x < \infty)$ is defined by

$$f(x;\xi) = \frac{1}{\xi}\exp(-\frac{x}{\xi})\,.$$

The PDF is characterized by a single parameter ξ. To generate the random variable $x(r)$ distributed according to the exponential PDF, let us set

$$F(x) = r\,,$$

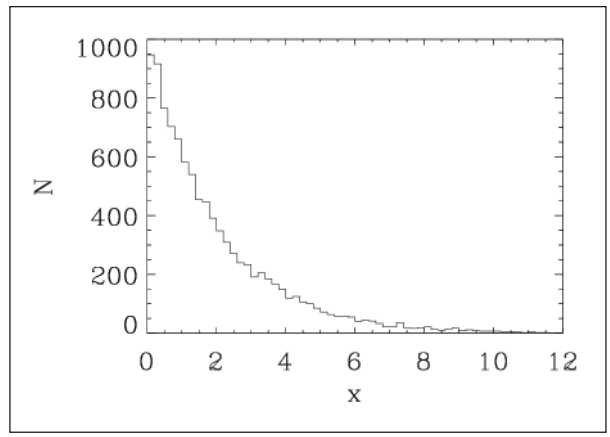

Figure A1. Histogram plot for the generation of the random variable x having exponential PDF $f(x)$ with $\xi = 2$ using the transformation method.

where $r \in [0, 1]$ and $F(x)$ is the CDF of the PDF $f(x)$ given by

$$F(x) = \int_0^\infty f(x';\xi)\mathrm{d}x' .$$

Therefore,

$$F(x) = r \Rightarrow x = -\xi \ln(1-r) .$$

But $(1-r)$ is distributed in the same way as r. So,

$$x = -\xi \ln r \Rightarrow x(r) = -\xi \ln r .$$

The variable $x(r)$ is distributed according to the exponential PDF $f(x;\xi)$ as given above. The histogram plot for the distribution of $x(r)$ with $\xi = 2$ is shown in *Figure* A1.

1.3 *Gaussian or Normal Distribution*

The Gaussian or normal PDF [2] of the continuous variable $x(-\infty < x < \infty)$ is defined by

$$f(x;\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right] .$$

The PDF has two parameters μ and σ^2. They correspond to the mean and variance of x, respectively. Using $\mu = 0$ and $\sigma = 1$, the standard Gaussian PDF is defined as

$$f(x;0,1) = \phi(x) = \frac{1}{\sqrt{2\pi}} \exp(-\frac{x^2}{2})$$

with the corresponding CDF

$$\Phi(x) = \int_{-\infty}^{x} \phi(x')\mathrm{d}x' .$$

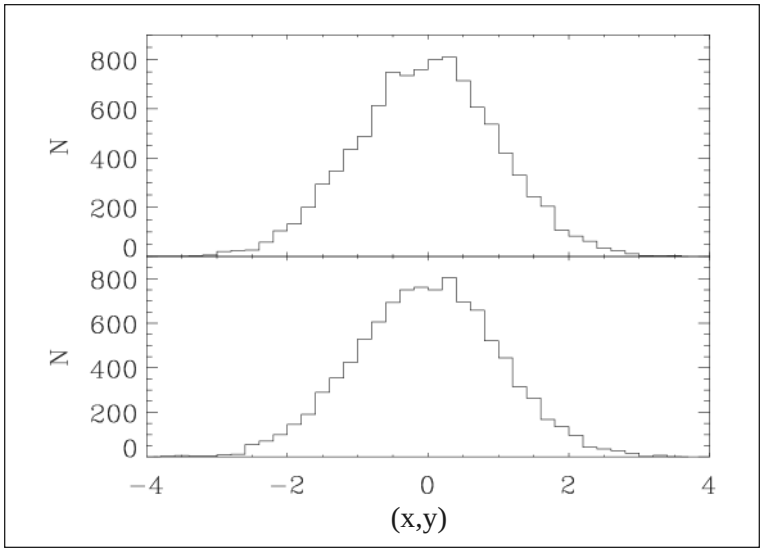

Figure A2. The upper and the lower panel show the histogram plots for the generation of the pair of random variables *x,y*, respectively, having the gaussian PDF *f* using the Box–Muller transformations.

In order to construct pairs of normally distributed random numbers, the following procedure may be adopted:

1. Obtain a pair of uniformly distributed random numbers (u_i, v_i).
2. Calculate $r_i = \sqrt{-2 \ln u_i}, \quad \theta_i = 2\pi v_i$.
3. The normally distributed variables are

$$x_i = r_i \cos\theta_i \,,$$
$$y_i = r_i \sin\theta_i \,.$$

The transformations given above are known as the Box–Muller transformations [3]. *Figure* A2 shows histogram plots for the generation of the pair of random variables (x, y) having the Gaussian PDF f using the Box–Muller transformations.

2. Acceptance-Rejection Method

Suppose we want to generate a random variable from a distribution with PDF f. If it turns out to be too difficult to simulate the value of the random variable using the transformation method, the acceptance-rejection method is a useful alternative [4]. Let $g(x)$ be another PDF defined in the support of $f(x)$ such that

$$f(x) \leq cg(x), \quad \forall x \,,$$

where $c > 0$ is a known constant. Suppose there exists a method to generate a random variable having PDF g, then according to the acceptance-rejection algorithm [2,3]:

1. Generate y from g.
2. Generate u from $U[0,1]$.
3. If $u \leq \frac{f(y)}{cg(y)}$ set $x = y$, else return to step 1.

It can be shown that x is a random variable from the distribution with PDF $f(x)$. The function $g(x)$ is also called majoring function [4]. It can be shown that the expected number of trials for an acceptance is c. Hence, for this method to be efficient, the constant c must be chosen such that rejection rate is low. A method to choose an optimum c is [3]

$$c = \max_x \frac{f(x)}{g(x)}.$$

Now, let us apply acceptance-rejection method to generate a random variable having PDF

$$f(x) = 12x(1-x)^2, \quad 0 < x < 1\,.$$

Since the random variable is concentrated in the interval $[0,1]$, let us consider the acceptance-rejection method with

$$g(x) = 1, \quad 0 < x < 1.$$

Therefore,

$$\frac{f(x)}{g(x)} = 12x(1-x)^2.$$

We need to determine the smallest constant c such that

$$\frac{f(x)}{g(x)} \leq c\,.$$

Now, we use calculus to determine the maximum value of $\frac{f(x)}{g(x)}$. It is found to be maximum at $x = \frac{1}{3}$. Therefore,

$$\frac{f(x)}{g(x)} \leq 12x(1-x)^2 \leq 12\frac{1}{3}(1-\frac{1}{3})^2 \leq \frac{16}{9} = c\,.$$

Hence,

$$\frac{f(x)}{cg(x)} = \frac{9}{16}12x(1-x)^2 = \frac{27}{4}x(1-x)^2.$$

The rejection procedure is as follows:

1. Generate random numbers $u_1, u_2 \sim U[0,1]$.
2. If $u_2 \leq \frac{27}{4}u_1(1-u_2)^2$ set $x = u_1$, else return to step 1.

The generation of samples corresponding to a PDF by acceptance-rejection method is shown in *Figure* A3.

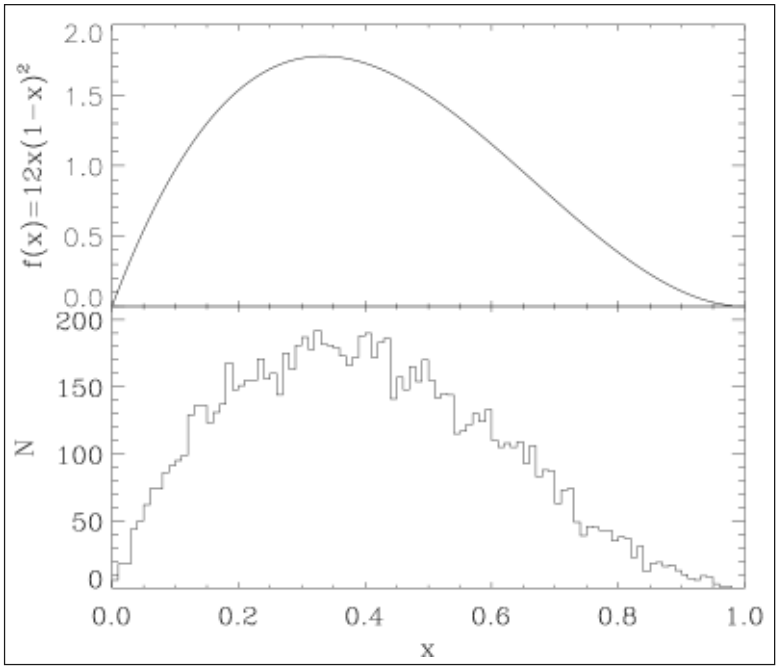

Figure A3. The upper panel shows the plot of the function $f(x) = 12x(1–x)^2$ as a function of x in the interval [0,1]. The lower panel shows the histogram plot for the generation of the random variable x having PDF $f(x)$ using the acceptance-rejection algorithm.

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Appendix B. Exercises for the Reader

1. Using a trial function of the form

$$\Psi_{\mathrm{T}}(\alpha) = \exp(-\alpha r^2),$$

show that the ground state energy of the H-atom (in units of $e = \hbar = m = 1$) is given by

$$E_{\mathrm{T}} = E_{\mathrm{min}}^{(\mathrm{VMC})} = -0.5.$$

2. Using a trial function of the form

$$\Psi_{\mathrm{T}} = x(x - L)\exp(\alpha x),$$

show that the ground state energy (in units of $e = \hbar = m = 1$) of a quantum particle of mass m moving in a one-dimensional box with walls at $x = 0$ and $x = L$, where $L = 2$, is

$$E_{\mathrm{T}} = E_{\mathrm{min}}^{(\mathrm{VMC})} = 1.249.$$