

Applications of the Variational Monte Carlo Method Using MATLAB

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Abstract

In this paper we present two examples to illustrate the application of the variational Monte Carlo method to quantum-mechanical problems by using the MATLAB program. The first problem is the one-dimensional harmonic oscillator and the second is the hydrogen atom. By a suitably chosen trial wave functions, the obtained results are in good agreement with the corresponding exact values.

1. Introduction

The variational Monte Carlo (VMC) method [1-13] has been applied successfully in nuclear, atomic, and molecular physics. It is one of the different techniques of the quantum Monte Carlo methods. It uses the Monte Carlo techniques for computing the integrals rise while applying the variational method in quantum mechanics. Also, the program MATLAB has been used extensively in the recent years in the solutions of many numerical problems in Mathematics, Physics, Chemistry, and Engineering researches. Thus, we are interested in the present paper by using the MATLAB program [14] in the numerical computations which result in applying the VMC method in solving problems in quantum mechanics. We shall discuss first the variational method, and then we will discuss the Monte Carlo techniques for integrals along with one sampling technique, namely; the Metropolis algorithm. We shall next solve the 1-dimensional harmonic oscillator problem and the hydrogen atom [15] by the variational method, and the VMC method.

2. The Variational Principle

We begin by a trial unknown wave function $\Psi(\mathbf{r})$. By the completion of the eigenstates of the Hamiltonian operator, we can express $\Psi(\mathbf{r})$ as follows:

$$\Psi(\mathbf{r}) = \sum_{n=1}^{\infty} a_n \psi_n(\mathbf{r})$$

where $\psi_n(\mathbf{r})$ are the eigenstates of the Hamiltonian in a certain domain R . Since $\Psi(\mathbf{r})$ is normalized, then

$$\int_R \Psi^* \Psi d\mathbf{r} = \int_R (\sum_m a_m^* \psi_m^*) (\sum_n a_n \psi_n) d\mathbf{r} = \sum_m \sum_n a_m^* a_n \int_R \psi_m^* \psi_n d\mathbf{r} = \sum_m \sum_n a_m^* a_n \delta_{mn} = 1$$

Hence

$$\sum_n |a_n|^2 = 1 \quad (2.1)$$

Now, we compute the energy of the state Ψ by Schrödinger's expectation value formula

$$\langle H \rangle = \frac{\int_R \Psi^* H \Psi d\mathbf{r}}{\int_R \Psi^* \Psi d\mathbf{r}} = \int_R \Psi^* H \Psi d\mathbf{r}, \quad \Psi \text{ is normalized}$$

Since H is a linear operator, we get

$$\begin{aligned}\langle H \rangle &= \int_{\mathbf{R}} (\sum_m a_m^* \psi_m^*) H (\sum_n a_n \psi_n) d\mathbf{r} = \int_{\mathbf{R}} (\sum_m a_m^* \psi_m^*) (\sum_n a_n H \psi_n) d\mathbf{r} \\ &= \int_{\mathbf{R}} (\sum_m a_m^* \psi_m^*) (\sum_n a_n E_n \psi_n) d\mathbf{r} = \sum_m \sum_n a_m^* a_n E_n \int_{\mathbf{R}} \psi_m^* \psi_n d\mathbf{r} \\ &= \sum_m \sum_n a_m^* a_n E_n \delta_{mn} = \sum_n |a_n|^2 E_n\end{aligned}$$

Since the ground state energy E_{gs} is the least energy. i.e. $E_{gs} \leq E_n$ for all $n = 1, 2, 3, \dots$, then

$$\langle H \rangle_{\psi} \geq E_{gs} \sum |a_n|^2$$

and from equation (2.1) we get

$$\langle H \rangle_{\psi} \geq E_{gs} \quad (2.2)$$

This is the variational principle, and it means that the energy of any arbitrary state Ψ is an upper bound of the ground state energy. With this principle in mind, the steps of the variational method are:

- (i) Pick a nice trial wave function Ψ with parameters a, b, \dots to be determined.
- (ii) Compute its energy $\langle H \rangle_{\psi}$. This will give a function of the parameters a, b, \dots
- (iii) Minimize $\langle H \rangle_{\psi}$ with respect to the parameters, then you get

$$\langle H \rangle_{\psi_{min}} \simeq E_{gs}$$

The following notes must be taken into consideration:

- (a) The choice of the trial wave function Ψ is up to the researcher, and it requires expertise and brilliance.
- (b) The variational method is used to estimate the ground state energy of the system. This must not be confused with the ground state itself. That is Ψ is not the ground state of the system.

3. The Variational Monte Carlo Method

The VMC method [1-4] can be considered as the variational method but with the use of the Monte Carlo technique for integration. In practice, the quantity:

$$\langle H \rangle_{\psi} = \frac{\int_{\mathbf{R}} \psi^* H \psi d\mathbf{R}}{\int_{\mathbf{R}} \psi^* \psi d\mathbf{R}} \quad (3.1)$$

is not easy to evaluate. It can even happen that it does not have a closed form. Hence the use of Monte Carlo. If we multiply and divide the integrals by Ψ , we get:

$$\langle H \rangle_{\psi} = \int_{\mathbf{R}} \frac{|\psi|^2}{\int_{\mathbf{R}} |\psi|^2 d\mathbf{R}} \frac{H\psi}{\psi} d\mathbf{R}$$

We put

$$\rho(\mathbf{R}) = \frac{|\psi|^2}{\int_{\mathbf{R}} |\psi|^2 d\mathbf{R}} \quad (3.2)$$

and

$$E_L(\mathbf{R}) = \frac{H\psi}{\psi} \quad (3.3)$$

In the above equations \mathbf{R} is the set of all possible coordinates \mathbf{R} . We call $\rho(\mathbf{R})$ the probability distribution function, and $E_L(\mathbf{R})$ the local energy function. Hence, the expectation value (3.1) becomes

$$\langle H \rangle_\psi = \int_{\mathbf{R}} \rho(\mathbf{R}) E_L(\mathbf{R}) d\mathbf{R} \quad (3.4)$$

with the property that

$$\int_{\mathbf{R}} \rho(\mathbf{R}) d\mathbf{R} = 1$$

we obtain

$$\langle H \rangle_\psi = \bar{E}_L(\mathbf{R}) \quad (3.5)$$

Now, we can estimate the expectation value of the local energy function by averaging its values at discrete N points $\{\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_N\}$. These points must be distributed by the probability distribution $\rho(\mathbf{R})$.

Thus, we have [6]

$$\langle H \rangle_\psi = \bar{E}_L(\mathbf{R}) \approx \frac{1}{N} \sum_{i=1}^N E_L(\mathbf{R}_i) \quad (3.6)$$

The problem now turns to how we could get these points distributed by this particular distribution. This problem is solved in statistics by the sampling techniques. By the theory of continuous random variables, this integral represents the expectation value of the local energy function according to the distribution $\rho(\mathbf{R})$ [6]

$$\langle H \rangle_\psi = \bar{E}_L(\mathbf{R}). \quad (3.7)$$

4. The Simple Harmonic Oscillator

4.1 The Simple Harmonic Oscillator Using the Variational Method

The simple harmonic oscillator has Hamiltonian given by

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2 \quad (4.1)$$

We will try to estimate the ground state energy of the harmonic oscillator in one dimension. A common trial function is of a Gaussian form

$$\psi = A e^{-ax^2} \quad (4.2)$$

where A is a normalization constant, and a is a parameter to be determined. Applying the normalization condition:

$$\int_{-\infty}^{\infty} \psi^* \psi dx = |A|^2 \int_{-\infty}^{\infty} e^{-2ax^2} = |A|^2 \sqrt{\frac{\pi}{2a}}$$

Thus, we have

$$|A|^2 = \sqrt{\frac{2a}{\pi}} \quad (4.3)$$

From (4.2) we obtain

$$\frac{d^2\psi}{dx^2} = 2aA[2ax^2 - 1]e^{-ax^2} \quad (4.4)$$

We will now compute the expectation value of the energy:

$$\begin{aligned}
\langle H \rangle_\psi &= \int_{-\infty}^{\infty} \psi^* H \psi \, dx = \int_{-\infty}^{\infty} \psi^* \left[\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 \right] \psi \, dx \\
&= \int_{-\infty}^{\infty} A^* e^{-ax^2} \left(\frac{-\hbar^2}{2m} 2aA[2ax^2 - 1]e^{-ax^2} + \frac{1}{2} m \omega^2 x^2 A e^{-ax^2} \right) dx \\
&= \frac{-\hbar^2 a |A|^2}{m} \int_{-\infty}^{\infty} [2ax^2 - 1] e^{-2ax^2} \, dx + \frac{|A|^2 m \omega^2}{2} \int_{-\infty}^{\infty} x^2 e^{-2ax^2} \, dx \\
&= \frac{-\hbar^2 a |A|^2}{m} \left(\frac{1}{2} \sqrt{\frac{\pi}{2a}} - \sqrt{\frac{\pi}{2a}} \right) + \frac{|A|^2 m \omega^2}{8a} \sqrt{\frac{\pi}{2a}}
\end{aligned}$$

Substituting for the value of A , we get:

$$\langle H \rangle_\psi = \frac{\hbar^2 a}{2m} + \frac{m \omega^2}{8a} \quad (4.5)$$

The next step is to minimize $\langle H \rangle_\psi$ with respect to the parameter a . This means that:

$$\begin{aligned}
\frac{d\langle H \rangle_\psi}{da} = 0, \text{ from which we obtain } \frac{\hbar^2}{2m} - \frac{m \omega^2}{8a^2} = 0. \text{ Hence,} \\
a = \frac{m \omega}{2\hbar}. \quad (4.6)
\end{aligned}$$

Computing the second derivative and substituting for a , we get:

$$\frac{d^2\langle H \rangle_\psi}{da^2} = \frac{2m \omega^2}{8a^3} = \frac{2\hbar^3}{m^2 \omega} > 0,$$

then $\langle H \rangle_\psi$ is minimum at a . Substituting for a into equation (4.5) we get the minimum energy

$$\langle H \rangle_{\psi_{\min}} = \frac{1}{2} \hbar \omega \quad (4.7)$$

This is exactly the ground state energy of the harmonic oscillator obtained by solving the problem analytically.

4.2 The Simple Harmonic Oscillator Using the VMC Method

We recall that the expectation value of the energy $\langle H \rangle_\psi$ with respect to a trial wave function ψ is expressed as [6]

$$\langle H \rangle_\psi = \int_x E_L(x) \rho(x) dx \quad (4.8)$$

It can be estimated as follows

$$\langle H \rangle_\psi = \bar{E}_L(x) \approx \frac{1}{N} \sum_{i=1}^N E_L(x_i) \quad (4.9)$$

where the points $\{x_i\}$ are distributed according to a probability distribution function $\rho(x)$ given by

$$\rho(x) = \frac{|\psi|^2}{\int_x |\psi|^2 dx} \quad (4.10)$$

and the function $E_L(x)$ is the local energy function and is given by $E_L(x) = \frac{H\psi}{\psi}$. A common trial function to begin with is of Gaussian form, we put one parameter α to calculate the minimum energy

$$\psi = e^{-\alpha x^2} \quad (4.11)$$

The distribution function is calculated simply as follows:

$$\rho(x) = \frac{e^{-2\alpha x^2}}{\int_{-\infty}^{\infty} e^{-2\alpha x^2} dx} = \sqrt{\frac{2\alpha}{\pi}} e^{-2\alpha x^2} \quad (4.12)$$

For simplicity and by a suitable choice of the physical units, we can put: $m = \hbar = \omega = 1$.

Acting on the trial wave function (4.11) by the Hamiltonian of the simple harmonic oscillator we get

$$H\psi = \left(\alpha + x^2 \left(\frac{1}{2} - 2\alpha \right) \right) e^{-\alpha x^2}$$

Hence, the local energy function is given by

$$E_L(x) = \alpha + x^2 \left(\frac{1}{2} - 2\alpha \right). \quad (4.13)$$

Our mission is to get the minimum of the energy. To do that in MATLAB [14], we introduce some values for the parameter α and compute the energy for each one, and finally we pick the minimum one. We use the Metropolis-Hastings algorithm [2] to estimate the value of the Hamiltonian for each α according to the Monte Carlo technique. We generate the random trial points given the point x by choosing them uniformly in the interval $(x - 2, x + 2)$. We implement all of these in the following code. We have made 20 samples, 500,000 points each.

```
seed = 1; rand('state', seed); %for reproducibility
a = [0.1:1:2];
x=[];
for i = [1:20];
targ = @(x) exp(-2*a(i)*x^2); %target distribution
proprnd = @(x) x+ 4*(rand - 0.5); %random number generator for new points uniformly in interval (x-4,
x+4)
proppdf = @(x,y) 1/8; %proposl density function
start = rand; %initialize
nsample = 500000; %# of points
sam = [start]; %the sample matrix
for j = [1:1:nsample-1];
xt = proprnd(sam(j)); %new point
r = (targ(xt)*proppdf(xt,sam(j))) / (targ(sam(j))*proppdf(sam(j),xt)); %calculate the ration
if r > rand;
sam(j+1) = xt; %accept
else
sam(j+1) = sam(j); %reject
end
end
x = [x ; sam]; %matrix of samples
end
E= []; %matrix of energy
for i = [1:20];
u = a(i) + ((x(i,:).^2) .* (0.5 - 2*(a(i)^2)));
h = sum(u)/nsample; %energy
E = [E ;h];
end
H = min(E)
r =find(E==H);
alpha = a(r)
```

and the output is

H=0.5000
alpha= 0.5000

We find the minimum energy is $\langle H \rangle_{\psi_{\min}} = \frac{1}{2}$ which is equal to the exact energy given in equation (4.7) providing that $m = \hbar = \omega = 1$ with relatively small number of iterations. This is because the harmonic oscillator is much simpler than any other problem in which we use the VMC method. Here, We can see a plot of a random sample of the 20 samples we made in Figure-1.

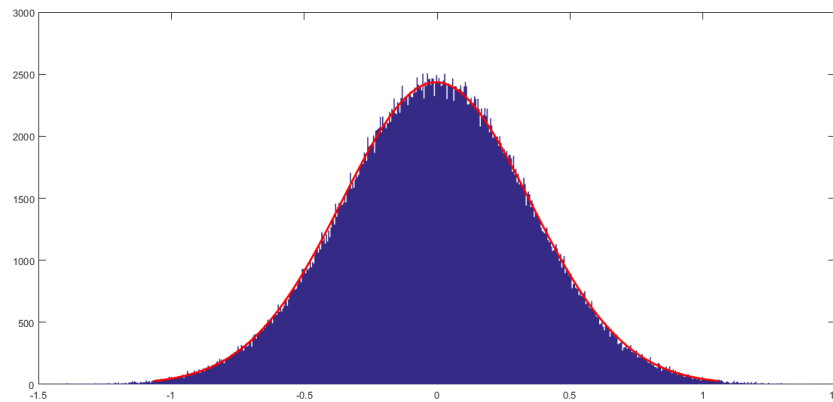


Figure-1 A random sample

If we plot the values of the energy for each value of α against the values of α we get the plot in the figure-2, and we are ensuring that the minimum energy is exactly at $\alpha = \frac{1}{2}$.

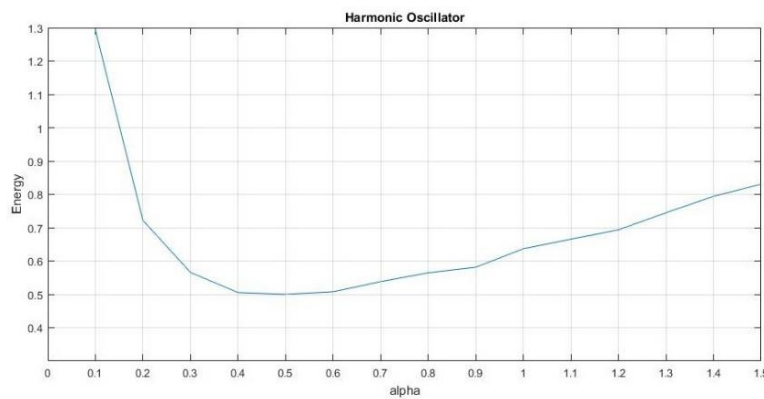


Figure-2 Energy of the harmonic oscillator as a function of alpha

5. The Hydrogen Atom

5.1 The Hydrogen Atom Problem

The Hydrogen atom is a two-body problem. We have a proton and an electron, so we have the Hamiltonian of the system as [15]

$$H = \frac{-\hbar^2}{2m_1} \nabla_1^2 - \frac{-\hbar^2}{2m_2} \nabla_2^2 - \frac{e^2}{4\pi\epsilon_0 r} \quad (5.1)$$

where ∇_1^2 and ∇_2^2 denote the Laplacian ∇^2 computed at the coordinates of the electron and the proton, respectively. m_1 is the mass of the electron, and m_2 is the proton mass. The third term is the electric potential which depends on the distance r between the electron and the proton where \mathbf{r}_1 and \mathbf{r}_2 are the coordinates of the electron and the proton, respectively. Hence, the complete solution for the Hydrogen atom expressed in terms of r, θ, ϕ is [15]

$$\psi_{lmn}(r, \theta, \phi) = A(\alpha r)^l e^{-\frac{1}{2}\alpha r} L_{n+l}^{2l+1}(\alpha r) Y_{l,m}(\theta, \phi) \quad (5.2)$$

where the constant A can be calculated by the normalization condition

$$\int_{r=0}^{\infty} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} |\psi_{lmn}|^2 r^2 \sin\theta dr d\theta d\phi = 1$$

The energy is given by

$$E_n = -\frac{\mu e^4}{2(4\pi^2\epsilon_0)^2 n^2 \hbar^2} \quad (5.3)$$

Putting the values of the constants in the right-hand side, we get the energy for the ground state ($n = 1$)

$$E_{gs} = -13.6057\text{eV} \quad (5.4)$$

This is the ground state energy of the hydrogen atom to the 4th decimal place. We shall approximate it in the next two sections.

5.2 The Hydrogen Atom in the Variational Method

We know that the hydrogen atom is spherically symmetric due to the symmetry of the electric potential around the nucleus

$$V(r) = \frac{e^2}{4\pi\epsilon_0 r} \quad (5.5)$$

So, a reasonable trial wave function can be taken as a function of the radial coordinate r

$$\psi = A e^{-\alpha r} \quad (5.6)$$

where A is a normalization constant, and α is a parameter to be determined. Applying the normalization condition:

$$\int_0^{\infty} \psi^* \psi r^2 dr = |A|^2 \int_0^{\infty} r^2 e^{-2\alpha r} dr = |A|^2 \left(\frac{1}{4\alpha^3}\right) = 1$$

we get

$$|A|^2 = 4\alpha^3 \quad (5.7)$$

Since ψ is a function of r only so $\nabla^2\psi$ in the spherical polar coordinates becomes

$$\nabla^2\psi = \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) \psi = \frac{1}{r^2} \frac{d}{dr} (-\alpha r^2 A e^{-\alpha r}) = A \left(\alpha^2 - \frac{2\alpha}{r} \right) e^{-\alpha r} \quad (5.8)$$

Assuming that the nucleus is fixed, then the Hamiltonian of the system is

$$H = \frac{-\hbar^2}{2m} \nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} \quad (5.9)$$

So that,

$$H = \frac{-\hbar^2}{2m} \left(\alpha^2 - \frac{2\alpha}{r} \right) - \frac{e^2}{4\pi\epsilon_0 r} \quad (5.10)$$

Computing the expectation value of the energy we get

$$\begin{aligned}\langle H \rangle_\psi &= \int_0^\infty \psi^* H \psi r^2 dr = \int_0^\infty e^{-\alpha r} \left[\frac{-\hbar^2 |A|^2}{2m} \left(\alpha^2 - \frac{2\alpha}{r} \right) e^{-\alpha r} - \frac{e^2 |A|^2}{4\pi\epsilon_0 r} e^{-\alpha r} \right] r^2 dr \\ &= |A|^2 \left[\frac{-\hbar^2 \alpha^2}{2m} \int_0^\infty e^{-2\alpha r} r^2 dr + \left(\frac{\hbar^2 \alpha}{m} - \frac{e^2}{4\pi\epsilon_0} \right) \int_0^\infty e^{-2\alpha r} r dr \right] \\ &= |A|^2 \left[-\frac{\hbar^2}{8m\alpha} + \left(\frac{\hbar^2 \alpha}{m} - \frac{e^2}{4\pi\epsilon_0} \right) \left(\frac{1}{4\alpha^2} \right) \right]\end{aligned}$$

Substituting for the value of A , we get:

$$\langle H \rangle_\psi = 4\alpha^3 \left[-\frac{\hbar^2}{8m\alpha} + \left(\frac{\hbar^2}{4m\alpha} - \frac{e^2}{16\pi\epsilon_0\alpha^2} \right) \right] = \left[\frac{\hbar^2 \alpha^2}{2m} - \frac{e^2 \alpha}{4\pi\epsilon_0} \right] \quad (5.11)$$

Now, we want to minimize the energy with respect to α ; $\frac{d\langle H \rangle_\psi}{d\alpha} = 0$, to obtain

$$\alpha = \frac{me^2}{4\pi\hbar^2\epsilon_0}. \quad (5.12)$$

Substituting this value in (5.11) we get the minimum value of the energy

$$\langle H \rangle_{\psi_{\min}} = \frac{-me^4}{2(4\pi\epsilon_0)^2\hbar^2} \quad (5.13)$$

This is again the same value of the analytical result.

It must be noted that it is not the case in every situation we can reach the true value of the ground state with just one parameter. In most cases, we get a poor estimation. We need to assume more parameters to get a good approximation.

5.3 The Hydrogen Atom in the VMC Method

We will assume that the nucleus is fixed. Since the Hydrogen atom is spherically symmetric about the nucleus, we put the trial function as a function of the distance between the electron and the proton. In the spherical coordinates, it will depend only on r . We put

$$\psi = e^{-\alpha r} \quad (5.14)$$

We will use the atomic units in which

$$m = \hbar = e = \frac{1}{4\pi\epsilon_0} = 1 \quad (5.15)$$

The expectation value is given by

$$\langle H \rangle_\psi = \frac{\int_0^\infty \psi^* H \psi r^2 dr}{\int_0^\infty |\psi|^2 r^2 dr}$$

Now, we apply the Monte Carlo technique by multiplying and dividing by ψ

$$\langle H \rangle_\psi = \int_0^\infty \frac{|\psi|^2}{\int_0^\infty |\psi|^2 r^2 dr} \left(\frac{H\psi}{\psi} \right) r^2 dr \quad (5.16)$$

This gives a distribution function

$$\rho(r) = \frac{|\psi|^2}{\int_0^\infty |\psi|^2 r^2 dr} \quad (5.17)$$

and a local energy function

$$E_L(r) = \frac{H\psi}{\psi} \quad (5.18)$$

Now the expectation value of the energy is the average of the local energy function of N points distributed according to $\rho(r)$

$$\langle H \rangle_{\psi} \approx \frac{1}{N} \sum_{i=1}^N E_L(r_i)$$

Calculating the distribution function

$$\rho(r) = \frac{e^{-2\alpha r}}{\int_0^{\infty} e^{-2\alpha r} r^2 dr} = \frac{1}{4\alpha^3} e^{-2\alpha r} \quad (5.19)$$

To calculate the local energy, recall the Hamiltonian of the hydrogen atom from equation (5.9). With the atomic units, it becomes

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

Since the trial function is a function of r only, then by expressing the operator ∇^2 in the spherical coordinates, we have

$$H = \frac{-1}{2} \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) - \frac{1}{r} \quad (5.20)$$

This gives us

$$E_L(r) = \frac{-\alpha}{2} \left(\alpha - \frac{2}{r} \right) - \frac{1}{r} \quad (5.21)$$

The following is the code for the hydrogen atom. It is the same as the harmonic oscillator code but with some modifications. the important one is that the values of r must be positive.

```

seed = 1; rand( 'state' , seed ); %for reproducibility
a = [0.1:0.1:2];
s=size(a);
r=[];
for i = [1:s(2)];
targ = @(r) (r^2)*exp(-2*a(i)*r); %target distribution
proprnd = @(r) abs(r+ 4*(rand - 0.5)); %random number generator for new points uniformly in interval
(r-4, r+4)
proppdf = @(r,y) 1/8; %proposl density function
start = rand; %initialize
nsample = 500000; %# of points
sam = [start]; %the sample matrix
for j = [1:1:nsample-1];
rt = proprnd(sam(j)); %new point
l = (targ(rt)*proppdf(rt,sam(j))) / (targ(sam(j))*proppdf(sam(j),rt)); %calculate the ration
if l > rand;
sam(j+1) = rt; %accept
else
sam(j+1) = sam(j); %reject
end
end
r = [r ; sam]; %matrix of samples
end
E= []; %matrix of energy
for i = [1:s(2)];
u = (-a(i)/2)*(a(i)- 2./ r(i,:)) - 1./r(i,:);
h = sum(u)/nsample; %energy
E = [E ;h];
end
H = min(E)
q =find(E==H);
alpha = a(q)

```

and the output is

H=-0.5000 alpha = 1

This is the exact value of the ground state energy of the hydrogen atom. However, in most cases when we do not have the exact form of the wave function of the problem under study, we do not get the exact value of the ground state energy by applying the VMC. Instead, we got a good approximation comparing to the experimental value of the energy. If we plot the energy as a function of the parameter variable α we get the plot in figure-3.

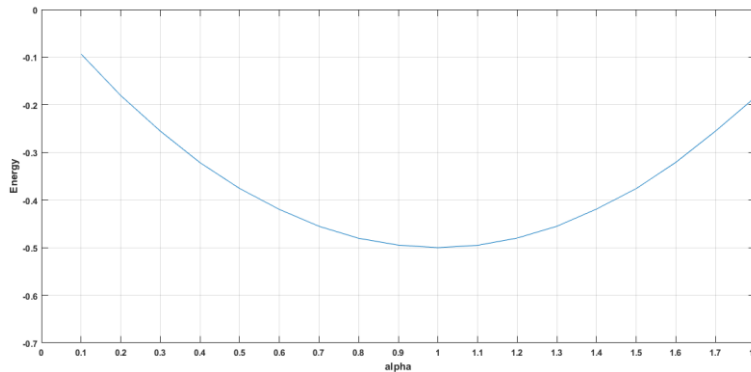


Figure-3 Energy of the hydrogen atom as a function of alpha

We must note that when using the VMC method with the Metropolis-Hastings algorithm [16], we did not use the normalization constant appeared in the denominator of the distribution function (5.19). This is because the Metropolis-Hastings algorithm samples the required distribution up to a constant. This is a powerful advantage of this method since it gives us the freedom of choosing any trial function without worrying about its complexity to calculate the normalization constant.

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