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MONTE CARLO SIMULATIONS

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Abstract: Techniques of Monte Carlo simulations are discussed and illustrated by applying them to solve different problems. The Hit-Or-Miss method and the Sample-Mean method are considered in detail. Special attention is paid to analyze the errors associated with each of the methods.

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1. Introduction

Monte Carlo [1, 2, 3, 4, 5, 6] simulation has become one of the most important computational tools in science and engineering disciplines. It has also found applications in the area of management and finance. The method rely generally on randomly sampling the population of interest. The name "Monte Carlo" came from a city in Monacco famous for its beautiful beaches and casinos.

We will discuss the techniques of the Monte Carlo methods. The use of the methods is illustrated by first applying them to compute definite integrals. Monte Carlo methods can be used in general to compute definite integrals of any dimension, d. A d-dimensional integral is one that involves d-fold integrals. The source of the error in a Monte Carlo simulation is purely statistically in nature and has nothing to do with the dimension of the integral. If N sample points are used in the simulation, then the error typically goes like $N^{-1/2}$. For small dimensions, say less than or equal to 3, and if the domain of integration is not too complicated, Monte Carlo methods cannot compete in efficiency and accuracy with traditional numerical methods such as trapezoidal and Simpson's rules [7], whose errors depend on the dimension of the integral, but usually decrease with increasing N faster than $N^{-1/d}$. However for $d >> 3$, Monte Carlo methods are often the only viable mean for computing integrals.

Our purpose here is to illustrate the basic ideas of Monte Carlo methods and will only work with one-dimensional integrals. However much of the discussions here can be trivially extended to higher dimensions.

We begin by defining here the problem of interest. Suppose $\rho(x)$ is a real valued function of a real variable, x, and $\rho(x) > 0$ for x in the domain $[a, b]$, our goal is to compute the definite integral of $\rho(x)$ from a to b

$$I = \int_a^b \rho(x)\, dx, \tag{1}$$

using a variety of Monte Carlo methods.

2. The Hit-Or-Miss Method

The first Monte Carlo method we will be discussing is the Hit-Or-Miss method. The method is based on the observation that, I, the integral of a function $\rho(x)$ from a to b, is given by the area bounded on top by $\rho(x)$, on the bottom by the x-axis, on the left by the vertical line $x = a$, and on the right by the vertical line $x = b$.

To compute this area by Monte Carlo simulation, we want to enclose this entire area within a rectangle. We choose an h that bound $\rho(x)$ within the interval $[a, b]$. That means that $h \geq \rho(x)$ for any x in $[a, b]$. Then the area of interest in entirely enclosed by the rectangle of height h between a and b.

Imagine that we sprinkle a thin layer of dust particles over this rectangle, covering it as uniformly as possible. The probability that a given particle lands inside the areas of interest is clearly given by the ratio, r, of the area I and the area of the rectangle, $(b - a)h$:

$$r = \frac{I}{(b-a)h}. \tag{2}$$

In a simulation, if we sprinkle a total of N dust particles and if N' of those land within the area of interest, then we expect the ratio N'/N to be given by r, barring statistical fluctuations, therefore

$$\frac{N'}{N} \approx r. \tag{3}$$

This result allows us to estimate the value of I from the simulation

$$I \approx (b-a)h\frac{N'}{N}. \tag{4}$$

The basic algorithm for the Hit-Or-Miss Method is:

1. Initialize N' to zero and N to a large positive integer.
2. Go through the following loop N times:
   (a) Randomly choose a point x in $[a, b]$, and
   (b) a point y in $[0, h]$.
   (c) If the point (x, y) lies within the area of interest, then increment N' by 1.
3. Compute $(b-a)h\frac{N'}{N}$ as an estimation for I.

Note that if u_1 and u_2 are 2 independent uniform deviates then we can let $x = (b-a)u_1 + a$ and $y = hu_2$. How do we actually determine whether or not the point (x, y) lies within the area of interest has a lot to do with the actual shape of the area under investigation.

2.1. An Example of the Hit-Or-Miss Method

As an example of the usage of the Hit-Or-Miss method we will revisit the problem of estimating the area of a unit circle by simulation.

This time, instead of enclosing the circle within a square of side 2, we will only consider the quarter circle that lies in the first quadrant. This entire area is enclosed by a square of height 1 between 0 and 1. Therefore we have $a = 0$, $b = 1$, and $h = 1$. The area of the enclosing rectangle (which in this case happens to be a square) has unit area and so $I \approx N'/N$.

In applying the basic algorithm for the Hit-Or-Miss method to the present problem, we let $x = u_1$ and $y = u_2$, and the point (x, y) lies within the area of interest if $(x^2 + y^2) \leq 1$. [This condition is exactly the same as the condition: $\sqrt{x^2 + y^2} \leq 1$, but it is much quicker to evaluate.]

Note that the function that we are integrating is actually given by $\rho(x) = \sqrt{1 - x^2}$, although the method does not explicitly use this function in this form. If $\rho(x)$ is a single-valued function, then we can rephrase the basic algorithm for the Hit-Or-Miss method in the following way.

An alternate way to express the above algorithm for the Hit-Or-Miss Method is:

1. Initialize N' to zero and N to a large positive integer.
2. Go through the following loop N times:
   (a) Let $x = (b - a)u_1 + a$.
   (b) Let $y = hu_2$.
   (c) Compute $\rho(x)$.
   (d) Increment N' by 1 if $y \leq \rho(x)$.
3. Compute $(b - a)h\frac{N'}{N}$ as an estimation for I.

In a realistic situation we do not know the exact answer for I, otherwise why do we want to compute it at all? However we are trying to learn the basic techniques of simulations and therefore it is a good idea to choose problems for which the exact answers are known. This way we can compare the results of the simulation with exact answers to gain confidence in the techniques and to gauge the accuracy of the methods.

For this particular problem, the exact answer for I is known because it represents the area of one quarter of a unit circle and so

$$I = \frac{\pi \cdot 1^2}{4} = \frac{\pi}{4}. \tag{5}$$

2.2. Error Analysis of the Hit-Or-Miss Method

In a computer simulation, it is important to be able to have a quantitative measure of how accurate the results of the simulations are. We will be able to do so by making use of the properties of normal random variables, in particular the Rule of the 3 σ's.

But first we must identify the random variable, X, of interest in the simulation. If we use a total of N points in the simulation, then there are N identical copies of the variable and the random variable of interest is then given by

$$\bar{X} = \frac{1}{N} \sum_{n=1}^{N} X_n. \tag{6}$$

We know from the Central Limit Theorem that $\bar{X}$ is a normal variable in the limit of large N. Moreover if the X_n have a mean μ and variance σ^2, then $\bar{X}$ has a mean μ and a variance σ^2/N. If variable X_n takes on the value x_n, for $n = 1, 2, ..., N$, then the sample mean, which we denote by μ', is given by

$$\mu' = \frac{1}{N}\sum_{n=1}^{N} x_n. \tag{7}$$

This μ' is an estimation of the actual mean μ, whose value is what the simulation attempts to obtain. For the present problem we are trying to find the ratio, r, of the number of points that fall within the area of interest to the total number of points used. The simulation estimates that r is given by N'/N. It is clear that

$$\frac{1}{N}\sum_{n=1}^{N} x_n = \frac{N'}{N}, \tag{8}$$

and therefore

$$\sum_{n=1}^{N} x_n = N'. \tag{9}$$

Consequently we are led to the choice of a discrete random variable, X, which takes on the value of 1 if the point falls within the area of interest, and the value of 0 if it falls outside.

Theoretically, X takes on the value of 1 with probability r, and takes on the value of 0 with probability $1 - r$:

x	1	0
$p(x)$	r	(1-r)

The accuracy of the result of the simulation for the value of the mean value, μ, is measured by the most probable error

$$\frac{0.6745\sigma}{\sqrt{N}}, \tag{10}$$

where $\sigma = \sqrt{V(X)}$ is the standard deviation of X. The value of σ is independent of the number of trials used in the simulation. It depends on the way simulation is carried out.

In practice we do not know the precise values of μ and σ. However we can obtain estimations of these values based on the sample obtained from the simulation. Estimating the mean μ from the data

$x_1, x_2, \ldots, x_n$ using the sample mean is of course the key part of the simulation. However we can also estimate the value for the variance σ^2 using

$$\sigma'^2 = \frac{1}{N-1} \sum_{n=1}^{N} (x_n - \mu')^2 \tag{11}$$

Notice that in the above estimation of the variance from the sample data, the sum is divided by $N - 1$ instead of N. This choice gives what is known as an unbiased estimator for the variance. [8]. Using σ' as an approximation for σ in Eq.(10), we have an estimation of the error in the value of μ'.

For the present problem, because the exact answer for the integral is known, the exact values for μ and σ can also be found because both quantities can be expressed in terms of r, the ratio of the area of interest to the area of the inscribing rectangle. The expected value $E(Y)$ can be calculated to be

$$E(X) = \sum_{x} xp(x) = 1 \cdot r + 0 \cdot (1 - r) = r = \mu, \tag{12}$$

which is to be anticipated. The expected value $E(X^2)$ is given by

$$E(X^2) = \sum_x x^2 p(x) = 1^2 \cdot r + 0^2 \cdot (1-r) = r, \tag{13}$$

and therefore the variance is given by

$$V(X) = \sigma^2 = E(X^2) - \mu^2 = r - r^2 = r(1-r). \tag{14}$$

With this value of σ, the probable error in estimating μ can be calculated from Eq.(10). The integral $I = (b-a)h\mu$ therefore has a probable error $I_{\text{error}}^{\text{HM}}$ of

$$\begin{aligned} I_{\text{error}}^{\text{HM}} &= 0.67(b-a)h\frac{\sigma}{\sqrt{N}} \qquad (15) \\ &= 0.67(b-a)h\sqrt{\frac{r(1-r)}{N}}. \end{aligned}$$

In this expression we can write r in terms of I using Eq.(2) to obtain

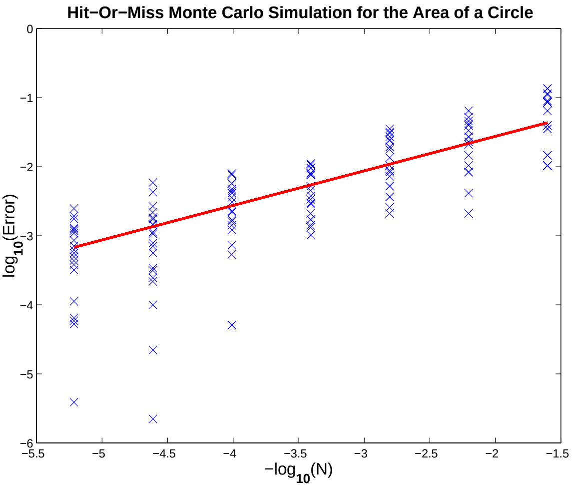
$$I_{\text{error}}^{\text{HM}} = 0.67\sqrt{\frac{I[(b-a)h - I]}{N}}. \tag{16}$$

Since the area of interest is enclosed here within a rectangle of height h, we see from Eq.(16) that the probable error is smallest if h is chosen to be the maximum of the integrand $\rho(x)$ within the interval $[a, b]$. A larger value for h can be used, however the probable error for I will be larger. In the case of the quarter circle, the probably error for I if the simulation is done using an h equal 4 is expected to be twice that for h equal to 1.

Next consider what happens if the simulation is performed not for a quarter circle, but for an entire circle. The integral I then represents the area of a full circle and an appropriate inscribing rectangle is a square of side equal to 2. The ratio, r, of the area of interest to the area of the inscribing rectangle, however remains unchanged. From Eq.(15) it is clear that the probable error for I is expected to be 4 times larger.

2.3. Application of the Hit-Or-Miss Method

We will now implement the above simulation using the Hit-Or-Miss method to estimate the area of a quarter circle of unit radius. We inscribe the area within a 1×1 square, and so $a = 0$, $b = 1$ and $h = 1$.



- **Behavior for a Fixed N**

One key feature of the Monte Carlo simulation is its stochastic characteristic. This can be seen by performing the simulation several times using a fixed value of N. The total number of uniform deviates needed for each simulation is $2N$, N for the x-coordinates and another N for the y-coordinates. Each run should use a different sequence of uniform deviates, otherwise identical results would be produced. This can be done by using the first $2N$ uniform deviates for the first run, and then using the next $2N$ uniform deviates for the second run, etc. Alternately we can use a different seed for the random number generator for each different run. Because of the stochastic nature of the Monte Carlo simulation, the results fluctuate from run to run. The amount of fluctuation of course has to do with the magnitude of the probable error, which will be investigated in detail below.

- **The $1/\sqrt{N}$ Convergence**

Next we want to verify the $1/\sqrt{N}$ convergence of Monte Carlo Simulations, as described by Eq.(10). The simulation will be repeated many times, each time using more and more points. To verify that the probable error for I should decrease with increasing N like $1/\sqrt{N}$, we note that the log of I_{error} should behave like

$$\log I_{\text{error}}^{\text{HM}} = -\frac{1}{2}\log N + \text{constant}. \tag{17}$$

Therefore a plot of $I_{\text{error}}^{\text{HM}}$ versus $-\log N$ should give approximately a straight line with a slope of one half.

3. The Sample-Mean Method

We describe here another method of performing Monte Carlo simulation called the sample-mean method. We begin by observing the fact that a function $\rho(x)$ of a continuous variable x in the domain $[a, b]$ has a mean or average value given by

$$< \rho >= \frac{\int_a^b \rho(x)dx}{\int_a^b dx} = \frac{1}{b-a}\int_a^b \rho(x)dx. \tag{18}$$

Consequently the integral

$$I = \int_a^b \rho(x)dx = (b-a) < \rho > . \tag{19}$$

In the sample-mean method, $< \rho >$ is estimated by uniformly and randomly sampling the function $\rho(x)$ within the interval $[a, b]$:

$$< \rho >\approx \frac{1}{N}\sum_{n=1}^{N} \rho(x_n), \tag{20}$$

where $x_n = (b-a)u_n + a$ and u_n are uniform deviates. [9]

3.1. Error Analysis of the Sample-Mean Method

We identify a continuous random variable Y, whose values, y, are given by $\rho(x)$ for x uniformly distributed in $[a, b]$. The random variable

$$\bar{Y} = \frac{1}{N}\sum_{n=1}^{N} Y_n \tag{21}$$

becomes a normal variable in the limit of large N. It has a mean $\mu_{\bar{Y}}$ which can be estimated from the result of N trials as

$$\begin{aligned} \mu_{\bar{Y}} = <\rho> &\approx \frac{1}{N}\sum_{n=1}^{N} y_n \\ &= \frac{1}{N}\sum_{n=1}^{N} \rho(x_n). \end{aligned} \tag{22}$$

This estimated mean value after multiplying by $(b-a)$ gives the integral, I. The variance of $\bar{Y}$ is

$$V(\rho) = <\rho^2> - (<\rho>)^2, \tag{23}$$

which can be estimated from the sample data using Eq.(20) for $< \rho >$ and

$$< \rho^2 > \approx \frac{1}{N} \sum_{n=1}^{N} \rho^2(x_n) \tag{24}$$

for $< \rho^2 >$.

The most probable error in I is then given by

$$I_{\text{error}}^{\text{SM}} = 0.67(b-a)\sqrt{\frac{V(\rho)}{N}}. \tag{25}$$

This can also be written as

$$I_{\text{error}}^{\text{SM}} = 0.67\sqrt{\frac{L\int \rho^2 \ dx - I^2}{N}}, \tag{26}$$

where $L = b - a$ is the length of the domain interval.

Note that the smaller the variance of the function is, the smaller is the probable error. Functions that vary little over the domain has small variances. In the limiting case of a constant function, where

$\rho(x) = c$ for all x in $[a, b]$,

$$V(\rho) = \frac{1}{b-a} \int_a^b (\rho(x) - <\rho>)^2 \, dx \tag{27}$$

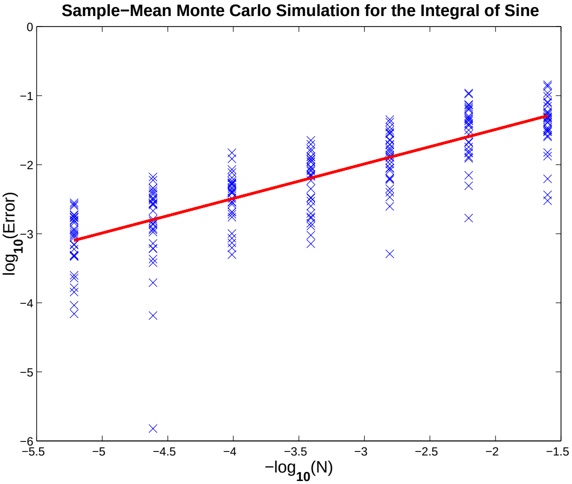
vanishes because $\rho(x)$ and $<\rho>$ are both equal c. Of course in that case the probable error is zero since Eq.(20) for the mean gives exactly c. The observation that the smaller the variation of the function $\rho(x)$ is within the domain, the smaller is the variance and therefore the smaller is the probable error provides us with important insight how to improve the efficiency of Monte Carlo simulations by techniques known as variance reductions.

3.2. Procedure for the Sample-Mean Method

The procedure for the sample-mean method is:

1. Initialize s_1 and s_2 to 0 and N to a large integer.
2. Go through the following loop N times:
   (a) Let $x_n = (b-a)u + a$.
   (b) Let $y_n = \rho(x_n)$.
   (c) Add y_n to s_1.
   (d) Add y_n^2 to s_2.
3. Estimate the mean $\mu' = \frac{s_1}{N}$.
4. Estimate the variance $V' = \frac{s_2}{N} - \mu'^2$.
5. Estimated the probable error for I: $0.67(b-a)\sqrt{\frac{V'}{N}}$.

3.3. Application of the Sample-Mean Method



We will apply the Sample-Mean method to compute the integral

$$I = \int_0^{\frac{\pi}{2}} \sin x \; dx. \tag{28}$$

For this problem, $a = 0$, $b = \pi/2$, and $\rho(x) = \sin x$.

This problem is so simple that it allows us to check the accuracy of the result of the simulation, as well as the accuracy of the estimation of the probable error because theoretically we know that

$$I = \int_0^{\frac{\pi}{2}} \sin x \; dx = -\left[\cos x\right]_0^{\frac{\pi}{2}} = 1, \tag{29}$$

and therefore we have $<\rho>= \frac{I}{b-a} = \frac{2}{\pi}$ exactly. Moreover we have

$$<\rho^2>= \frac{1}{b-a} \int_a^b \rho^2(x) = \frac{2}{\pi} \int_0^{\frac{\pi}{2}} \sin^2 x \; dx = \frac{1}{2}, \tag{30}$$

and therefore the variance is given exactly by

$$V(\rho) = \frac{1}{2} - \left(\frac{2}{\pi}\right)^2 . \tag{31}$$

Thus our analysis shows that the probable error is given by

$$I_{\text{error}}^{\text{SM}} = 0.67\sqrt{\frac{\frac{\pi^2}{8} - 1}{N}}. \tag{32}$$

It is interesting to compare the above theoretical estimate of the error of the Sample-Mean method with that of the Hit-Or-Miss method. We find

$$\frac{I_{\text{error}}^{\text{SM}}}{I_{\text{error}}^{\text{HM}}} = \sqrt{\frac{\frac{\pi^2}{8} - 1}{\frac{\pi}{2} - 1}} \approx 0.64, \tag{33}$$

and therefore the probable error of the Sample-Mean method is 36% less than that of the Hit-Or-Miss method.

Another way to make comparison between the errors obtained by these two methods is to assume that we use N^{HM} points for the Hit-Or-Miss method, and N^{SM} points for the Sample-Mean method, and equate the theoretical estimates of the errors. Solving for N^{SM} we find that

$$N^{\text{SM}} = \frac{\frac{\pi^2}{8} - 1}{\frac{\pi}{2} - 1} N^{\text{HM}} \approx 0.41 N^{\text{HM}}. \tag{34}$$

Thus the Sample-Mean method is a little more that twice as fast as the Hit-Or-Miss method.

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$$x_n = a + \frac{b-a}{N} n,$$

for $n = 1, 2, ..., N$, then the method becomes a rectangular approximation of the integral in numerical analysis. See, for example, W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery *Numerical Recipes*, Second Edition, Ch. 4, p. 123-155 (Cambridge University Press, 1992).

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