MONTE CARLO METHODS

Jonathan Pengelly

February 26, 2002

1 Introduction

This tutorial describes numerical methods that are known as Monte Carlo methods. It starts with a basic description of the principles of Monte Carlo methods. It then discusses four individual Monte Carlo methods, describing each individual method and illustrating their use in calculating an integral. These four methods have been implemented in my example program 8.2, and the results from these are used in my discussion on each method. This discussion looks at the principles behind each method. It also looks at the approximation error for each method and compares each different method's approximation accuracy. After this, the tutorial discusses how Monte Carlo methods can be used for many different types of problem, that are often not so obviously suitable to Monte Carlo methods. We then discuss the reasons why Monte Carlo is used, attempting to illustrate the advantages of this group of methods. Finally, I discuss how Monte Carlo methods relate to the field of Computer Vision and give examples of Computer Vision applications that use some form of Monte Carlo methods. Note that the appendix includes a basic mathematics overview, the program code and results that are referred to in section 3 and some focus questions involving Monte Carlo methods. This tutorial does contain a moderate content of mathematical and statistical concepts and syntax. The basic mathematics overview is an attempt to describe some of the more familiar concepts and syntax in relation to this tutorial and thus a quick initial review of this section may improve the understandability and clarity of it.

2 Basic Description

Monte Carlo methods provide approximate solutions to a variety of mathematical problems by performing statistical sampling experiments. They can be loosely defined as statistical simulation methods, where statistical simulation is defined in quite general terms to be any method that utilizes sequences of random numbers to perform the simulation. Thus Monte Carlo methods are a collection of different methods that all basically perform the same process. This process involves performing many simulations using random numbers and probability to get an approximation of the answer to the problem. The defining characteristic of Monte Carlo methods is its use of random numbers in its simulations. In fact, these methods derive their collective name from the fact that Monte Carlo, the capital of Monaco, has many casinos and casino roulette wheels are a good example of a random number generator.

The Monte Carlo simulation technique has formally existed since the early 1940s, where it had applications in research into nuclear fusion. However, only with the increase in computer technology and power has the technique become more widely used. This is because computers are now able to perform millions of simulations much more efficiently and quickly than before. This is an important factor because it means that the technique can provide an approximate answer quickly and to a higher level of accuracy, because the more simulations that you perform then the more accurate the approximation is (This point is illustrated in the next section when we compare approximation error for different numbers of simulations).

Note that these methods only provide a approximation of the answer. Thus the analysis of the approximation error is a major factor to take into account when evaluating answers from these methods. The attempt to minimise this error is the reason there are so many different Monte Carlo methods. The various methods can have different levels of accuracy for their answers, although often this can depend on certain circumstances of the question and so some method's level of accuracy varies depending on the problem. This is illustrated well in the next section where we investigate four different Monte Carlo methods and compare there answers and the accuracy of their approximations.

3 Monte Carlo Techniques

One of the most important uses of Monte Carlo methods is in evaluating difficult integrals. This is especially true of multi-dimensional integrals which have few methods for computation and thus are suited to getting an approximation due to their complexity. It is in these situations that Monte Carlo approximations become a valuable tool to use, as it may be able to give a reasonable approximation in a much quicker time in comparison to other formal techniques.

In this section, we look at four different Monte Carlo methods to approach the problem of integral calculation. We investigate each method by giving a basic description of its individual procedure and then attempt to give a more formal mathematical description. We also discuss the example program that is included with this tutorial. It has implemented all four methods that we discuss, and also has results from these different methods in integrating an example function.

Before we discuss our first method it must be brought to the reader's attention the reasons why we are discussing four different Monte Carlo methods. The first point in explaining this, is to acknowledge that there are many considerations when using Monte Carlo techniques to perform approximations. One of the chief concerns is to be able to get as accurate an approximation as possible. Thus, for each method we discuss their associated error statistics (the variance is discussed). There is also the consideration of what technique is most suitable to the problem and so will get the best results. For example, a curve that has many plateaus (flat sections) may be very suitable to a stratified sampling method because the flat sections will have very low variance. Thus, we discuss four different Monte Carlo methods, because they all have their individual requirements and benefits. Probably the most important consideration, for the methods are the accuracy of their approximations because the more accurate the approximation, the less samples are needed to reach a specific level of accuracy.

3.1 Crude Monte Carlo

The first method for discussion is crude Monte Carlo. We are going to use this technique to solve the integral I.

$$I = \int_{a}^{b} f(x)dx \tag{1}$$

A basic description of this method is that you take a number, N, of random samples where a i = s (sample value) i = b. For each random sample s, we find the function value f(s) for the function f(x). We sum all of these values, and divide by N to get the mean value from our samples. We then multiply this value by the interval (b-a) to get the integral. This can be represented as -

$$I = \frac{(b-a)}{N} \sum_{i=1}^{N} f(x_i)$$
 (2)

Now, the next part to describe is the accuracy of this approximation technique, because otherwise the answer will not be meaningful without a description of its uncertainty. In my implementation, I did a very simple, one-dimensional example. I found the variance of my sample by finding the mean of all of my N-groups of samples. I then substituted the information into the equation to determine the variance. The sample variance equation is -

$$s^{2} = \frac{1}{n-1} \sum_{i=1}^{N} (x_{i} - x)^{2}$$
(3)

Using this information you can determine the confidence intervals of your method and determine how accurate your answer is. This information about our implementation example, is discussed further on in the tutorial.

3.2 Acceptance - Rejection Monte Carlo

The next method for discussion is Acceptance - Rejection Monte Carlo. This is the easiest technique to explain and understand. However, it is also the technique with the least accurate approximation out of the four discussed.

A basic description of the Acceptance-Rejection method is that you have your integral as before. In the (a,b) interval for any given value of x the function you find the upper limit. You then enclose this interval with a rectangle that is high enough to be above the upper limit, so we can be sure that the entire function for this interval is within the rectangle. We now begin taking random points within the rectangle and evaluate this point to see if it is below the curve or not. If the random point is below the curve then it is treated as a successful sample. Thus, you take N random points and perform this check, remembering to keep count of the number of successful samples there have been. Now, once you have finished sampling, you can approximate the integral for the interval (a,b) by finding the area of the surrounding rectangle. You then multiply this area by the number of successful samples over the total number of samples, and this will give you an approximation of the interval (a,b). This is illustrated more clearly in the diagram.

Mathematically, we can say that the ratio of the area below the function f(x) and the whole area of the rectangle (Max(f(x)) * (b-a)) is approximately the ratio of the successful samples (k) and the whole number (N) of samples taken. Therefore

$$\int_{a}^{b} f(x)dx \approx \frac{k}{N}M(b-a)$$
(4)

To find the accuracy of the approximation, I have used the same variance technique as for the Crude Monte Carlo method. This analysis shows that the Acceptance-Rejection method gives a less accurate approximation than crude monte carlo.

3.3 Stratified Sampling

The basic principle of this technique is to divide the interval (a,b) up into subintervals. You then perform a crude monte carlo approximation on each subinterval.



Figure 1: Acceptance-Rejection Monte Carlo method. We see the surrounding rectangle (red lines) for the interval (a,b). We would now randomly sample points within this rectangle to see if they are underneath the function line.

This is illustrated in this diagram.

The reason you might use this method is that now instead of finding the variance in one big go, you can find the variance by adding up the variances of each subinterval. This may sound like you are just doing a long-winded performance of the Crude Monte Carlo algorithm but if you have a function that is step-like or that has periods of flat, then this method could be well-suited. This is because if you did an integration of a sub-interval that was very flat then you are going to get a very small variance value. Thus this is the advantage of the stratified sampling method, you get to split the curve into parts that could have certain advantageous properties when evaluating them on their own. Mathematically we can represent the integration as -

$$\int_{a}^{b} f(x)dx = \int_{a}^{c} f(x)dx + \int_{c}^{b} f(x)dx$$
(5)

Note that this equation is when the interval (a,b) has been broken into two sub-intervals (a,c) and (c,b).

3.4 Importance Sampling

The last method we look at is importance sampling. This is the most difficult technique to understand out of the four techniques. In fact, before any attempt to explain the basic principles behind this method, we will discuss a sort of link from the last technique (stratified sampling) to the concepts behind importance sampling.

Now in the figure we see that the four sub-intervals are quite different. I1 sees the value of f(x) staying very constant. However, as we progress across to B, we see the value of f(x) becoming larger than the fairly steady curve of I1. Now these larger values of f(x) are going to have more impact on the value of the integral. So should we not do more samples in the area where there is the highest values. By doing this, we will get a better approximation of a sub-interval that contributes more to the integral than the other sub-intervals. We won't skew the results either, because you still have to get the total integral by adding every sub-intervals together, all you have is a more accurate approximation of an important sub-interval of the curve.

This leads in to the method of importance sampling. This method gets its name because it attempts to do more samples at the areas of the function that are more important. The way it does this is by bringing in a probability distribution function (pdf). All this is, is a function that attempts to say which areas of the function in the interval should get more samples. It does this by having a higher probability in that area. This diagram can be used as reference during my explanation.



Figure 2: Stratified Sampling Monte Carlo method. This diagram sees the function interval (a,b) divided into four equal sized intervals - (I1, I2, I3, I4).



Figure 3: Importance Sampling Monte Carlo method. Notice that this graph shows both f(x) and a probability distribution function (p(x)).

Now first of all, note that we can define the integral equation as the following because they are equal -

$$\int_{a}^{b} f(x)dx = \int_{a}^{b} \frac{f(x)}{p(x)} p(x)dx \tag{6}$$

p(x) is the probability distribution function. Note that the integral of p(x) over (a,b) is always equal to 1 and that for no value of x within the interval (a,b) will p(x) evaluate to 0. The question is what do we do with p(x) now that we have put it into the equation. Well, we can use it so that when perform our samples of the curve f(x) within the interval (a,b), we can make the choices taking into account the probability of that particular sample getting selected. For example, according to the example graph about half of the probability curve area is in the last quarter of the interval (a,b). Therefore, when we choose samples we should do it in a way so that half of the samples get taken in this area of the interval.

Now, you may be wondering why we should do this? and how we can do it without jeopardising the accuracy of our approximation? Well, the reason why we should do this, is that if we have chosen a good probability distribution function, then it should have a higher probability for samples to be selected at the important parts of the interval (the parts where the values are highest). Thus, we will spend more effort getting an accurate approximation of the important parts of the curve. But, this will affect the accuracy of our approximation because we will hopefully have a set of samples that focuses on certain parts of the curve. However, we counteract this by giving the value of f(x) / p(x) for every individual sample. This acts as a counterbalance to our unbalanced sampling technique. Thus the end result is a Monte Carlo method that effectively samples the important parts of the curve (as long as it is a good probability distribution function) and then scales this sampling to give an approximation of the integral of f(x). Note again that the success of this method in getting a more accurate approximation is entirely dependent on selecting a good p(x). It has to be one that makes it more likely that a sample will be in an area of the interval(a,b) where the curve f(x) has a higher than the average value (and is thus more important to the approximation).

This method is effective in reducing error when it does have a good pdf because it samples the important parts of the curve more (due to the increased probability of a sample being selected in an important area). Thus it can get a good approximation of these important parts which lowers variance because these important parts are defined so because they have a larger effect on the overall approximation value.

3.5 Program Implementation and Discussion

These methods that are discussed previously are all important methods that do have some key differences. The last two methods are able to improve the accuracy of the approximations greatly, however they do need to have suitable conditions. In the case of importance sampling, it needs a good probability distribution function to come up with an effective approximation. In the case of stratified sampling it can come up with a much more accurate approximation if the shape of the curve is suitable and can be broken up into sections, with some being relatively flat thus allowing a very accurate approximation for that sub-interval. The first two methods, which are really the two basic Monte Carlo methods, are important to know as they both are used as the basis in more complex techniques.

The program implemented all four algorithms, and used them on the function illustrated in the following figure.

Our results did agree with our predictions. The acceptance-rejection method was the most inaccurate. Crude Monte Carlo was the next least effective approximation model. Then the importance sampling model was next with the Stratified Model being the most efficient model in my program. On reflection, this is a sensible result, because the Stratified Model splits the interval into four sub-intervals and two of these sub-intervals have a constant value of 1 (thus a variance of 0). Another contributing factor is in the fact that my probability distribution function models the function effectively enough but a better pdf would have resulted in more accurate results.

Note that a full print out of the results and the program code is in the Appendix. Here is a summary table of the variance results from the program. Note that in my implementation, I also created a hybrid method which was based on the one that I mentioned as a lead in to the discussion on Importance sampling. However, the results for this method were disappointing, although I think it was a fault in implementation because the method sounds feasible. I have included in the results table, although I am sure it should be able to approximate better than the standard stratified sampling model.

I B	
Implementation Results	
Monte Carlo Method	Variance
Crude Monte Carlo	0.022391
Acceptance/Rejection	0.046312
Stratified Sampling	0.011871
Hybrid Model	0.018739
Importance Sampling	0.0223



Figure 4: Program Implementation functions. f(x) is on the top. p(x) is on the bottom.

4 Other Applications for Monte Carlo Techniques

The previous section went into detail about the use of various Monte Carlo methods to evaluate integrals. However Monte Carlo techniques can be applied to many different forms of problems. In fact, Monte Carlo techniques are widely used in physics and chemistry to simulate complex reactions and interactions. This section is to illustrate the use of the basic Monte Carlo algorithm in another form of problem. It is a fairly simplistic example, however it illustrates Monte Carlo being used from a different perspecitive. This form of problem can also be seen in the focus questions in the appendix.

In this example, we have to imagine a coconut shy. We want to determine the probability that if we take 10 shots at the coconut shy we will have an even number of hits. The only fact that we know is that there is a 0.2 probability of having a hit with a single shot. We can work out the answer to this question using Monte Carlo by performing a large number of simulations of taking 10 shots at the coconut shy. We can then count all of the simulations that have an even number of hits and put that number over the total number of simulations. This gives us an approximation of the probability of getting an even number of hits when we take 10 shys at the coconuts.

This example illustrates the use of the Monte Carlo algorithm for a different sort of problem. You may wonder where the use of random numbers is involved in this process. Well, as we know the probability of getting a hit with a single shot, we can use some random process to determine if each shot in each simulation is successful. For example, we could use a random number between 0 and 1 to simulate a shot at the coconuts. If the random number is between 0 and 0.2 then we can call it a hit, otherwise we can count it as a loss. (Note that the probability still stays at 0.2 to score a hit with a single shot). Thus now we can do all of the simulations just by generating random numbers and using these as our single shots at the coconuts.

Thus this is a simple illustration of using the principle behind Monte Carlo methods and applying it to a different form of problem to come out with an effective approximation of the answer. Note that this example is so simple that Monte Carlo techniques would not be a sensible choice in this situation because the actual answer can be worked out with much less effort than performing a few hundred thousand simulations. However Monte Carlo techniques are more valuable when the problem is highly complex and where the effort required to get the actual answer is larger than the amount of effort required to get a reasonable approximation through simulation.

5 Why use Monte Carlo techniques?

Two of the main reasons why we use monte carlo methods are because of their antialiasing properties and their ability to approximate quickly an answer that would be very time-consuming to find out the answer too if we were using methods to determine the exact answer.

This last point refers to the fact that Monte Carlo methods are used to simulate problems that are too difficult and time-consuming to use other methods for. An example is in the use of Monte Carlo techniques in integrating very complex multidimensional integrals. This is a task that other processes can not handle well, but which Monte Carlo can.

The first point refers to the fact that since Monte Carlo methods involve a random component in the algorithm, then this goes some way to avoiding the problems of anti-aliasing (only for certain applications). An example that was brought to my attention was that of finding the area of the black squares on a chess board. Now, if I was using an acceptance-rejection method to attack this problem, I should come out with a fair approximation, due to the fact that I would be going to random points on the chessboard. However what would happen if I was trying to do the same process but I used an algorithm that moved to a certain next point a set distance away and then cotinued to do this, thus not having any random point selection. Well, the potential problem is that this person may have a bad step size and may overevaluate or underevaluate the number of successful trials he has, thus inevitably giving a poor approximation.

These are two solid reasons why people use Monte Carlo techniques. Other possible reasons could include its ease in simulating complex physical systems in the fields of physics, engineering and chemistry.

6 How does this relate to Computer Vision?

Now from the above descriptions, we can see the value of Monte Carlo methods are their ability to give reasonable approximations for problems that can be very complex and time and resource consuming to solve. But how can this ability be used in the field of Computer Vision?

The area of computer vision that I first found Monte Carlo methods being mentioned was object tracking. The article that I found used a Monte Carlo technique discussed an algorithm called CONDENSATION - Conditional Density Propagation for Visual Tracking.

This technique was invented to handle the problem of tracking curves in dense visual clutter. Thus it tracks outlines and features of foreground objects, modeled as curves, as they move in substantial clutter, and in fact does this at a fairly quick, efficient rate.

Basically, the algorithm has a cycle in which it is trying to predict the state that the object is in. It models the state an object is in and then as the picture moves ahead a frame, it trys to guess what likely states the object is now in. The big advantage with this technique is that it keeps multiple hypothesis of the object state open, thus allowing for a bit more flexibility with fixing incorrect guesses as to the object state.

Now, the computer holds these guesses as to what the state is going to be as probability distribution functions. In this case the areas of the curve with higher probability are the states the computer thinks are going to be next. The last step is where Monte Carlo Methods come into the procedure. This is where the computer randomly samples from this probability distribution function (which is guessing at the state of the object). It then checks these samples with image data to see if they support any of the states of the object at all. The more accurate the sample, then the more successfully weighted the sample response is.

Thus once you are finished taking the samples you now have the new probability distribution for the new frame of movement which will reflect the probable parameter state that the object is in.

Another article that I found used Monte Carlo methods involved Object Recognition. It used Monte Carlo methods to solve a complex integral that related back to do with the probability that something was being falsely recognised as the object.

So, there are two examples of Computer Vision's use for Monte Carlo methods. I am sure that they have many applications in other areas of Computer Vision. Especially, with their ability to give accurate approximations to complex integrals, as integral calculus is used in many different areas of Computer Science.

7 Conclusion

Monte Carlo methods are a very broad area of mathematics. They allow us to get reasonable approximations of very difficult problems through simulation and the use of random numbers. I discussed four of these methods that can be used in the evaluation of integrals. I then discussed my implementations of these methods and discussed my program results. Finally, I gave two examples of Monte Carlo methods being used within the field of Computer Science.

8 Appendix

8.1 Appendix A - Basic Mathematics Overview

8.1.1 Sigma Notation

$$\sum_{n=1}^{10} \tag{7}$$

The Greek letter, sigma, is very often used in mathematics to represent the sum of a series. It is a shorthand notation. An example is -

$$\sum_{n=1}^{10} 3n$$
 (8)

This is shorthand for the series starting with the first term and ending with the tenth term of 3n. Thus it equals = 3(1) + 3(2) + 3(3) + 3(4) + 3(5) + 3(6) + 3(7) + 3(8) + 3(9) + 3(10) = 165

The symbol 3n is called the summand, the numbers 1 and 9 are the limits of the summation, and the symbol n is the index.

8.1.2 Variance and Standard Deviation

The variance is a measure of how spread out a distribution is. It is computed as the average squared deviation of each number from its mean.

For example, for the numbers 1, 2, and 3 the mean is 2 and the variance is:

$$\frac{(1-2)^2 + (2-2)^2 + (3-2)^2}{3} = 0.667$$
(9)

The formula for the variance in a population where m is the mean and N is the number of scores is -

$$s^{2} = \frac{1}{N} \sum_{i=1}^{N} (X_{i} - \mu)^{2}$$
(10)

When the variance is computed in a sample you multiply by 1/(N-1) instead.

8.2 Appendix B - Program Code and Results

I have included my code and output from my program. It is attached to this tutorial.

8.3 Appendix C - Focus Question

8.3.1 Background

A student exits his COSC 453 lecture in a bewildered state. He is at position 4 on the map. He has four possible choices of direction in which to go but he is so bewildered that he is equally likely to choose each direction (thus a probability of 0.25 of heading in any particular direction). Now at each position on the outside of the map, the student will find an activity to do for the afternoon thus when a student reaches one of these boundary positions he stops. The four points in the middle of the map (4,5,8,9) the bewildered student is still looking for something to do for the afternoon and once is equally likely to head in any one of the four directions available (even back to the point he just came from).

8.3.2 Question

Using the Monte Carlo method, describe how you would find out an approximation of the probability that a student leaving his COSC 453 lecture will find it to one of the two pubs on the map.

8.3.3 Key

- 1 = Back to the flat
 - 2 = Back to the graphics lab to do some study
 - 3 = Back to the AI lab to do some study
 - 4 = Starting position A junction with four possible next moves
 - 5 = A junction with four possible next moves
 - 6 = Poppa's Pizza to get some lunch
 - 7 =Goes to the dental school for an appointment
 - 8 = A junction with four possible next moves
 - 9 = A junction with four possible next moves
 - 10 = The Garden Sports Tavern (A pub)
 - 11 = The Captain Cook (Also a pub)
 - 12 = The Union to participate in a student protest

8.4 Appendix D - Project Sources

I have used a variety of sources to help develop my knowledge on Monte Carlo methods. They could prove to be helpful for anybody looking to do some extra reading on the topic. Here is a list of material that I have used but not directly referenced.



Figure 5: Map of the states for the question. Note that each outside state is a destination and is not able to be left.

Internet

-http://wwitch.unl.edu/zeng/joy/mclab/mcintro.html

-http://stud4.tuwien.ac.at/

-http://csep1.phy.ornl.gov/CSEP/MC/MC.html

Books

- Introduction to the Monte-Carlo Method, Author = Istvan Manno, Publisher = AKADEMIAI KIADO, Budapest, Year = 1999

- The Monte Carlo Method, Editor = Yu. A. Shreider, Publisher = Pergamon Press, Year = 1966

-The Monte Carlo Method of Evaluating Integrals, Author = Daniel T. Gillespie, Publisher = Naval Weapons Center, Year = 1975