1

Introduction

1.1 A brief history of the Monte Carlo method

In this section we outline the important historical developments in the evolution of the Monte Carlo method. This section is just for fun; feel free to skip over it to the next chapter if you’re not interested.

The idea of Monte Carlo calculation is a lot older than the computer. The name “Monte Carlo” is relatively recent—it was coined by Nicolas Metropolis in 1949—but under the older name of “statistical sampling” the method has a history stretching back well into the last century, when numerical calculations were performed by hand using pencil and paper and perhaps a slide-rule. As first envisaged, Monte Carlo was not a method for solving problems in physics, but a method for estimating integrals which could not be performed by other means. Integrals over poorly-behaved functions and integrals in high-dimensional spaces are two areas in which the method has traditionally proved profitable, and indeed it is still an important technique for problems of these types. To give an example, consider the function

\[ f(x) \equiv \sin^2 \frac{1}{x} \]  

which is pictured in Figure 1.2. The values of this function lie entirely between zero and one, but it is increasingly rapidly varying in the neighbourhood of \( x = 0 \). Clearly the integral

\[ I(x) \equiv \int_0^x f(x') \, dx' \]  

which is the area under this curve between 0 and \( x \), takes a finite value somewhere in the range \( 0 < I(x) < x \), but it is not simple to calculate this value exactly because of the pathologies of the function near the origin.
Figure 1.1  The pathological function \( f(x) \equiv \sin^2 \frac{1}{x} \), whose integral with respect to \( x \), though hard to evaluate analytically, can be evaluated in a straightforward manner using the Monte Carlo integration technique described in the text.

However, we can make an estimate of it by the following method. If we choose a random real number \( h \), uniformly distributed between zero and \( x \), and another \( v \) between zero and one and plot on Figure 1.2 the point for which these are the horizontal and vertical coordinates, the probability that this point will be below the line of \( f(x) \) is just \( I(x)/x \). It is easy to determine whether the point is in fact below the line: it is below it if \( h < f(v) \). Thus if we simply pick a large number \( N \) of these random points and count up the number \( M \) which fall below the line, we can estimate \( I(x) \) from

\[
I(x) = \lim_{N \to \infty} \frac{Mx}{N}.
\]  

(1.3)

You can get an answer accurate to one figure by taking a thousand points, which would be about the limit of what one could have reasonably done in the days before computers. Nowadays, even a cheap desktop computer can comfortably run through a million points in a few seconds, giving an answer accurate to about three figures. In Figure 1.3 we have plotted the results of such a calculation for a range of values of \( x \). The errors in this calculation are smaller than the width of the line in the figure.\(^1\)

A famous early example of this type of calculation is the experiment known as “Buffon’s needle” (Dörrie 1965), in which the mathematical constant \( \pi \) is determined by repeatedly dropping a needle onto a sheet of paper ruled with evenly spaced lines. The experiment is named after Georges-Louis Leclerc, Comte de Buffon who in 1777 was the first to show that if we throw a needle of length \( l \) completely at random onto a sheet of paper ruled with lines a distance \( d \) apart, then the chances that the needle will fall so as to intersect one of the lines is \( 2l/\pi d \), provided that \( d \geq l \). It was Laplace in 1820 who then pointed out that if the needle is thrown down \( N \) times and is observed to land on a line \( M \) of those times, we can make an estimate of \( \pi \) from

\[
\pi = \lim_{N \to \infty} \frac{2Nl}{Md}.
\]  

(1.4)

Perhaps the connection between this and the Monte Carlo evaluation of integrals is not immediately apparent, but it will certainly become clear

\(^{1}\)In fact there exist a number of more sophisticated Monte Carlo integration techniques which give more accurate answers than the simple “hit or miss” method we have described here. A discussion can be found in the book by Kalos and Whitlock (1986).
if you try to derive Equation (1.44) for yourself, or if you follow Dörrie’s derivation.) A number of investigators made use of this method over the years to calculate approximate values for $\pi$. The most famous of these is Mario Lazzarini, who in 1901 announced that he had calculated a value of $3.1415929$ for $\pi$ from an experiment in which a $2\frac{1}{2}$ cm needle was dropped 3408 times onto a sheet of paper ruled with lines 3 cm apart. This value, accurate to better than three parts in ten million, would be an impressive example of the power of the statistical sampling method were it not for the fact that it is almost certainly faked. Badger (1994) has demonstrated extremely convincingly, that, even supposing Lazzarini had the technology at his disposal to measure the length of his needle and the spaces between his lines to a few parts in $10^7$ (a step necessary to ensure the accuracy of Equation (1.44)), still the chances of his finding the results he did were poorer than three in a million; Lazzarini was imprudent enough to publish details of the progress of the experiment through the 3408 castings of the needle, and it turns out that the statistical “fluctuations” in the numbers of intersections of the needle with the ruled lines are much smaller than one would expect in a real experiment. All indications are that Lazzarini forged his results. However, other, less well known attempts at the experiment were certainly genuine, and yielded reasonable figures for $\pi$: 3.1596 (Wolf 1850), 3.1553 (Smith 1855). Apparently, performing the Buffon’s needle experiment was for a while quite a sophisticated pastime amongst Europe’s intellectual gentry.

With the advent of mechanical calculating machines at the end of the nineteenth century, numerical methods took a large step forward. These machines increased enormously the number and reliability of the arithmetic operations that could be performed in a numerical “experiment”, and made the application of statistical sampling techniques to research problems in physics a realistic possibility for the first time. An early example of what was effectively a Monte Carlo calculation of the motion and collision of the molecules in a gas was described by William Thomson (later Lord Kelvin) in 1901. Thomson’s calculations were aimed at demonstrating the truth of the equipartition theorem for the internal energy of a classical system. However, after the fashion of the time, he did not perform the laborious analysis himself, and a lot of the credit for the results must go to Thomson’s secretary, William Anderson, who apparently solved the kinetic equations for more than five thousand molecular collisions using nothing more than a pencil and a mechanical adding machine.

Aided by mechanical calculators, numerical methods, particularly the
method of finite differences, became an important tool during the First World War. The authors recently heard the intriguing story of the Herculean efforts of French mathematician Henri Soudée, who in 1916 calculated firing tables for the new 400 mm cannons being set up at Verdun, directly from his knowledge of the hydrodynamic properties of gases. The tables were used when the cannons were brought to bear on the German-occupied Fort de Douaumont, and as a result the fort was taken by the allies. Soudée was later honoured by the French. By the time of the Second World War the mechanical calculation of firing angles for large guns was an important element of military technology. The physicist Richard Feynman tells the story of his employment in Philadelphia during the summer of 1940 working for the army on a mechanical device for predicting the trajectories of planes as they flew past (Feynman 1985). The device was to be used to guide anti-aircraft guns in attacking the planes. Despite some success with the machine, Feynman left the army’s employ after only a few months, joking that the subject of mechanical computation was too difficult for him. He was shrewd enough to realize he was working on a dinosaur, and that the revolution of electronic computing was just around the corner. It was some years however before that particular dream would become reality, and before it did Feynman had plenty more chance to spar with the mechanical calculators. As a group leader during the Manhattan Project at Los Alamos he created what was effectively a highly pipelined human CPU, by employing a large number of people armed with Marchant mechanical adding machines in an arithmetic assembly line in which little cards with numbers on were passed from one worker to the next for processing on the machines. A number of numerical calculations crucial to the design of the atomic bomb were performed in this way.

The first real applications of the statistical sampling method to research problems in physics seem to have been those of Enrico Fermi, who was working on neutron diffusion in Rome in the early 1930s. Fermi never published his numerical methods—apparently he considered only the results to be of interest, not the methods used to obtain them—but according to his influential student and collaborator Emilio Segrè those methods were, in everything but name, precisely the Monte Carlo methods later employed by Ulam and Metropolis and their collaborators in the construction of the hydrogen bomb (Segrè 1980).

So it was that when the Monte Carlo method finally caught the attention of the physics community, it was again as the result of armed conflict. The important developments took place at the Los Alamos National Laboratory in New Mexico, where Nick Metropolis, Stanislaw Ulam and John von Neumann gathered in the last months of the Second World War shortly after the epochal bomb test at Alamagordo, to collaborate on numerical calculations to be performed on the new ENIAC electronic computer, a mammoth, room-
filing machine containing some 18,000 triode valves, whose construction was nearing completion at the University of Pennsylvania. Metropolis (1980) has remarked that the technology that went into the ENIAC existed well before 1941, but that it took the pressure of America’s entry into the war to spur the construction of the machine.

It seems to have been Stan Ulam who was responsible for reinventing Fermi’s statistical sampling methods. He tells of how the idea of calculating the average effect of a frequently repeated physical process by simply simulating the process over and over again on a digital computer came to him whilst huddling over a pack of cards, playing patience\(^2\) one day. The game he was playing was “Canfield” patience, which is one of those forms of patience where the goal is simply to turn up every card in the pack, and he wondered how often on average one could actually expect to win the game. After abandoning the hopelessly complex combinatorics involved in answering this question analytically, it occurred to him that you could get an approximate answer simply by playing a very large number of games and seeing how often you win. With his mind never far from the exciting new prospect of the ENIAC computer, the thought immediately crossed his mind that he might be able to get the machine to play these games for him far faster than he ever could himself, and it was only a short conceptual leap to applying the same idea to some of the problems of the physics of the hydrogen bomb that were filling his work hours at Los Alamos. He later described his idea to John von Neumann who was very enthusiastic about it, and the two of them began making plans to perform actual calculations. Though Ulam’s idea may appear simple and obvious to us today, there are actually many subtle questions involved in this idea that a physical problem with an exact answer can be approximately solved by studying a suitably chosen random process. It is a tribute to the ingenuity of the early Los Alamos workers that, rather than plunging headlong into the computer calculations, they considered most of these subtleties right from the start.

The war ended before the first Monte Carlo calculations were performed on the ENIAC. There was some uncertainty about whether the Los Alamos laboratory would continue to exist in peacetime, and Edward Teller, who was leading the project to develop the hydrogen bomb, was keen to apply the power of the computer to the problems of building the new bomb, in order to show that significant work was still going on at Los Alamos. Von Neumann developed a detailed plan of how the Monte Carlo method could be implemented on the ENIAC to solve a number of problems concerned with neutron transport in the bomb, and throughout 1947 worked with Metropolis on preparations for the calculations. They had to wait to try their ideas out however, because the ENIAC was to be moved from Philadelphia where it

\(^2\)Also called “solitaire” in the USA.
was built to the army’s Ballistics Research Laboratory in Maryland. For a modern computer this would not be a problem, but for the gigantic ENIAC, with its thousands of fragile components, it was a difficult task, and there were many who did not believe the computer would survive the journey. It did, however, and by the end of the year it was working once again in its new home. Before von Neumann and the others put it to work on the calculations for the hydrogen bomb, Richard Clippinger of the Ballistics Lab suggested a modification to the machine which allowed it to store programs in its electronic memory. Previously a program had to be set up by plugging and unplugging cables at the front of the machine, an arduous task which made the machine inflexible and inconvenient to use. Von Neumann was in favour of changing to the new “stored program” model, and Nick Metropolis and von Neumann’s wife, Klari, made the necessary modifications to the computer themselves. It was the end of 1947 before the machine was at last ready, and Metropolis and von Neumann set to work on the planned Monte Carlo calculations.

The early neutron diffusion calculations were an impressive success, but Metropolis and von Neumann were not able to publish their results, because they were classified as secret. Over the following two years however, they and others, including Stan Ulam and Stanley Frankel, applied the new statistical sampling method to a variety of more mundane problems in physics, such as the calculation of the properties of hard-sphere gases in two and three dimensions, and published a number of papers which drew the world’s attention to this emerging technique. The 1949 paper by Metropolis and Ulam on statistical techniques for studying integro-differential equations is of interest because it contained in its title the first use of the term “Monte Carlo” to describe this type of calculation. Also in 1949 the first conference on Monte Carlo methods was held in Los Alamos, attracting more than a hundred participants. It was quickly followed by another similar meeting in Gainesville, Florida.

The calculations received a further boost in 1948 with the arrival at Los Alamos of a new computer, humorously called the MANIAC. (Apparently the name was suggested by Enrico Fermi, who was tiring of computers with contrived acronyms—he claimed that it stood for “Metropolis and Neumann Invent Awful Contraption”. Nowadays, with all our computers called things like XFK–23/z we would no doubt appreciate a few pronounceable names.) Apart from the advantage of being in New Mexico rather than Maryland, the MANIAC was a significant technical improvement over the ENIAC which Presper Eckert (1980), its principal architect, refers to as a “hastily built first try”. It was faster and contained a larger memory (40 kilobits, or 5 kilobytes in modern terms). It was built under the direction of Metropolis, who had been lured back to Los Alamos after a brief stint on the faculty at Chicago by the prospect of the new machine. The design was based
on ideas put forward by John von Neumann and incorporated a number of
technical refinements proposed by Jim Richardson, an engineer working on
the project. A still more sophisticated computer, the MANIAC 2, was built
at Los Alamos two years later, and both machines remained in service until
the late fifties, producing a stream of results, many of which have proved to
be seminal contributions to the field of Monte Carlo simulation. Of partic-
ular note to us is the publication in 1953 of the paper by Nick Metropolis,
Marshall and Arianna Rosenbluth, and Edward and Mici Teller, in which
they describe for the first time the Monte Carlo technique that has come to
be known as the Metropolis algorithm. This algorithm was the first example
of a thermal “importance sampling” method, and it is to this day easily the
most widely used such method. We will be discussing it in some detail in
Chapter 3. Also of interest are the Monte Carlo studies of nuclear cascades
performed by Antony Turkevich and Nick Metropolis, and Edward Teller’s
work on phase changes in interacting hard-sphere gases using the Metropolis
algorithm.

The exponential growth in computer power since those early days is by
now a familiar story to us all, and with this increase in computational re-
sources Monte Carlo techniques have looked deeper and deeper into the
subject of statistical physics. Monte Carlo simulations have also become
more accurate as a result of the invention of new algorithms. Particularly in
the last twenty years, many new ideas have been put forward, of which we
describe a good number in the rest of this book.