Monte Carlo

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Abstract
The Monte Carlo method is a technique for solving, by use of their statistical analogues, deterministic or stochastic mathematical problems that cannot be solved using traditional closed-form algebraic means. The method was married to the earliest computers at the Manhattan Project. We characterise statistical sampling, outline a broad range of problems, and explore a means of determining the value of π. Absent truly random sequences of numbers, alternatives are used. The Markov Chain Monte Carlo method has led to a revolution in the application of Bayesian statistics. Applications in management, the social sciences, and computer simulations are addressed.

Definition
Monte Carlo
The Monte Carlo method is, broadly, a technique that solves mathematical problems by solving their statistical analogues, by subjecting random numbers to numerical processes. The method uses statistical sampling to obtain solutions to deterministic or stochastic problems that cannot readily be solved using closed-form techniques.

Monte Carlo

The Monte Carlo method is a technique for solving, by use of their statistical analogues, deterministic or stochastic mathematical problems that are not amenable to solution using traditional closed-form algebraic means. In one type of problem, the Monte Carlo method consists in formulating a game of chance or a stochastic (probabilistic) process that produces a random variable whose expected value is the deterministic solution to a certain problem. An approximation to the expected value is then obtained by means of sampling from the resulting distribution (Bauer, 1968). The primary source of error in the approximation is due to the fact that only a finite sample can be taken, although the greater the number of samples, the lower the error, as in the Buffon Needle example below.

It is also possible to estimate other moments from the sample distribution, especially useful when the problem is not deterministic: a second type of problem occurs in non-parametric econometrics, when the conditions required for an analytical probability distribution are not satisfied (for example, the error term is skewed) or when the mathematics for a statistic is intractable (for instance, the difference between two sample medians). In these cases and others, Monte Carlo simulation can be used to estimate the sampling distribution of a statistic empirically (Mooney, 1997).

As well as assessing the distribution of a new statistic, the Monte Carlo method can be used to assess the robustness of an empirical or simulated analysis to variations in initial conditions or other definitions of the pseudo-population, the set of samples. The method can also be used to search for theoretical formulations of newly constructed statistics. As a computationally intensive technique, Monte Carlo is almost always performed using computers.

Origins

Polymath Stanislaw Ulam faced a tough problem. At the Manhattan Project to develop the atomic bomb in the 1940s, he needed to determine answers to the collective patterns of neutron emissions possibly leading to a chain reaction. Although he knew the basic properties of the motion of such neutrons moving in the medium, try as he might he could not derive closed-form expressions for their equations of motion, including the possibilities of colliding with nuclei. The stochastic calculus required was too complex. And yet the success of the project, and perhaps of the war, depended on solving this problem.

It occurred to Ulam that he could solve it without deriving an explicit, closed-form solution. Rather, he could start a simulation of a neutron's trajectory, and then choose its successive velocities by selecting from the experimentally determined probability distributions at each impact. And then repeat the exercise many times: no two trajectories would be identical, but each would satisfy the experimental probability distributions. The distribution of paths derived using this statistical sampling would give him the answer sought, and the greater the number of paths, the more reliable the distribution. Ulam's first simulations were painstakingly performed with a calculator, but his insights led John von Neumann to arrange for these simulations to be performed on ENIAC, one of the earliest digital computers (Eckhardt, 1987). Although the method had been known (as 'statistical sampling') and used previously, it was not until the advent of such computers that it became practicable. It was named after the casino in Monaco, apparently frequented by Ulam's uncle (Metropolis, 1987).[1]

Buffon's Needle

To give a mundane example of the first type of problem: we can use the statistical sampling of the Monte Carlo method to derive ever more precise estimates of the value of π, by measuring the frequency of a pin, dropped at random, in falling across one of a pair of parallel lines, the Buffon Needle problem (Ramaley, 1969).

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1. Like Stan Ulam, the author too was struggling with the stochastic calculus of newly constructed statistic, the State Similarity Measure (Marks, 2013), when he too realised that he could simulate with a Monte Carlo sampling from a (pseudo) random number generator to compare the output from his simulations and from historical market data with randomly generated data.

Consider a needle of length $2N$ dropped at random between two parallel lines D units apart, where $2N < D$. Let x be the distance from the centre of the needle to the nearer of the two lines. The probability P of the needle crossing the nearer line is given by the product of the two independent probabilities, P_1 and P_2, where P_1 is the probability that the needle could cross the line if oriented appropriately (i.e., that $x < N$), and P_2 is the probability that a randomly oriented needle with its centre $x < N$ from the line crosses the line.

The probability P_1 is given by the ratio $2N/D < 1$. The probability P_2 is given by the ratio of the angle 2ϕ to π, the semi-circle (in radians), where ϕ is the angle as shown in Figure 1.

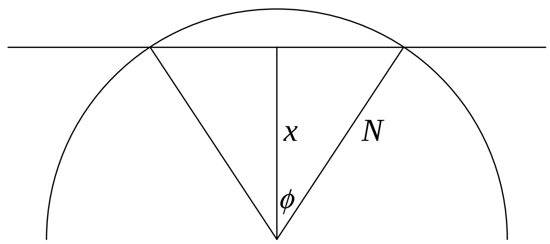

Figure 1 : The Buffon Needle problem

Since $\cos\phi = \frac{x}{N}$, then $\phi = \arccos\frac{x}{N}$. Probability P_2 is given by integrating x between 0 and N: $P_2 = \frac{2}{\pi}\int_0^N \arccos\frac{x}{N}\,dx$. Let $y \equiv \frac{x}{N}$, then $P_2 = \frac{2}{\pi}\int_0^1 \arccos y\,dy = \frac{2}{\pi}$. Therefore the probability P that the needle dropped at random between the parallel lines will cross a line is given by $P_1 \times P_2 = \frac{4N}{\pi D}$. If the needle's length is half the distance between the lines (i.e., $2N = \frac{1}{2}D$), then $P = \frac{1}{\pi}$.

Given this derivation, we can estimate the value of π by randomly dropping a needle of length 1 between a pair of parallel lines 2 units apart, and tallying the frequency of the needle crossing a line. The sample mean of this frequency tends to $1/\pi$. The greater the number of samples, the better the estimate, i.e., the more reliable the number obtained. This is an example of using the Monte Carlo method to estimate a deterministic value without using computers.

How could we simulate the Buffon Needle problem? We could choose two numbers, r and θ, that are random, uniformly distributed between 0 and 1. Tally the frequency of the joint event of, first, $r < 2N/D$ (i.e. the needle could cross the nearer line), and, second, $\theta < \frac{2}{\pi}\arccos\left(\frac{D}{2N}r\right)$ (i.e. the needle crosses the nearer line). The frequency of this event will tend to $4N/\pi D$ as the number of samples increases. Of course, this simulation requires the use of a trigonometric function and the number we seek, π. The attraction of the actual needle-dropping is that these things are implicit in the problem set-up, which can also be seen as a way in which the two uniform probability distributions are transformed into the joint event whose frequency is a simple function of the number we seek, π.

In general, there are two ways to use uniform distributions to generate the desired non-uniform distributions (Eckhardt, 1987). First, parametrically, using the inverse of the desired function: if g is the desired function, then one applies the inverse function $f(x) = g^{-1}(x)$ to a uniform distribution of random numbers, x. Second, if it is difficult or impossible to form the inverse function (perhaps there are only empirical samples of function $g(x)$), then use von Neumann's 'acceptance-rejection' technique, using two uniformly distributed random variables, as seen in the simulation of the Buffon Needle example above.

This transformation of uniformly distributed random variables into variables whose non-uniform distributions reflect the phenomena under examination is essential for the Monte Carlo method. If the only information we have is historical data, then, rather than fitting the data to a known distribution (which, for complex processes is unlikely to be correct), it is far better to rely on non-parametric techniques to use this data to derive simulation results, as did Ulam in 1944. See the non-parametric bootstrap techniques below.

Pseudo-Random and Quasi-Random Sequences

Judd (1998) reminds us that truly random sequences are difficult to construct, and so rarely used in Monte Carlo methods.[2] Instead, almost all Monte Carlo implementations use *pseudo-random sequences*, that is, deterministic sequences that seem to be random in that they display some properties satisfied by random sequences. Two basic properties are zero serial correlation and the correct frequency of runs, both of which the pseudo-random sequences generated by some algorithm should come close to satisfying to be useful for the Monte Carlo method. But for some purposes, *quasi-random sequences* (or *low-discrepancy sequences*) might be preferable: although they lack the serial independence of pseudo-randoms, they present a much more uniform coverage of the domain, avoiding clusters and gaps in the patterns of a finite sequence.

Stochastic Estimation, Bootstrapping, and Markov Chain Monte Carlo

As mentioned above, we can use Monte Carlo to derive estimates of the parameters of stochastic processes. In particular, we can derive the sampling distribution in three ways, where 'bootstrap' generally refers to replicating an experiment by resampling from a given distribution function (parametric) or from observed data (non-parametric) (Rizzo & Albert, 2010): parametric bootstrap: repeated sampling from a given probability distribution; ordinary bootstrap: resampling with replacement from an observed sample (non-parametric); and permutation bootstrap: applying resampling without replacement (non-parametric).

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2. The recent development of affordable, practical, true random-number generators, based on quantum physics is a breakthrough (ID Quantique, 2010).

The use of Monte Carlo bootstrapping has allowed the widespread use of the Markov Chain Monte Carlo methods of numerically calculating multi-dimensional integrals, by deriving correlated random samples, where the Markov chain is constructed so as to have the integrand as its equilibrium. MCMC methods include (uncorrelated) random walk Monte Carlo methods. MCMC has enabled the practical use of Bayesian statistics, and is also used in computational physics, biology, and linguistics (Diaconis, 2009).[3]

Uses in Management and the Social Sciences

Following Metropolis & Ulam's 1949 article, Monte Carlo was soon used by statisticians and econometricians. The first uses by management scientists were for railroad car management (Crane et al., 1955), investment in heavy industry (Jones & Lee, 1955), and air traffic control (Blumstein, 1957). Agricultural economists (Willis et al., 1969) were amongst the first social scientists to use the method, although Hammersley & Morton (1954) offered a problem from archæology. The first suggestion for the use of the Monte Carlo method in strategic management was (future Nobel Laureate) Sharpe (1969).

With the rise of computational simulation models in strategy, and in particular the use of agent-based models (Tesfatsion & Judd, 2006), Monte Carlo methods have facilitated the modelling of market interactions of heterogeneous firms and other economic actors. Such models might rely on random numbers, first, to generate exogenous events, and, second, to initialise the attributes of the agents, subject to a statistical distribution.

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3. MCMC is another valuable side-product of the Manhattan Project; see Metropolis et al. (1953).

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