3. Monte Carlo - introduction

3.1. Definition

[Own knowledge, Antti Kuronen's lecture; http://www-groups.dcs.st-andrews.ac.uk/ history/HistTopics/Pi_through_the_ages.html]

In the widest sense of the term, **Monte Carlo** (MC) simulations mean any simulation (not even necessarily a *computer* simulation) which utilizes random numbers in the simulation algorithm.

The term "Monte Carlo" does indeed come from the famous casinos in Monte Carlo. When study of MC methods became in earnest in the 1940's and 1950's, someone thought of the likeness of using random numbers to the randomness in the games at the casino, and named the method thereafter.

Another closely related term is **stochastic** simulations, which means the same thing as Monte Carlo simulations. Even though stochastic would seem to be a more descriptive term, since the chances of misunderstandings are much smaller, Monte Carlo is more widely used probably for no better reason that that it sounds more exciting.

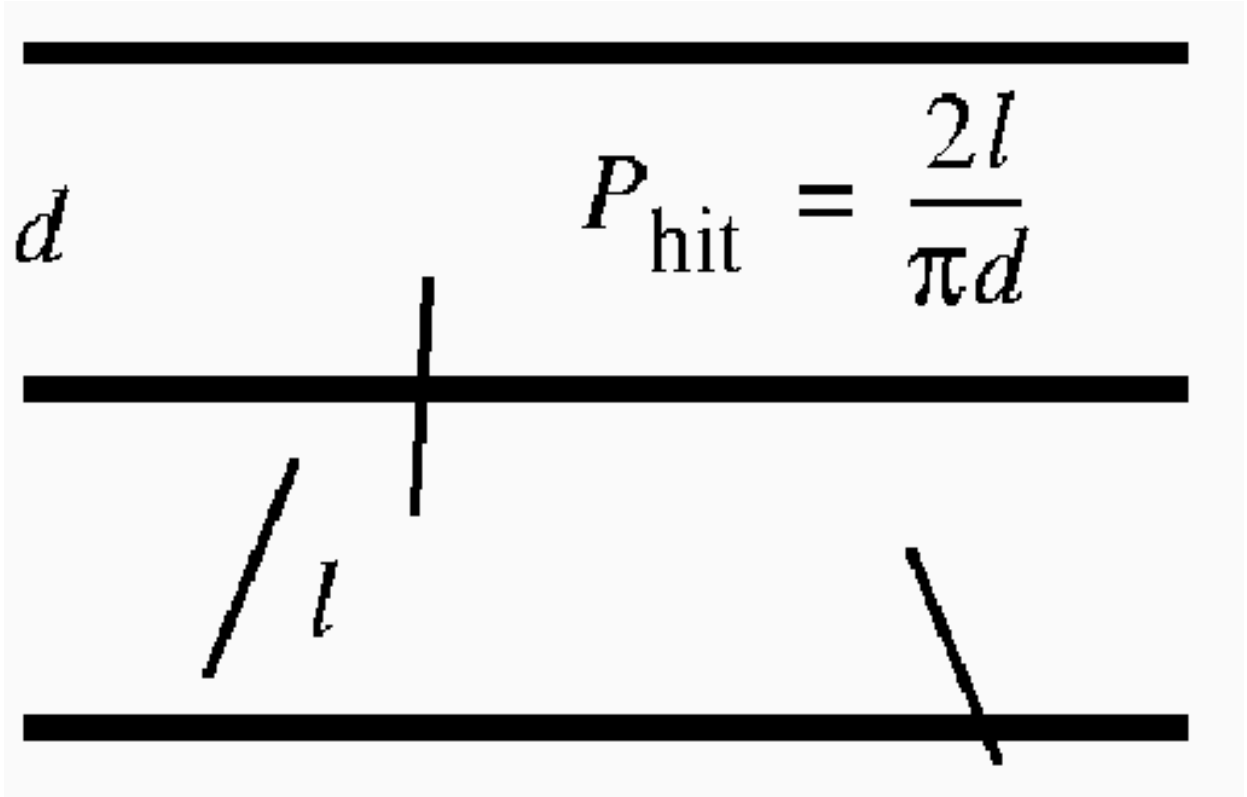
The idea of using randomness to obtain an answer to a scientific problem is actually much older than computers.

3.2. Very brief history

It was Buffon (1707 - 1788) who found out that if one has a uniform grid of parallel lines, distance d apart, and if one drops a needle of length $l < d$ on the grid, the probability that the needle falls across a line is

$$P_{hit} = \frac{2l}{\pi d}$$

(Proving this is left as an exercise).

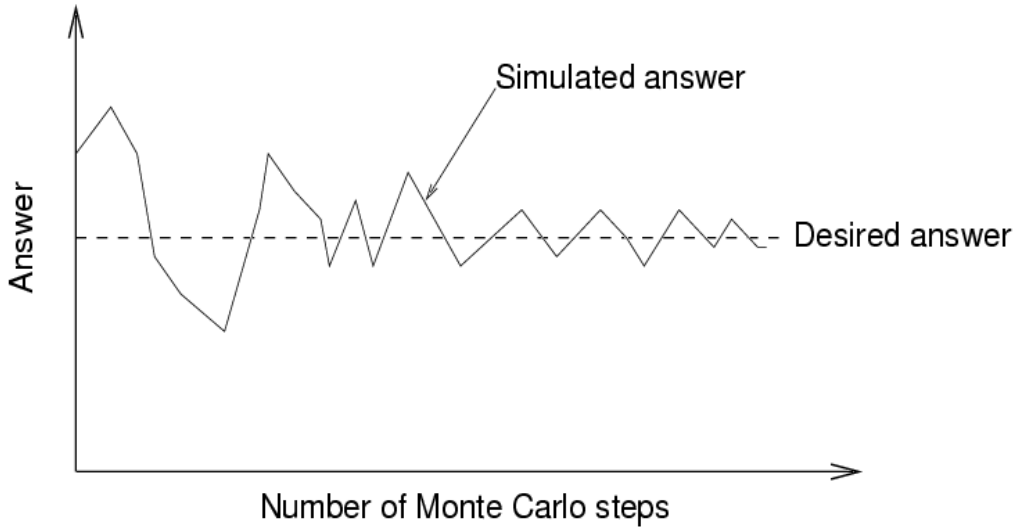


Various people have tried to calculate π by throwing needles. The most remarkable result was that of Lazzarini (not Lazzerini) (1901), who made 3408 tosses and got

$$\pi = \frac{355}{113} = 3.1415929$$

This outcome is suspiciously good.

This actually nicely illustrates a potential pitfall in MC simulations. If you know in advance the answer you want to get, and start doing MC to obtain it looking after every step at your intermediate answer, your result will behave something like follows:



So if you stop the simulation exactly when you happen to cross the 'right answer' line, you will get the right answer! But doing this is of course utterly wrong.

In practice, people seldom do MC simulations knowing the answer in advance (what would be the point of the simulation). But a more dangerous and common pitfall is that you e.g. wish for a low, or high, value, you stop the simulation at a value in one of the ends.

So pretty obviously, what Lazzarini did is stop his needle throwing when he got the accurate answer, which explains the strange number 3408 of tosses.

To avoid this pitfall, one should always decide in advance how many MC steps to do.

Since Buffon's needle, random numbers were used now and then in statistics, e.g. by Student (in connection with developing the distribution which carries his name). But the wide use began really in the 1940's, in connection with the Manhattan project. Semi-mechanical computers were used to model the diffusion of neutrons in fissile materials by Ulam and von Neumann. This work soon lead to the more widespread use of such methods in other, less explosive, problems in physics; already in 1948 Fermi, Metropolis, and Ulam obtained Monte Carlo estimates for the eigenvalues of the Schrödinger equation. [http://stud2.tuwien.ac.at/ e9527412/history.html]

3.3. Terminology

The term "MC" is actually extremely wide, and there is much overlap.

To give a concrete example, the molecular dynamics simulations which describe atomistic motion are in principle completely deterministic in nature. But in practice, one often uses random numbers in MD as well. The initial atom velocities are usually given randomly, so this brings in an MC character. But only because of this MD simulations are not called MC.

But in more advanced cases MD is often used within an MC scheme. As a concrete example, consider for instance a radiation physics problem: we have a particle which impacts on a lattice. (FIGURE DRAWN ON LECTURE). The outcome (how deep in and where does it go) will be strongly dependent on the impact position. Hence one needs to simulate numerous (tens – thousands) of events to get a comprehensive picture of what can happen, and collect statistics. The initial impact positions are chosen randomly, so the set of simulations forms an MC simulation. The whole scheme could be called MC-MD (but usually is not).

I list here some of the more common MC terms in Physics and briefly describe what they are.

Metropolis MC

A simulation algorithm, central to which is the formula which determines whether a process should happen or not. Originally used for simulating atom systems in an NVT thermodynamic ensemble, but nowadays generalized to many other problems.

Simulated annealing

The Metropolic MC idea generalized to optimization, i.e. finding minima or maxima in a system. This can be used in a very wide range of problems, many of which have nothing to do with physics.

Thermodynamic MC

MC when used to determine thermodynamic properties, usually of atomic systems.

Lattice MC, LMC

MC used on a lattice. In condensed matter physics this is used to distinguish MC done on crystal lattices from those done in a random/amorphous medium

Kinetic MC, KMC

MC used to simulate activated processes, i.e. processes which occur with an exponential probability

$$e^{-E_a/k_BT}$$

Typical example is the migration of defects in a solid. This can be done either in a non-directional system, or on a lattice. In the latter case one could also talk about lattice kinetic MC.

Variational MC, VMC

Diffusion MC, DMC

These terms, although very wide in principle, are nowadays used often to signify a variety of electronic structure calculations where MC techniques are used to obtain the ground state electron configuration. Sometimes the terms are used without specifying that one deals with electronic structure, which may lead to confusion as "diffusion MC" obviously could mean many other things as well.

Quantum Monte Carlo, QMC

Another term which is used in many different contexts. One is that the electronic structure calculation methods VMC and DMC are often called QMC. Another is that quantum mechanical

simulations of spin systems (which does not necessarily relate to electronic structure-determining calculations in any direct way) are also called QMC...

MC for radiation effects

In the field of ion irradiation, a method used often to calculate the depth to which an ion penetrates in a solid selects the position of the next colliding atom randomly. Hence this is clearly a variety of MC. Unfortunately it is common usage to call this method $only$ MC, to distinguish with methods where the next colliding atom has a fixed lattice position, the so called BCA (binary collision approximation) method.

This usage is extremely misleading, for three main reasons. 1. There are a zillion other MC methods, as seen from the list above. 2. Also the lattice-based BCA methods are MC since the initial atom position is random, and 3. Also the "MC" method is a binary collision method, i.e. a BCA method

A more recommended usage would to talk about MC-BCA vs. crystal BCA.

In general, these examples emphasize that one should avoid using any XXXMC term and abbreviation without (at least in the beginning of the text) clearly defining precisely which context it is related to.