Shooting blindly

Finally, we would like to show how one can use random numbers to perform calculations. This technique is called the **Monte Carlo** method, since it has a lot in common with a casino, in which chance plays a decisive role. The method was invented by Stanislaw Ulam; when recovering from a serious illness he took to playing the solitaire game Canfield. While trying to calculate the probability of winning, Ulam came to the conclusion that it would be much easier to play a hundred times and use the outcomes of the games to approximate the chance of winning, rather than to calculate the exact result by means of rather complex combinatorial calculations. This simple yet brilliant observation is the basic idea of the Monte Carlo method.

A simple application of this method is in the calculation of area under the graph of a function $f(x)$ over the range (a, b); in other words, the calculation of the **integral** of $f(x)$ from a to b. In order to achieve this, we generate some random points within the given range, calculate the average value of f at these

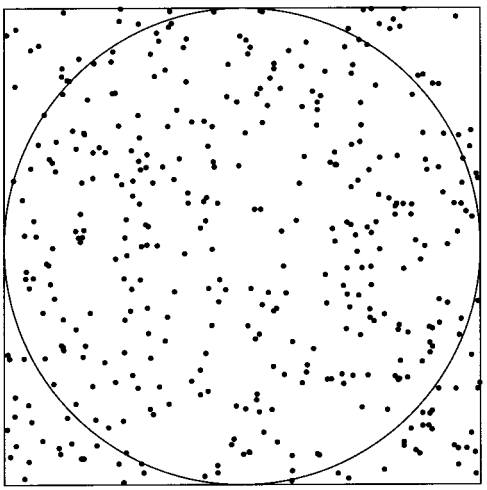


Fig. 3.4 Calculating π using the Monte Carlo method. Here 315 out of 400 points lay inside the circle. This gives the approximate value $\pi \approx 4 \cdot 315/400 = 3.15$.

points, and multiply it by the length of the range. This method is not the best for calculating integrals of one-dimensional functions; however, it does start to pay off with multiple integrals—when the function depends on more than one variable i.e., $f(x_1, x_2, \ldots, x_n)$, and we need to calculate the volume of an $(n + 1)$-dimensional solid under the curve.

The Monte Carlo method can also be used to approximate the value of π. If we inscribe a circle of radius 1 into a square of side 2, then the ratio of the area of the circle to the area of the square is $\pi/4$. We can therefore generate random points from within the square and note which of them fall within the circle (see Fig. 3.4). As we keep performing such trials, the ratio of the number of points inside the circle to the total number of trials should approach $\pi/4$. This example serves solely to illustrate the principle of the method, since there exist far better algorithms for determining π.

Another example of how the Monte Carlo method leads quickly to an approximate solution is our last approach to the Bertrand problem presented earlier in this chapter. Arriving at the exact solution required long and tedious calculations, while finding the approximate result by writing a program based on the Monte Carlo method took just a few minutes.

The program **Ulam** illustrates how the Monte Carlo method can be used to calculate integrals of a given function within a given range.

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!

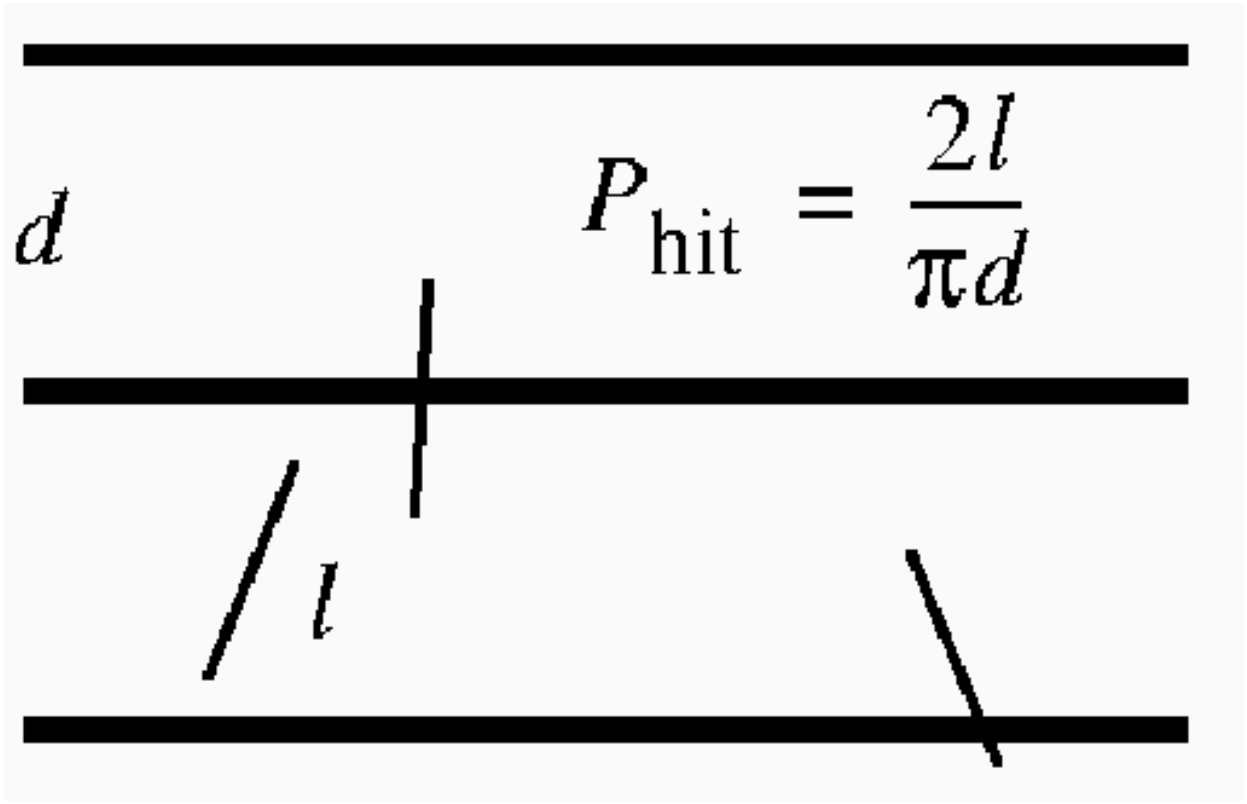
The idea of using randomness to obtain an answer to a scientific problem is actually much older than computers.

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).



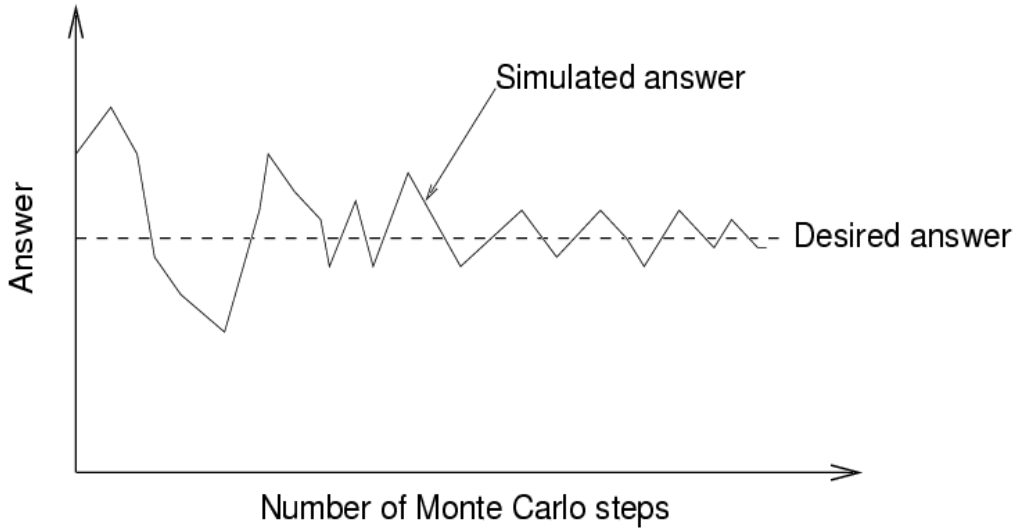
Various people have tried to calculate π by throwing needles. The most remarkable result was that

of Lazzarini (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 (see links on web page). Exactly where and how it began and where the name originates from is hard to pin down exactly.

This is rather obviously is related to the fact that the beginnings were closely related to the Manhattan project, and publication of results was not the number one priority there....

If you check the web for this, be careful: some sources are in direct contradiction to others.

Two early crucial papers are:

Note on census-taking in Monte Carlo calculations E. Fermi and R.D. Richtmyer 1948. A declassified report by Enrico Fermi. From the Los Alamos Archive.

The Monte Carlo Method N. Metropolis and S. Ulam 1949 Journal of the American Statistical Association, 44, 335 (1949)

The name apparently originates with Metropolis, who says that he invented it in 1945 inspired by Stan Ulam's gambling uncle who "just had to go to Monte Carlo" [Metropolis, N. "The Beginning of the Monte Carlo Method." Los Alamos Science, No. 15, p. 125, http://jackman.stanford.edu/mcmc/metropolis1.pdf]

3.3. MC now, and intent of this course

Nowadays MC methods are also used widely outside of mathematics, statistics, and physics. There are uses in:

- Optimization (any field where it is needed)

- Social sciences: there is even a book called "Monte Carlo Simulation (Quantitative Applications in the Social Sciences)"

- Economics: citation from the description of the book "Monte Carlo Methods in Financial Engineering":

"Monte Carlo Methods are among the most broadly applicable and thus most powerful tools for valuing derivatives securities and measuring their risks. "

Common to all of the wide areas where MC is used is that one in any of them one has to be able

to generate random numbers efficiently. Many of the basic MC methods, such as MC integration and generation of synthetic data, are also used in a wide range of sciences.

The intent of this course "Basics of MC" is specifically to go through the basic MC tools which can be used in a wide range of sciences. MC methods in physics are dealt with on the continuation course "MC simulations in physics".

3.4. 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.

I list here some of the more common MC terms 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:

Markov Chain MC, MCMC

A generelized version of Metropolis MC, used to generate a sequence of points in some known distribution.

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

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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...

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.