The Monte Carlo method

Introduction

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The origin of the Monte Carlo method

The Monte Carlo method is a numerical method of solving mathematical, physical, etc., problems by means of random sampling.

It is conventionally assumed to be born in 1949 when the paper *The Monte Carlo method* was published:

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The term *Monte Carlo* is due to the name of town Monte Carlo in the Principality of Monaco which is famous for its casino. The point is that the roulette is one of the simplest mechanical devices for generation of random numbers.

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Example

To clarify the idea behind the Monte Carlo method, let us consider a simply example.

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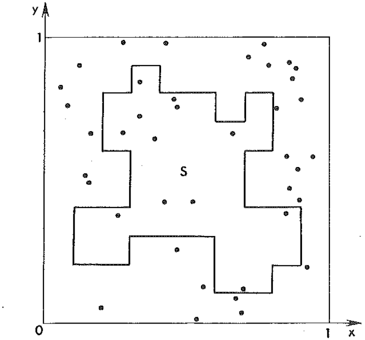

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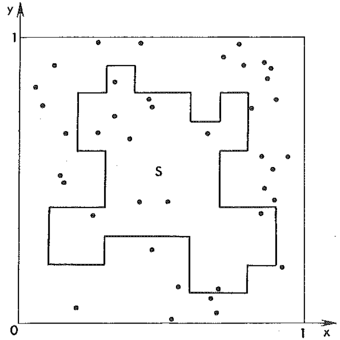

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Example

It is obvious that the area of S should be equal approximately to the ratio N'/N.

In our example $N = 40$ of which $N' = 12$ is inside S, thus

$$\frac{N'}{N} = \frac{12}{40} = 0.30,$$

while the true area of S is 0.35. Obviously, our approximation would become better, if we used more random points.

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In practise the Monte Carlo (MC) method is not used to calculate areas of flat figures, as there are much better methods, though a bit more complicated, which are much better in this respect.
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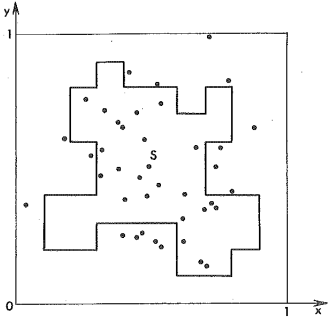
More about the example

How the random points should actually be selected?

Consider our example once more, but this time imagine that we fix our figure on the wall and let some dart player to hit it with darts from some distance.



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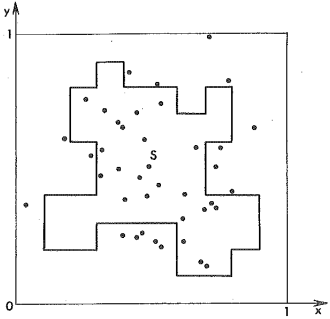

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Random variables

The term *random variable*, in its commonplace sense is used to emphasize that we do not know what specific value this variable will assume.

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Discrete random variables

A random variable ξ which takes on values from a discrete set $\{x_1, x_2, ..., x_n\}$ is specified by the table

$$\xi = \begin{pmatrix} x_1 & x_2 & \dots & x_n \\ p_1 & p_2 & \dots & p_n \end{pmatrix},$$

where $p_1, p_2, ..., p_n$ are the corresponding probabilities.
Denote the probability that the random variable ξ will be equal to x_i by

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Condition 2 means that in each trial ξ must assume one of the values $x_1, x_2, ..., x_n$.

The quantity

$$\boldsymbol{M}\xi = \sum_{i=1}^{n} x_i p_i$$

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Basic properties of the expected value

If c is an arbitrary non-random number, then

$$\begin{aligned} \boldsymbol{M}(\xi + c) &= \boldsymbol{M}\xi + c, \\ \boldsymbol{M}(c\xi) &= c\boldsymbol{M}\xi. \end{aligned}$$

If ξ and η are two arbitrary random variables, then

$$\boldsymbol{M}(\xi + \eta) = \boldsymbol{M}\xi + \boldsymbol{M}\eta.$$

The quantity

$$\boldsymbol{D}\xi = \boldsymbol{M}[(\xi - \boldsymbol{M}\xi)^2]$$

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Practical importance of $\boldsymbol{M}\xi$ and $\boldsymbol{D}\xi$

If in the course of many observations of the random variable ξ we obtain a set of values $\xi_1, \xi_2, ..., \xi_N$, each of them being equal to one of the numbers $x_1, x_2, ..., x_n$, then the arithmetic mean of these numbers will be close to $\boldsymbol{M}\xi$, i.e.

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The following relations are valid for independent random variables ξ and η

$$\begin{aligned} \boldsymbol{M}(\xi\eta) &= \boldsymbol{M}\xi \cdot \boldsymbol{M}\eta, \\ \boldsymbol{D}(\xi + \eta) &= \boldsymbol{D}\xi + \boldsymbol{D}\eta. \end{aligned}$$

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Example. Let us consider a random variable κ which is the number of points obtained in a single throw of a die. It can be represented by the following table

$$\kappa = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} \end{pmatrix}.$$

Let us find the expected value and variance of κ.

$$\boldsymbol{M}\kappa = \sum_{i=1}^{6} x_i p_i = 1 \cdot \frac{1}{6} + 2 \cdot \frac{1}{6} + ... + 6 \cdot \frac{1}{6} = 3.5,$$

$$\boldsymbol{D}\kappa = \boldsymbol{M}(\kappa^2) - (\boldsymbol{M}\kappa)^2 = 1^2 \cdot \frac{1}{6} + 2^2 \cdot \frac{1}{6} + ... + 6^2 \cdot \frac{1}{6} - 3.5^2 = 2.917.$$

Example. Let us consider a random variable θ which is a single toss of a coin, assuming that a toss of heads brings 3 points an that of tails brings 4 points. It can be represented by the following table

$$\theta = \begin{pmatrix} 3 & 4 \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}.$$

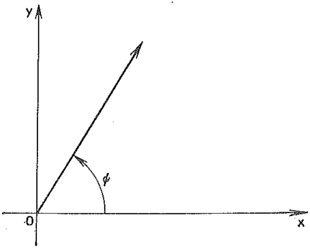
The expected value and variance of θ are

$$\boldsymbol{M}\theta = \sum_{i=1}^{2} x_i p_i = 3 \cdot \frac{1}{2} + 4 \cdot \frac{1}{2} = 3.5,$$

$$\boldsymbol{D}\theta = \boldsymbol{M}(\theta^2) - (\boldsymbol{M}\theta)^2 = 3^2 \cdot \frac{1}{2} + 4^2 \cdot \frac{1}{2} - 3.5^2 = 0.25.$$

We see that $\boldsymbol{M}\theta = \boldsymbol{M}\kappa$, but $\boldsymbol{D}\theta < \boldsymbol{D}\kappa$. The inequality can be easily understood, as the maximum deviation of θ from the mean 3.5 is ± 0.5, while the maximum deviation of κ from the mean is ± 2.5.

Let us assume that a certain amount of radium is placed on a plane at the origin of the coordinates. An α-particle is emitted in each decay of a radium atom. The direction of motion of this particle will be characterized by an angle ψ, see the figure below.



Since any direction of emission is possible, the random variable ψ can assume any value fro 0 to 2π.

We shall call a random variable ξ *continuous* if it takes on any value out of a certain interval (a, b).

A continuous random variable ξ is defined by specifying the interval (a, b) of its variation and the function $p(x)$ called the *probability density* of the random variable ξ.

The physical meaning of $p(x)$ is the following. Let (a', b') be an arbitrary interval contained within (a, b), i.e. $a \leq a'$ and $b' \leq b$. Then the probability that ξ falls inside (a', b') is given by the integral

$$\boldsymbol{P}\{a' < \xi < b'\} = \int_{a'}^{b'} p(x)dx.$$

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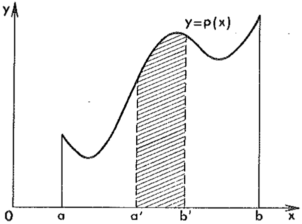
The integral $\int_{a'}^{b'} p(x)dx$ is equal to the hatched area in the following figure.



The set of values of ξ can be any interval. The cases when $a = -\infty$ as well as $b = +\infty$ are also possible.

Continuous random variables

However, the density $p(x)$ must satisfy two conditions, similar to those of probabilities p_i in the case of a discrete random variable:

1. the density $p(x)$ is positive: $p(x) > 0$,
2. the integral of the density $p(x)$ over the whole interval (a, b) is equal to 1:

$$\int_a^b p(x)dx = 1.$$

The value

$$\boldsymbol{M}\xi = \int_a^b xp(x)dx$$

is called *expected* or *mean value* of the continuous random variable.

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We will mention here only one more expression for the expected value of a function of ξ. Let us assume that the random variable ξ is characterized by the probability density $p(x)$ and consider an arbitrary continuous function $f(x)$. We introduce a random variable $\eta = f(\xi)$. It can be shown that

$$\boldsymbol{M} f(\xi) = \int_a^b f(x) p(x) dx.$$

We must emphasize that in general $\boldsymbol{M} f(\xi) \neq f(\boldsymbol{M}\xi)$.

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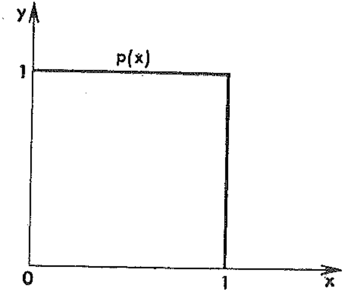
A random variable γ, defined on the interval $(0, 1)$ with the density $p(x) = 1$ is said to be *uniformly distributed* in $(0, 1)$, see the figure below.



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Indeed, for any interval (a', b') within $(0, 1)$ the probability that γ will take on the value within (a', b') is equal to

$$\int_{a'}^{b'} p(x)dx = b' - a',$$

i.e. to the length of this interval. If, in particular, we divide the interval $(0, 1)$ into an arbitrary number of intervals of equal length, the probability of γ falling within one of these intervals will be the same. Note that

$$\boldsymbol{M}\gamma = \int_0^1 xp(x)dx = \int_0^1 xdx = \frac{1}{2},$$

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