Basic MonteCarlo concepts

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1 Probability distributions
   - Binomial
   - Poisson
   - Normal

2 Generation of a continuous random variable
   - Inverse transform method
   - Acceptance-rejection method

3 The Monte Carlo method
   - Central Limit Theorem
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• It is a discrete distribution which was introduced by the swiss mathematician Jacob Bernoulli (1654-1705).
• Let’s consider a discrete variable, which has two possible results, with probabilities $p$ and $q = 1 - p$. The probability to obtain $x$ results of the first type after $N$ measurements of the variable is

$$P(x) = \frac{N!}{x!(N-x)!} p^x q^{(N-x)}$$

with the following mean value and standard deviation

$$\bar{x} = Np$$

$$\sigma = \sqrt{Npq} = \sqrt{Np(1-p)}$$

Therefore it’s a **discrete distribution defined by two parameters:** $N$ and $p$.

http://demonstrations.wolfram.com/BinomialProbabilityDistribution/
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It was introduced by Siméon Denis Poisson (1781-1840) during its studies on criminal matter. It describes a discrete random variable $x$ which tallies the number of occurrences of a given type which take place during a time interval.

It’s the limiting case of a binomial distribution when $N \to \infty$, $p \to 0$, being $\overline{x} = Np$ its only parameter.

The Poisson distribution is discrete and is fully characterized by its mean value $\overline{x}$.

$$p_{\overline{x}}(x) = \frac{\overline{x}^x}{x!} e^{-\overline{x}}$$

http://demonstrations.wolfram.com/PoissonDistribution/

http://demonstrations.wolfram.com/BinomialApproximationToAPoissonRandomVariable/
Let’s consider the disintegration of a radioactive atomic nucleus with probability per unit time $\lambda$. Ultimately, we will resort to differential calculus, therefore being $dt$ the differential time interval and $t$ the total elapsed time.

$$t = N \times dt$$

$$N \to \infty$$

$$dt \to 0$$

each sampling of the random variable (disintegration: does it happen? or doesn’t it happen?) corresponds to a time interval $dt$ with probability of success (i.e. it happens)

$$p = \lambda \times dt$$

which evidently fulfills

$$p \to 0$$
In these conditions ($N \to \infty$ and $p \to 0$) the binomial distribution tends to the Poisson distribution (also known as *Law of rare events*).

The condition to satisfy this statistics is that the probability of *success* in each sampling be small, which is obviously accomplished since each sampling corresponds to a differential time interval $dt$.

Let $p_x(t)$ be the probability of $x$ successes (disintegrations) in a given interval $[0, t]$. In this case

$$p_x(t + dt) = p_x(t)(1 - \lambda dt) + p_{x-1}(t)\lambda dt$$

from which it follows

$$\frac{dp_x}{dt} = \frac{p_x(t + dt) - p_x(t)}{dt} = \lambda [p_{x-1}(t) - p_x(t)]$$

which solution is

$$p_x(t) = \frac{(\lambda t)^x}{x!}e^{-\lambda t}$$
Evidently the average number of successes is

$$\bar{x} = \lambda t$$

which leads to the most usual representation

$$p_{\bar{x}}(x) = \frac{\bar{x}^x}{x!} e^{-\bar{x}}$$

It’s straightforward to demonstrate

$$\bar{x}^2 = \bar{x}^2 + \bar{x}$$

i.e. $\sigma = \sqrt{\bar{x}}$.

The Poisson distribution is discrete and fully characterized by its mean value $\bar{x}$.

The rare events condition has been implicitly applied when the probability of simultaneous occurrence of two disintegrations in the same time interval $dt$ has been neglected.
In our differential treatment this condition is met, since

\[ p = \lambda dt \longrightarrow 0 \]

For this reason the Poisson distribution plays a key rôle in the simulations by the MonteCarlo method of processes in which the probability of occurrence per unit time or unit length is known (for instance, the radioactive disintegration and processes taking place during radiation transport through matter).
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The normal distribution (also called *Gauss* distribution)

\[
p_{\bar{x}, \sigma}(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\bar{x})^2}{2\sigma^2}}
\]

is characterized by two parameters: the mean value \( \bar{x} \) and the standard deviation \( \sigma \).

The Poisson distribution tends to the normal for large values of the mean value \( \bar{x} \), therefore becoming:

\[
p_{\bar{x}}(x) = \frac{\bar{x}^x}{x!} e^{-\bar{x}} \rightarrow \frac{1}{\sqrt{2\pi\bar{x}}} e^{-\frac{(x-\bar{x})^2}{2\bar{x}}}
\]

The *standard* normal distribution corresponds to the situation where \( \bar{x} = 0 \) and \( \sigma = 1 \)

\[
p_{\text{standard}}(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}
\]

http://demonstrations.wolfram.com/TheNormalDistribution/

http://demonstrations.wolfram.com/NormalApproximationToAPoissonRandomVariable/
Calculations with *Mathematica*

Figura: $\bar{x} = 5$

$x_0 = 5$

$x_{min} = x_0 - 2 \sqrt{x_0}$

$x_{max} = x_0 + 2 \sqrt{x_0}$

$\text{Tabla} = \text{Table}[[i, \text{Poisson}[i]], \{i, x_{min}, x_{max}\}]$

$g1 = \text{ListPlot}[\text{Tabla}, \text{PlotStyle} \rightarrow \{\text{PointSize}[0.015]\}, \text{DisplayFunction} \rightarrow \text{Identity}$

$g2 = \text{Plot}[\text{Gaus}[x], \{x, x_{min}, x_{max}\}$

$\text{PlotStyle} \rightarrow \{\text{RGBColor}[1, 0, 0]\}, \text{DisplayFunction} \rightarrow \text{Identity}$

$\text{show}[g1, g2, \text{DisplayFunction} \rightarrow \$\text{DisplayFunction}$]$
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The goal is to generate values of $\xi$ with probability density $p(x)$, defined in the interval $[x_1, x_2]$. It can be shown that

$$\int_{x_1}^{\xi} p(x) \, dx = \gamma$$

where $\gamma$ is uniformly in $[0, 1]$. Therefore, provided a random number generator is available, the problem reduces to solve the above integral equation.

http://demonstrations.wolfram.com/TheMethodOfInverseTransforms/
PROOF

Let’s define

\[ y(x) = \int_{x_1}^{x} p(x) \, dx \]

which is monotonically increasing (\( y'(x) = p(x) > 0 \)) with \( y(x_1) = 0 \) and \( y(x_2) = 1 \).

It follows that \( y(x) = \text{valor} \) has a unique solution

If \( x \in (a, b) \Rightarrow y(x) \in [y(a), y(b)] \)

\[ \Downarrow \]

\[ P [a < \xi < b] = P [y(a) < \gamma < y(b)] \]

Since \( \gamma \) is uniformly distributed:

\[ P [y(a) < \gamma < y(b)] = \frac{y(b) - y(a)}{y(x_2) - y(x_1)} = \frac{y(b) - y(a)}{\int_{a}^{b} p(x) \, dx} = y(b) - y(a) = \int_{a}^{b} p(x) \, dx \]

Therefore \( P [a < \xi < b] = \int_{a}^{b} p(x) \, dx \)
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The inverse transform method may be unpractical if:

- The integral of \( p(x) \) cannot be solved analytically.
- The probability density \( p(x) \) is known graphically or is tabulated.

**Method:** let’s consider \( \xi \) defined in \([x_1, x_2]\) and its probability density \( p(x) \leq M_0 \), then the values of \( \xi \) can be sampled as follows:

1. A point \( \Gamma \) of coordinates \((\eta', \eta'')\) is built from two values \( \gamma' \) and \( \gamma'' \) of the random variable uniformly distributed in \([0, 1]\):
   \[
   \eta' = x_1 + \gamma'(x_2 - x_1) \\
   \eta'' = \gamma'' M_0
   \]

2. If the point \( \Gamma \) is below the curve \( y = p(x) \), then \( \xi = \eta' \). Otherwise a new pair of values \((\gamma', \gamma'')\) is sampled and the procedure is repeated until the above condition is fulfilled.
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Generation of a gaussian distribution (inverse transform method)

Figure: Inverse transform method. CPU time Mathematica: 103 seconds
Generation of a gaussian distribution (acceptance-rejection method)

Figure: Acceptance-rejection method. CPU time Mathematica: 10 seconds
2D uniform distribution

\[ 1 = \int_0^R \int_0^{2\pi} P(r, \phi) dr d\phi = \int_0^R \int_0^{2\pi} p(r, \phi) r dr d\phi \]

Uniform distribution:

\[ \Rightarrow p(r, \phi) = C \quad \Rightarrow 1 = C \int_0^R \int_0^{2\pi} r dr d\phi \]

\[ C = \frac{1}{\pi R^2} \quad \Rightarrow P(r, \phi) dr d\phi = \frac{r dr d\phi}{\pi R^2} \]

**Figura:** Polar coordinates

The distribution in \( r \):

\[ P_r(r) dr = \left[ \int_0^{2\pi} P(r, \phi) d\phi \right] dr = \frac{2r dr}{R^2} \]

The distribution in \( \phi \):

\[ P_\phi(\phi) d\phi = \left[ \int_0^R P(r, \phi) dr \right] d\phi = \frac{d\phi}{2\pi} \]
Therefore for sampling the $r$ and $\phi$ values, being $\gamma$ a continuous uniformly distributed random variable in $[0, 1]$ (random number generator in mathematical libraries available in all major scientific languages, as FORTRAN and C++):

\[
\int_0^r P_r(r') dr' = \gamma = \frac{2}{R^2} \int_0^r r' dr' = \frac{r^2}{R^2} \Rightarrow r = R \sqrt{\gamma}
\]

\[
\int_0^\phi P_\phi(\phi') d\phi' = \gamma' = \frac{1}{2\pi} \int_0^\phi d\phi' = \frac{\phi}{2\pi} \Rightarrow \phi = 2\pi \gamma'
\]
Mathematica calculations

- distribución radial uniforme (2D)

```mathematica
<< Graphics'Graphics'
puntos = Table[Sqrt[Random[]], {i, 1, 10000}],
PolarListPlot[puntos]
```

- distribución radial pseudouniforme (2D)

```mathematica
psu = Random[]
puntos2 = Table[Sqrt[Random[]], {i, 1, 10000}],
PolarListPlot[puntos2]
```

**Figura:** Uniform 2D distribution

**Figura:** Pseudouniform 2D distribution
3D uniform distribution

The distribution in $r$:

$$P_r(r)dr = \left[ \int_0^\pi \int_0^{2\pi} P(r, \theta, \phi)d\theta d\phi \right] dr = \frac{3r^2dr}{R^3}$$

The distribution in $\theta$:

$$P_\theta(\theta)dr = \left[ \int_0^R \int_0^{2\pi} P(r, \theta, \phi)d\theta d\phi \right] d\theta = \frac{\text{sen}(\theta)d\theta}{2}$$

The distribution in $\phi$:

$$P_\phi(\phi)d\phi = \left[ \int_0^R \int_0^{\pi} P(r, \theta, \phi)d\theta d\phi \right] d\phi = \frac{d\phi}{2\pi}$$

Uniform distribution: $p(r, \theta, \phi) = C \Rightarrow 1 = C \int_0^R \int_0^\pi \int_0^{2\pi} r^2 \text{sen}(\theta) dr d\theta d\phi \Rightarrow C = \frac{3}{4\pi R^3} \Rightarrow P(r, \theta, \phi) dr d\theta d\phi = \frac{3r^2 \text{sen}(\theta) dr d\theta d\phi}{4\pi R^3}$

Figura: Spherical coordinates
3D uniform distribution (cont.)

Therefore, for sampling the $r$, $\theta$ and $\phi$ values, being $\gamma$ a continuous uniformly distributed random variable in $[0, 1]$ (random number generator generator in mathematical libraries available in all major scientific languages, as FORTRAN and C++):

$$
\int_0^r P_r(r')dr' = \gamma = \frac{3}{R^3} \int_0^r r'^2 dr' = \frac{r^3}{R^3} \Rightarrow r = R\gamma^{1/3}
$$

$$
\int_0^\theta P_\theta(\theta')d\theta' = \gamma' = \frac{1}{2} \int_0^\theta \text{sen}(\theta')d\theta' = \frac{1}{2(1 - \cos(\theta))} \Rightarrow \theta = \arccos(2\gamma' - 1)
$$

$$
\int_0^\phi P_\phi(\phi')d\phi' = \gamma'' = \frac{1}{2\pi} \int_0^\phi d\phi' = \frac{\phi}{2\pi} \Rightarrow \phi = 2\pi\gamma''
$$
distribución radial uniforme (3D)

```
puntos = Table[Random[]^0.3, {i, 1, 10000}],
<< Graphics'Graphics3D'

z[i_] := (Random[])^0.3
theta[i_] := ArcCos[1 - 2 Random[]]
phi[i_] := Random[] 2 Pi

puntos = Table[{z[i] Sin[theta[i]] Cos[phi[i]],
               z[i] Sin[theta[i]] Sin[phi[i]],
               z[i] Cos[theta[i]]}, {i, 0, 64 Pi, Pi/20}]

ScatterPlot3D[puntos]
```

Figura: Uniform distribution

---

distribución radial pseudouniforme (3D)

```
x2[i_] := Random[]
theta[i_] := ArcCos[1 - 2 Random[]]
phi[i_] := Random[] 2 Pi

puntos2 = Table[{x2[i] Sin[theta[i]] Cos[phi[i]],
                 x2[i] Sin[theta[i]] Sin[phi[i]],
                 x2[i] Cos[theta[i]]}, {i, 0, 64 Pi, Pi/20}]

ScatterPlot3D[puntos2]
```

Figura: Pseudouniform distribution
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The Monte Carlo method

Theorem

Given N independent, equal, random variables:

\[ \xi_1, \xi_2, \ldots, \xi_N \]

\[ \bar{\xi}_1 = \bar{\xi}_2 = \ldots = \bar{\xi}_N = m \]

\[ \Delta \xi_1 = \Delta \xi_2 = \ldots = \Delta \xi_N = \sigma \]

and being \( \rho \) their sum

\[ \rho_N = \sum_{i=1}^{N} \xi_i \quad \bar{\rho}_N = \sum_{i=1}^{N} \bar{\xi}_i = Nm \quad \Delta \rho_N = \sqrt{N} \sigma \]

for large \( N \), \( \rho \) is a random normal variable (i.e. distributed according to Gauss law) with the above parameters

\[ P[a \leq \rho_N \leq b] \approx \int_{a}^{b} p_{\rho_N}(x) \, dx \quad \text{con} \quad p_{\rho_N}(x) = \frac{1}{\sqrt{2\pi} \Delta \rho_N} e^{-\frac{(x-\bar{\rho}_N)^2}{2\Delta \rho_N^2}} \]
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It is a direct application of the Central Limit Theorem. The goal is to calculate a magnitude \( m \) (for instance, the number of neutrons which get through a given material thickness). The method consists in:

1. Take \( N \) equal and independent random variables (which ultimately are the \( N \) Monte Carlo samplings or histories).

\[
\xi_1, \xi_2, \ldots, \xi_N
\]

\[
\bar{\xi}_1 = \bar{\xi}_2 = \ldots = \bar{\xi}_N = m
\]

\[
\Delta \xi_1 = \Delta \xi_2 = \ldots = \Delta \xi_N = \sigma
\]

2. Calculated their mean value:

\[
\bar{\xi} = \frac{\rho_N}{N} = \frac{\sum_{i=1}^{N} \xi_i}{N}
\]

According to the Central Limit Theorem, it follows:

\[
P[Nm - 3\sigma \sqrt{N} \leq \rho_N \leq Nm + 3\sigma \sqrt{N}] \approx 0.997
\]

\[
P[m - 3\frac{\sigma}{\sqrt{N}} \leq \frac{\rho_N}{N} \leq m + 3\frac{\sigma}{\sqrt{N}}] \approx 0.997
\]

\[
P[\frac{1}{N} \sum_{i=1}^{N} \xi_i - m < 3\frac{\sigma}{\sqrt{N}}] \approx 0.997
\]
Basically, a MonteCarlo calculation is a *numerical experiment* which uses random number generators to simulate the physical quantities, which are sampled according to probability distributions (Physics models).
Evidently, the larger the number $N$ of *samplings*, the closer will be the *experimental* average (by MonteCarlo) to the *theoretical* mean value, which strictly would ask for $N \to \infty$.

In a typical application a huge number of events takes place, for instance a beam of particles with intensity $10^{10}$ p/s impinges on a macroscopic target, which contains of the order of the Avogadro number ($6.02 \times 10^{23}$) of scattering centers.

As a direct consequence of the Central Limit Theorem the *quality* of the Montecarlo simulation is proportional to $\sqrt{N}$, since the relative error goes as $\sigma/\sqrt{N}$, where $\sigma$ is the standad deviation; from this follows the limitation coming from the available computational power.
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Calculation of $\pi$

- The numerical integration by geometrical \textit{(acceptance-rejection)} method was at the origin of the MonteCarlo calculations.
- We will start with a simple geometrical example for calculating the value of $\pi$.
- From the figure, it’s obvious that the area of the circle within one of the quadrants is $r=1$ is $\pi/4$. 
Let’s imagine that we throw darts against the figure.

After a high enough number of throws, the number of hits (impacts within the circle) will be approx. proportional to the area of the circle.

In other words, the ratio of hits over total number of throws will be $\pi/4$.

If we actually carry out this experiment, we would verify that a very large number of throws (well above 1000) is needed in order to reach an acceptable estimation of $\pi$.

For this very reason it’s much better to carry the experiment *virtually* with a computer by using a random number generator within this very simple algorithm.

The quality of the estimation will depend on the quality of the random number generator and the number of iterations (*virtual throws*).
Distribution law from Poisson statistics

If $\Sigma$ is the probability per unit length for a certain process to occur, that leads to the Poisson distribution of the number of occurrences which take place within the length interval $[0, \ell]$:

$$p_x(\ell) = \frac{(\Sigma \ell)^x e^{-\Sigma \ell}}{x!}$$

Nevertheless, in a numerical simulation by the Monte Carlo method what we do really need is the occurrence probability of the first success within the interval $[\ell, \ell + d\ell]$:

**Distribution law of the length**

$$l_1(\ell)d\ell = p_0(\ell) \Sigma d\ell = e^{-\Sigma \ell} \Sigma d\ell$$

where

- $p_0(\ell)$ is the non-occurrence probability within the interval $[0, \ell]$.
- $\Sigma d\ell$ is the occurrence probability of a single success within the interval $[\ell, \ell + d\ell]$. 
By applying the inverse transform method:

Sampling algorithm

\[ \ell = -\frac{1}{\sum} \ln \gamma \]

where \( \gamma \) is a random variable uniformly distributed in \([0, 1]\).

The same applies for distribution of occurrence times (for instance, in radiactive disintegration) provided that the disintegration constant (probability per unit time) is known.
Neutron transport

In this simple example only two processes are considered:

- elastic scattering
- absorption

Therefore there are 3 possibilities after transportation through the slab:

- reflection (probability: $p^-$)
- absorption (probability: $p^0$)
- transmission (probability: $p^+$)

The macroscopic cross section is defined as the probability per unit path length of a neutron experiencing a collision. $\Sigma = \sigma \rho$, where $\sigma$ is the cross section of the process and $\rho$ is the density of targets.

$$\Sigma = \frac{1}{\lambda} = \Sigma_{abs} + \Sigma_{disp} \quad (2)$$

being $\lambda$ the mean free path of a neutron in the slab material.
### Probability distributions

#### Generation of a continuous random variable

The **Monte Carlo** method

**Concept**

#### Examples

**sampling of \( \lambda \)**

\( \lambda \): random variable with distribution function

\[
p(\lambda) = \frac{1}{\lambda} e^{-\frac{1}{\lambda} \lambda} = \sum e^{-\sum \lambda}
\]

By applying the inverse transform method:

\[
\lambda = -\frac{1}{\sum} \ln \gamma
\]

**sampling of \( \theta \)**

\( \theta \): random variable with distribution function:

\[
P_\theta(\theta)dr = \frac{\sin(\theta)d\theta}{2}
\]

By applying the inverse transform method:

\[
\theta = \arccos(1 - 2\gamma)
\]

**Method (after the k-th collision the neutron is in position \( z_k \))**

1. Sampling of \( \lambda \): \( \lambda_k = -\frac{1}{\sum} \ln \gamma \)
2. Sampling of \( \theta \): \( \theta_k = \arccos(2\gamma' - 1) \)
3. The new position is calculated: \( z_{k+1} = z_k + \lambda_k \cos(\theta_k) \)
4. If \( z_{k+1} > h \Rightarrow \text{transmitted neutron} \Rightarrow N^+ = N^+ + 1 \)
5. If \( z_{k+1} < 0 \Rightarrow \text{reflected neutron} \Rightarrow N^- = N^- + 1 \)
6. If \( 0 < z_{k+1} < h \Rightarrow \text{the neutron is still inside}:
   
   - If \( \gamma'' < \frac{\Sigma_{\text{abs}}}{\sum} \Rightarrow N^0 = N^0 + 1 \) (captured neutron)
   - Otherwise return to point 1 and repeat the process

Finally: \( p^+ = \frac{N^+}{N} \); \( p^0 = \frac{N^0}{N} \); \( p^- = \frac{N^-}{N} \).
Potential problem

A problem may arise if after N repetitions few particles (if any) survive (bad statistics).

Solution: weighting method

1. Instead of considering individual neutrons, an initial bunch made of $\omega_0$ neutrons is created.
   - In a given interaction, ($k$), in average
     - $\omega_{k-1} \frac{\Sigma_{abs}}{\Sigma}$ are absorbed.
     - $\omega_{k-1} \frac{\Sigma_{disp}}{\Sigma}$ is are scattered.

2. $\omega_{k-1} \frac{\Sigma_{abs}}{\Sigma}$ is added to $N^0$ (absorbed particles) and the process is repeated with the remaining bunch, with weight $\omega_{k-1} \frac{\Sigma_{disp}}{\Sigma}$, moving in the same direction.

- All former formulae apply, substituting $\omega_{k+1} = \omega_k \frac{\Sigma_{disp}}{\Sigma}$ as the part of the bunch which survives after each collision ($\omega_k$ is the weight of the neutron).
- The initial weight is $\omega_0 = 1$.
- In this way a trajectory never ends in an absorption: there is always a remnant, which is a fractionary quantity, obviously proportional to the transmission probability.
- In these circumstances, this method noticeably improves the efficiency of the simulation.