

Monte Carlo methods

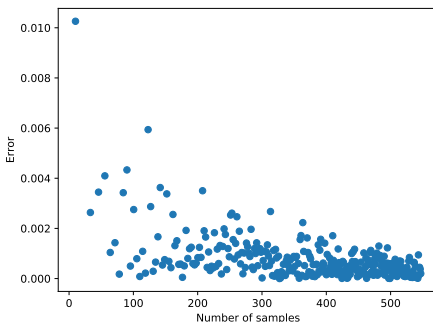
November 15, 2020

Objective

- ▶ We will discuss Monte Carlo methods
- ▶ It will be sometimes technical.
- ▶ However you don't need to understand all technical details in order to apply these ideas to the project (if you are interested in doing so, which is not mandatory).
- ▶ We will discuss possible applications to the game.

Defining the problem

- Facing a random process, we would like to compute its **expected value**.



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- ▶ Facing a random process, we would like to compute its **expected value**
- ▶ For instance
 - ▶ what is the mean amount of rain one can expect in october in Paris ?
 - ▶ how much time should I expect to wait when taking the metro ?
 - ▶ If I play a game, what is my expected gain ?

Defining the problem

- ▶ We are in a situation where we have some information about the random process.
 - ▶ We know its **probability density** or **distribution**.

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 - ▶ We know its **probability density** or **distribution**.
 - ▶ However, it is not straightforward to explicitly compute the **expected value**.
 - ▶ We will need to compute an **approximate value** for the expectation.

Defining the problem

- ▶ The Monte-Carlo method uses **simulated random variables** to compute such an approximate value.

Question

- ▶ But why should we use a method involving randomness ?

Overview

Expected values

The Monte Carlo Method

- The law of large numbers

- Central limit theorem

- Random variables simulations

Why is Monte-Carlo useful ?

- Notion of algorithmic complexity

Application to the game

Expected values

- ▶ Let us study the **expected value**

Expected values

- ▶ The **expected value** (or expectation) is a **weighted average** of a random variable.

Example 1

- ▶ The expected value is a **weighted average** of a random variable.
- ▶ What is the expectation of a single throw of an unbiased dice ?



Figure: Dice

Example 2

- ▶ Propose a probability law for the waiting time of the metro and compute the expected value.

Exercises on probabilities

- ▶ Exercise I
- ▶ Exercise II

Formal definition

- Is the random variable X can take a finite number of values x_i with probabilities p_i , then the expected value is :

$$E(X) = \sum_{i=1}^n p_i x_i \quad (1)$$

Deterministic computation

Exercise 1: Computing an expected value.

- ▶ Let us consider the following situation. We have n computers.
 - ▶ Computer 1 transmits a message to computer 2.
 - ▶ Computer 2 transmits the received message to computer 3.
 - ▶ ...

Deterministic computation

Exercise 1: Computing an expected value.

- ▶ Let us consider the following situation. We have n computers.
 - ▶ Computer 1 transmits a message to computer 2.
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 - ▶ ...
- ▶ At each step, the probability that there is a mistake in the transmission is p .

Deterministic computation

Exercise 1: Computing an expected value.

- ▶ Let us consider the following situation. We have $n + 1$ computers.
 - ▶ Computer 1 transmits a message to computer 2.
 - ▶ Computer 2 transmits the received message to computer 3.
 - ▶ ...
- ▶ At each step, the probability that there is a mistake in the transmission is p .
- ▶ Let X be the total number of mistakes done during the transmission to the last computer. (we have n transmissions between n computers)

Deterministic computation

Exercise 1: Computing an expected value.

- ▶ What is the law of X ?
- ▶ ie: for each $k \in [0, n]$, what is $P(X = k)$?

Deterministic computation

Exercise 1: Computing an expected value.

- ▶ Can we check that our result is correct ?
- ▶ We need that :
 - ▶ $\forall k \ p_k \geq 0$
 - ▶ $\sum_{k=0}^n p_k = 1$

Deterministic computation

Exercise 1 : Computing an expected value.

- ▶ Please write a program that computes the expected value of X !

Law of X

- ▶ This law is called the **binomial law**

Remark

- ▶ If X is a random variable, any function $f(X)$ of X is also a random variable.

Generalisation

- ▶ Up to now, we studied **discrete, finite** random variables.

Generalisation

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- ▶ But we often encounter **continuous** random variables.

Generalisation

- ▶ Up to now, we studied **discrete, finite** random variables.
- ▶ But we often encounter **continuous** random variables.
- ▶ The gaussian law $\mathcal{N}(\mu, \sigma^2)$ is continuous, defined by a **density** $f(x)$.

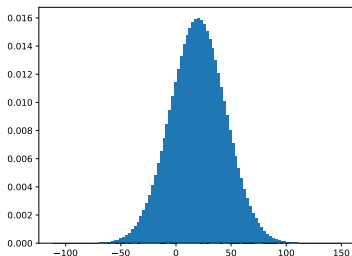


Figure: Normalized histogram

Expected value of continuous variables

- How can we express the expected value of a continuous variable X that has a density $f(X)$?

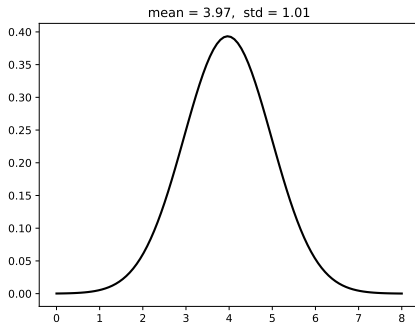


Figure: Probability density (normal law)

Expected value of continuous variables

- ▶ How can we express the expected value of a continuous variable $X \in \mathbb{R}$ that has a density $f(X)$.



$$E(X) = \int_{\mathbb{R}} xf(x)dx \quad (2)$$

Expected value of continuous variables

- For instance the expected value for the gaussian law writes :

$$E(X) = \int_{\mathbb{R}} x \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2} dx = ? \quad (3)$$

Careful !

- ▶ Sometimes the expected value does not exist !

Careful !

- ▶ Sometimes the expected value does not exist !
- ▶ Can you think of examples ?

Careful !

- ▶ Let us consider the random variable Y defined by
 - ▶ $Y = e^{X^3}$
 - ▶ where $X \sim N(\mu, \sigma^2)$

Careful !

- ▶ Let us consider the random variable Y defined by
 - ▶ $Y = e^{X^3}$
 - ▶ where $X \sim N(\mu, \sigma^2)$
- ▶ The expected value would be

$$\int_{\mathbb{R}} e^{x^3} \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2} dx = +\infty \quad (4)$$

- ▶ There is **no expected value**

Variance

- ▶ The **variance** of a random variable is a measure of the variations around the mean.

Variance

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$$V(X) = E((X - E(X))^2) \quad (5)$$

Exercise 2 : Famous rule

- Please show that :

$$V(X) = E(X^2) - E(X)^2 \quad (6)$$

Back to our problem

- ▶ Until now, we studied random variables where we can either explicitly compute the expectation, or write a very simple program to compute it.

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- ▶ Until now, we studied random variables where we can either explicitly compute the expectation, or write a very simple program to compute it.
- ▶ But we are interested in a situation where it is not easy to compute the expectation. For instance when we want the expectation of some function g of a random variable of density f :

$$E[g(X)] = \int_{\mathbb{R}} f(x)g(x)dx \quad (7)$$

Objective

- We want an approximation of this object :

$$E[g(X)] = \int_{\mathbb{R}} f(x)g(x)dx \quad (8)$$

Objective

- ▶ We want an approximation of this object :

$$E[g(X)] = \int_{\mathbb{R}} f(x)g(x)dx \quad (9)$$

- ▶ Several methods exist :
 - ▶ Deterministic methods
 - ▶ Random methods (such as Monte-Carlo)

Random methods

- ▶ Now let us discuss today's topic, the Monte Carlo method

The law of large numbers

- ▶ The fundamental idea behind the Monte Carlo method is the following theorem

Theorem

Let $(X_n)_{n \in \mathbb{N}}$ be a sequence of real random variables, independent and identically distributed. We assume that $E(|X_1|) < +\infty$. Then

$$\frac{X_1 + \cdots + X_n}{n} \xrightarrow[n \rightarrow +\infty]{a.s.} E(X) \quad (10)$$

The law of large numbers

- ▶ Let us apply this idea to our problem. If X is a random variable distributed with a probability density $f(x)$. We want to compute, the expectation $E[g(X)]$ for some function g .
- ▶ Is $(X_i)_{i \in \mathbb{N}}$ is a sequence of **i.i.d** random variables with density f , then

$$\frac{1}{n} \sum_{i=1}^n g(X_i) \rightarrow E[g(X)] \quad (11)$$

Remark

- If we simply want to compute the expectation $E[X]$, then

$$\frac{1}{n} \sum_{i=1}^n X_i \rightarrow E[X] \quad (12)$$

Method

- So all we need to do is being able to **simulate** i.i.d. random variables with the relevant density f .

Applying Monte Carlo

Exercise 3 : Computing an expectation

We want an estimation of the expected value of the **kinetic energy** of a set of particles.

We assume the energy E_c of a given particle writes

$$E_c = \frac{1}{2}mv^2 \quad (13)$$

Where m is the mass of the particle (identical for all particles) and v its speed.

We unrealistically assume that the speed is **uniformly distributed** on $[0, 1000]$ meters per second. The order of magnitude is ok, but not the shape of the distribution.

Use a Monte-Carlo method in order to compute the expected kinetic energy.

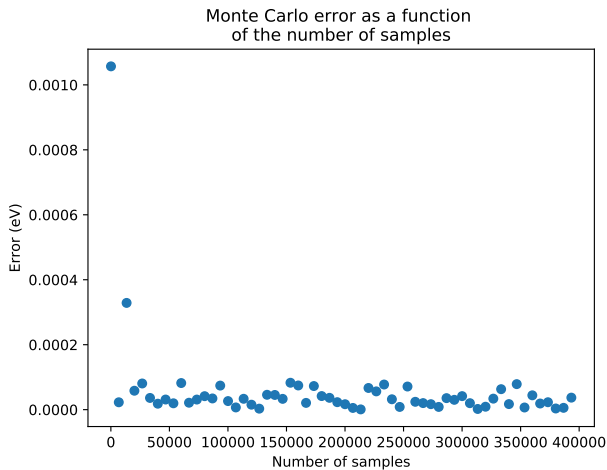
We assume $m = 2e^{-26} \text{ Kg}$.

Applying Monte Carlo

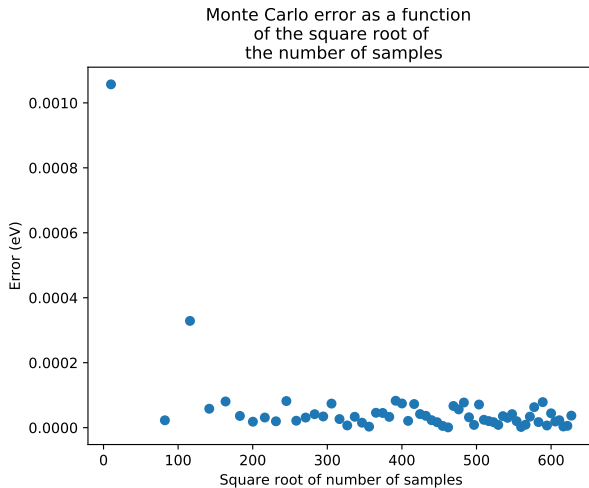
Exercise 3 : Computing an expectation

- ▶ Please plot the **error of the estimation** as a function of the number of samples used.

Applying Monte Carlo



Applying Monte Carlo



Error and number of samples

- ▶ We need a result that tells us how much simulation we need to perform in order to trust our result.

Speed of convergence

- ▶ How many variables X_i should we simulate ?
- ▶ i.e : what n should we choose ?

Central limit theorem

- ▶ This theorem tells us that with the same hypothesis as before **and** a new condition $E(X_1^2) < +\infty$:

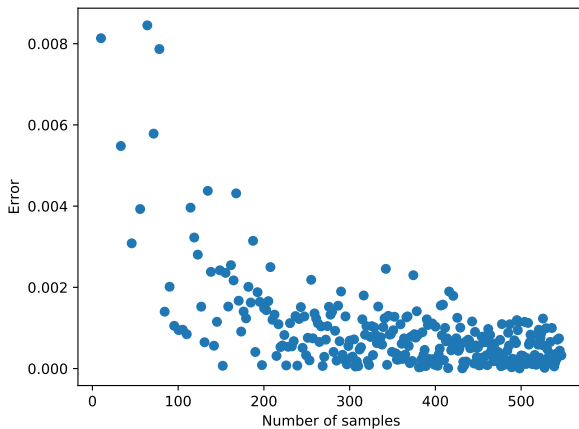
$$\frac{\sqrt{n}}{\sigma} \left(\frac{X_1 + \cdots + X_n}{n} - E(X_1) \right) \xrightarrow[n \rightarrow +\infty]{distribution} \mathcal{N}(0, 1) \quad (14)$$

Error

- ▶ The theorem tells us that the error decays as a function of \sqrt{n}

Error

Monte Carlo error as a function of the square root of number of simulated variables



Central limite theorem

- ▶ Let ϵ_n be the error $(\frac{X_1 + \dots + X_n}{n} - E(X_1))$
- ▶ The Central limit theorem tells us that **in distribution**,

$$\frac{\sqrt{n}}{\sigma} \epsilon_n \xrightarrow[n \rightarrow +\infty]{distribution} \mathcal{N}(0, 1) \quad (15)$$

Central limite theorem

Exercise 4 : Value of n

- ▶ Let ϵ_n be the error $(\frac{X_1 + \dots + X_n}{n} - E(X_1))$
- ▶ The Central limit theorem tells us that **in distribution**,

$$\frac{\sqrt{n}}{\sigma} \epsilon_n \xrightarrow[n \rightarrow +\infty]{\text{distribution}} \mathcal{N}(0, 1) \quad (16)$$

- ▶ For what value of n can we say that the error is smaller than 0.01 with probability 0.95 ?

Central limit theorem

For n sufficiently large :

$$P(|\frac{\sqrt{n}}{\sigma}\epsilon_n| \leq 1.96) \sim P(|\mathcal{N}(0,1)| \leq 1.96) = 0.95 \quad (17)$$

Central limit theorem

For n sufficiently large :

$$P\left(\left|\frac{\sqrt{n}}{\sigma}\epsilon_n\right| \leq 1.96\right) \sim P(|\mathcal{N}(0,1)| \leq 1.96) = 0.95 \quad (18)$$

Which we can write :

$$P(|\epsilon_n| \leq \frac{1.96 \times \sigma}{\sqrt{n}}) \sim 0.95 \quad (19)$$

Remark

- ▶ The variance σ of the random variables appears in the estimator !

Simulation of non uniform random variables

- Let us now assume that we need the expectation of a random variable that is **not uniform**.

Cumulative distribution function

- To do so, we will need the Cumulative distribution function

$$F(x) = P(X \leq x) \quad (20)$$

Cumulative distribution function

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- F is monotonically increasing

Pseudo inverse

- We introduce the pseudo inverse F^{-1} .

$$\forall u \in [0, 1], F^{-1}(u) = \inf\{y \in \mathbb{R}, F(y) \geq u\} \quad (22)$$

Pseudo inverse

- We can show that $\forall u \in [0, 1], x \in \mathbb{R}$

$$F^{-1}(u) \leq x \Leftrightarrow u \leq F(x) \quad (23)$$

Pseudo inverse

- ▶ We can show that $\forall u \in [0, 1], x \in \mathbb{R}$

$$F^{-1}(u) \leq x \Leftrightarrow u \leq F(x) \quad (24)$$

- ▶ and that if U is a uniform law on $[0, 1]$, then the random variable $F^{-1}(U)$ is a random variable with a cumulative distribution function of F .

Exponential law

Exercise 5 : Computing a pseudo inverse.

- ▶ Let us introduce the **exponential law**.
- ▶ Its density is

$$f(x) = \lambda \exp(-\lambda x) \quad (25)$$

for $x \geq 0$ and 0 otherwise.

- ▶ Please compute its cumulative distribution function.

Exponential law

Exercise 5 : Computing a pseudo inverse.

- ▶ Let us introduce the **exponential law**.
- ▶ Its density is

$$f(x) = \lambda \exp(-\lambda x) \quad (26)$$

for $x \geq 0$ and 0 otherwise.

- ▶ Please compute its cumulative distribution function F .
- ▶ What is the pseudo-inverse of F ?

Monte Carlo II

Exercise 6 : Computing an expectation.

- ▶ Let us consider the lifespan of a transistor. We will say that this lifespan is a random variable T following an exponential law of parameter $\frac{1}{3}$. Let us assume (unrealistically) that the user could process T^2 tasks using the machine.
- ▶ Please use the Monte Carlo method in order to approximate the expectation of this random variable.

Deterministic vs stochastic ?

- ▶ So which method is better : deterministic or stochastic ?

Algorithmic complexity

- ▶ The **complexity** of an algorithm is a measure of its **cost**. It is the number of elementary operations necessary for the algorithm to run.

Complexity examples

- ▶ 1) What is the complexity of enumerating all the elements in a set of size n ?

Complexity examples

- ▶ 2) What is the complexity of enumerating all the subsets elements in a set of size n ?

Complexity examples

- ▶ 3) What is the complexity searching a given name in a stack of **ranked** n folders ?

Complexity examples

- ▶ 4) What is the complexity of enumerating all the permutations of a set of size n ?

Complexities

- ▶ linear, polynomial complexities are OK
- ▶ exponential complexities are not OK

Monte Carlo vs deterministic complexity

- ▶ Let n be the number of simulated variables for MC and the number of steps for the Riemann method (deterministic)
- ▶ Let d be the **dimensionality** of the problem (we worked with dimension 1). If you work with **random vectors** the dimension might be > 1 .

Monte Carlo vs deterministic complexity

- ▶ $n \simeq$ computation cost
- ▶ Deterministic method : the error depends on $n^{-\frac{1}{d}}$.
- ▶ Monte Carlo : the error depends on $n^{-\frac{1}{2}}$.

Monte Carlo vs deterministic complexity

- ▶ $n \simeq$ computation cost
- ▶ Deterministic method : the error depends on $n^{-\frac{1}{d}}$.
- ▶ Monte Carlo : the error depends on $n^{-\frac{1}{2}}$.
- ▶ Which method is better ?

Monte Carlo vs deterministic

- ▶ Monte Carlo is better is the dimension is bigger than 3.
- ▶ Its precision does not depend on the dimensionality.
- ▶ Monte Carlo is mostly used in large dimensions when the precision required is smaller.
- ▶ The speed of convergence is in $\frac{1}{\sqrt{n}}$ which is quite slow.

- └ Why is Monte-Carlo useful ?
- └ Notion of algorithmic complexity

Speeding up Monte Carlo

- ▶ There are several methods to accelerate the convergence
- ▶ The most famous one is the **Variance reduction method**

Speeding up Monte Carlo

- ▶ There are several methods to accelerate the convergence
- ▶ The most famous one is the **Variance reduction method**
- ▶ The idea is to use, instead of X , another random variable with the same expectation but with smaller variance.

$$E[Y] = E[X], \quad V(Y) \leq V(X) \quad (27)$$

Monte Carlo and game

- How could we apply these ideas when building a fantom or an inspector ?



Monte Carlo and game

- We could compute the probability of winning after being in some state s with a Monte Carlo approximation.



Monte Carlo and game

- ▶ We could compute the probability of winning after being in some state s with a Monte Carlo approximation.
- ▶ Example of state to consider : (I, N) where :
 - ▶ I is the number of isolated suspects.
 - ▶ N is the number of non-isolated ones.



Monte Carlo and game

- ▶ We could compute the probability of winning after being in some state s with a Monte Carlo approximation.
- ▶ Example of state to consider : (I, N) where :
 - ▶ I is the number of isolated suspects.
 - ▶ N is the number of non-isolated ones.
- ▶ But other choices are possible.

