

# Chapter 2. Computer Simulations and Monte Carlo Methods

## 1 Monte Carlo Methods and Random Number Generators

**Monte Carlo (MC) methods** are methods of approximation (estimation) based on computer simulations involving random numbers. And yes!, the name *does* come from the famous casino in Monaco (probability distributions involved in gambling are often complicated, but they can be estimated via simulations).

The main purpose of simulations is estimating quantities whose direct computation is complicated, expensive, time consuming, dangerous, or plainly impossible (think space shuttle launch, spread of a virus or disease, performance of a medical device or procedure, etc.). MC methods are mostly used for computation of probabilities, expected values and other distribution characteristics, but they can also be used to estimate lengths, areas, volumes, integrals, irrational numbers (like  $\pi$ ,  $e$ ,  $\sqrt{2}$ ), etc.

Recall that probability can be defined as a *long-run proportion* (relative frequency). With the help of random number generators, computers can actually simulate a “long run”. The longer the run is simulated, the more accurate the results obtained.

Some examples include:

- **Forecasting**, i.e. making reasonably remote predictions for weather, profit, stock prices, costs, etc. For a time  $n$ , we estimate  $X_n$  from the (already known) variables  $X_1, X_2, \dots, X_{n-1}$ . Controlling the length of this do-loop, we can obtain forecasts for the next days, weeks, months or years.
- **Signal transmission (percolation)**. Consider a network of nodes (a graph), some nodes connected, others not. A signal is sent from a certain node. Once a node  $k$  receives a signal, it sends it along each of its output lines with some probability  $p_k$ . After a certain period of time, one wishes to estimate the proportion of nodes that received a signal, the probability for a certain node to receive it, etc. That would mean generating Bernoulli variables with probability  $p_k$ . Spread of a disease or a computer virus, spread of fire through a forest would fit such a model.
- **Queuing systems (server facilities)**. A queuing system is described by a number of random variables. It involves spontaneous arrivals of jobs, their random waiting time, assignment to

servers, their random service and departure time; some jobs may exit prematurely, others may not enter the system if it appears full, also, intensity of the incoming traffic and the number of servers on duty may change during the day. One wants to be able to evaluate a queuing system's vital performance characteristics, such as a job's average waiting time, average length of a queue, the proportion of customers who had to wait, the proportion of "unsatisfied customers" (that exit prematurely or cannot enter), the proportion of jobs spending more than a certain time in the system, the expected usage of each server, the average number of available (idle) servers at the time when a job arrives, and so on.

Implementation of MC methods reduces to generation of random variables from given distributions. All mathematical and statistical software packages (Matlab, Maple, Mathematica, SAS, R, Splus, SPSS, Minitab, Excel, etc.) have built-in procedures for generating random variables from the most common (discrete or continuous) distributions. As it turns out, the main job is that of generating random numbers from a Uniform distribution, in fact, from a *Standard Uniform* distribution. These can then be used to generate random numbers from *any* given distribution.

However, generating *truly random* Uniformly distributed numbers is not an easy task and is an ongoing research area in Modern Statistics. More often, *pseudo-random* (deterministic) numbers are generated, i.e. a long list of numbers. The user specifies a random number *seed* that points to the location from which the list will be read. Often each seed is generated within the system, to improve the quality of random numbers.

## 2 Discrete Methods

These are methods for generating some simple discrete variables, most being specific to certain distributions, by using their interpretation and relationship with other variables, rather than their definition (pdf or cdf).

From here on, we denote by  $U \in U(0, 1)$  a Standard Uniform variable. Let us recall the pdf and cdf (equation (5.10) in Chapter 1, Lecture 2):

$$f_U(x) = \begin{cases} 1, & x \in [0, 1] \\ 0, & x \notin [0, 1] \end{cases}, \quad F_U(x) = \begin{cases} 0, & x \leq 0 \\ x, & 0 < x \leq 1 \\ 1, & x \geq 1. \end{cases} \quad (2.1)$$

**Bernoulli Distribution**  $Bern(p), p \in (0, 1)$ 

Recall that a Bernoulli distribution models the occurrence (or nonoccurrence) of an event (success), with a given probability  $p$ .

Let  $U$  be a Standard Uniform variable. That means its value is in  $(0, 1)$ , just like the value of  $p$ . Then define

$$X = \begin{cases} 1, & U < p \\ 0, & U \geq p \end{cases}, \quad (2.2)$$

i.e. define “success” as  $(U < p)$  (and, obviously, “failure” as  $(U \geq p)$ ). Let us check that this is indeed a Bernoulli variable with parameter  $p$ . We have

$$P(X = 1) = P(U < p) = F_U(p) = p,$$

by (2.1), since  $p \in (0, 1)$ . So  $X$  has the desired distribution.

**Algorithm 2.1.**

Read  $p \in (0, 1)$

$U = rand$ ;

$X = (U < p)$ ;

Now we can use this simple way of simulating success/failure with a given probability, for all the variables that are defined in terms of that.

**Binomial Distribution**  $B(n, p), n \in \mathbb{N}, p \in (0, 1)$ 

Recall (Remark 5.2 in Chapter 1, Lecture 2) that a  $B(n, p)$  variable is the sum of  $n$  independent  $Bern(p)$  variables.

**Algorithm 2.2.**

Read  $n \in \mathbb{N}, p \in (0, 1)$

$U = rand(n, 1)$ ;

$X = sum(U < p)$ ;

**Geometric Distribution**  $Geo(p), p \in (0, 1)$ 

A Geometric variable counts the number of failures that occurred before the 1<sup>st</sup> success. We can simulate that.

**Algorithm 2.3.**

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Read  $p \in (0, 1)$ 
 $X = 0$ ; % initial number of failures
while  $rand \geq p$  % while there are failures
     $X = X + 1$ ; % count number of failures
end % stop at the first success

```

**Remark 2.4.** Obviously, the same algorithm can be used to simulate a  $Y \in SGeo(p)$  variable, as well.  $Y$  is the number of *trials* needed to get the 1<sup>st</sup> success, so simply let  $Y = X + 1$  in Algorithm 2.3.

**Negative Binomial (Pascal) Distribution**  $NB(n, p), n \in \mathbb{N}, p \in (0, 1)$ 

Again, we use the same Remark 5.2 (in Chapter 1, Lecture 2), which states that a  $NB(n, p)$  variable is the sum of  $n$  independent  $Geo(p)$  random variables.

**Algorithm 2.5.**

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Read  $n \in \mathbb{N}, p \in (0, 1)$ 
 $X = \text{zeros}(1, n)$ ;
for  $i = 1 : n$  % generate  $n$   $Geo(p)$  variables
    while  $rand \geq p$  % while there are failures
         $X(i) = X(i) + 1$ ; % count number of failures
    end % stop at the first success
end
 $Y = \text{sum}(X)$ ; % the sum is a  $NBin(n, p)$  variable

```

**Arbitrary Discrete Distribution**

Let  $X$  be an arbitrary discrete random variable with pdf

$$X \begin{pmatrix} x_1 & x_2 & \dots \\ p_1 & p_2 & \dots \end{pmatrix}, \quad \sum p_i = 1. \quad (2.3)$$

We generalize the idea that was used to generate a  $Bern(p)$  variable. There, we basically divided the interval  $[0, 1]$  into the disjoint subintervals  $[0, p)$  and  $[p, p + (1 - p)]$ . We can do the same for *any* number of subintervals.

**Algorithm 2.6.**

- Read  $x_i, p_i, i = 1, 2, \dots$
- Divide the interval  $[0, 1]$  into subintervals

$$\begin{aligned}
A_1 &= [0, p_1) \\
A_2 &= [p_1, p_1 + p_2) \\
A_3 &= [p_1 + p_2, p_1 + p_2 + p_3) \\
&\dots \\
A_i &= [p_1 + \dots + p_{i-1}, p_1 + \dots + p_i) \\
&\dots
\end{aligned}$$

Then  $\text{length}(A_i) = p_i$ , for a finite or countably infinite number of values  $x_i$ .

- Get  $U \in U(0, 1)$ .
- If  $U \in A_i$ , then let  $X = x_i$ .

Then, we have

$$\begin{aligned}
P(X = x_i) &= P(U \in A_i) = P(p_1 + \dots + p_{i-1} \leq U < p_1 + \dots + p_{i-1} + p_i) \\
&= F_U(p_1 + \dots + p_{i-1} + p_i) - F_U(p_1 + \dots + p_{i-1}) \\
&= p_1 + \dots + p_{i-1} + p_i - (p_1 + \dots + p_{i-1}) \\
&= p_i,
\end{aligned}$$

so  $X$  has indeed pdf (2.3).

**Example 2.7.** Let us use Algorithm 2.6 to generate a variable with pdf

$$X \begin{pmatrix} 0 & 1 & 2 & \dots \\ p_0 & p_1 & p_2 & \dots \end{pmatrix}, \quad \sum_{i \in \mathbb{N}} p_i = 1.$$

Recall that for a discrete random variable, the cdf is computed as  $F(x) = P(X \leq x) = \sum_{x_i \leq x} p_i$ ,

so in this case,

$$F(k) = \sum_{i \leq k} p_i = p_0 + p_1 + \dots + p_k, \quad k = 0, 1, \dots,$$

so to check if  $U \in A_k$ , we check that  $F(k-1) \leq U < F(k)$ .

### Algorithm

Read  $p_0, p_1, \dots$

Get  $U \in U(0, 1)$

$i = 0$ ; % initial value of  $X$

$F = p_0$ ; % initial value of cdf  $F(0)$

while  $U \geq F$  % check if  $U \in A_i$

$i = i + 1$ ;

$F = F + p_i$ ; % new value of cdf,  $F(i+1)$

end % the while loop ends when  $U < F(i)$

$X = i$ ;

## 3 Inverse Transform Method

This is a method used when we want to generate a random variable whose cdf  $F$  does not have a very complicated form. It is based on the following result:

**Theorem 3.1.** *Let  $X$  be a continuous random variable with cdf  $F : \mathbb{R} \rightarrow \mathbb{R}$ . Then  $U = F(X) \in U(0, 1)$ .*

*Proof.* So,  $F$  is the cdf of  $X$ , i.e.  $F(x) = P(X \leq x)$ , for all  $x \in \mathbb{R}$ .

We will show that  $U$  has the  $U(0, 1)$  pdf, by starting with its cdf and then taking its derivative.

First off, let us notice that, being a cdf,  $F(x) \in [0, 1]$ , for all  $x \in \mathbb{R}$  and, thus, all the values of  $U$  are in  $[0, 1]$ .

Secondly,  $X$  being a continuous random variable, there exists an interval  $[a, b] \subseteq \mathbb{R}$  such that :

- $F : [a, b] \rightarrow [0, 1]$  is strictly increasing (therefore one-to-one),
- $F(x) = 0, \forall x < a$  and
- $F(x) = 1, \forall x > b$ .

Hence, its inverse  $F^{-1} : [0, 1] \rightarrow [a, b]$  exists.

Now, let us consider the cdf,  $F_U$ . Let  $x \in \mathbb{R}$ .

If  $x < 0$ , then  $F_U(x) = P(U \leq x) = P(\text{impossible event}) = 0$ . Hence,  $f_U(x) = F'_U(x) = 0$ .

If  $x > 1$ , then  $F_U(x) = P(U \leq x) = P(\text{sure event}) = 1$  and thus,  $f_U(x) = F'_U(x) = 0$ .

For  $x \in [0, 1]$ , we have

$$F_U(x) = P(U \leq x) = P(F(X) \leq x) = P(X \leq F^{-1}(x)) = F(F^{-1}(x)) = x.$$

Then  $f_U(x) = F'_U(x) = 1$  and  $U \in U(0, 1)$ . □

As a consequence, to generate a continuous random variable with given cdf  $F$ , we generate a variable  $U \in U(0, 1)$  and let

$$X = F^{-1}(U). \quad (3.1)$$

Indeed, then the cdf of  $X$  is

$$F_X(x) = P(X \leq x) = P(F^{-1}(U) \leq x) = P(U \leq F(x)) = F_U(F(x)) = F(x),$$

for all  $x \in \mathbb{R}$ , the last assertion following from (2.1) and the fact that  $F(x) \in [0, 1]$ . Thus  $X$  has the desired cdf  $F$ .

**Example 3.2.** Use the ITM to generate a random variable  $X$  with pdf

$$f(x) = \frac{1}{2}(x+1), \quad x \in [-1, 1]. \quad (3.2)$$

Then use the value  $U = 0.16$  to generate a value for  $X$ .

**Solution** First, we find the cdf  $F(x) = \int_{-\infty}^x f(t)dt$ .

If  $x < -1$ , obviously  $F(x) = 0$  (the integrand is 0).

If  $x \in [-1, 1]$ , we have

$$\begin{aligned} F(x) &= \frac{1}{2} \int_{-1}^x (t+1)dt = \frac{1}{2} \left( \frac{1}{2}t^2 + t \right) \Big|_{-1}^x \\ &= \frac{1}{2} \left( \frac{1}{2}x^2 + x + \frac{1}{2} \right) = \frac{1}{4}(x+1)^2. \end{aligned}$$

If  $x > 1$ , then  $F(x) = \frac{1}{2} \int_{-1}^1 (t+1)dt = \int_{\mathbb{R}} f(t)dt = 1$ .

So,

$$F(x) = \begin{cases} 0, & x < -1 \\ \frac{1}{4}(x+1)^2, & -1 \leq x \leq 1 \\ 1, & x > 1 \end{cases}.$$

The graph of the cdf  $F$  is shown in Figure 1. One can see that  $F : [-1, 1] \rightarrow [0, 1]$  is one-to-one and surjective, so the inverse  $F^{-1} : [0, 1] \rightarrow [-1, 1]$  exists. We find it by solving  $F(x) = y$  for  $x$ , i.e.  $x = F^{-1}(y)$ .

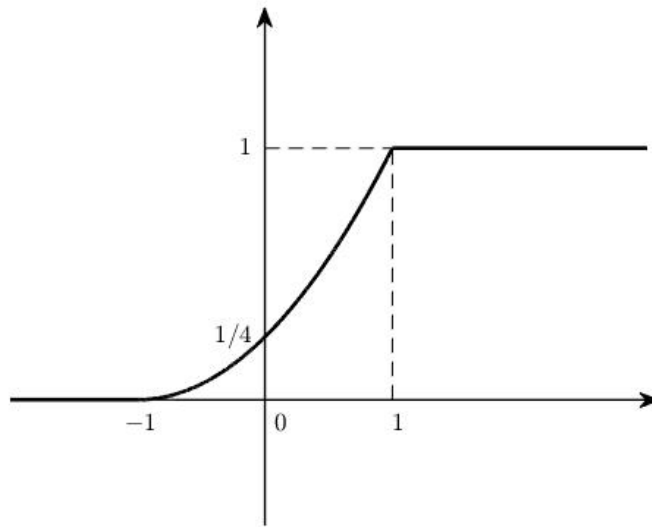


Fig. 1: Function  $F$  in Example 3.2

We have

$$\begin{aligned}\frac{1}{4}(x+1)^2 &= y, \\ (x+1)^2 &= 4y, \\ x+1 &= \sqrt{4y}, \\ x &= 2\sqrt{y} - 1,\end{aligned}$$

so,  $F^{-1}(y) = 2\sqrt{y} - 1$ , for  $y \in [0, 1]$ .

Then we generate  $X$  from  $U$  by

$$X = F^{-1}(U) = 2\sqrt{U} - 1.$$

For the value  $U = 0.16$ , we get  $X = 2 \cdot 0.4 - 1 = -0.2$ . ■

**Example 3.3.** Use the ITM to generate  $X \in \text{Exp}(\lambda)$ ,  $\lambda > 0$ .

**Solution** For  $X \in \text{Exp}(\lambda)$ , the pdf and cdf are given by

$$f(x) = \lambda e^{-\lambda x}, x \geq 0 \text{ and } F(x) = 1 - e^{-\lambda x}, x \geq 0,$$

respectively (see equation (5.14), Chapter 1, Lecture 2).



So, we find the inverse of the cdf

$$\begin{aligned}
F(X) &= U, \\
1 - e^{-\lambda X} &= U, \\
e^{-\lambda X} &= 1 - U, \\
-\lambda X &= \ln(1 - U), \\
X_1 &= -\frac{1}{\lambda} \ln(1 - U).
\end{aligned} \tag{3.3}$$

Now, algebraically, we cannot simplify this expression, but we can notice the following:

$$U \in U(0, 1) \iff 1 - U \in U(0, 1).$$

Indeed, we see that for  $x \in [0, 1]$ ,

$$\begin{aligned}
F_{1-U}(x) &= P(1 - U \leq x) = P(U \geq 1 - x) = 1 - P(U < 1 - x) \\
&= 1 - F_U(1 - x) \stackrel{(2.1)}{=} 1 - (1 - x) = x = F_U(x).
\end{aligned}$$

Then, by taking the derivative,  $f_{1-U}(x) = f_U(x)$ , so we can replace  $U$  by  $1 - U$  in (3.3) and get

$$X_2 = -\frac{1}{\lambda} \ln(U). \tag{3.4}$$

Notice that since  $U, 1 - U \in (0, 1)$ , we have that both  $\ln(U), \ln(1 - U) < 0$  and, thus,  $X_1, X_2 > 0$ , as they should be. ■

### Discrete Inverse Transform Method

We can see that the previous algorithm seems to have one major fault, namely, that it is not applicable to discrete random variables, since in this case, the cdf  $F$  is not injective and, thus, not invertible. This problem can be overcome, by adjusting the algorithm the following way. In equation (3.1), we will take

$$X = F^{-1}(U) = \min\{x \mid F(x) \geq U\}. \tag{3.5}$$

This is known as the *generalized inverse* function. So, in Figure 2, we have

$$\begin{aligned} X_1 &= F^{-1}(U_1) = \min\{x \mid F(x) \geq U_1\} = x_1, \text{ here } F(x_1) = U_1, \\ X_2 &= F^{-1}(U_2) = \min\{x \mid F(x) \geq U_2\} = x_2, \text{ here } F(x_2) > U_2. \end{aligned}$$

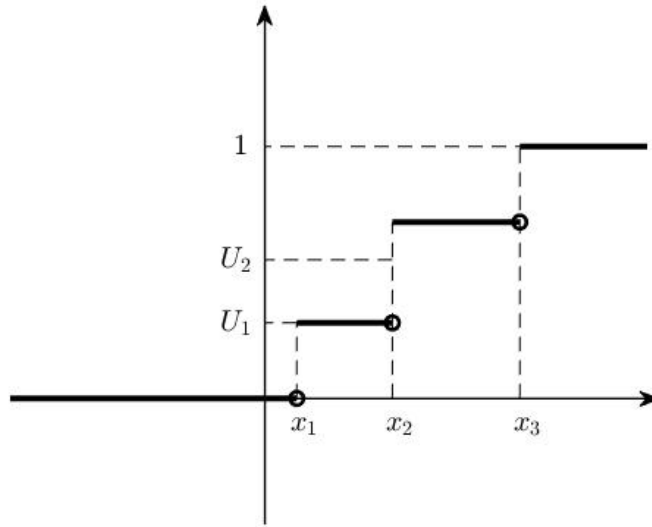


Fig. 2: Generalized inverse

**Example 3.4.** Let us revisit Geometric and Shifted Geometric variables and generate them using the DITM.

**Solution** To keep computations simple, we generate a  $SGeo(p)$  variable first and then adjust it accordingly to get a  $Geo(p)$  variable.

For  $X \in SGeo(p)$ ,  $p \in (0, 1)$ , recall the cdf (Chapter 1, Lecture 2):

$$F(x) = 1 - q^x = 1 - (1 - p)^x, \quad x \in \mathbb{N}.$$

We use (3.5) to find  $X$ :

$$\begin{aligned}
1 - (1 - p)^x &\geq U, \\
(1 - p)^x &\leq 1 - U, \\
x \ln(1 - p) &\leq \ln(1 - U), \\
x &\geq \frac{\ln(1 - U)}{\ln(1 - p)}, \text{ since } \ln(1 - p) < 0.
\end{aligned}$$

The smallest integer value satisfying this is the ceiling function value. Also, as before,  $1 - U$  can be replaced by  $U$ . Thus, a variable  $X \in SGeo(p)$  is generated by

$$X = \left\lceil \frac{\ln(U)}{\ln(1 - p)} \right\rceil. \quad (3.6)$$

For a  $X \in Geo(p)$  variable, with cdf  $F(x) = 1 - (1 - p)^{x+1}$ , the same computations lead to

$$X = \left\lceil \frac{\ln(U)}{\ln(1 - p)} - 1 \right\rceil. \quad (3.7)$$

■

**Remark 3.5.** Notice how similar formula (3.6) is to (3.4), which gives the simulation of an  $Exp(\lambda)$  variable. If  $\lambda = -\ln(1 - p)$ , then the generated  $SGeo(p)$  variable is just the ceiling of the  $Exp(\lambda)$  one. In other words, the ceiling of an Exponential variable has Shifted Geometric distribution. This just shows, again, the strong analogy between the two distributions.