Exercise – Understanding the theory of inverse transform sampling

1. Aim of the exercise

The aim of this exercise is to understand the theory behind the method of inverse transform sampling.

2. Theory

The aim of the inverse transformation method is to provide a way of drawing from a cumulative distribution function (CDF) $F(x)$ that is not straightforward to sample from directly. Packages for random number generation in programming software typically cover only the most simple and widely used probability distributions. However, there exist uncountably many distributions beyond these. Under certain restrictive conditions, the inverse transformation method is the most natural technique for drawing from a non-standard CDF. First, the distribution must be valid, meaning its total probability adds up to one.

Second, the CDF must have a formula we can write out directly. This requirement is satisfied for many theoretical distributions, such as the exponential or normal, where F has a closed form.

Third, the method requires that the inverse of the CDF can be written in closed form. This is restrictive because only some distributions admit such an explicit formula. For example, the exponential distribution does, while the normal distribution does not.

Fourth, the inverse of a function is only defined when the function is injective, meaning that distinct inputs do not lead to the same output. Many CDFs, especially those of discrete distributions, are not injective because they contain flat regions between jumps. In these regions, different x values yield the same $F(x)$. In these cases the inverse does not exist, and the generalized inverse is used.

The generalized inverse of the CDF F of a random variable X is defined as follows:

$$F^{-1}(y) := \inf\{x : F(x) \geq y\}, \tag{1}$$

where $y \in [0, 1]$. Figure 1 provides the geometric interpretation of the generalized inverse. A number y between 0 and 1 is chosen, representing a height on the vertical axis of the CDF. A horizontal line is drawn at this level until it intersects the graph of $F(x)$. The intersection point indicates where the CDF first reaches or exceeds the chosen level y. Projecting this point down to the horizontal axis gives the value x, which is the generalized inverse $F^{-1}(y)$.

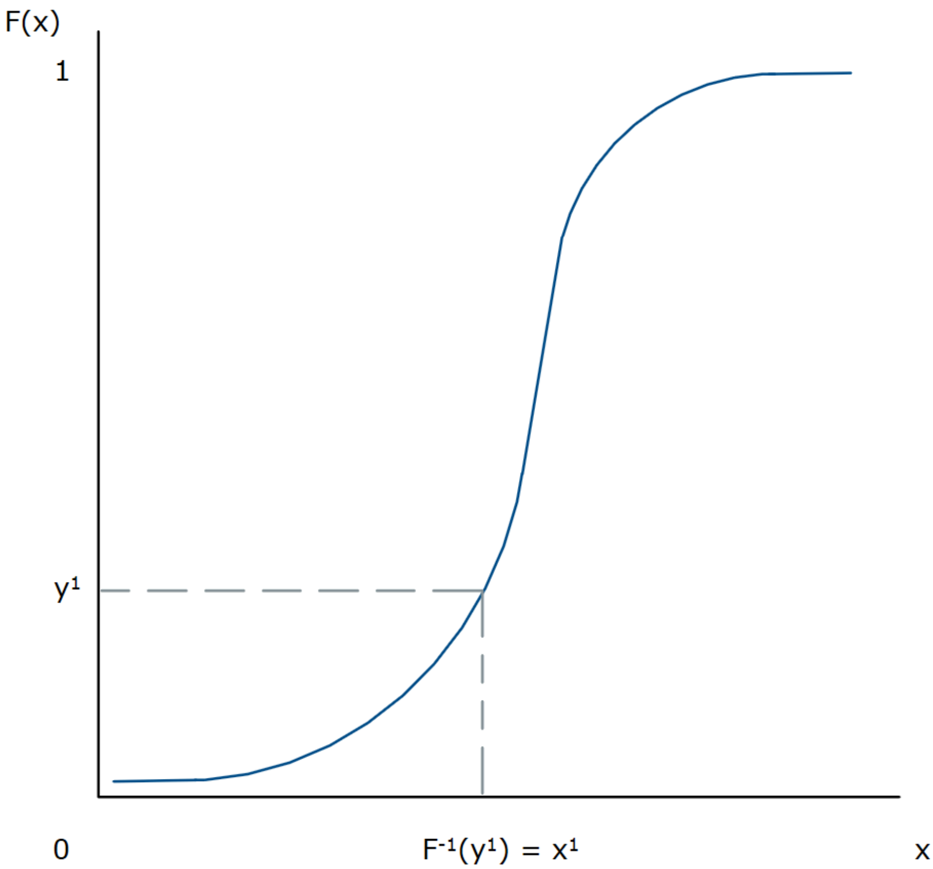

Figure 1: Geometric interpretation of the generalized inverse of a CDF.

That is, the inverse function tries to find the x such that $F(x) = y$, but this fails whenever multiple x values correspond to the same y. The generalized inverse function avoids this ambiguity by assigning a unique value, namely the infimum of $\{x : F(x) \geq y\}$. In this way the generalized inverse function remains well-defined, even in the presence of flat regions in the CDF.

To illustrate the definition, suppose $X \sim \text{Bernoulli}(0.3)$. The probability mass function is

$$P(X = x) = \begin{cases} 0.7 & \text{if } x = 0, \\ 0.3 & \text{if } x = 1, \\ 0 & \text{otherwise.} \end{cases}$$

The CDF is

$$F(x) = \begin{cases} 0 & \text{for } x < 0, \\ 0.7 & \text{for } 0 \leq x < 1, \\ 1 & \text{for } x \geq 1. \end{cases}$$

Notice that the CDF remains constant at the level 0.7 for all x in the interval $[0, 1)$. As a result, $F^{-1}(0.7)$ gives more than one possible x value, which makes the inverse ambiguous. The generalized inverse resolves this ambiguity. Consider $y = 0.7$. The set

$$\{x : F(x) \geq 0.7\}$$

contains all $x \geq 0$. The infimum of this set is 0, and therefore the generalized inverse is

$$F^{-1}(0.7) = 0.$$

From this reasoning we obtain the generalized inverse CDF:

$$F^{-1}(y) = \begin{cases} 0 & \text{for } 0 \leq y \leq 0.7, \\ 1 & \text{for } 0.7 < y \leq 1. \end{cases}$$

This means that the plateau at 0.7 is resolved by assigning $y = 0.7$ to $x = 0$. Similarly, larger values of y are mapped to $x = 1$.

With these definitions in place, we can now formally state the inverse transformation method.

Theorem 1. *To generate a random variable X with (normalized) CDF F, draw $U \sim$ Unif$(0, 1)$ and calculate $X = F^{-1}(U)$.*

The theorem says that to sample from F, we first draw a uniform random number U on $[0, 1]$ and then evaluate it at the inverse of F. In other words, the uniform draw selects a probability level, and the inverse CDF converts that level into the corresponding value of the random variable X.

The method works because the CDF F maps values of X into probabilities on $[0, 1]$, and the uniform distribution provides a random draw from this same interval. For $U \sim \text{Unif}(0, 1)$ we have $\mathbb{P}(U \leq u) = u$ for $u \in [0, 1]$, meaning U selects a probability level at random. Evaluating this draw at the inverse of F converts the chosen probability level back into the corresponding realization of X.

Proof. The argument relies only on the definition of the generalized inverse of F and the fact that for $U \sim \text{Unif}(0,1)$ we have $\mathbb{P}(U \leq u) = u$ for $u \in [0,1]$. Then

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

Therefore, $X = F^{-1}(U)$ has distribution function F. ∎

The method applies only to one-dimensional, that is, univariate distributions. For multivariate distributions, with two or more variables, the situation is different. The CDF assigns probabilities to regions in space, not single points, so a single probability value can correspond to many possible outcomes. The implication is that the inverse is not uniquely defined in the multivariate case.

3. Final notes