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.

The method has a few basic requirements that must be satisfied. 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 expressed in closed form. This condition is restrictive, since only certain distributions admit such an explicit formula. For example, the exponential distribution does, whereas the normal distribution does not. In the latter case, numerical routines provided by software packages such as MATLAB can approximate the inverse, making it possible to apply the method when no analytic expression exists.

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 $y \in [0, 1]$. 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.

As an example, suppose $X \sim$ 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

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

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

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

contains all $x \ge 0$. 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:

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

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 $\mathbb{P}(U \le u) = u$ 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.

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

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Note that the step

$$\mathbb{P}(F^{-1}(U) \le x) = \mathbb{P}(U \le F(x))$$

follows directly from the definition of the generalized inverse. That is, the event $\{F^{-1}(U) \le x\}$ is the same as the event $\{U \le F(x)\}$. This means that instead of requiring $F(x) = y$, which might fail or be ambiguous on plateaus, we allow $F(x) \ge y$ and then take the smallest such x. This ensures the equivalence holds for all CDFs and guarantees uniqueness even when F has flat regions.

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