The Inverse CDF Method

(Chapter 3)

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Stats 102C: Introduction to Monte Carlo Methods

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Outline

1. The Inverse CDF Method
   - Example 1: Uniform Distribution ($\mathrm{Unif}(a, b)$)
   - Example 2: Exponential Distribution ($\mathrm{Exp}(\lambda)$)
   - Example 3: Polynomial Density
   - Example 4: Geometric Distribution ($\mathrm{Geom}(p)$)

2. Sampling from Finite Discrete Distributions
   - Example 5: Finite Discrete Distribution
   - Example 6: Bivariate Finite Discrete Distribution

generate $U \sim$ uniform $\longrightarrow$ X by use $F^{-1}(U)$

Introduction

One of the fundamental tools required in computational statistics is the ability to simulate random variables from various probability distributions.

Uniform Assumption: We assume that we can generate samples from $\mathrm{Unif}(0,1)$, the uniform distribution on the interval $(0,1)$:

$$\text{PDF of } \mathrm{Unif}(0,1)\text{: } f(x) = \begin{cases} 1 & \text{for } x \in (0,1) \\ 0 & \text{otherwise} \end{cases}$$

Can we start from this assumption to generate samples from other distributions?

Cumulative Distribution Function

Recall:

Definition

Let X denote a continuous random variable with PDF $f(x)$. The **cumulative distribution function (CDF)** of X is

$$F(x) := P(X \leq x) = \int_{-\infty}^{x} f(t)\,\mathrm{d}t.$$

What is the range of values that $F(x)$ can take?

$0 \leq F(x) \leq 1$

$\rightarrow U = F(X) \sim$ uniform $[0, 1]$

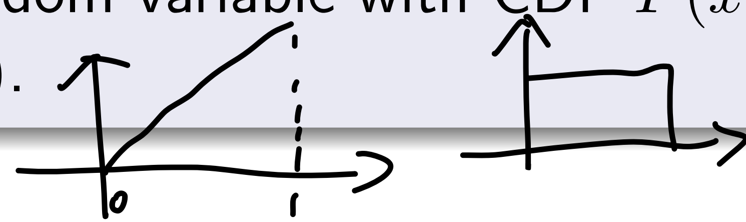
$F: X \longrightarrow$ uniform

The Probability Integral Transformation

The CDF of X maps the support of X onto the unit interval $[0, 1]$. In fact, even more is true.

Theorem (Probability Integral Transformation)

If X is a continuous random variable with CDF $F(x)$, then $U = F(X) \sim \text{Unif}(0, 1)$.



In other words, F transforms X into $\text{Unif}(0, 1)$. If we start with $\text{Unif}(0, 1)$, can we transform back to X?

The Inverse CDF Transformation

Theorem (The Inverse CDF Transformation)

Let X be a continuous random variable with CDF $F(x)$. Define the **inverse CDF transformation** u: probability

for some t F(X<t)=u

$$F^{-1}(u) := \min\{t : F(t) \geq u\}, \quad \text{for } 0 < u < 1.$$

t

If $U \sim \mathrm{Unif}(0,1)$, then $F^{-1}(U) \sim F(x)$.

CDF

Proof.

If $U \sim \mathrm{Unif}(0,1)$, then, for all $x \in \mathbb{R}$,

$$\begin{aligned} P[F^{-1}(U) \leq x] &= P[\min\{t : F(t) \geq U\} \leq x] \\ &= P[U \leq F(x)] \\ &= F(x). \end{aligned}$$

$F^{-1}(U) = X$

Therefore $F^{-1}(U)$ has the same distribution as X, as desired. □

U~ unifm [0, 1]

The Inverse CDF Method

The Inverse CDF (or Inverse Transform) Method

Goal: Generate samples from $X \sim F(x)$. $x_1\ x_2 \cdots x_n$ (CDF)

Step
1. Derive the inverse CDF $F^{-1}(u)$. $X = F^{-1}(u) \sim F(x)$
2. Generate $U \sim \text{Unif}(0, 1)$.
3. Then $X = F^{-1}(U) \sim F(x)$.

Know $f(x) \to F(x) \to F^{-1}(u)$

- The inverse CDF transform gives us a way to start with $\text{Unif}(0, 1)$ and generate from general distributions.
- An easy method to apply, as long as the inverse CDF is easy to compute.
- The method can be applied to generate from continuous or discrete random variables.

Example 1: Uniform Distribution ($\mathrm{Unif}(a,b)$)

$X \sim \text{uniform}(a, b)$

- Let $f(x)$ denote the probability density function of $\mathrm{Unif}(a,b)$:

$$f(x) = \begin{cases} \dfrac{1}{b-a} & \text{for } x \in (a,b) \\ 0 & \text{otherwise} \end{cases}$$

- The CDF of $\mathrm{Unif}(a,b)$ is then $a \le X \le b$

$$F(x) = \int_a^x 1 \cdot \frac{1}{b-a}\,\mathrm{d}t = \frac{x-a}{b-a}, \quad \text{for } a \le x \le b.$$

$$X \cdot \frac{1}{b-a}\Big|_a^x = \frac{1}{b-a}(x-a)$$

$$= \frac{x-a}{b-a}$$

- How can we sample from $\mathrm{Unif}(a,b)$?

$f(x) = \frac{1}{b-a} \rightarrow F(x) = \frac{x-a}{b-a} \rightarrow F^{-1}(u) = x$

Example 1: Uniform Distribution ($\mathrm{Unif}(a, b)$)

Inverse CDF Method for $\mathrm{Unif}(a, b)$: $X = F^{-1}(u)$

1. Derive the inverse CDF $F^{-1}(u)$. $F(x) = u$

   Set $F(x) = u$ and solve for x:

$$\begin{aligned} F(x) &= u \\ \frac{x-a}{b-a} &= u \\ x &= a + (b-a)u \end{aligned}$$

   So $F^{-1}(u) = a + (b-a)u$. (inverse cdf) $\sim F(x)$

2. Generate $U \sim \mathrm{Unif}(0, 1)$.

3. Then $X = a + (b-a)U \sim \mathrm{Unif}(a, b)$.

Example 2: Exponential Distribution ($\mathbf{Exp}(\boldsymbol{\lambda})$)

- Let $f(x)$ denote the PDF of the exponential distribution with rate parameter λ:

$$\underline{f(x) = \lambda e^{-\lambda x},} \quad \text{for } x \geq 0.$$

- The CDF of $\mathrm{Exp}(\lambda)$ is then

$$F(x) = \int_0^x \lambda e^{-\lambda t}\,\mathrm{d}t = 1 \underline{- e^{-\lambda x},} \quad \text{for } x \geq 0.$$

- How can we sample from $\mathrm{Exp}(\lambda)$?

Example 2: Exponential Distribution ($\mathrm{Exp}(\lambda)$)

Inverse CDF Method for $\mathrm{Exp}(\lambda)$: $X = F^{-1}(u)$

1. Derive the inverse CDF $F^{-1}(u)$.

   $F(x) = u$

   Set $F(x) = u$ and solve for x:

   $1 - e^{-\lambda x} = u$

   $$\begin{aligned} F(x) &= u \\ 1 - e^{-\lambda x} &= u \\ x &= -\frac{1}{\lambda}\log(1-u) \end{aligned}$$

   $x = \frac{1}{-\lambda}\log(1-u)$

   So $F^{-1}(u) = -\frac{1}{\lambda}\log(1-u)$.

   $X = F^{-1}(u) = -\frac{1}{\lambda}\log(\underbrace{1-u}_{u})$

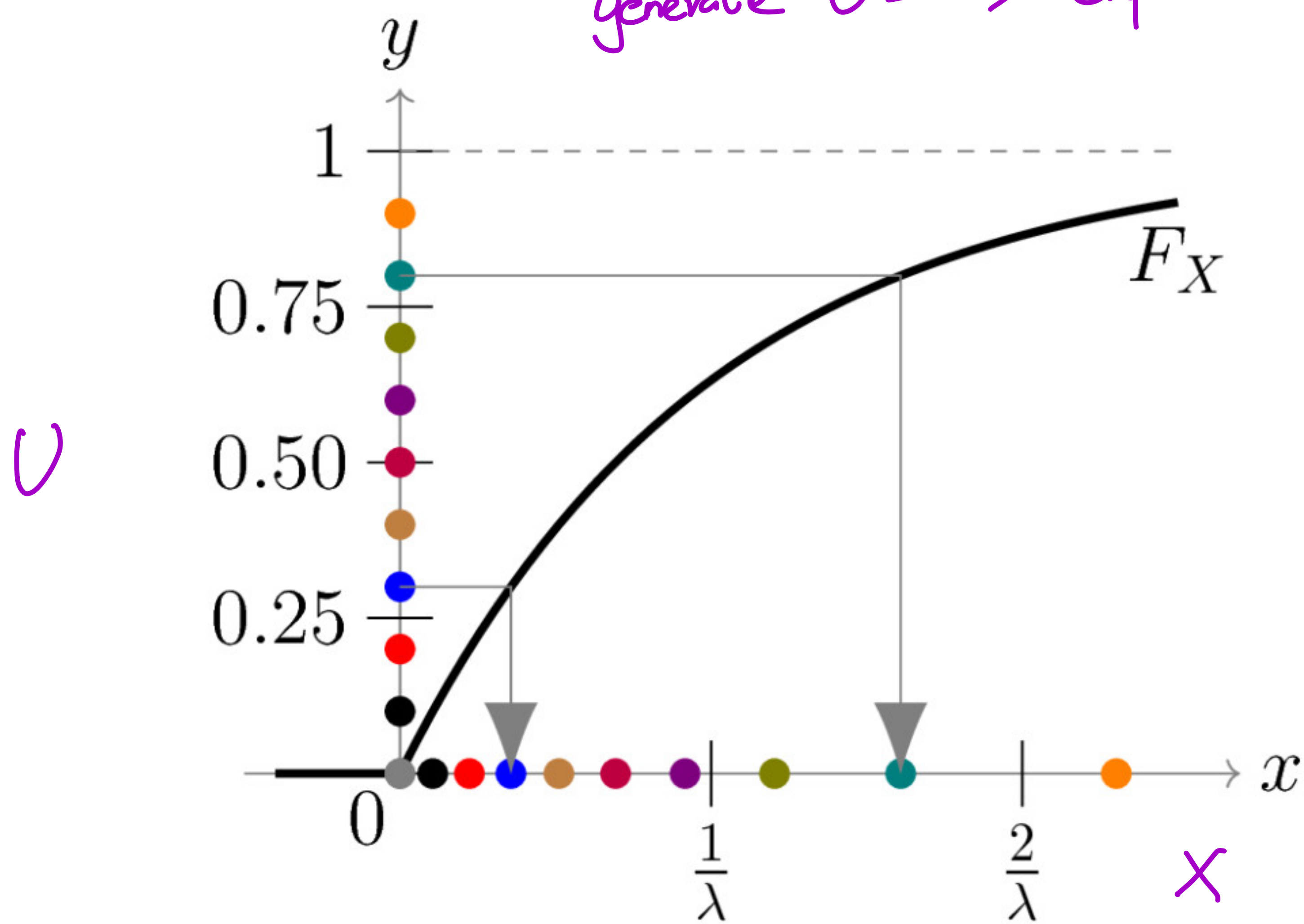
2. Generate $U \sim \mathrm{Unif}(0,1)$.

   Notice that $1 - U \sim \mathrm{Unif}(0,1)$ has the same distribution as U.

3. Then $\overset{F^{-1}(u)}{X} = -\frac{1}{\lambda}\log U \sim \mathrm{Exp}(\lambda)$.

Example 2: Exponential Distribution ($\text{Exp}(\lambda)$)

generate $U \longrightarrow$ exp



Source: `https://commons.wikimedia.org/wiki/File:Inverse_transformation_method_for_exponential_distribution.jpg`

Exercise: Let $f(x)$ be the PDF defined by

$$f(x) = k\frac{(x-a)^{k-1}}{(b-a)^k}, \quad \text{for } k > 0,\ a \le x \le b.$$

Use the inverse CDF to describe how to sample from this distribution.

A Special Case: Set $a = 0$, $b = 1$.

- The PDF simplifies to

$$f(x) = kx^{k-1}, \quad \text{for } x \in [0, 1].$$

(Beta (k, 1))

a=k b=1

- The CDF is

$$F(x) = \int_0^x f(t)\,\mathrm{d}t = \int_0^x kt^{k-1}\,\mathrm{d}t = t^k\Big|_0^x = x^k. \quad = u$$

$x = u^{\frac{1}{k}}$

- The inverse CDF is then $F^{-1}(u) = u^{1/k}$.

$F(x) = x^k \to F^{-1}(u) = x$

$F(x) = u = x^k$

$x = u^{\frac{1}{k}} = F^{-1}(u)$

$F^{-1}(u) = u^{\frac{1}{k}} \sim F(x)$

$= (u^{-1})(u^{k})$

The **Beta distribution**, $\mathrm{Beta}(a, b)$, with parameters a and b has PDF defined by

$k = \frac{\Gamma(k+1)}{\Gamma(k)+\Gamma(1)}$ $a = k$ $b = 1$

$$f(x) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} x^{a-1}(1-x)^{b-1}, \quad \text{for } x \in [0, 1],$$

$x^{k-1}(1-x)^{0} = x^{k-1}$

where $\Gamma(z) = \int_0^\infty x^{z-1} e^{-x}\, \mathrm{d}x$ is the gamma function.

How does the previous example relate to this well known distribution?

$\Gamma(a) = (a-1)!$

$\Gamma(1) = (1-1)! = 0$

$\frac{\Gamma(k+1)}{\Gamma(k)\Gamma(1)} = \frac{k \cdot k-1 \cdots 1}{k-1 \cdot k-2 \cdots 1+0} = k$.

Example 3: Polynomial Density

- We can rewrite the PDF from the previous example as
$$f(x) = kx^{k-1} = kx^{k-1}(1-x)^0,$$
so this PDF describes a $\mathrm{Beta}(k,1)$ distribution.

- In particular,
$$\frac{\Gamma(k+1)}{\Gamma(k)\Gamma(1)} = k.$$

- Verifies the identity: $\Gamma(n) = (n-1)!$ if n is a positive integer.

- It can be helpful to recognize the densities of well known distributions for computing integrals (as we will see later).

$f(x) = kx^{k-1} \sim \mathrm{Beta}(k, 1)$

$\boxed{\text{discrete}}$

- The probability mass function (PMF) of a geometric random variable $X \sim \mathrm{Geom}(p)$ with parameter p can be written as

$$P(X = k) = (1 - p)p^k, \quad \text{for } k = 0, 1, 2, \ldots.$$

F·F·F· . . F · S

k : # of failure before success

(1-p) = success

p = failure

- The CDF of X is then

$$F(x) = \sum_{k=0}^{[x]} P(X = k) = 1 - p^{[x]+1},$$

where $[x]$ is the integer part of x.

- How can we sample from $\mathrm{Geom}(p)$?

Example 4: Geometric Distribution ($\text{Geom}(p)$)

1. Derive the inverse CDF $F^{-1}(u)$.

   We need to be careful for discrete distributions, since the inverse CDF may not be well defined.

   For $u \in (0,1)$,

$$F^{-1}(u) = \min\{t : F(t) \geq u,\ t = 0, 1, 2, \ldots\}.$$

   For any $t = 0, 1, 2, \ldots,$

$$\begin{aligned} F(t) &\geq u \\ F(t) = 1 - p^{\lfloor t \rfloor + 1} &\geq u \\ \underbrace{\lfloor t \rfloor \geq \frac{\log(1-u)}{\log p} - 1.} & \end{aligned}$$

$$t \geqslant \left\lceil \frac{\log(1-u)}{\log p} - 1 \right\rceil$$

Example 4: Geometric Distribution ($\mathrm{Geom}(p)$)

Inverse CDF Method for $\mathrm{Geom}(p)$:

1. $$F^{-1}(u) = \min\left\{t : [t] \geq \frac{\log(1-u)}{\log p} - 1\right\} = \left[\frac{\log(1-u)}{\log p}\right]$$
2. Generate $U \sim \mathrm{Unif}(0,1)$.
3. Then $X = \left[\dfrac{\log(1-U)}{\log p}\right] \sim \mathrm{Geom}(p)$.

$$X = \left[\frac{\log U}{\log p}\right] \sim \mathrm{Geom}(p)$$

Outline

1. The Inverse CDF Method

   infinite $\begin{cases} \text{continuous} \\ \text{discrete} \end{cases}$

   - Example 1: Uniform Distribution ($\mathrm{Unif}(a, b)$)
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Example 5: Finite Discrete Distribution

- Let X denote a discrete random variable with PMF given by

X	1	2	3
$P(X = x)$	0.2	0.5	0.3

$1 \times 0.2 + 2 \times 0.5 + 3 \times 0.3$

$= 0.2 + 1 + 0.9 = 2.1$

- The CDF $F(x) = P(X \leq x)$ is a discontinuous step function. For example,

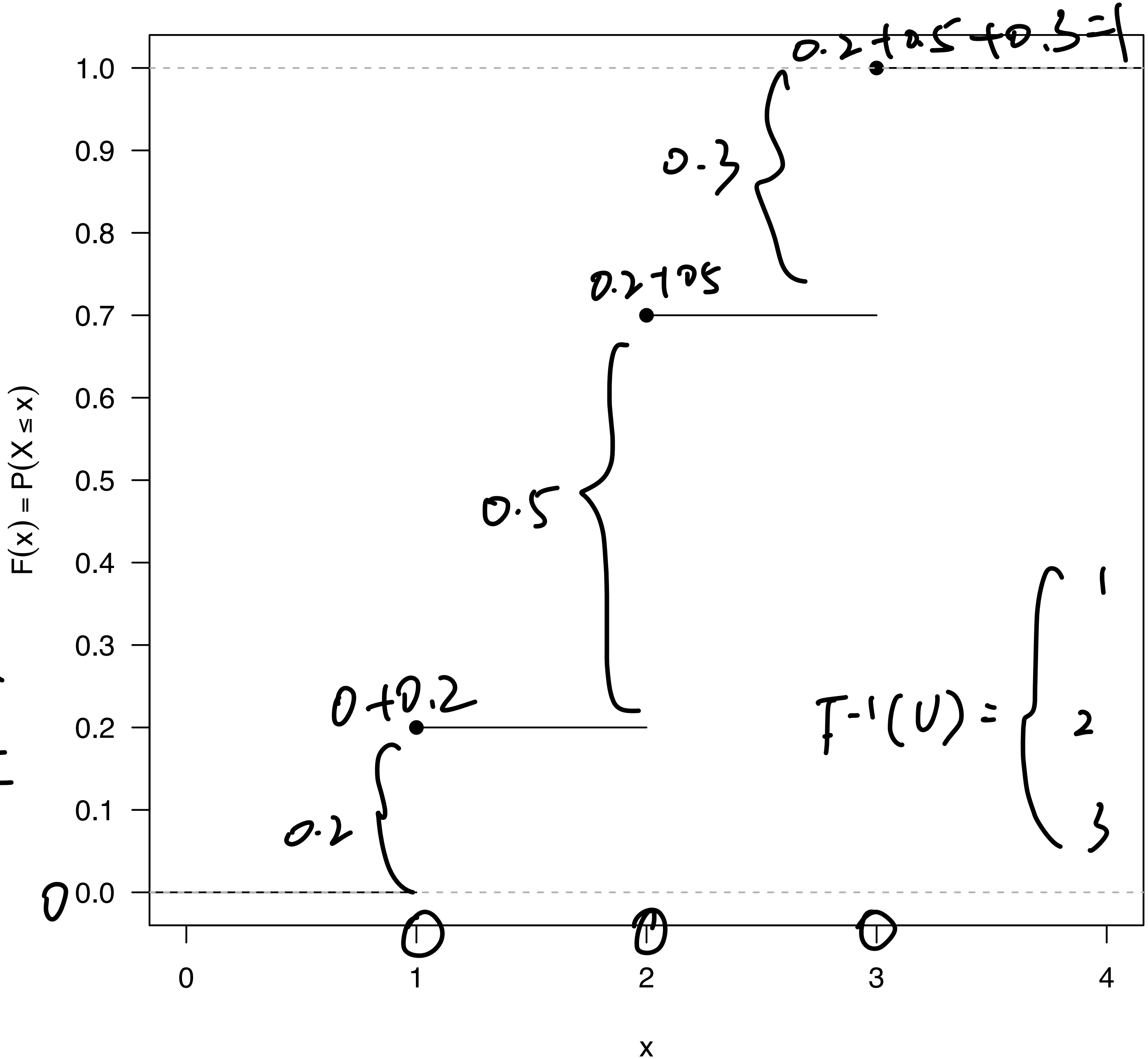
$$F(2) = P(X \leq 2) = P(X = 1) + P(X = 2).$$

$0.2 + 0.5 = 0.7$

The graph of $F(x)$ is shown on the next slide.

- How do we use the inverse CDF method to sample from this distribution?

Example 5: Finite Discrete Distribution



U

↑

CDF

$$F^{-1}(U) = \begin{cases} 1 & 0<U\le 0.2 \\ 2 & 0.2<U\le 0.7 \\ 3 & 0.7<U\le 1 \end{cases}$$

Value

X

R Code for the plot:

11 22222 333 0.2 0.5 0.3

```
> X <- rep(c(1, 2, 3), c(2, 5, 3))

> plot(ecdf(X),
+       ylab = expression(F(x) == P(X <= x)),
+       main = "",
+       las = 1
+       )
> axis(2, at = seq(0.1, 0.9, by = 0.2), las = 1)
```

1 1 2 2 2 2 2 3 3 3

min value

Example 5: Finite Discrete Distribution

1. Derive the inverse CDF $F^{-1}(u)$.

   For $u \in (0,1)$,

   $$F^{-1}(u) = \min\{t : F(t) \geq u\}.$$

   So

   $$F^{-1}(u) = \begin{cases} 1 & \text{for } 0 < u \leq 0.2 \\ 2 & \text{for } 0.2 < u \leq 0.7 \\ 3 & \text{for } 0.7 < u < 1 \end{cases}.$$

$$X = F^{-1}(U) = \begin{cases} 1 \\ 2 \\ 3 \end{cases}$$

Example 5: Finite Discrete Distribution

Inverse CDF Method for a finite discrete distribution:

1. $$F^{-1}(u) = \begin{cases} 1 & \text{for } 0 < u \leq 0.2 \\ 2 & \text{for } 0.2 < u \leq 0.7 \\ 3 & \text{for } 0.7 < u < 1 \end{cases}.$$

2. Generate $U \sim \mathrm{Unif}(0, 1)$.

3. Then $X = F^{-1}(U)$, where:

$$F^{-1}(U) = \begin{cases} 1 & \text{if } 0 < U \leq 0.2 & \text{with pr. } P(0 < U \leq 0.2) = 0.2 \\ 2 & \text{if } 0.2 < U \leq 0.7 & \text{with pr. } P(0.2 < U \leq 0.7) = 0.5 \\ 3 & \text{if } 0.7 < U < 1 & \text{with pr. } P(0.7 < U \leq 1) = 0.3 \end{cases}$$

Sampling from Finite Discrete Distributions

- We can use the same procedure (the inverse CDF method) to sample from general finite discrete distributions.
- Let X denote a discrete random variable with PMF given by

$$P(X = x_k) = p_k, \quad \text{for } k = 1, 2, \ldots, m.$$

X	x_1	x_2	$\cdots$	x_m
$P(X = x_k)$	p_1	p_2	$\cdots$	p_m

m values

sum(pi) = 1

- Let $F_j = p_1 + p_2 + \cdots + p_j = \sum_{k=1}^{j} p_k$, for $j = 1, 2, \ldots, m$, → more than 1, but u ~ (0,1)

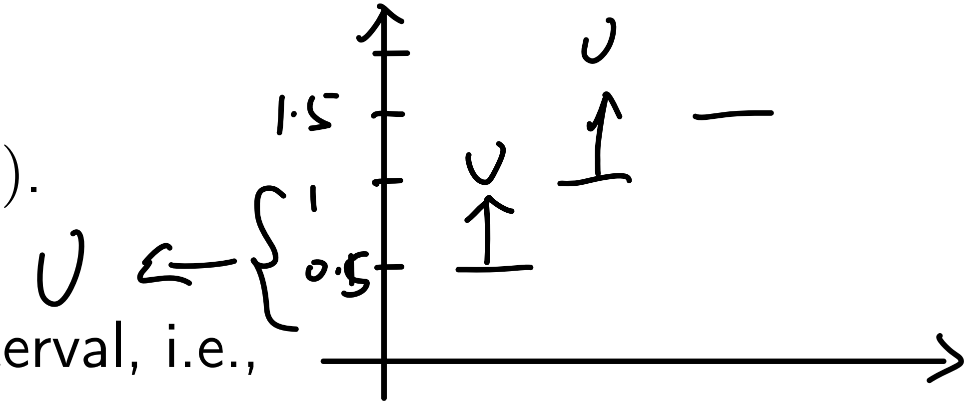
$p_1 + p_2 + \cdots p_{j-1}$

and $F_m = 1$.

F(last) = 1

Sampling from Finite Discrete Distributions

$P(X=x)$



1. Generate $U \sim \mathrm{Unif}(0,1)$.

2. If U is in the kth subinterval, i.e.,

$$F_{k-1} < U \leq F_k,$$

then $X = x_k$.

Can we show that X has the distribution we want?

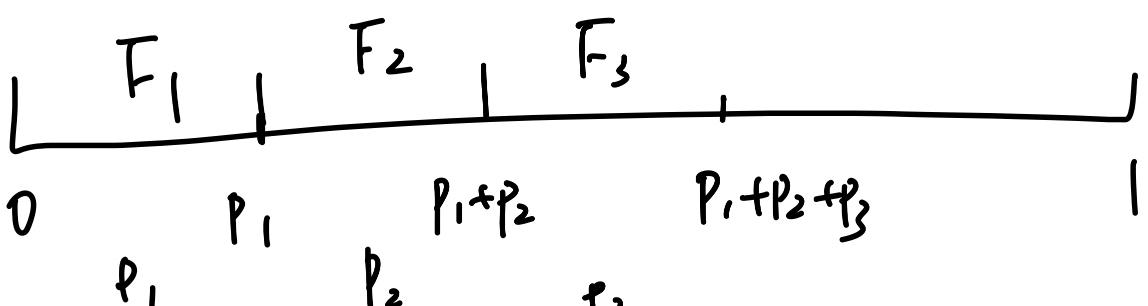
Sampling from Finite Discrete Distributions

Proof (Inverse CDF Method for Finite Discrete Distributions).

Since

$$
\begin{aligned}
P(X = x_k) &= P(F_{k-1} \le U \le F_k) \\
&= F_k - F_{k-1} \\
&= (\cancel{p_1 + p_2 + \cdots} + p_k) - (\cancel{p_1 + p_2 + \cdots + p_{k-1}}) \\
&= p_k,
\end{aligned}
$$

then X has the desired distribution. □



Example 6: Bivariate Finite Discrete Distribution

$P(x, y)$

- Let X and Y have a joint PMF given by:

(0,0) (0,1)

$X \backslash Y$	0	1
0	0.2	0.6
1	0.1	0.1

(1,0) (1,1)

- How can we sample from this distribution?

F_1	F_2	F_3	F_4
(0,0)	(0,1)	(1,0)	(1,1)
0.2	0.6	0.1	0.1

$\longrightarrow$

$F_1 = 0.2$

$F_2 = 0.2 + 0.6$

$F_3 = 0.2 + 0.6 + 0.1$

$F_4 = 1$

Example 6: Bivariate Finite Discrete Distribution

We can apply the previous result by mapping the pairs of X and Y onto the unit interval $(0,1)$.

Let $p_{xy} = P(X = x, Y = y)$. Define:

$$\begin{aligned} F_1 &= p_{00} &= 0.2 \\ F_2 &= p_{00} + p_{01} &= 0.8 \\ F_3 &= p_{00} + p_{01} + p_{10} &= 0.9 \\ F_4 &= p_{00} + p_{01} + p_{10} + p_{11} &= 1 \end{aligned}$$

1. Generate $U \sim \mathrm{Unif}(0,1)$.
2. Then:

$$(X,Y) = \begin{cases} (0,0) & \text{if } 0 < U \leq F_1 \\ (0,1) & \text{if } F_1 < U \leq F_2 \\ (1,0) & \text{if } F_2 < U \leq F_3 \\ (1,1) & \text{if } F_3 < U < F_4 \end{cases}$$

We can verify that $P(X = x, Y = y) = p_{xy}$.