### STATISTICAL INFERENCE (MA862)Lecture Slides Topic 1: Monte Carlo Simulation

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## Example

- Let we want to estimate the average distance between two randomly selected points in a region.
- Let X = (X<sub>1</sub>, X<sub>2</sub>) and Y = (Y<sub>1</sub>, Y<sub>2</sub>) be independent and uniformly distributed two points drawn from a finite rectangle R = [0, a] × [0, b].
- The Euclidean distance between these two points is

$$Z = d(X, Y) = \sqrt{(X_1 - Y_1)^2 + (X_2 - Y_2)^2}.$$

• We need E(Z).

$$E(Z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2} \\ \times f_{X_1, X_2}(x_1, x_2) f_{Y_1, Y_2}(y_1, y_2) dx_1 dx_2 dy_1 dy_2$$

## Example

 We can approximate E(Z) by sampling pair points (X<sub>i</sub>, Y<sub>i</sub>), i = 1, 2, ..., n, form R and then calculating the average

$$\frac{1}{n}\sum_{i=1}^n d(\boldsymbol{X}_i, \boldsymbol{Y}_i).$$

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## Simple Monte Carlo

- In a simple Monte Carlo problem, we express the quantity we want to know as the expected value of a random variable Y, such as µ = E(Y).
- Generate values  $Y_1, \ldots, Y_n$  independently from the distribution of Y.
- Take their average

$$\widehat{\mu}_n = \frac{1}{n} \sum_{i=1}^n Y_i$$

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as an estimate of  $\mu$ .

## Simple Monte Carlo

- In many examples, Y = h(X).
- X has a PMF/PDF p(x) (known).
- f is a real-valued function defined over the support of X.

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## Justification of Simple MC

• The strong law of large numbers:

$$\mathbb{P}\left(\lim_{n\to\infty}|\widehat{\mu}_n-\mu|=0\right)=1.$$

• Loosely speaking, the SLLNs says that the error in approximation will be very small if we increase *n*.

## Random Number Generation

- Our aim is to generate random number from appropriate distribution.
- Basic step of a random number generation from a distribution is to generate random numbers from Uniform distribution U(0, 1).
- The PDF of a random variable having U(0, 1) distribution is

$$f(x) = egin{cases} 1 & ext{if } 0 < x < 1 \ 0 & ext{otherwise.} \end{cases}$$

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## Uniform Random Numbers Generation

- To generate random numbers from a process that according to well established understanding of physics is truly random.
- Radioactive particle emission, that are thought to be truly random.
- Such process has it's own draw back.
- Therefore, people use Pseudo-random numbers (computer generated).
- We will not discuss it in detail, as almost all software has a routine to generate pseudo-random numbers from U(0, 1).
- Now-onward, the pseudo-random number will be referred as random number.

### Uniform Random Numbers Generation

• A linear congruence generator (LCG):

$$x_{i+1} = ax_i \mod m, \quad u_{i+1} = \frac{x_{i+1}}{m}, \quad i = 0, 1, 2, \ldots$$

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- The multiplier *a* and the modulus *m* are integer constants.
- The initial value (seed)  $x_0$  is called seed.
- $x_0$  is an integer between 1 and m-1.
- LCG is a deterministic recurrence relation.

### Uniform Random Numbers Generation

• The general linear congruence generator (GLCG):

$$x_{i+1} = (ax_i + c) \mod m, \quad u_{i+1} = \frac{x_{i+1}}{m}, \quad i = 0, 1, 2, \ldots$$

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• *a*, *m* and *c* are appropriate integers.

## Non-uniform Random Number Generation

• Method for transforming random numbers from U(0, 1) distribution to samples from other required distributions.

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- The two most widely used general techniques are:
  - 1 Inverse Transform Method.
  - 2 Acceptance Rejection Method.

• The inverse transform method is based on the following theorem.

**Theorem 1:** Let *F* be a CDF. Define the quasi-inverse of *F* by

$$\mathcal{F}^{-1}(u) = \inf \left\{ x \in \mathbb{R} : \mathcal{F}(x) \geq u 
ight\} \quad ext{for } 0 < u < 1.$$

Let  $U \sim U(0, 1)$  and  $X = F^{-1}(U)$ . Then, the CDF of X is F.

{x ∈ ℝ : F(x) ≥ u} is non-empty and has a lower bound for all u ∈ (0, 1).

- Want a sample from the CDF F(x). That means that we want to generate a random variable X with the property that P(X ≤ x) = F(x) for all x ∈ ℝ.
- Using above theorem, we have the following algorithm.

Algorithm 1 Inverse Transform Method

1: Generate U from U(0, 1) distribution.

2: Set 
$$X = F^{-1}(U)$$
.

3: Return X.

- In principle, this algorithm can be used to generate random number from any distribution.
- However, there are computational aspects. We generally use this algorithm if  $F^{-1}$  is in closed form and easy to compute.

**Example 1:** (Generation from exponential distribution) The PDF is

$$f(x) = egin{cases} \lambda e^{-\lambda x} & ext{if } x > 0 \ 0 & ext{otherwise.} \end{cases}$$

Example 2: (Generation from Arc Sin Law) Consider the CDF

$$F(x) = rac{2}{\pi} ext{ arc sin } \sqrt{x} \ , \ 0 \leq x \leq 1.$$

Example 3: (Generation from Rayleigh Distribution) The CDF is

$$F(x) = 1 - e^{-2x(x-b)} \ , \ x \ge b.$$

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**Lemma 1:** F and  $F^{-1}$  both are non-decreasing. **Lemma 2:**  $F F^{-1}(u) \ge u$  for all  $u \in (0, 1)$ . **Lemma 3:**  $F^{-1}F(x) \le x$  for all  $x \in \mathbb{R}$ . **Lemma 4:** For  $x \in \mathbb{R}$  and 0 < u < 1,  $F(x) \ge u$  if and only if  $F^{-1}(u) \le x$ .

**Example 4:** Generation from a Bernoulli distribution with probability of success p(q = 1 - p).

$$F_X(x) = \begin{cases} 0 & \text{if } x < 0 \\ q & \text{if } 0 \le x < 1 \\ 1 & \text{if } x \ge 1. \end{cases} \text{ and } F^{-1}(u) = \begin{cases} 0 & \text{if } 0 < u < q \\ 1 & \text{if } q \le u < 1. \end{cases}$$

#### **Algorithm 2** Generation from *Bernoulli*(*p*)

- 1: generate U from U(0, 1).
- 2: **if** U < 1 p **then**
- 3: Set  $X \leftarrow 0$ .
- 4: **else**
- 5: Set  $X \leftarrow 1$ .
- 6: **end if**
- 7: **return** *X*

**Example 5:** Generation from a discrete distribution with finite support.

• Consider a DRV X whose support is  $c_1 < c_2 < c_3 < \cdots < c_N$ .

• Let 
$$p_i = P(X = c_i), i = 1, 2, 3 \dots, N$$
.

• Set 
$$q_0 = 0$$
 and  $q_i = \sum_{j=1}^{i} p_j$ ,  $i = 1, 2, 3 ..., N$ .

**Algorithm 3** Inversion Transformation Method for Discrete Random Variable with Finite Support

- 1: Generate a uniform  $U \sim U(0, 1)$ .
- 2: Find  $K \in \{1, 2, ..., N\}$  such that  $q_{K-1} < U \le q_K$ .
- 3: Return  $c_K$ .

# Acceptance-Rejection Method

- We want to generate random number from a PDF *f* (target distribution).
- Let g (candidate distribution) be a PDF such that for all  $x \in \mathbb{R}$  and for some  $c \geq 1$

$$f(x) \leq cg(x).$$

- The technique to generate random number from g is known.
- Then we can use the following algorithm to generate random number from *f*.

#### Algorithm 4 Acceptance Rejection Method

- 1: repeat
- 2: generate X from distribution g.
- 3: generate U from U(0, 1).
- 4: until  $U \leq \frac{f(X)}{cg(X)}$
- 5: **return** X

**Example 6:** Generation random number from  $Gamma(\alpha, \beta)$ . The PDF of the distribution is

$$f(x) = rac{eta^{lpha}}{\Gamma(lpha)} x^{lpha - 1} e^{-eta x} \quad ext{for } x > 0.$$

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We will consider generation from Gamma(α, 1) for α > 0.

Case I :  $0 < \alpha < 1$ . Take

$$g(x) = \begin{cases} \frac{x^{\alpha-1}}{A} & \text{if } 0 < x < 1 \\ \frac{e^{-x}}{A} & \text{if } x \ge 1, \end{cases}$$

where  $A = \frac{1}{\alpha} + \frac{1}{\epsilon}$ .

• Then,  $f(x) \leq cg(x)$ , where  $c = \frac{A}{\Gamma(\alpha)}$ .

• The CDF corresponding to g is

$$G(x) = egin{cases} rac{x^lpha}{lpha A} & ext{if } 0 < x < 1 \ 1 - rac{e^{-x}}{A} & ext{if } x \geq 1. \end{cases}$$

Now,

$$G^{-1}(u) = \begin{cases} (\alpha A u)^{\frac{1}{\alpha}} & \text{if } 0 < u < \frac{1}{\alpha A} \\ -\ln A - \ln(1-u) & \text{if } \frac{1}{\alpha A} \le u < 1. \end{cases}$$

**Algorithm 5** Generation from  $Gamma(\alpha, 1)$  for  $0 < \alpha < 1$ 

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- 1: repeat
- 2: generate  $U_1$  from U(0, 1)
- 3: if  $U < \frac{1}{\alpha A}$  then
- 4: Set  $X \leftarrow (\alpha AU)^{\frac{1}{\alpha}}$
- 5: **else**

6: Set 
$$X \leftarrow -\ln A - \ln (1 - U)$$

7: end if

- 8: generate  $U_2$  from U(0, 1)
- 9: until  $cg(X)U_2 \leq f(X)$

10: **return** *X* 

Case II: 
$$\alpha$$
 is a positive integer.  
• Let  $X_i \stackrel{i.i.d.}{\sim} Exp(1)$  for  $i = 1, 2, ..., n$ .  
• Then  $\sum_{i=1}^{n} X_i \sim Gamma(n, 1)$ .

**Algorithm 6** Generation from  $Gamma(\alpha, 1)$ ,  $\alpha$  is a positive integer

1: Set 
$$n \leftarrow \alpha$$
 and  $Y \leftarrow 0$ 

2: while  $n \neq 0$  do

3: generate U from 
$$U(0, 1)$$

- 4: Set  $X \leftarrow -\ln(U)$
- 5:  $Y \leftarrow Y + X$
- 6:  $n \leftarrow n-1$
- 7: end while
- 8: return Y

Case III:  $\alpha > 1$  and not an integer.

- Let  $X \sim Gamma(\alpha_1, \beta)$  and  $Y \sim Gamma(\alpha_2, \beta)$ .
- ▶ Suppose that *X* and *Y* are independent.
- Then  $X + Y \sim \text{Gamma}(\alpha_1 + \alpha_2, \beta)$ .
- $\lfloor x \rfloor$ : the integer part of the positive real number x.
- $\{x\}$ : the fractional part of the positive real number x.

$$\blacktriangleright \ \alpha = \lfloor \alpha \rfloor + \{ \alpha \}.$$

**Algorithm 7** Generation from  $Gamma(\alpha, 1)$  when  $\alpha > 1$  and  $\alpha$  is not an integer

- 1: generate Y from  $Gamma(\{\alpha\}, 1)$  using Algorithm 5
- 2: generate X from  $Gamma(\lfloor \alpha \rfloor, 1)$  using Algorithm 6
- 3: Z = X + Y
- 4: **return** *Z*

## Acceptance-Rejection Method

**Theorem 2:** Let *f* and *g* be two PDFs such that

 $f(x) \leq cg(x)$  for all  $x \in \mathbb{R}$  and for some  $c \geq 1$ .

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Then X generated by Algorithm 4 has PDF f.

## Technique based on Transformation

### **Example 7:** Generation of random number from $Beta(\alpha, \beta)$ .

- $X \sim \text{Gamma}(\alpha_1, \beta)$
- $Y \sim Gamma(\alpha_2, \beta)$
- $\blacktriangleright$  X and Y are independent

• Then 
$$\frac{X}{X+Y} \sim Beta(\alpha_1, \alpha_2)$$
.

### **Algorithm 8** Generation from $Beta(\alpha_1, \alpha_2)$ distribution

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- 1: generate X from  $Gamma(\alpha_1, \beta)$
- 2: generate Y from  $Gamma(\alpha_2, \beta)$

3: 
$$Z = \frac{X}{X + Y}$$
  
4: return Z

# Technique based on Transformation

### **Example 8:** Generation of random number from $N(\mu, \sigma^2)$

- $\blacktriangleright U_1, U_2 \overset{i.i.d.}{\sim} U(0, 1)$
- Define

 $Z_1 = \sqrt{-2 \ln U_1} \cos (2\pi U_2)$  and  $Z_2 = \sqrt{-2 \ln U_1} \sin (2\pi U_2)$ .

- ▶ Then  $Z_1, Z_2 \stackrel{i.i.d.}{\sim} N(0, 1)$
- ► This transformation is called Box-Muller transformation.

**Algorithm 9** Box-Muller Method to generate from N(0, 1)

1: generate  $U_1$  and  $U_2$  from U(0, 1)2:  $R \leftarrow \sqrt{-2 \ln U_1}$ 3:  $\theta \leftarrow 2\pi U_2$ 4:  $Z_1 \leftarrow R \cos(\theta)$ 5:  $Z_2 \leftarrow R \sin(\theta)$ 6: return  $(Z_1, Z_2)$ .

# Technique based on Transformation

### **Example 9:** Generation from *Geometric*(*p*).

► The PMF is given by

$$P(X = i) = p(1 - p)^{i}$$
 for  $i = 0, 1, 2, ...$ 

• Let Y be an exponential random variable with mean  $\frac{1}{\lambda}$ .

▶ Take 
$$W = \lfloor Y \rfloor$$
. Then

$$P(W=i)=e^{-i\lambda}\left(1-e^{-\lambda}
ight) ext{ for } i=0,\,1,\,2,\,\ldots.$$

• 
$$W \sim Geometric(1 - e^{-\lambda})$$
.

### **Algorithm 10** Generation from *Geometric*(*p*)

1: generate U from U(0, 1)

2: 
$$X \leftarrow \left\lfloor \frac{\ln U}{\ln(1-p)} \right\rfloor$$
  
3: **return** X.

## Error in Monte Carlo Integration

- Both laws of large numbers tell us that Monte Carlo will eventually produce an error as small as we like.
- They do not tell us how large *n* has to be for this to happen.
- They also do not say for a given sample  $Y_1, \ldots, Y_n$  whether the error is likely to be small.
- The situation improves markedly when Y has a finite variance.
- Suppose that Var(Y) = σ<sup>2</sup> < ∞.</li>
- The mean of  $\widehat{\mu}_n$  is  $\mathbb{E}(\widehat{\mu}_n) = \frac{1}{n} \sum_{i=1}^n \mathbb{E}(Y_i) = \mu$ .
- The variance of  $\hat{\mu}_n$  is  $Var(\hat{\mu}_n) = \mathbb{E}((\hat{\mu}_n \mu)^2) = \frac{\sigma^2}{n}$ .
- The variance of  $\hat{\mu}$  may be considered as (average) error in  $\hat{\mu}$  for approximating or estimating  $\mu$ .
- For fixed *n*, the variance increases as  $\sigma$  increases.
- The variance decreases as n increases for fixed  $\sigma$ .
- The root mean squared error of  $\widehat{\mu}_n$  is  $\sqrt{Var(\widehat{\mu}_n)} = \frac{\sigma}{\sqrt{n}}$ .