

Lecture 7: Monte Carlo Methods

Ziyu Shao

School of Information Science and Technology
ShanghaiTech University

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Outline

- 1 History of Monte Carlo
- 2 Sampling: Random Variable Generation
- 3 Sampling: Random Vector Generation
- 4 Monte Carlo Integration
- 5 Asymptotic Analysis: Law of Large Numbers
- 6 Non-asymptotic Analysis: Inequalities

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Motivation I

If you can not calculate a probability or expectation exactly, then you have three powerful strategies:

- Simulations using Monte Carlo Methods
- Approximations using limiting theorems
 - ▶ Poisson approximation: The Law of Small Numbers
 - ▶ Sample mean limit: The Law of Large Numbers
 - ▶ Normal approximation: The Central Limit Theorem
- Bounds (upper and lower bounds) on probability using inequalities.

Motivation II

Probability
Math



Statistics
Science

Monte Carlo
Computing

Monte Carlo Methods

- One of the top ten algorithms for science and engineering in 20th century
- Monte Carlo Methods, Simplex Method, Fast Fourier Transform, Quicksort, QR Algorithm...

Widely Applications

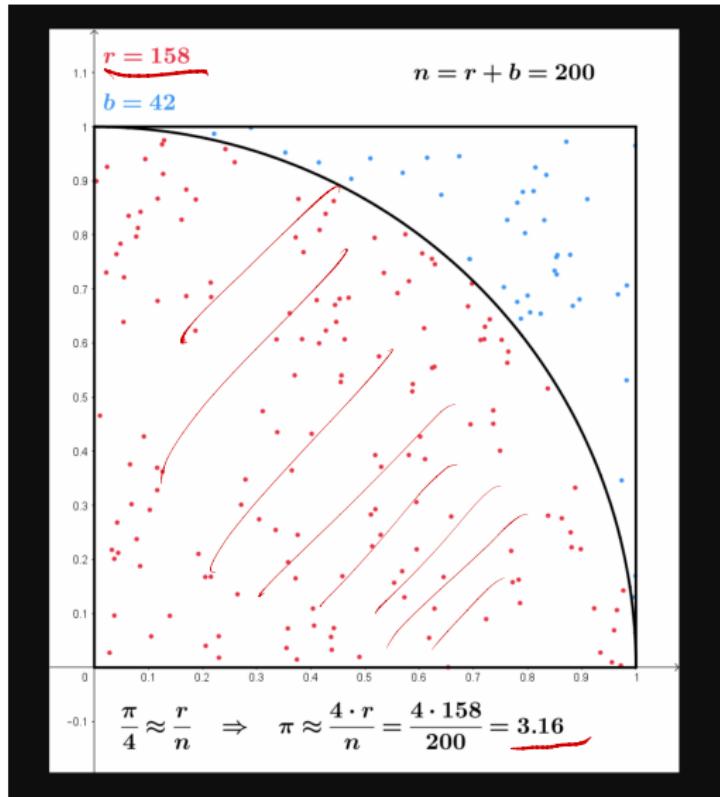
Monte Carlo methods have been used in various tasks, including

- Sampling from the underlying probability distribution $f(x)$ and simulating a random system
- Sampling from posterior distribution for bayesian inference
- Estimation through numerical integration

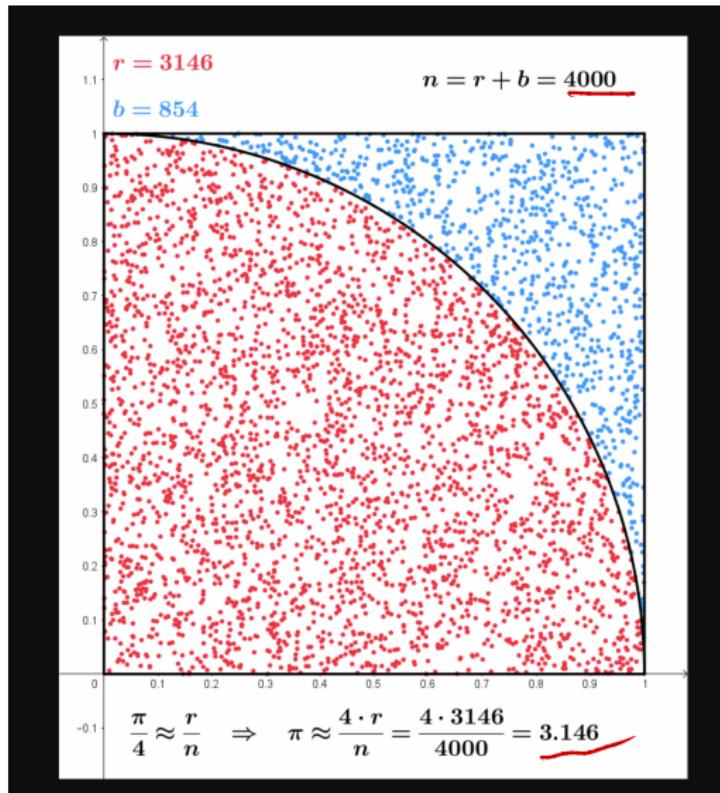
$$c = E_{\pi}(h(x)) = \int f(x)h(x)dx.$$

- Optimizing a target function to find its maxima or minima

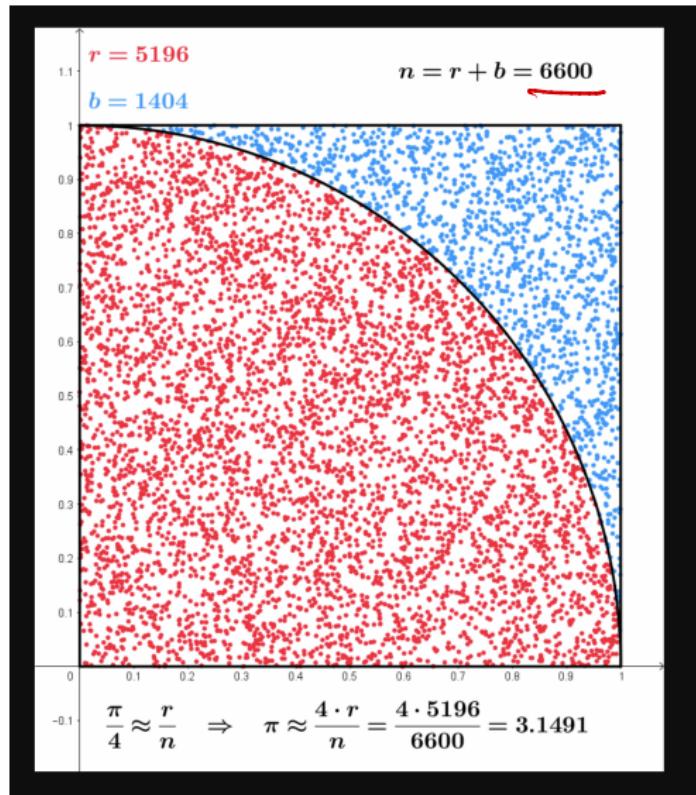
Classical Example: Estimation of π



Classical Example: Estimation of π



Classical Example: Estimation of π



History



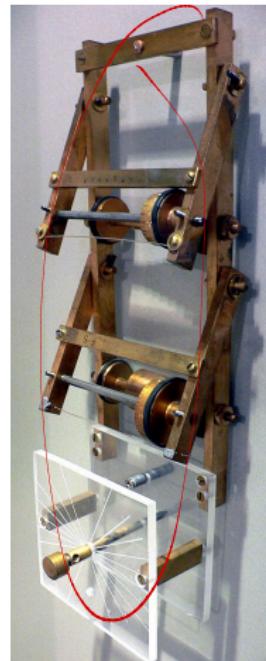
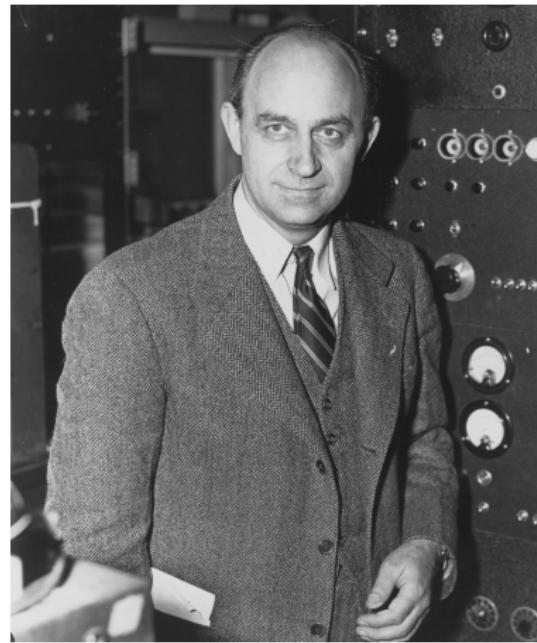
Monte Carlo Methods

- Basic Monte Carlo methods: formally proposed by Stanislaw Ulam & John Von Neumann in 1940s at Los Alamos National Lab (Named after a casino in Monaco)



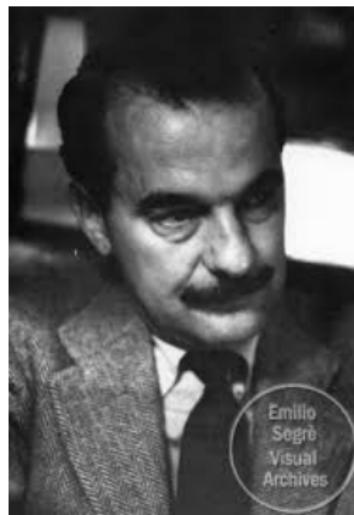
Monte Carlo Trolley

- Analog computer invented by Enrico Fermi in 1946



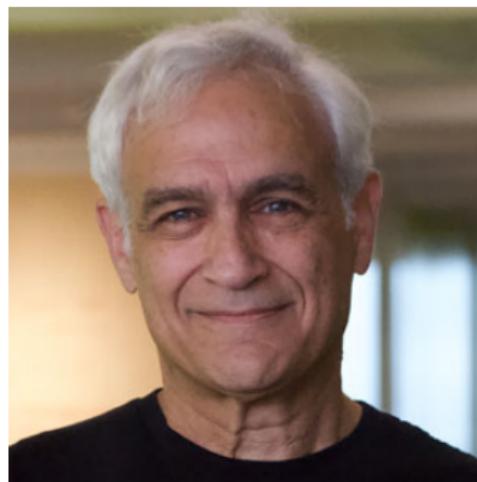
Markov Chain Monte Carlo Methods

- Metropolis-Hastings Algorithm: formally proposed by Nicholas Metropolis et al in 1950s at Los Alamos National Lab, then extended in 1970 by Wilfred Keith Hastings



Markov Chain Monte Carlo Methods

- Gibbs Sampling Algorithm: proposed in 1984 by brothers Stuart Geman (1949-) and Donald Geman (1943-).
- Gibbs sampling is named after the physicist Josiah Willard Gibbs (1839-1903), in reference to an analogy between the sampling algorithm and statistical physics.

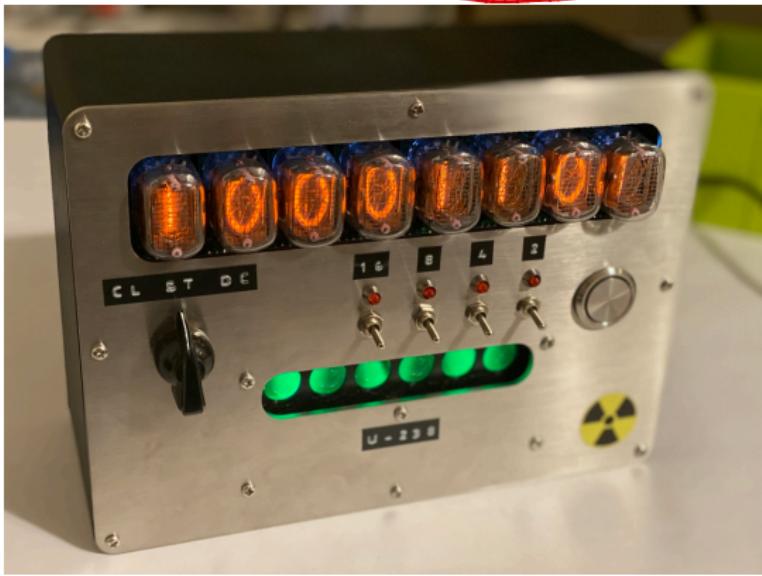


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Randomness Generation

- Earlier days: manual techniques including coin flipping, dice rolling, card shuffling, and roulette spinning
- Early days: physical devices including noise diodes and Geiger counters (https://github.com/nategri/chernobyl_dice)



Randomness Generation

- The prevailing belief: only mechanical or electronic devices could produce truly random sequences
- The book: A Million Random Digits With 100,000 Normal Deviates (based on Uranium radiation) RAND
- Current days: computer simulation with deterministic algorithms, also called pseudorandom number generator

Unif(0,1)

Sampling

- Assuming an algorithm is available for generating $\text{Unif}(0, 1)$ random numbers
- Two elementary methods for generating random variables (or samples)
 - ▶ Inverse-transform method: operates on the CDF
 - ▶ The acceptance-rejection method: operates on the PDF (or PMF)

Inverse Transform Method

- Given a $\text{Unif}(0, 1)$ r.v., we can construct an r.v. with any continuous distribution we want.
- Conversely, given an r.v. with an arbitrary continuous distribution, we can create a $\text{Unif}(0, 1)$ r.v.
- Other names:
 - ▶ probability integral transform
 - ▶ inverse transform sampling
 - ▶ the quantile transformation
 - ▶ the fundamental theorem of simulation

Inverse Transform Method: Recall

Theorem

Let F be a CDF which is a continuous function and strictly increasing on the support of the distribution. This ensures that the inverse function F^{-1} exists, as a function from $(0, 1)$ to \mathbb{R} . We then have the following results.

- ① Let $U \sim \text{Unif}(0, 1)$ and $X = F^{-1}(U)$. Then X is an r.v. with CDF F .
- ② Let X be an r.v. with CDF F . Then $F(X) \sim \text{Unif}(0, 1)$.

Algorithm Inverse-Transform Method: PDF Case

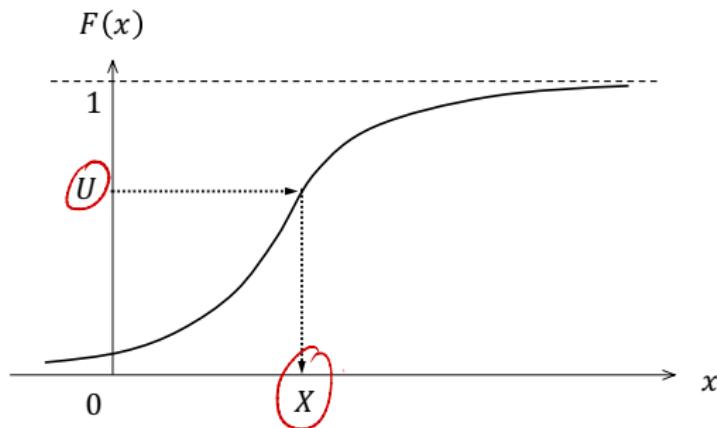
input: Cumulative distribution function F .

output: Random variable X distributed according to F .

1: Generate U from $\text{Unif}(0, 1)$.

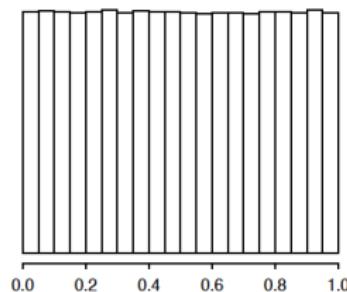
2: $X \leftarrow F^{-1}(U)$

3: **return** X

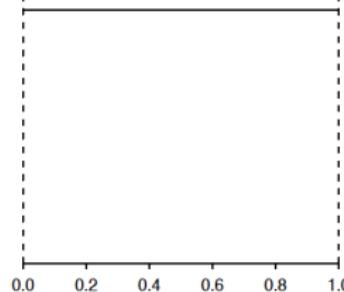


Histogram & PDF: Example

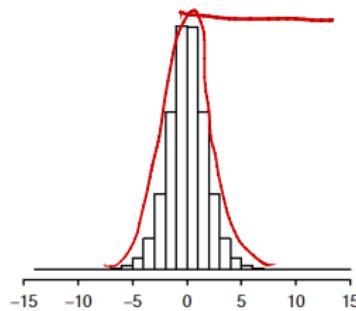
Histogram of u



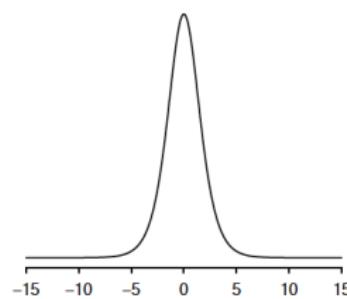
Unif(0,1) PDF



Histogram of $\log(u/(1-u))$



Logistic PDF



Box-Muller Method: Recall

$$1^{\circ}. U \sim \text{Unif}(0, 2\pi) = 2\pi \text{ Unif}(0, 1)$$

$$U_2 \sim \text{Unif}(0, 1), \quad U = \underline{2\pi U_2}$$

Let $U \sim \text{Unif}(0, 2\pi)$, and let $T \sim \text{Expo}(1)$ be independent of U .

Define $X = \sqrt{2T} \cos U$ and $Y = \sqrt{2T} \sin U$. Then X and Y are independent, and their marginal distributions are standard normal distribution.

$$2^{\circ}. F_T(t) = 1 - e^{-t}, t > 0 \Rightarrow F_T^{-1}(u) = -\ln(1-u)$$

Algorithm Normal Random Variable Generation: Box-Muller Approach

$$U_1 \sim \text{Unif}(0, 1), \quad -\ln(1-U_1) \sim \text{Expo}(1)$$

output: Independent standard normal random variables X and Y .

- 1: Generate two independent random variables, U_1 and U_2 , from $\text{Unif}(0, 1)$.
- 2: $X \leftarrow (-2 \ln U_1)^{1/2} \cos(2\pi U_2)$
- 3: $Y \leftarrow (-2 \ln U_1)^{1/2} \sin(2\pi U_2)$
- 4: **return** X, Y

$$\sqrt{-2 \ln U_1}$$

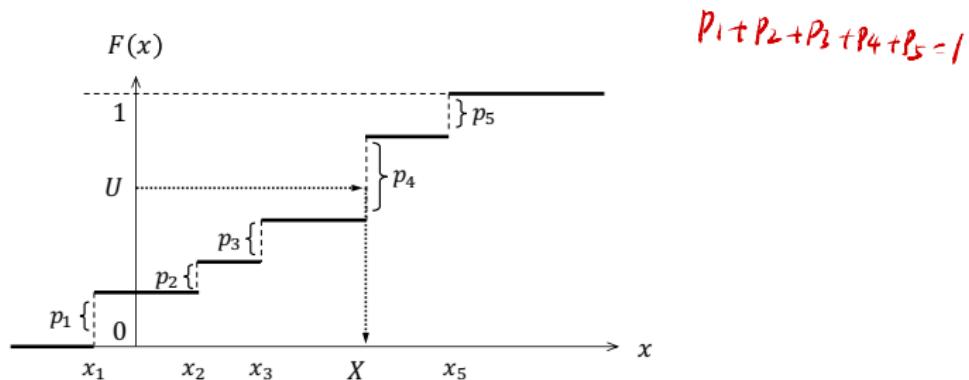
$$U_1 \sim 1-U_1$$

$$T := -\ln U_1$$

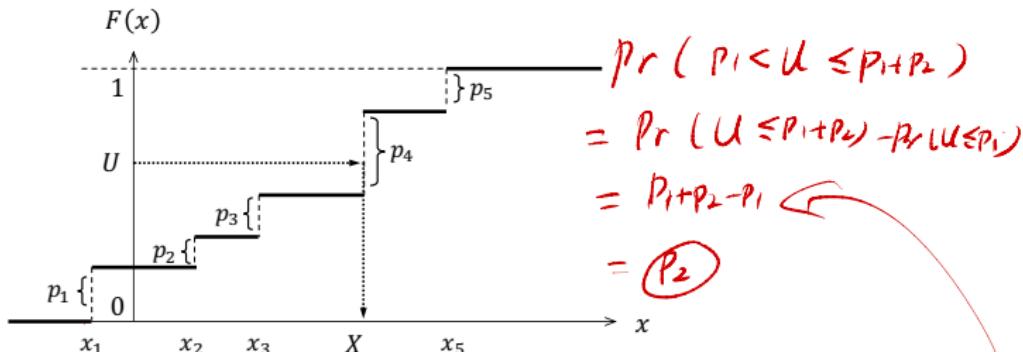
Inverse Transform Method for Discrete Distribution

- Example: PMF with $P(X = x_j) = p_j, j = 1, 2, 3, 4, 5$,
 $x_1 < x_2 < x_3 < x_4 < x_5$.
- CDF with

$$F(x_k) = P(X \leq x_k) = \sum_{j=1}^k P(X = x_j) = \sum_{j=1}^k p_j, k = 1, 2, 3, 4, 5.$$



Inverse Transform Method for Discrete Distribution



- $U \sim \text{Unif}(0, 1)$:

$$\Pr(0 < U \leq p_1) = \Pr(U \leq p_1) = (p_1) = \underline{P(X=x_1)}$$

$$X = \begin{cases} x_1 & \text{if } 0 < U \leq p_1 \\ x_2 & \text{if } p_1 < U \leq p_1 + p_2 \\ x_3 & \text{if } p_1 + p_2 < U \leq p_1 + p_2 + p_3 \\ x_4 & \text{if } p_1 + p_2 + p_3 < U \leq p_1 + p_2 + p_3 + p_4 \\ x_5 & \text{if } p_1 + p_2 + p_3 + p_4 < U \leq 1 \end{cases}$$

Inverse Transform Method for Discrete Distribution

Generalization
of Inverse Transform

$$F^{-1}(u) = \inf \{x : F(x) \geq u\}$$

Algorithm Inverse-Transform Method: PMF Case

input: Discrete cumulative distribution function F with monotonic sequence $\{x_j\}$

output: Discrete random variable X distributed according to F .

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

2: Find the smallest positive integer, k , such that $U \leq F(x_k)$. Let $X \leftarrow x_k$.

3: return X

$$\underline{k-1} \quad \underline{U > F(x_{k-1})}$$

$$\begin{aligned} & \Pr(F(x_{k-1}) < U \leq F(x_k)) \\ &= \Pr(U \leq F(x_k)) - \Pr(U \leq F(x_{k-1})) \\ &= F(x_k) - F(x_{k-1}) = \sum_{j=1}^k p_j - \sum_{j=1}^{k-1} p_j = p_k \end{aligned}$$

Bernoulli Distribution

$$x_1 = 0, x_2 = 1$$

- Bernoulli distribution $\text{Bern}(p)$ with PMF:
 $P(X = 1) = p, P(X = 0) = 1 - p, 0 < p < 1.$

$$\begin{array}{l} F(x_1) = 1-p, \\ \text{or} \\ F(x_2) = 1, \end{array}$$

Algorithm Inverse-Transform Method: PMF Case

input: $p \in (0, 1)$

output: Discrete random variable $X \sim \text{Bern}(p)$

- 1: Generate $U \sim \text{Unif}(0, 1)$.
 - 2: If $U \leq 1 - p$, then $\underline{X \leftarrow 0}$
 - 3: Else $\underline{X \leftarrow 1}$
 - 4: **return** X
-

Inverse Transform Method for Discrete Distribution

Algorithm Inverse-Transform Method: PMF Case

input: PMF $\{p_j\}$ for distribution with non-monotonic sequence
 $\{x_j\}$

output: Discrete random variable X distributed according to PMF $\{p_j\}$.

- 1: Generate $U \sim \text{Unif}(0, 1)$.
- 2: Find the positive integer, k , such that

$$\sum_{j=1}^{k-1} p_j < U \leq \sum_{j=1}^k p_j.$$

(k)

- 3: **return** $X = x_k$
-

Bernoulli Distribution

$$X_1 = 1, X_2 = 0$$

- Bernoulli distribution $\text{Bern}(p)$ with PMF:

$$P(X = 1) = p, P(X = 0) = 1 - p, 0 < p < 1.$$

Algorithm Inverse-Transform Method: PMF Case

input: $p \in (0, 1)$

output: Discrete random variable $X \sim \text{Bern}(p)$

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

2: If $U \leq p$, then $X \leftarrow 1$

3: Else $X \leftarrow 0$

4: **return** X

Acceptance-Rejection Method

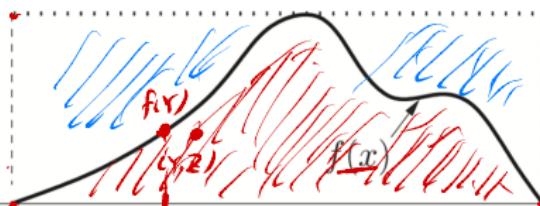
③ Acceptance-Rejection: if $Z \leq f(Y)$; Accept (Y, Z) .

Red A

$$= \{(y, z) : a \leq y \leq b, 0 \leq z \leq f(y)\}$$

④ $(Y^*, Z^*) \in \text{Red A}$

$$f_{Y^*, Z^*}(y, z) = \frac{1}{\text{Area}(\text{Red})} = 1 \quad Y \Rightarrow f_{Y^*(y)} = \int_0^b f_{Y^*, Z^*}(y, z) dz$$



① Objective PDF $f: X \in [a, b]$, $\text{C} \geq \sup_x f(x)$

$$\int_a^b f(x) dx = 1 \quad \text{Area}(\text{Red}) =$$

② $Y \sim \text{Unif}(a, b)$

$Z \sim \text{Unif}(0, c)$ independent

(Y, Z) uniform over the Rectangle.

Algorithm Acceptance-Rejection Algorithm

Step 1: Generate $Y \sim \text{Unif}(a, b)$.

$$= \int_0^{f(y)} 1 \cdot dz = f(y)$$

Step 2: Generate $Z \sim \text{Unif}(0, c)$.

$$\Rightarrow Y^* \sim f$$

Step 3: If $Z \leq f(Y)$, set $X = Y$. Otherwise go back to step 1.

Acceptance-Rejection Method

$$\textcircled{2} \quad Y \sim g; Z \sim \text{unif}(0, c \cdot g(Y)).$$

$$\Rightarrow f_{Y,Z}(y,z) = f_Y(y) \cdot f_{Z|Y}(z|y)$$

$$= g(y) \cdot \frac{1}{c \cdot g(y)} = \frac{1}{c}$$

$$= \frac{1}{\text{Area(Triangle)}}.$$

$$\Rightarrow (Y, Z)$$

$$\sim \text{unif}(\text{Triangle})$$

$$\textcircled{3} \quad (Y^*, Z^*) \in \text{Red } A. \quad \sim \text{unif}(A).$$

Algorithm Acceptance-Rejection Algorithm

Step 1: Generate $Y \sim g$.

$Z | Y=y \sim \text{unif}(0, c \cdot g(y))$

Step 2: Generate $Z \sim \text{Unif}(0, c \cdot g(Y))$.

Step 3: If $Z \leq f(Y)$, set $X = Y$. Otherwise go back to step 1.

$$\text{Unif}(0, c \cdot g(Y)) \leq f(Y) \Leftrightarrow c \cdot g(Y) \cdot \text{Unif}(0,1) \leq f(Y)$$

$$\Leftrightarrow \text{Unif}(0,1) \leq \frac{f(Y)}{c \cdot g(Y)}$$



Acceptance-Rejection Method

$f = g$
Supporting set

- Suppose one can generate samples (relatively easily) from PDF g
- How can random samples be simulated from PDF f ?

Algorithm Acceptance-Rejection Algorithm

Let c denote a constant such that $c \geq \sup_y \frac{f(y)}{g(y)}$. Then:

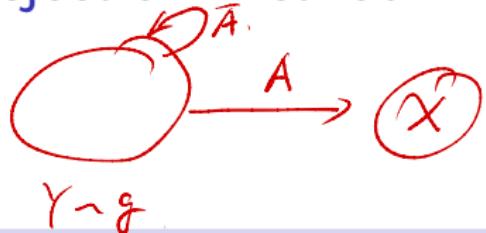
Step 1: Generate $Y \sim g$.

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

Step 3: If $U \leq \frac{f(Y)}{c \cdot g(Y)}$, set $X = Y$. Otherwise go back to step 1.

Acceptance-Rejection Method

(ii)



of iterations

$$N \sim F_S(p)$$

$$P = P(A) = \frac{1}{c}$$

$$\Rightarrow E(N) = \frac{1}{p} = c$$

Theorem

- (i) The random variable generated by the Acceptance-Rejection method has the desired PDF f.
- (ii) The number of iterations of the algorithm that are needed is a first-success random variable with mean c.
- (iii) $c \geq 1$ ✓

Proof (i). event $A = "U \leq \frac{f(Y)}{C \cdot g(Y)}"$, $f_{Y|A}(y|A) = \underline{\underline{f(y)}}_{\text{desired pdf}}$

$$f_{Y|A}(y|A) = \frac{P(A|Y=y)}{P(A)} f_Y(y).$$

unnormalized

$$1^{\circ} P(A|Y=y) = P(U \leq \frac{f(y)}{C \cdot g(y)} | Y=y) = P(U \leq \frac{f(y)}{C \cdot g(y)})$$

$$= P(U \leq \frac{f(y)}{C \cdot g(y)}) = \frac{f(y)}{C \cdot g(y)}$$

(C $\geq \sup_y \frac{f(y)}{g(y)}$)
 $\Rightarrow \frac{f(y)}{C \cdot g(y)} \leq 1.$

$$2^{\circ} P(A) \stackrel{\text{LopP}}{\approx} \int P(A|Y=y) \cdot g(y) dy = \int \frac{f(y)}{C \cdot g(y)} g(y) dy$$

$$= \frac{1}{C} \int f(y) dy = \frac{1}{C} \cdot \leq 1 \Rightarrow C \geq 1.$$

$$\Rightarrow f_{Y|A}(y|A) = \frac{P(A|Y=y)}{P(A)} \cdot \underline{\underline{f_Y(y)}} = \frac{\frac{f(y)}{C \cdot g(y)}}{\frac{1}{C}} \cdot g(y) = f(y).$$

$\Rightarrow X \sim f.$

Proof

Example: Beta Distribution

$$X \sim \text{Beta}(2, 4), \quad f(x) = 20x(1-x)^3, \quad 0 < x < 1$$

- An r.v. X is said to have the *Beta distribution* with parameters a and b , $a > 0$ and $b > 0$, if its PDF is

$$f(x) = \frac{1}{\beta(a, b)} x^{a-1} (1-x)^{b-1}, \quad 0 < x < 1,$$

where the constant $\beta(a, b)$ is chosen to make the PDF integrate to 1. We write this as $X \sim \text{Beta}(a, b)$. $a=b=1, f(x) \propto \text{constant}$.

- Beta distribution is a generalization of uniform distribution.
- Use the Acceptance-Rejection Method to generate a random variable with distribution Beta(2, 4)

Solution

$$f(x) = 20x(1-x)^3, 0 < x < 1$$

① $g : \text{Unif}(0,1)$, $g(x) = 1, 0 < x < 1$.

$$C \geq \sup_{y \in [0,1]} \frac{f(y)}{g(y)} = \sup_{y \in [0,1]} \frac{20y(1-y)^3}{1} = \sup_{y \in [0,1]} 20y(1-y)^3. \Rightarrow y^* = \frac{1}{4}$$
$$\Rightarrow C \geq \frac{135}{64}. \text{ choose } C = \frac{135}{64}.$$

② $\Rightarrow 0 < y < 1$, $\frac{f(y)}{C \cdot g(y)} = \frac{20y(1-y)^3}{\frac{135}{64} \cdot 1} = \frac{256}{27} y(1-y)^3$.

Step 1 : Generate $Y \sim \text{Unif}(0,1)$.

Step 2 : Generate $U \sim \text{unif}(0,1)$

Step 3 : If $U \leq \frac{f(Y)}{C \cdot g(Y)} = \frac{256}{27} Y(1-Y)^3$, set $X=Y$.

otherwise reject Y , go back to step 1.

Solution

Example: Normal Distribution

① $Z \sim N(0,1)$. $(-\infty, +\infty)$

$$\underline{X=|Z|} \quad (0, +\infty)$$

$$P(X \leq x) = P(|Z| \leq x) = 2P(0 \leq Z \leq x) = 2 \int_0^x \frac{1}{\sqrt{\pi}} e^{-z^2} dz$$

$$= \int_0^x \sqrt{\frac{2}{\pi}} e^{-z^2} dz \Rightarrow f_X(x) = \sqrt{\frac{2}{\pi}} e^{-\frac{1}{2}x^2}, 0 < x < \infty$$

② choose $g \sim \text{Exp}(1)$. $g(x) = e^{-x}, 0 < x < \infty$.

- Use the Acceptance-Rejection Method to generate a random variable with distribution $N(0, 1)$

$$C \geq \sup_y \frac{f(y)}{g(y)} = \sup_y \sqrt{\frac{2}{\pi}} e^{-\frac{1}{2}y^2} / e^{-y} = \sup_y \sqrt{\frac{2}{\pi}} e^{-\frac{1}{2}(y-1)^2 + \frac{1}{2}} = \sqrt{\frac{2e}{\pi}}$$

$$\Rightarrow y^* = 1, \text{ choose } C = \sqrt{\frac{2e}{\pi}}$$

$$\Rightarrow \frac{f(y)}{C \cdot g(y)} = e^{1(y - \frac{1}{2}y^2 - \frac{1}{2})} = e^{-\frac{1}{2}(y-1)^2}$$

Solution ③

Step 1 : Generate $Y \sim \text{Exp}(1)$

2 : $\dots \sim U \sim \text{unif}(0,1)$

3 : If $U \leq e^{-\frac{1}{2}(Y-1)^2}$, set $X = Y$.

otherwise return to Step 1.

$X \sim \mathcal{N}(0,1)$

Step 4 : generate $u' \sim \text{unif}(0,1)$

Box-Muller

Acceptance-Rejection

$$Z = \begin{cases} X & \text{if } u' \leq \frac{1}{2} \\ -X & \text{otherwise.} \end{cases}$$

$$\underline{Z \sim \mathcal{N}(0,1)}$$

Solution

Outline

- 1 History of Monte Carlo
- 2 Sampling: Random Variable Generation
- 3 Sampling: Random Vector Generation $f(x,y,z) = \underline{f(x)} \cdot \underline{f(y|x)} \cdot \underline{f(z|x,y)}$
- 4 Monte Carlo Integration
- 5 Asymptotic Analysis: Law of Large Numbers
- 6 Non-asymptotic Analysis: Inequalities

Change of Variables

Theorem

Let $\mathbf{X} = (X_1, \dots, X_n)$ be a continuous random vector with joint PDF $f_{\mathbf{X}}(x)$, and let $\mathbf{Y} = g(\mathbf{X})$ where g is an invertible function from \mathbb{R}^n to \mathbb{R}^n . Let $y = g(\mathbf{x})$ and suppose that all the partial derivatives $\frac{\partial x_i}{\partial y_j}$ exists and are continuous, so we can form the **Jacobian matrix**

$$\frac{\partial \mathbf{x}}{\partial \mathbf{y}} = \begin{pmatrix} \frac{\partial x_1}{\partial y_1} & \frac{\partial x_1}{\partial y_2} & \cdots & \frac{\partial x_1}{\partial y_n} \\ \vdots & \vdots & & \vdots \\ \frac{\partial x_n}{\partial y_1} & \frac{\partial x_n}{\partial y_2} & \cdots & \frac{\partial x_n}{\partial y_n} \end{pmatrix}$$

Also assume that the determinant of the Jacobian matrix is never 0. Then the joint PDF of \mathbf{Y} is

$$f_{\mathbf{Y}}(y) = f_{\mathbf{X}}(x) \left| \frac{\partial \mathbf{x}}{\partial \mathbf{y}} \right|$$

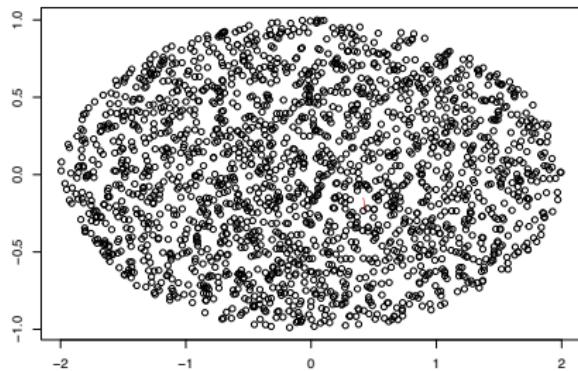
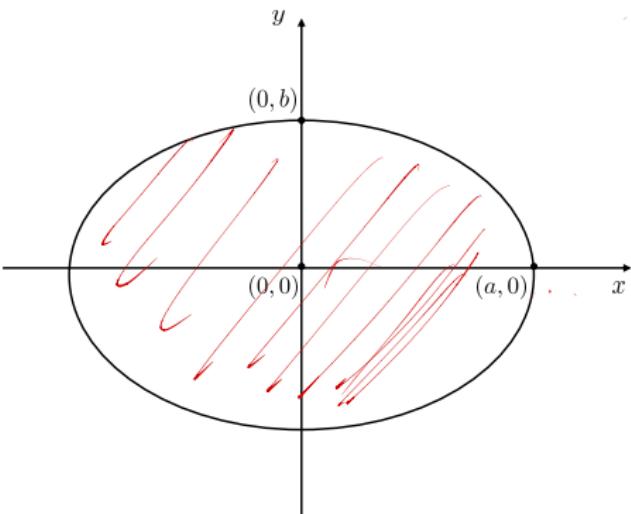
Example: Generate Uniform Distribution over An Ellipse

objective PDF $f_{X,Y}(x,y) = \frac{1}{\pi \cdot a \cdot b} \quad \theta(x,y) \in E_2(a,b)$

- Ellipse:

$$x = \rho \cdot a \cdot \cos \theta \quad \rho \in [0,1] ; \theta \in [0,2\pi]$$

$$E_2(a,b) = \left\{ (x,y) \in \mathbb{R}^2 : \left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right)^2 \leq 1 \right\}$$



Solution ① Jacobi Matrix

$$\begin{bmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} \end{bmatrix} = \begin{bmatrix} a \cos \theta & -r a \sin \theta \\ b \sin \theta & r b \cos \theta \end{bmatrix}$$

$$J = \det(J) \checkmark, J = r a b.$$

$$\Rightarrow f_{R,\Theta}(r, \theta) = f_{x,y}(x, y) \cdot |J| = \frac{1}{\pi a b} r a b = \frac{1}{\pi}, r \in [0, 1], \theta \in [0, \pi].$$

$$\Rightarrow f_R(r) = \int_0^{2\pi} \frac{1}{\pi} d\theta = 2\pi, 0 \leq r \leq 1 \Rightarrow F_R(r) = \underline{r^2}, 0 \leq r \leq 1.$$

$$f_\Theta(\theta) = \int_0^{2\pi} \frac{1}{\pi} d\theta = \frac{1}{2\pi}, 0 \leq \theta \leq 2\pi. \quad \theta \sim \text{Unif}(0, 2\pi)$$

$$\Rightarrow f_{R,\Theta}(r, \theta) = f_R(r) \cdot f_\Theta(\theta), R, \Theta \text{ independent.}$$

(R) $\cdot F_R^{-1}(z) = \sqrt{z}, 0 \leq z \leq 1;$

Solution ②

U_1, U_2 independent Uniform

$$X = a \sqrt{U_1} \cos(2\pi U_2)$$

$$Y = b \sqrt{U_1} \sin(2\pi U_2)$$

$$\underline{(X, Y)}$$

Solution

Change of Variables

$A : n \times n$

$$\det(ATA) = \det^2(A)$$

Theorem

Let $\mathbf{X} = (X_1, \dots, X_n)$ be a continuous random vector with joint PDF $f_{\mathbf{X}}(x)$, and let $\mathbf{Y} = g(\mathbf{X})$ where g is a function from \mathbb{R}^n to \mathbb{R}^m . Let $y = g(x)$ and we have the Jacobian matrix $\frac{\partial \mathbf{x}}{\partial \mathbf{y}}$. The corresponding Gram matrix is

$$\mathbf{G} = \left(\frac{\partial \mathbf{x}}{\partial \mathbf{y}} \right)^T \frac{\partial \mathbf{x}}{\partial \mathbf{y}}.$$

Then the joint PDF of \mathbf{Y} is

$$f_{\mathbf{Y}}(y) = f_{\mathbf{X}}(x) \sqrt{\det(\mathbf{G})}$$

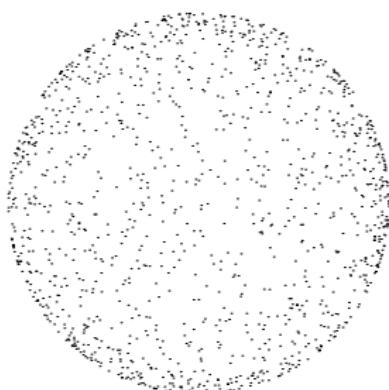
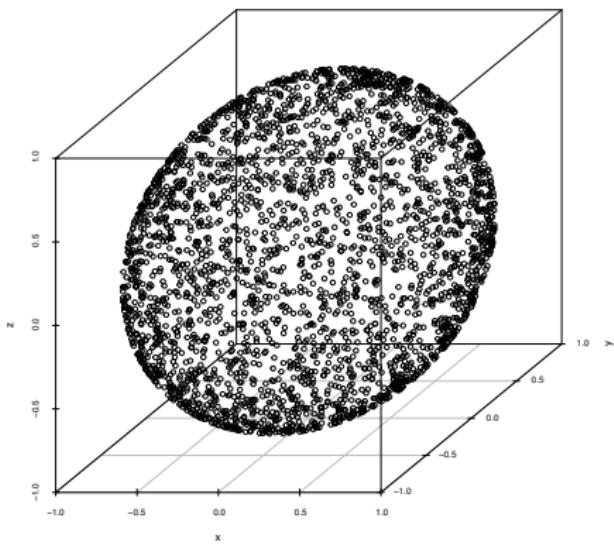
Example: Generate Uniform Distribution over A

Sphere

$$\text{Ball } B_3(r) = \{(x,y,z) \in \mathbb{R}^3 : x^2 + y^2 + z^2 \leq r^2\}$$

- Sphere:

$$S_2(r) = \{(x, y, z) \in \mathbb{R}^3 : x^2 + y^2 + z^2 = r^2\}.$$



Solution ① $f_{x,y,z}(x,y,z) = \frac{1}{4\pi r^2}$ ($(x,y,z) \in S_{out}$).

$$\begin{cases} x = r \sin \theta \cos \phi \\ y = r \sin \theta \sin \phi \\ z = r \cos \theta \end{cases} \quad \begin{array}{l} \theta \in [0, \pi], \\ \phi \in [0, 2\pi], \end{array} \quad \underline{(x,y,z)} \rightarrow \underline{(\theta, \phi)}$$

Jacobi Matrix $M = \begin{bmatrix} \frac{\partial x}{\partial \theta} & \frac{\partial x}{\partial \phi} \\ \frac{\partial y}{\partial \theta} & \frac{\partial y}{\partial \phi} \\ \frac{\partial z}{\partial \theta} & \frac{\partial z}{\partial \phi} \end{bmatrix} = \begin{bmatrix} r \cos \theta \cos \phi & -r \sin \theta \sin \phi \\ r \cos \theta \sin \phi & r \sin \theta \cos \phi \\ -r \sin \theta & 0 \end{bmatrix}$

Gram matrix $G = M^T M = \begin{bmatrix} r^2 & 0 \\ 0 & r^2 \sin^2 \theta \end{bmatrix} \Rightarrow \det(G) = r^4 \sin^2 \theta.$

$$\Rightarrow f_{\theta, \phi}(\theta, \phi) = f_{x,y,z}(x,y,z) \cdot \sqrt{\det(G)} = \frac{1}{4\pi r^2} \cdot r^2 \sin \theta = \frac{1}{4\pi} \sin \theta$$

$\theta \in [0, \pi]$
 $\phi \in [0, 2\pi]$

Solution ② $f_{\theta}(\theta) = \int_0^{2\pi} f_{\theta,\phi}(\theta, \phi) d\phi = \frac{1}{2} \sin \theta ; 0 \leq \theta \leq \pi.$

$$F_{\theta}(\theta) = \int_0^{\theta} f_{\theta}(s) ds = \left(\frac{1-\cos \theta}{2} \right), 0 \leq \theta \leq \pi.$$

$$f_{\phi}(\phi) = \frac{1}{2\pi} ; 0 \leq \phi \leq 2\pi ; \Rightarrow f_{\theta,\phi}(\theta, \phi) = f_{\theta}(\theta) f_{\phi}(\phi)$$

θ and ϕ independent. ; $\phi \sim \text{Unif}(0, 2\pi) = 2\pi \text{ Unif}(0, 1);$

$$\underline{F_{\theta}^{-1}(s) = \arccos(1-2s)}, 0 \leq s \leq 1$$

Note: if $\theta = \arccos(1-2s) \Rightarrow \cos \theta = 1-2s$

$$\sin^2 \theta = 1 - \cos^2 \theta = 1 - (1-2s)^2 = 4s(1-s)$$

$$\Rightarrow \sin \theta > 0 ; \Rightarrow \underline{\sin \theta = 2\sqrt{s(1-s)}}$$

Solution ③

independently generate $U_1, U_2 \sim \text{Uniform}$

$$\left\{ \begin{array}{l} X \leftarrow r \cdot 2\sqrt{U_1(1-U_1)} \cdot \cos(2\pi U_2) \\ Y \leftarrow r \cdot 2\sqrt{U_1(1-U_1)} \cdot \sin(2\pi U_2) \\ Z \leftarrow r \cdot (1-2U_1) \end{array} \right.$$

Outline

- 1 History of Monte Carlo
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Monte Carlo Integration

~~E(X)~~

$$\underline{x}_1, \dots, \underline{x}_n : \frac{1}{n} (x_1 + \dots + x_n)$$
$$E[g(x)] \quad g(x_1), \dots, g(x_n) : \frac{1}{n} (g(x_1) + \dots + g(x_n))$$

- We can use the sample mean to approximate the expectation:

$$\underline{E[g(X)]} \approx \frac{1}{n} \sum_{i=1}^n g(X_i). \quad X \sim \text{Unif}(a, b).$$

- Now we have integration

$$\int_a^b g(x) dx = (b - a) \int_a^b g(x) \cdot \frac{1}{b - a} dx. \quad f(x) \cdot \text{PDF}$$
$$= (b - a) \int_a^b g(x) dx = (b - a) E[g(X)]$$

- Drawing n samples (empirical samples) from Unif(a, b):

$$\underline{X_1, X_2, \dots, X_n \sim \text{Unif}(a, b)}.$$

$$\pi(b-a) \cdot \frac{1}{n} (g(x_1) + \dots + g(x_n))$$

- Monte Carlo Integration:

$$\int_a^b g(x) dx \approx \frac{1}{n} \sum_{i=1}^n g(X_i) (b - a).$$

Monte Carlo Integration

Example: π as An Integration

Evaluate the integration

$$\int_0^1 \frac{4}{1+x^2} dx.$$

- $g(x) = 4/(1+x^2)$, $0 < x < 1$. $a=0, b=1$
- X_1, \dots, X_n : samples from $\text{Unif}(0, 1)$.
- Monte Carlo Integration:

$$\int_0^1 \frac{4}{1+x^2} dx \approx \frac{1}{n} \sum_{i=1}^n \left(\frac{4}{1+X_i^2} \right)$$

Example

Evaluate the integration

$$\int_0^4 \sqrt{x + \sqrt{x + \sqrt{x + \sqrt{x}}}} dx.$$

- Corresponding

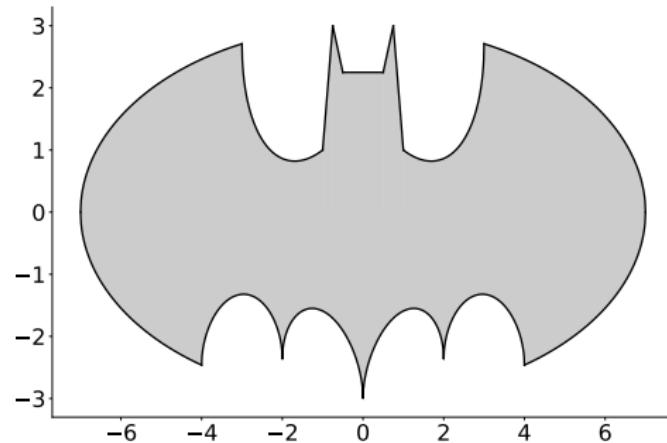
$$g(x) = \sqrt{x + \sqrt{x + \sqrt{x + \sqrt{x}}}}$$

- X_1, \dots, X_n : samples from $\text{Unif}(0, 4)$. $a=0, b=4$
- Monte Carlo Integration:

$$\int_0^4 \sqrt{x + \sqrt{x + \sqrt{x + \sqrt{x}}}} dx \approx \frac{4}{n} \sum_{i=1}^n \sqrt{X_i + \sqrt{X_i + \sqrt{X_i + \sqrt{X_i}}}}$$

Example: Area of Batman Curve

- Challenging and Fun
- <https://mathworld.wolfram.com/BatmanCurve.html>



Example: Estimation of Probability

- Indicator: bridge between expectation and probability
- Given event A :

$$\underline{I_A(x)} = \begin{cases} 1 & \text{if } x \in A \\ 0 & \text{Otherwise} \end{cases}.$$

- For random variable X :

$$\underline{P(X \in A)} = 1 \cdot P(X \in A) + 0 \cdot P(X \notin A)$$
$$= \underline{E(I_A(X))}$$

$$\approx \frac{1}{n} \sum_{i=1}^n I_A(X_i).$$

$x_1, \dots, x_n \sim X$

Example: Estimation of π

generate n points $(X_1, Y_1), \dots, (X_n, Y_n)$

① event A_i : "the i^{th} point lands within the circle", $\Leftrightarrow \{X_i^2 + Y_i^2 \leq 1\}$

$$-1 \leq X_i \leq 1$$

$$-1 \leq Y_i \leq 1$$

② $I_{A_i} = Z_i$

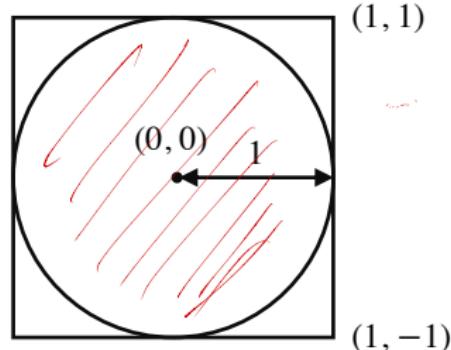
$$P(Z_i = 1) = P(A_i) = \frac{\pi \cdot 1}{4} = \frac{\pi}{4}$$

$$P(Z_i = 0) = 1 - \frac{\pi}{4}$$

$$\Rightarrow E(Z_i) = P(Z_i = 1) = \frac{\pi}{4}$$

$$Z_1, \dots, Z_n \sim \underbrace{\text{Bern}(\frac{\pi}{4})}_{(-1, -1)}$$

$$\Rightarrow E(Z) = \frac{\pi}{4}$$



$$\Rightarrow \pi = 4E(Z) \approx 4 \cdot \underbrace{\frac{1}{n}(Z_1 + \dots + Z_n)}_{}$$

Example: Estimation of π

Example: Estimation of π

Useful Tools: Importance Sampling

- Standard Monte Carlo integration is great if you can sample from the target distribution (i.e. the desired distribution)
- But what if you can't sample from the target?
- **Importance Sampling:** draw the sample from a proposal distribution and re-weight the integral using importance weights so that the correct distribution is targeted

Importance Sampling

$$H = \underline{E_f[h(Y)]} = \int \underline{h(y)f(y)dy}$$

- h is some function and f is the PDF of random variable Y
- When the PDF f is difficult to sample from, importance sampling can be used
- Rather than sampling from f , you specify a different PDF g , as the proposal distribution.

$$\underline{H = \int h(y)f(y)dy} = \int h(y) \frac{f(y)}{g(y)} g(y)dy = \int \boxed{\frac{h(y)f(y)}{g(y)}} g(y)dy$$

Importance Sampling

g is a PDF.

$$H = E_f[h(Y)] = \int \frac{h(y)f(y)}{g(y)} dy = E_g\left[\frac{h(Y)f(Y)}{g(Y)}\right]$$

- Hence, given an iid sample Y_1, \dots, Y_n from PDF \underline{g} , our estimator of H becomes

$$\hat{H} = \frac{1}{n} \sum_{j=1}^n \frac{h(Y_j)f(Y_j)}{g(Y_j)}$$

Example: Gaussian Tail Probability

$$P(-3 < Y < 3) = 0.997$$

Method 1: $C = P(Y > 8) = \frac{E[I(Y > 8)]}{f(Y_1, \dots, Y_n)}$

$C \approx 0$

$$\approx \frac{1}{n} \sum_{j=1}^n I(Y_j > 8)$$

$$f(Y_1, \dots, Y_n) \sim N(0, 1)$$

$$h(y) = I(Y > 8) = \begin{cases} 1 & \text{if } y > 8 \\ 0 & \text{otherwise} \end{cases}$$

Evaluate the probability of rare event $c = \underline{\mathbb{P}(Y > 8)}$, where $\underline{Y \sim N(0, 1)}$.

choose $g \sim N(8, 1)$, $Y_1, \dots, Y_n \sim g$.

Method 2:

importance sampling

$$\begin{aligned} C &\approx \frac{1}{n} \sum_{j=1}^n \frac{h(Y_j) f(Y_j)}{g(Y_j)} = \frac{1}{n} \sum_{j=1}^n I(Y_j > 8) \cdot \frac{\frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2} Y_j^2}}{\frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2} (Y_j - 8)^2}} \\ &= \frac{1}{n} \sum_{j=1}^n I(Y_j > 8) \cdot e^{-8Y_j + 32} \end{aligned}$$

$$n = 50000 \rightarrow C \approx 6.025 \times 10^{-16}$$

Solution

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$$n \rightarrow \infty$$

Sample Mean: Recall

Definition

Let X_1, \dots, X_n be i.i.d. random variables with finite mean μ and finite variance σ^2 . The *sample mean* \bar{X}_n is defined as follows:

$$\bar{X}_n = \frac{1}{n} \sum_{j=1}^n X_j.$$

The sample mean \bar{X}_n is itself an r.v. with mean μ and variance σ^2/n .

$$n \rightarrow \infty$$

$$\sigma^2/n \rightarrow 0$$

Strong Law of Large Numbers (SLLN)

$$\int_a^b g(x)dx \approx \frac{b-a}{n} \sum_{i=1}^n g(x_i) \Rightarrow \frac{b-a}{n} \sum_{i=1}^n g(x_i) \xrightarrow{\text{w.p.1}} \int_a^b g(x)dx.$$

x_1, \dots, x_n i.i.d. unif(a,b).

(1) x_1, \dots, x_n i.i.d. g = continuous function.

$g(x_1), \dots, g(x_n)$ i.i.d.

$$E[g(x_i)] = \int_a^b g(x) \cdot \frac{1}{b-a} dx.$$

Theorem

The sample mean \bar{X}_n converges to the true mean μ pointwise as $n \rightarrow \infty$, with probability 1. In other words, the event $\bar{X}_n \rightarrow \mu$ has probability 1.

(2) By SLLN $\frac{g(x_1) + \dots + g(x_n)}{n} \xrightarrow[n \rightarrow \infty]{\text{w.p.1}} E[g(x)] = \int_a^b g(x) \frac{1}{b-a} dx$

$$\Rightarrow \frac{(b-a)}{n} \sum_{i=1}^n g(x_i) \xrightarrow[n \rightarrow \infty]{\text{w.p.1}} \int_a^b g(x)dx.$$

Weak Law of Large Numbers (WLLN)

$$\begin{aligned} X_n &\xrightarrow{\text{a.s.}} 0 & X_n &\xrightarrow{\text{P}} 0 \\ X_n &\xrightarrow{\text{w.p.1}} 0 & \lim_{n \rightarrow \infty} P(|X_n - 0| > \varepsilon) &= 0 \\ P(\lim_{n \rightarrow \infty} X_n = 0) &= 1 & \forall \varepsilon > 0. \end{aligned}$$

X_n = { 1 w.p. $\frac{1}{n}$
0 w.p. $1 - \frac{1}{n}$.



Theorem

For all $\epsilon > 0$, $P(|\bar{X}_n - \mu| > \epsilon) \rightarrow 0$ as $n \rightarrow \infty$. (This form of convergence is called convergence in probability).

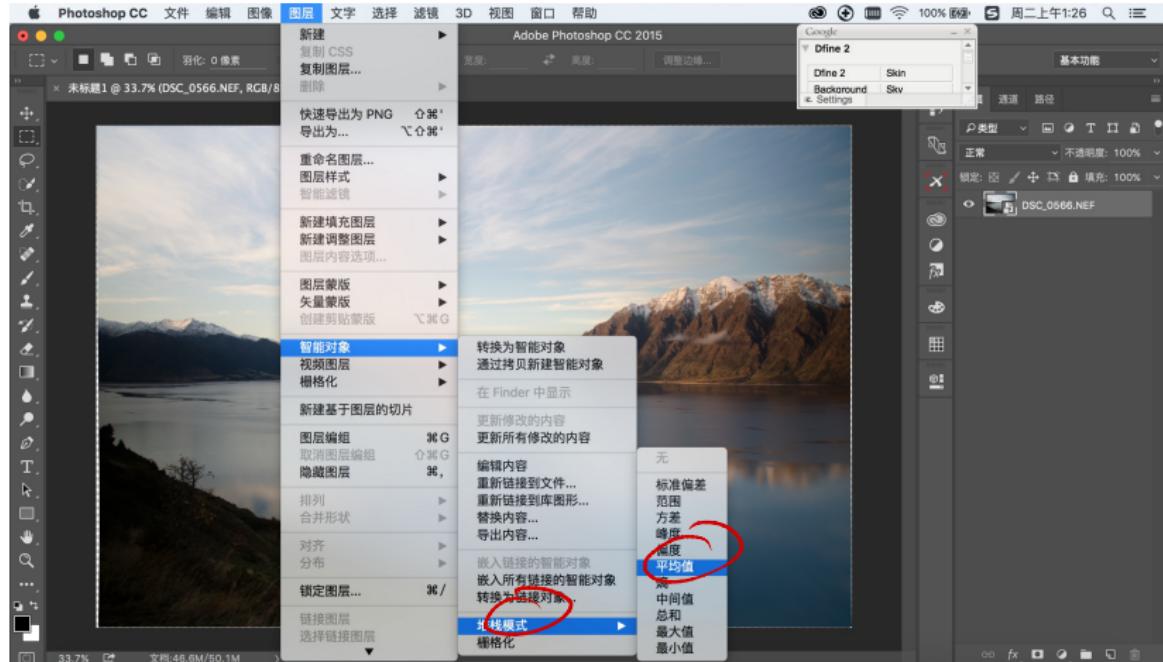
$$\begin{aligned} \lim_{n \rightarrow \infty} P(|X_n - 0| > \varepsilon) &= P(X_n > \varepsilon) & (\varepsilon > 1) \\ &= \overbrace{P(X_n = 1)}^{0 < \varepsilon < 1} & = 0 \\ &= \frac{1}{n} & \xrightarrow{n \rightarrow \infty} 0. \end{aligned}$$

$X_n \xrightarrow{\text{P}} 0.$

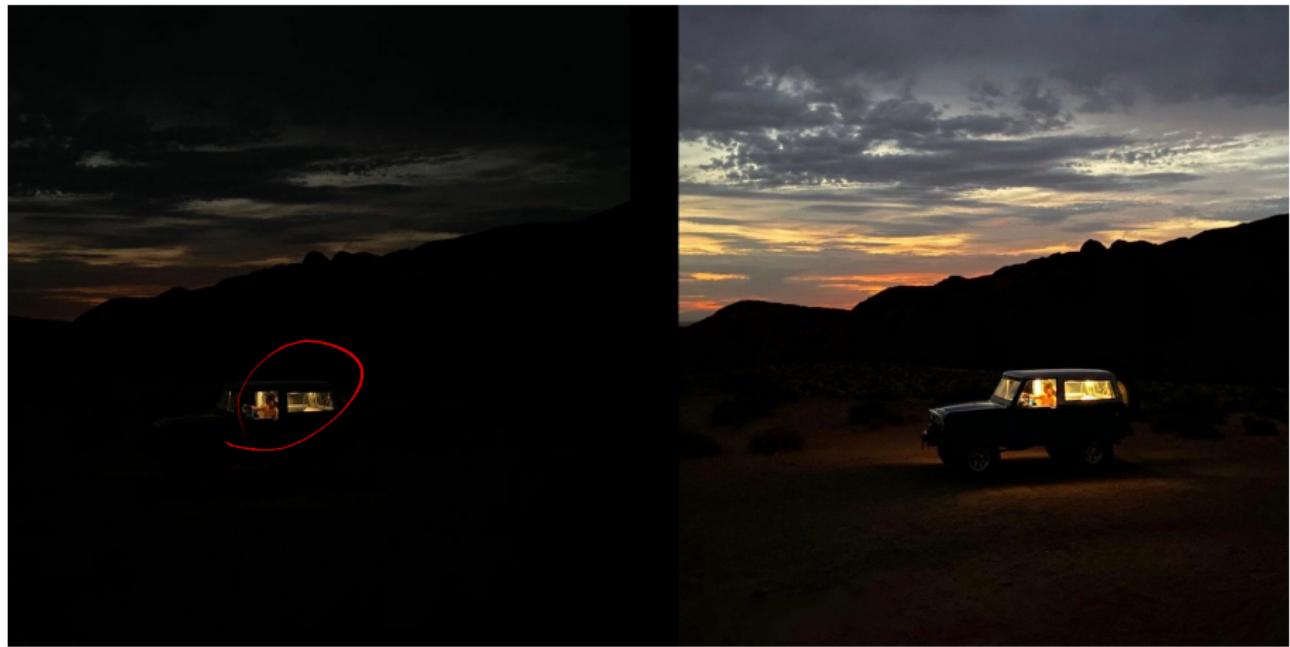
Widely Applications: Photo Stacking with PC



Widely Applications: Photo Stacking with PC



Widely Applications: Night Model with Smart Phone



Widely Applications: Photo Stacking with Smart Phone



Widely Applications: Photo Stacking with Smart Phone



Widely Applications: Photo Stacking with Smart Phone



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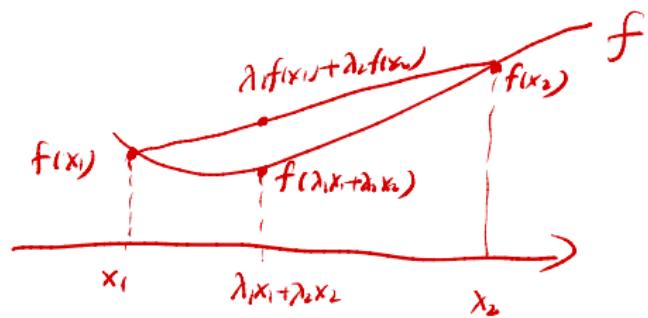
Cauchy-Schwarz Inequality: Recall

Theorem

For any r.v.s X and Y with finite variances,

$$|E(XY)| \leq \sqrt{E(X^2) E(Y^2)}.$$

Jensen's Inequality



If f is a convex function, $0 \leq \lambda_1, \lambda_2 \leq 1, \lambda_1 + \lambda_2 = 1$, then for any x_1, x_2 ,

$$f(\lambda_1 x_1 + \lambda_2 x_2) \leq \lambda_1 f(x_1) + \lambda_2 f(x_2).$$

Jensen's Inequality

Theorem

Let X be a random variable. If g is a convex function, then $E(g(X)) \geq g(E(X))$. If g is a concave function, then $E(g(X)) \leq g(E(X))$. In both cases, the only way that equality can hold is if there are constants a and b such that $g(X) = a + bX$ with probability 1.

Quick Examples

$$\left. \begin{array}{l} g \text{ is convex ; } E[g(X)] \geq g(E(X)) \\ g \text{ is concave ; } E[g(X)] \leq g(E(X)) \end{array} \right\} \begin{array}{l} g'' \geq 0 \\ \text{Convex} \end{array}$$

1^o. $g(x) = x^2$, $x \in \mathbb{R}$; convex; $\Rightarrow E[x^2] \geq (E(x))^2$ ✓

$$\text{Var}(x) = E(x^2) - E(x)^2 \geq 0.$$

2^o. $g(x) = \frac{1}{x}$, $x > 0$; convex; $\Rightarrow E[\frac{1}{x}] \geq \frac{1}{E(x)}$ ✓

3^o. $g(x) = \log x$, $x > 0$; concave; $\Rightarrow E[\log x] \leq \log(E(x))$.

Entropy

- Let X be a discrete r.v. whose distinct possible values are a_1, a_2, \dots, a_n , with probabilities p_1, p_2, \dots, p_n respectively (so $p_1 + p_2 + \dots + p_n = 1$).
- The *entropy* of X is defined as follows:
$$H(X) = \sum_{j=1}^n p_j \log_2 (1/p_j).$$
- Using Jensen's inequality, show that the maximum possible entropy for X is when its distribution is uniform over a_1, a_2, \dots, a_n , i.e., $p_j = 1/n$ for all j .
- This makes sense intuitively, since learning the value of X conveys the most information on average when X is equally likely to take any of its values, and the least possible information if X is a constant.

Proof ① Construct a random variable Y . s.t

$$Y = \begin{cases} \frac{1}{p_1} & \text{w.p. } p_1 \\ \frac{1}{p_2} & \text{w.p. } p_2 \\ \vdots & \\ \frac{1}{p_n} & \text{w.p. } p_n \end{cases} \Rightarrow E(Y) = \frac{1}{p_1} \cdot p_1 + \frac{1}{p_2} \cdot p_2 + \dots + \frac{1}{p_n} \cdot p_n = n$$

$$\textcircled{2} H(X) \triangleq \sum_{j=1}^n p_j \log_2 \frac{1}{p_j} = \underbrace{E[\log_2 Y]}_{\text{w.p. } p_1, \dots, p_n} \leq \log_2 E[Y] = \log_2 n.$$

$$\text{w.p. } p_1, \dots, p_n \Rightarrow \max_{p_1, \dots, p_n} H(X) \leq \log_2 n$$

$$\textcircled{3} \text{ when } X \sim \text{Dunif}(\frac{1}{n}), p_1 = p_2 = \dots = p_n = \frac{1}{n}; H(X) = \sum_{j=1}^n \frac{1}{n} \cdot \log_2 n = \log_2 n.$$

$$\Rightarrow \max_{p_1, \dots, p_n} H(X) \geq \log_2 n \Rightarrow \max_{p_1, \dots, p_n} H(X) = \log_2 n$$

Kullback-Leibler Divergence

Let $\mathbf{p} = (p_1, \dots, p_n)$ and $\mathbf{r} = (r_1, \dots, r_n)$ be two probability vectors (so each is nonnegative and sums to 1). Think of each as a possible PMF for a random variable whose support consists of n distinct values. The *Kullback-Leibler* divergence between \mathbf{p} and \mathbf{r} is defined as

$$D(\mathbf{p}, \mathbf{r}) = \sum_{j=1}^n p_j \log_2 (1/r_j) - \sum_{j=1}^n p_j \log_2 (1/p_j).$$

Show that the Kullback-Leibler divergence is nonnegative.

Proof ① $D(P, r) = \sum_{j=1}^n p_j \log_2 \frac{r_j}{p_j} - \sum_{j=1}^n p_j \log_2 \frac{p_j}{r_j} = \sum_{j=1}^n p_j \log_2 \frac{p_j}{r_j}$

 $= -\frac{\sum_{j=1}^n p_j \log_2 \frac{r_j}{p_j}}{\sum_{j=1}^n p_j}$

② Construct a random variable Y . s.t.

$P(Y = \frac{r_j}{p_j}) = p_j, j = 1, 2, \dots, n.$

$\Rightarrow E(Y) = \sum_{j=1}^n \frac{r_j}{p_j} \cdot p_j = \sum_{j=1}^n r_j = 1$

③ $D(P, r) = -E[\log_2 Y] \geq -\log_2 E(Y) = -\log_2 1 = 0$

Markov's Inequality

Concentration Inequality

Chebyshev
Markov Lapunov

$$P(|X - E(X)| \geq a) \leq \frac{1}{\frac{a^2}{E[X]^2}} = \frac{1}{e^a}$$

Theorem

For any r.v. X and constant $a > 0$,

$$P(|X| \geq a) \leq \frac{E|X|}{a}.$$

Proof

$$\boxed{P(|X| \geq a) \leq \frac{1}{a} E[|X|], \quad a > 0}$$

① $Y = \frac{1}{a} |X| \geq 0 : \quad \underline{I(Y \geq 1)} \leq Y \quad \begin{cases} Y \geq 1 & LHS \\ 0 \leq Y < 1 & RHS \end{cases}$

$$\Rightarrow \underline{E[I(Y \geq 1)]} \leq E[Y]$$

$$\Rightarrow P(Y \geq 1) \leq E[Y] = E\left[\frac{1}{a}|X|\right] = \frac{1}{a} E[|X|].$$

$$\begin{aligned} & P\left(\frac{|X|}{a} \geq 1\right) \\ & \leq \\ & P(|X| \geq a) \end{aligned}$$

Chebyshev's Inequality

$$P(|X-\mu| \geq a) = P(|X-\mu|^2 \geq a^2)$$

Markov's Inequality

$$\leq \frac{1}{a^2} E(|X-\mu|^2) = \frac{1}{a^2} \text{Var}(x)$$

Theorem

Let X have mean μ and variance σ^2 . Then for any $a > 0$, $P(|X-\mu| \geq a) \leq \frac{\sigma^2}{a^2}$

$$P(|X-\mu| \geq a) \leq \frac{\sigma^2}{a^2}. \quad O\left(\frac{1}{a^2}\right)$$

Application: \bar{X}_n Sample mean : $E(\bar{X}_n) = \mu$; $\text{Var}(\bar{X}_n) = \frac{1}{n} \sigma^2$

$$P(|\bar{X}_n - \mu| \geq a) \leq \frac{1}{a^2} \text{Var}(\bar{X}_n) = \frac{\sigma^2}{(n \cdot a^2)} \xrightarrow{n \rightarrow \infty} 0$$

$$\bar{X}_n \xrightarrow{P} \mu.$$

$$O\left(\frac{1}{n}\right)$$

Proof

Chernoff's Inequality

$$\forall t > 0 \quad P(X \geq a) = P(e^{tX} \geq e^{ta})$$

Martingale Inequality

\leq

$$\frac{E[e^{tX}]}{e^{ta}} f(t)$$

Theorem

For any r.v. X and constants $a > 0$ and $t > 0$,

$$P(X \geq a) \leq \frac{E(e^{tX})}{e^{ta}} f(t) \xrightarrow{\text{MGF.}}$$

$$\forall t > 0 \quad P(X \geq a) \leq f(t)$$

$$\Rightarrow P(X \geq a) \leq \inf_{t > 0} f(t)$$

Proof

Chernoff's Technique

$$\forall t < 0 ; P(X \leq a) = P(tx \geq ta)$$

$$= P(e^{tx} \geq e^{ta}) \leq \frac{E[e^{tx}]}{e^{ta}} \cdot f(t)$$

Theorem

For any r.v. X and constants a ,

$$P(X \geq a) \leq \inf_{t>0} \frac{E(e^{tX})}{e^{ta}}$$

$$P(X \leq a) \leq \inf_{t<0} \frac{E(e^{tX})}{e^{ta}}.$$

Proof

Example: Normal Distribution

① MGF of X : $M_X(t) = e^{\mu t + \frac{1}{2}\sigma^2 t^2}$

② $P(X > a) \leq \inf_{t > 0} \frac{E[e^{tx}]}{e^{ta}} = \inf_{t > 0} f(t)$

Given $X \sim \mathcal{N}(\mu, \sigma^2)$, for arbitrary constant $a > \mu$, find the Chernoff bound on $\underline{P}(X > a)$.

$$f(t) = \frac{E[e^{tx}]}{e^{ta}} = \frac{M_X(t)}{e^{ta}} = e^{\frac{1}{2}\sigma^2 t^2 + (\mu - \alpha)t}$$
$$= e^{\frac{1}{2}\sigma^2 \left[\underline{(t + \frac{\mu - \alpha}{\sigma^2})^2} - \frac{(\mu - \alpha)^2}{\sigma^2} \right]} \quad t^* = \frac{\alpha - \mu}{\sigma^2} > 0$$

$$\Rightarrow P(X > a) \leq f(t^*) = e^{-\frac{(\alpha - \mu)^2}{2\sigma^2}}$$

$$\alpha = \mu + \varepsilon$$

$$\mathcal{O}(e^{-\varepsilon^2})$$

$$\Rightarrow P(X > \mu + \varepsilon) \leq e^{-\frac{\varepsilon^2}{2\sigma^2}} \Rightarrow P(X - \mu > \varepsilon) \leq e^{-\frac{\varepsilon^2}{2\sigma^2}}$$

Solution

Hoeffding Bound

$$E\left(\frac{1}{n} \sum_{i=1}^n X_i\right) = \mu$$

Theorem

Let the random variables X_1, X_2, \dots, X_n be independent with $E(X_i) = \mu$, $a \leq X_i \leq b$ for each $i = 1, \dots, n$, where a, b are constants. Then for any $\epsilon \geq 0$,

$$\mathbb{P}\left(\left|\frac{1}{n} \sum_{i=1}^n X_i - \mu\right| \geq \epsilon\right) \leq 2e^{-\frac{2n\epsilon^2}{(b-a)^2}}.$$

$\epsilon \uparrow \downarrow$
 $n \uparrow \downarrow$

$$\mathbb{P}(|\bar{X}_n - \mu| \geq \epsilon) \leq \frac{o(e^{-\epsilon^2})}{\sqrt{n}}$$

Application: Parameter Estimation

$$\begin{aligned} p \in [\hat{p} - \epsilon, \hat{p} + \epsilon] &\Leftrightarrow \hat{p} - \epsilon \leq p \leq \hat{p} + \epsilon \\ &\Leftrightarrow -\epsilon \leq p - \hat{p} \leq \epsilon \\ &\Leftrightarrow -\epsilon \leq \hat{p} - p \leq \epsilon \Leftrightarrow |\hat{p} - p| \leq \epsilon \end{aligned}$$

Instead of predicting a single value \hat{p} for the parameter p , we are given an interval that is likely to contain the parameter:

Definition

$\delta = 0.05$

A $1 - \delta$ confidence interval for a parameter p is an interval $[\hat{p} - \epsilon, \hat{p} + \epsilon]$ such that

$$Pr(p \in [\hat{p} - \epsilon, \hat{p} + \epsilon]) \geq 1 - \delta.$$

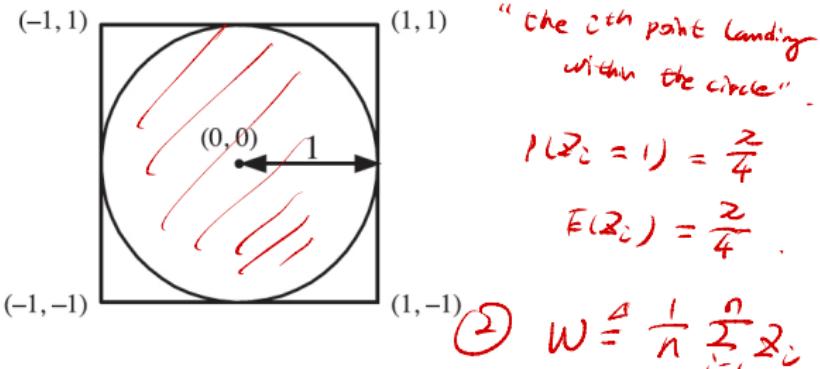
$$\begin{aligned} Pr(|\hat{p} - p| \leq \epsilon) &\geq 1 - \delta \\ \Rightarrow Pr(|\hat{p} - p| > \epsilon) &\leq \underline{\delta} \end{aligned}$$

Application Example: Monte Carlo Method for Estimation π

① (x_2, y_2) ($-1 \leq x_2 \leq 1, -1 \leq y_2 \leq 1$)

Circle: $\{ (x, y) : x^2 + y^2 \leq 1 \}$

Z_2 : indicator of the event



② $W \triangleq \frac{1}{n} \sum_{c=1}^n Z_c$

- A point chosen uniformly at random in the square has probability $\pi/4$ of landing in the circle

$$E(W) = \frac{\pi}{4}.$$

③ $\hat{\pi} = 4W = 4 \cdot \frac{1}{n} \sum_{c=1}^n Z_c$

Confidence Interval of π .

Example: Monte Carlo Method for Estimation π

③ $n \rightarrow \infty$, $\hat{\pi} \rightarrow \pi$ (w.p.1).

Z_1, \dots, Z_n i.i.d.

Param($\frac{Z}{4}$)

$$\Pr(|\hat{\pi} - \pi| \geq \varepsilon) = \Pr(|4W - \pi| \geq \varepsilon)$$

$$= \Pr\left(|W - \frac{\pi}{4}| \geq \frac{\varepsilon}{4}\right) = \Pr\left(\left|\frac{1}{n} \sum_{i=1}^n Z_i - E(Z)\right| \geq \frac{\varepsilon}{4}\right)$$

~~Hoeffding's inequality~~

$$\frac{\text{Var}\left(\frac{1}{n} \sum_{i=1}^n Z_i\right)}{\left(\frac{\varepsilon}{4}\right)^2} = \frac{\frac{2}{n}(1-\frac{2}{n})}{\left(\frac{\varepsilon}{4}\right)^2 \cdot n}$$

Hoeffding's inequality

$$\text{bound} \leq 2 \cdot e^{-\frac{2n(\frac{\varepsilon}{4})^2}{(1-\frac{2}{n})^2}} = \frac{2e^{-\frac{1}{8}n\varepsilon^2}}{n} = \delta$$

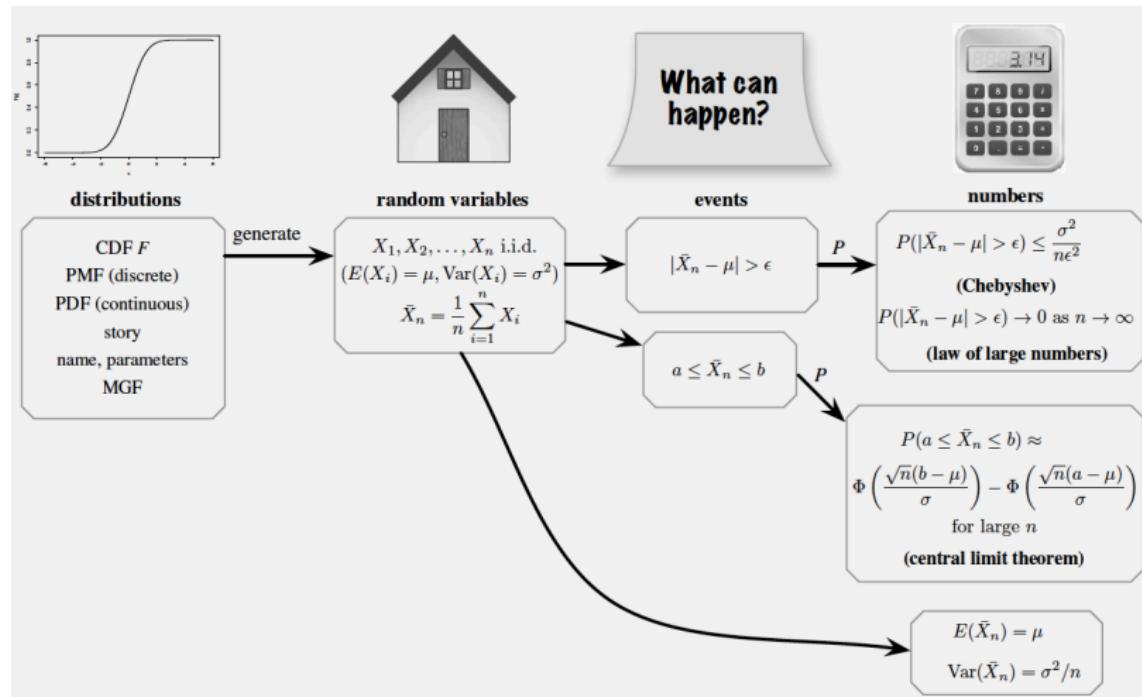
$$\Rightarrow \varepsilon = \sqrt{\frac{8 \ln(\frac{1}{\delta})}{n}}$$

$\delta = 0.05$

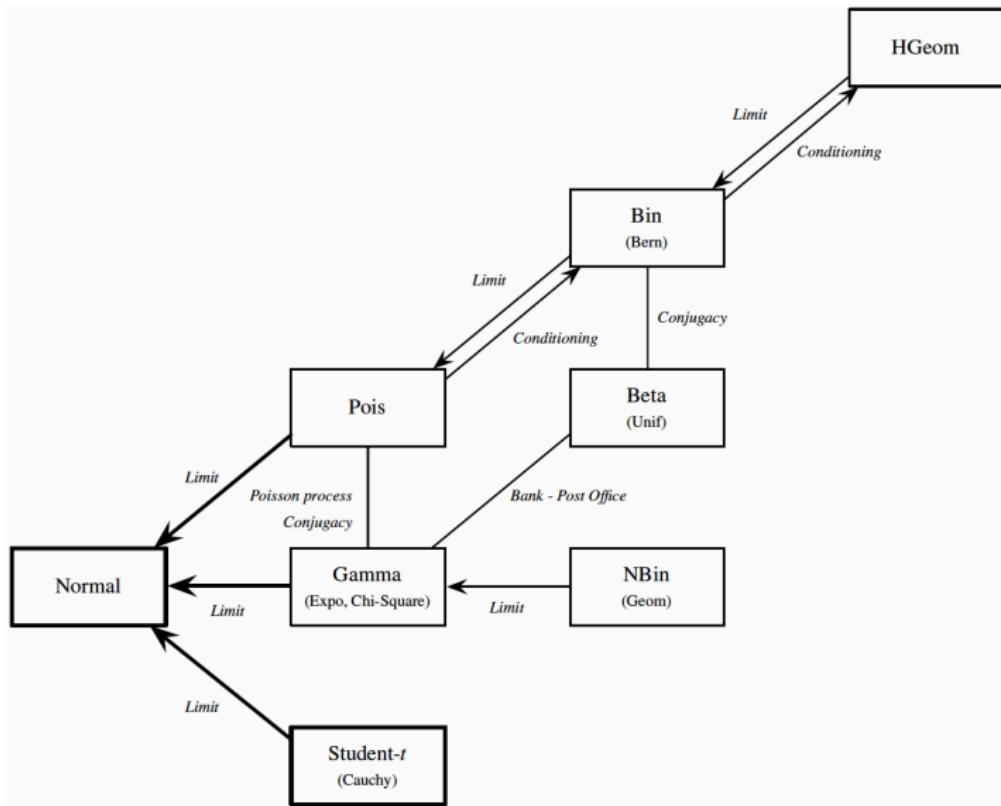
$$\Rightarrow \Pr\left(\pi \in \left(\hat{\pi} - \sqrt{\frac{8 \ln(\frac{1}{\delta})}{n}}, \hat{\pi} + \sqrt{\frac{8 \ln(\frac{1}{\delta})}{n}}\right)\right) \geq 1 - \delta$$

Example: Monte Carlo Method for Estimation π

Summary 1



Summary 2



References

- Chapter 10 of **BH**
- Chapter 5 of **BT**