

統計計算與模擬

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第二單元：隨機變數模擬

<http://csyue.nccu.edu.tw>



以下分配的亂數如何產生？

The 10 examples of Discrete Random Variables are the following;

1. The number of outcomes of tossing a fair coin.
2. The number of students inside the classroom.
3. The number of honors during the school year.
4. The number of covid cases on a daily basis.
5. The number of patients in a ward.
6. The number of vaccine dosages.
7. The number of eggs sold in a day.
8. The number of recoveries from Novel Corona Virus 19 in a week.
9. The number of equations used to solve a problem.
10. The number of items during the examination.

The 10 examples of Continuous Random Variables are the following;

1. The distance from your school to your home.
2. The minimum salary of an employee.
3. The height requirement to become a flight attendant.
4. The minimum weight before obesity.
5. The average grades you during a semester.
6. The amount you invested for the future.
7. The temperature during the wet season.
8. The minimum temperature to store the vaccines.
9. The amount of water that a box can contain.
10. The amount of air pressure in a tank.

常見的隨機變數產生方式

(Random Numbers from certain Distribution)

均勻分配以外的隨機變數通常藉由下列方法，透過均勻亂數產生。

- Inverse Transform Method
- Composition Method
- Rejection (and Acceptance) Method
- Alias Method
- Table Method

註：二維以上變數的模擬也類似，但需要矩陣的輔助，將在下一單元介紹。

Normal Distribution

- 與均勻分配類似，常態分配是最常用到的分配，常見的常態分配亂數產生法：

(Random numbers from normal distribution is one of the popular choices for simulation.)

→ $\sum_{i=1}^{12} U_i - 6$ (僅為近似，only approximation)

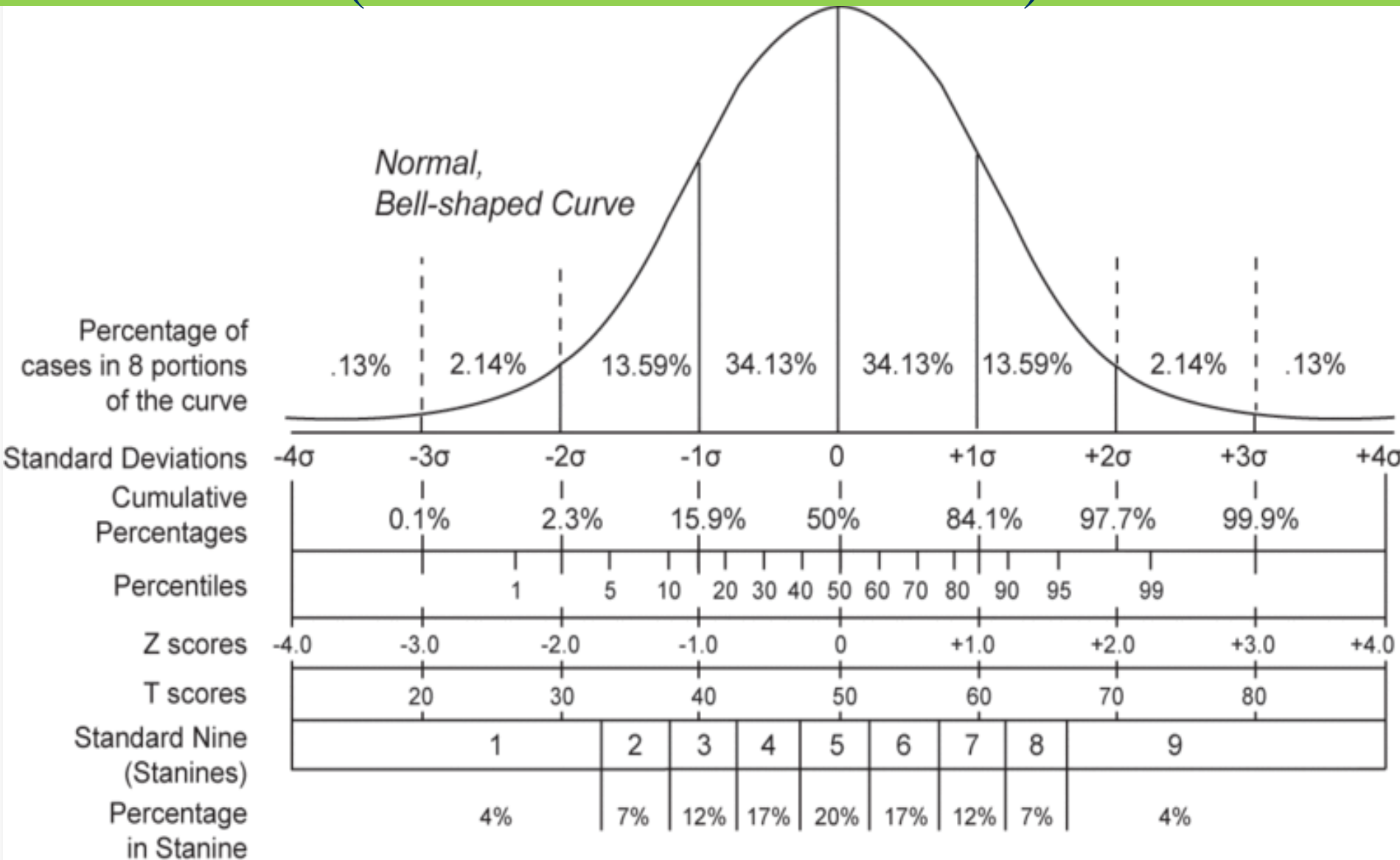
→ Box-Muller

→ Polar

→ Ratio-of-uniforms

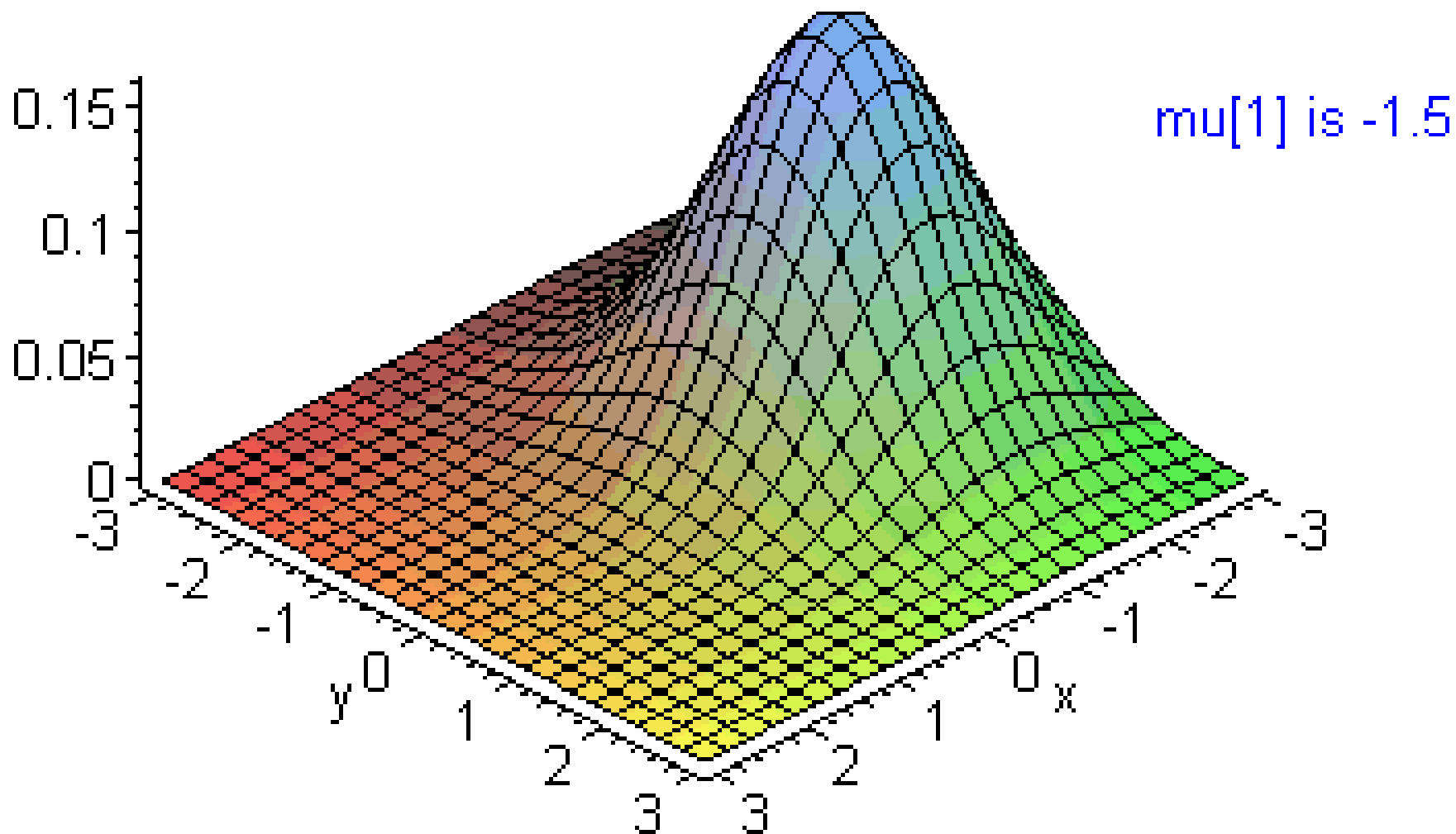
常態分配的重要特性

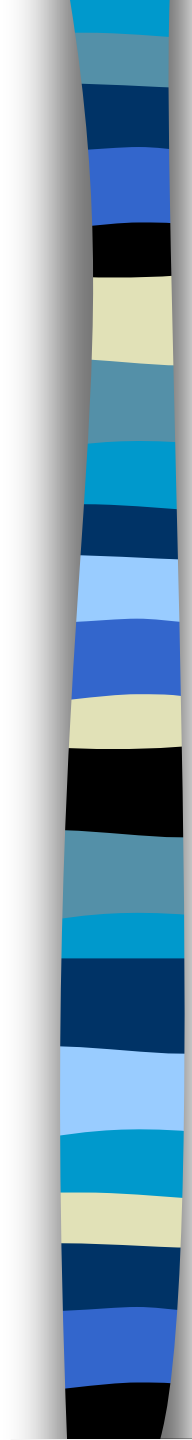
(About normal distribution)



二維與多維常態分配

(Bivariate and Multivariate Normal Distribution)





- $Y = \sum_{i=1}^{12} U_i - 6$ (近似法)

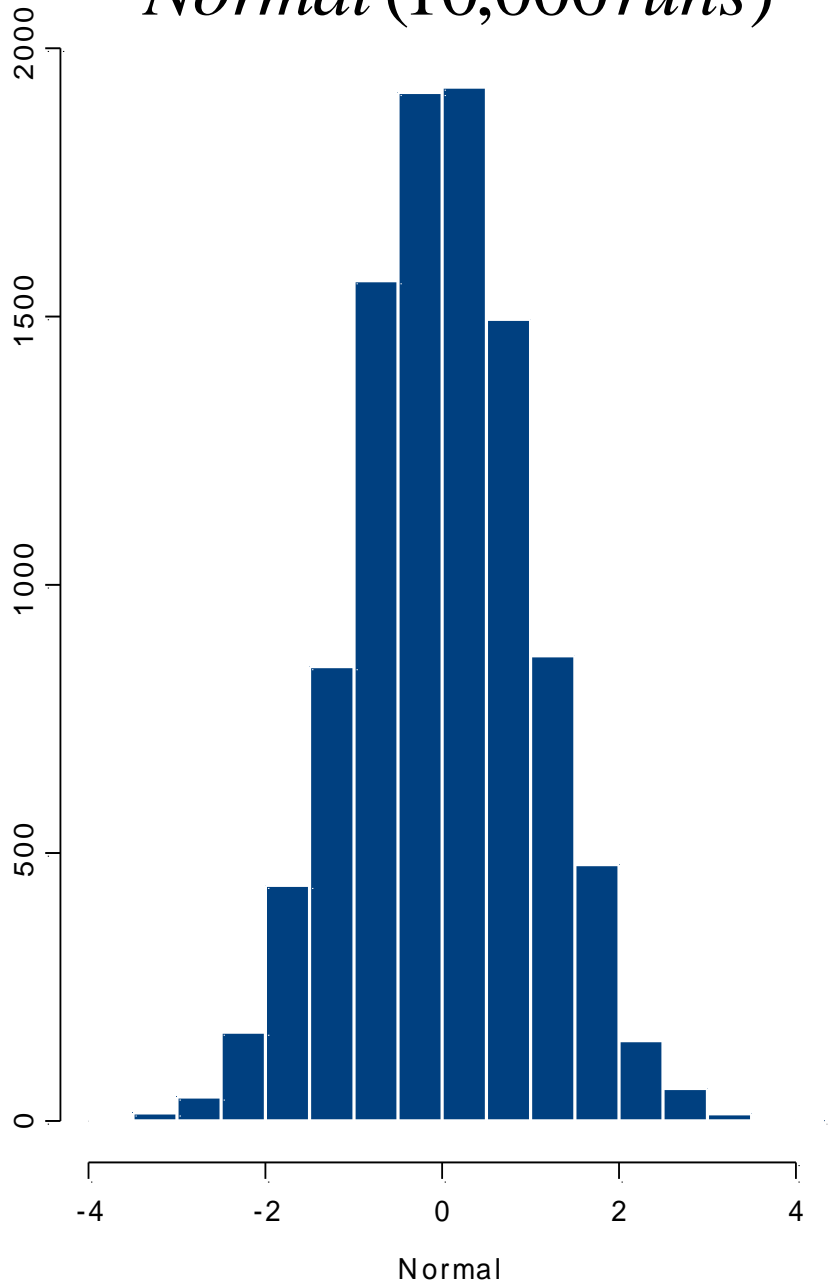
→ 因為 Y 的期望值與變異數等於

$$E(Y) = E\left(\sum_{i=1}^{12} U_i\right) - 6 = 6 - 6 = 0$$

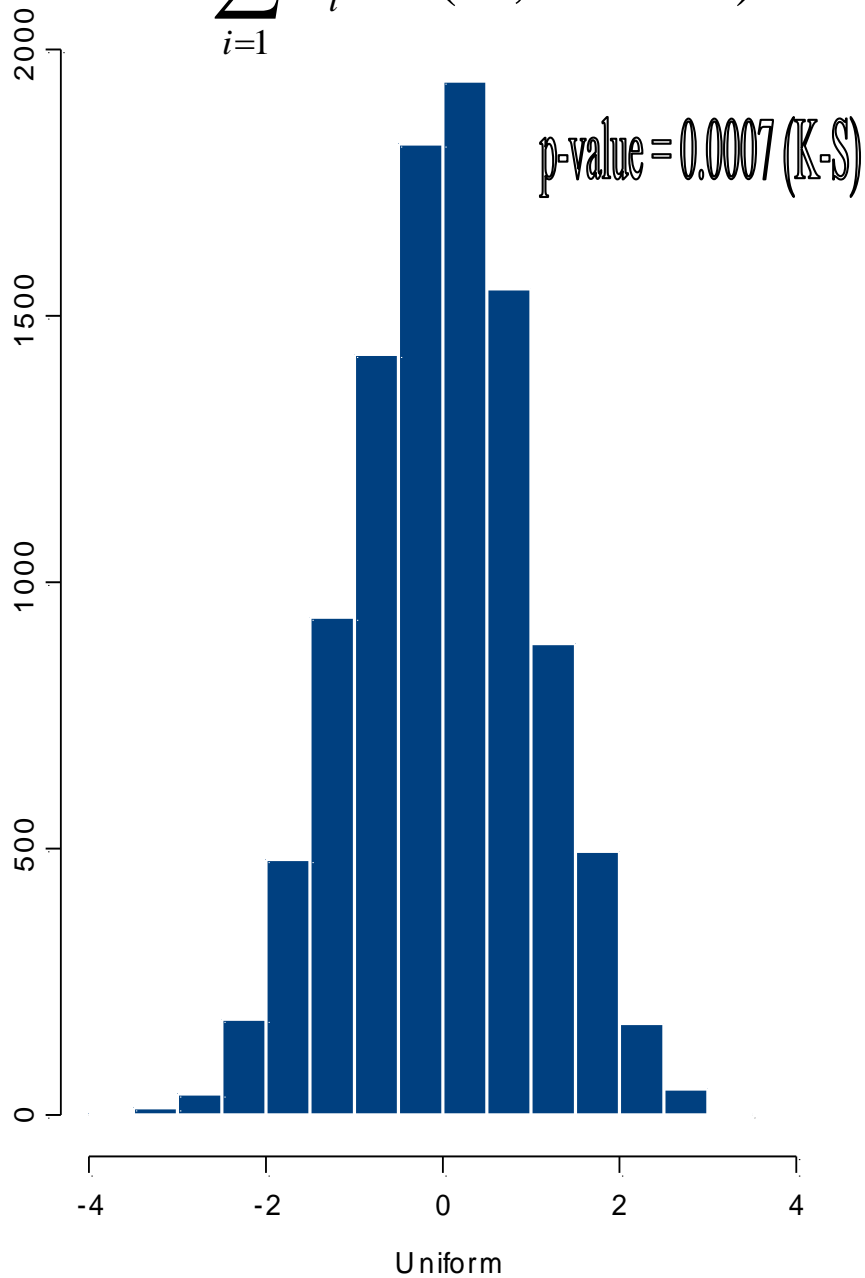
$$Var(Y) = 12 \cdot Var(U_i) = 12 \cdot \frac{1}{12} = 1$$

與標準常態分配相同。

Normal (10,000 runs)



$$\sum_{i=1}^{12} U_i - 6 \text{ (10,000 runs)}$$





- Box and Muller (1958)

→ The best known “exact” method for the normal distribution.

- Algorithm

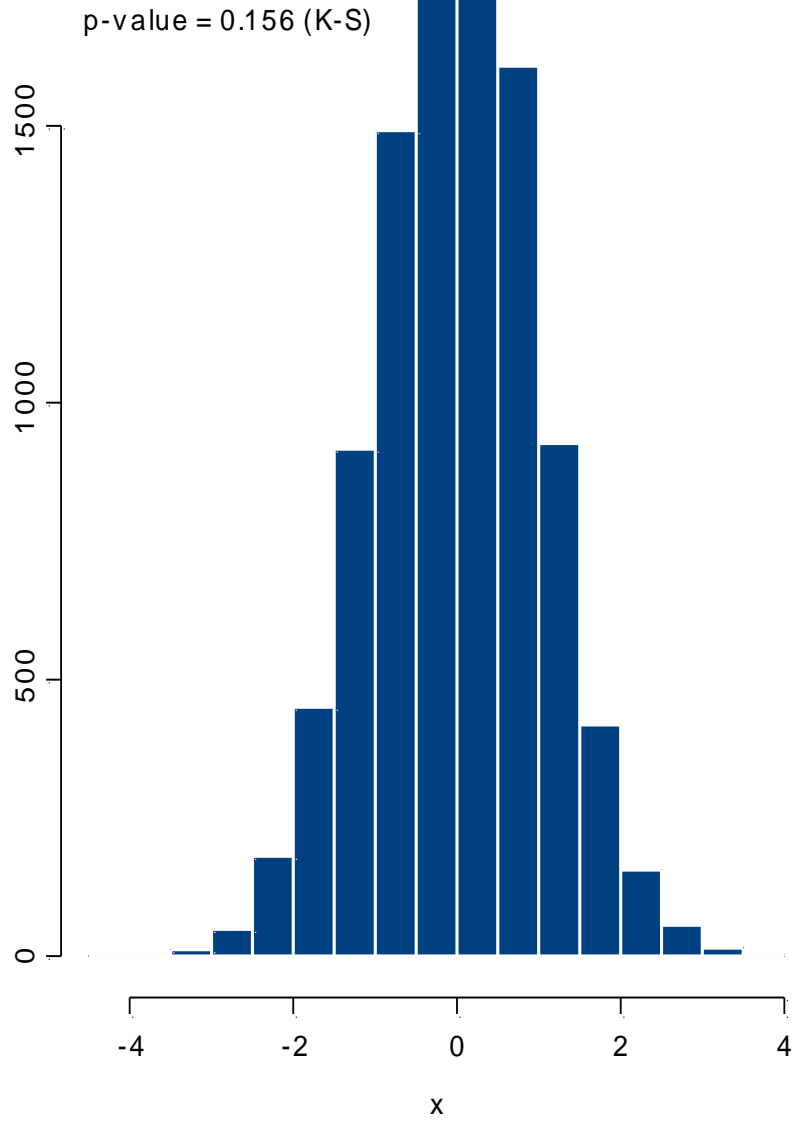
1. Generate $U_1, U_2 \sim U(0,1)$

2. Let $\theta = 2\pi U_1$

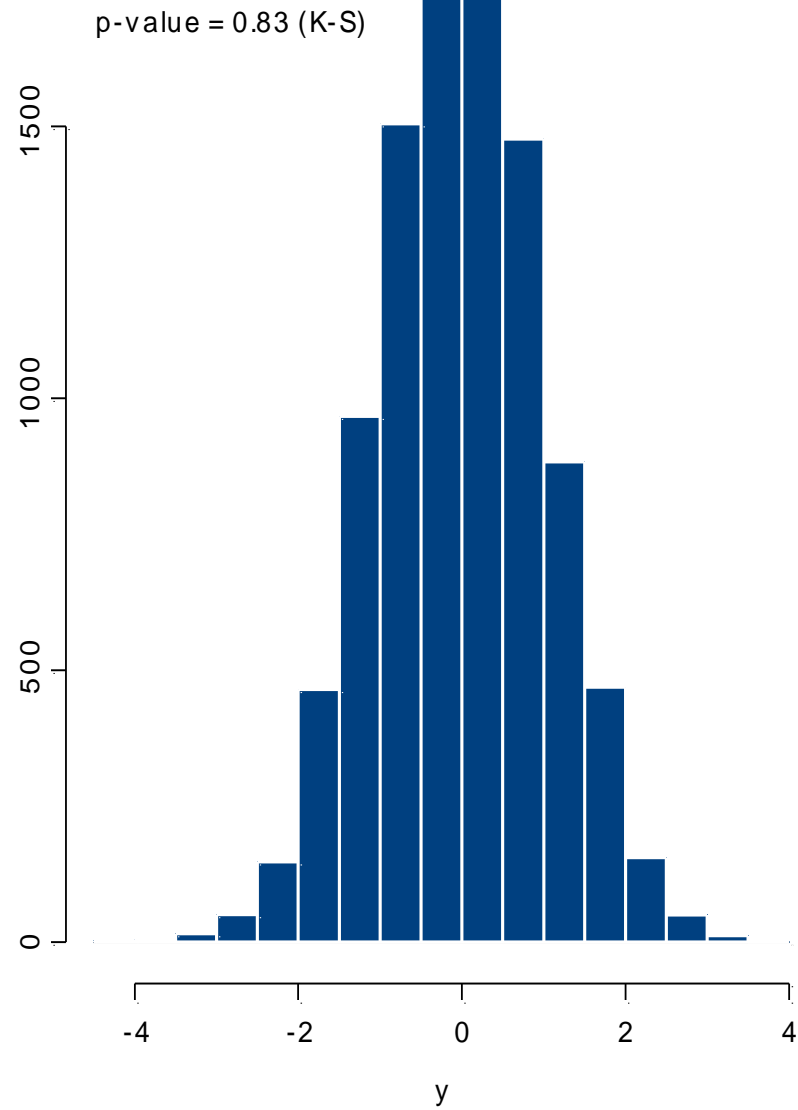
$$E = -\log U_2 \quad \& \quad R = \sqrt{2E}$$

3. Then $X = R \cos \theta$ and $Y = R \sin \theta$ are independent standard normal variables.

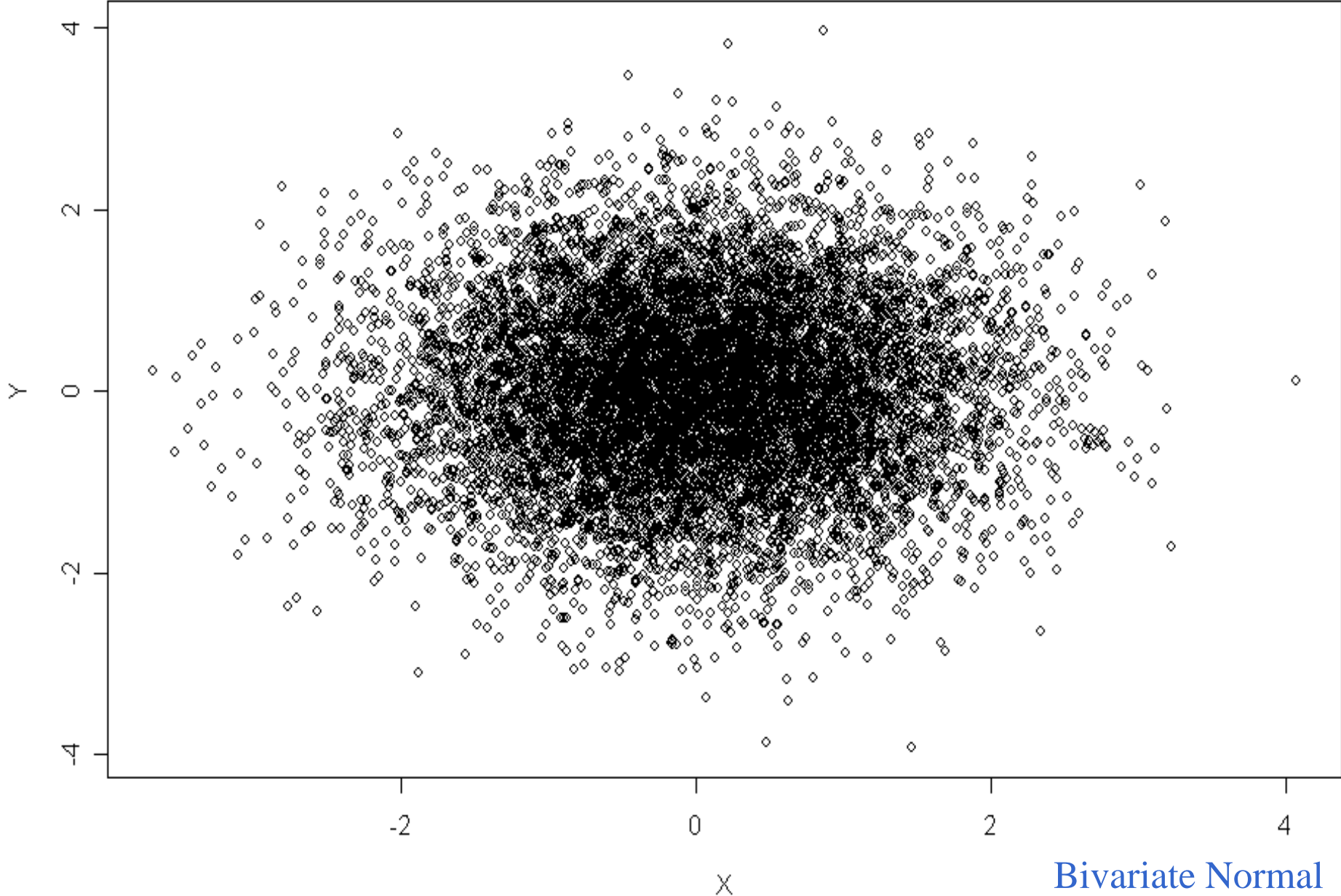
Box-Muller (10,000 runs)



correlation(X,Y)=-0.0039



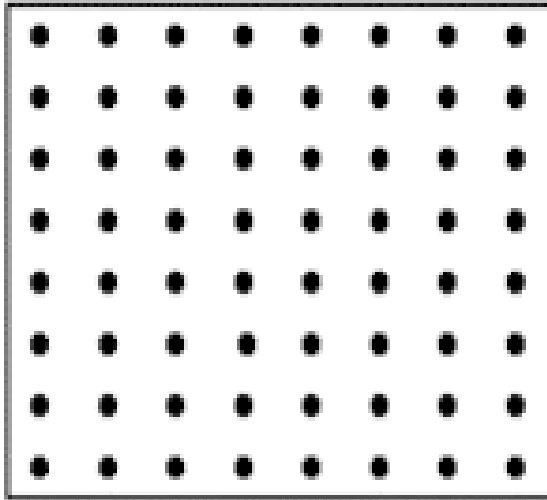
Scatter Plot of Box-Muller



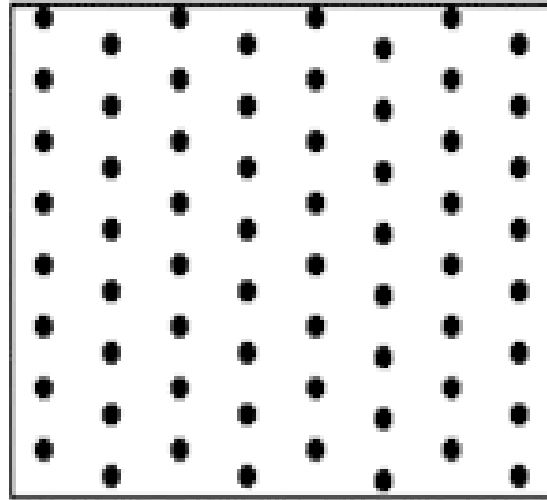
Bivariate Normal

二維觀察值的可能特性

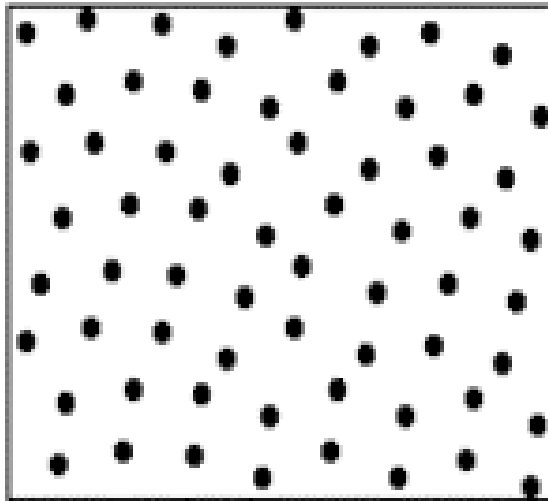
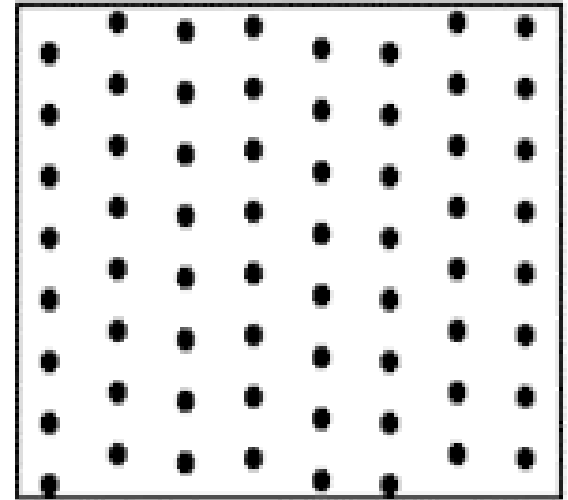
REGULAR



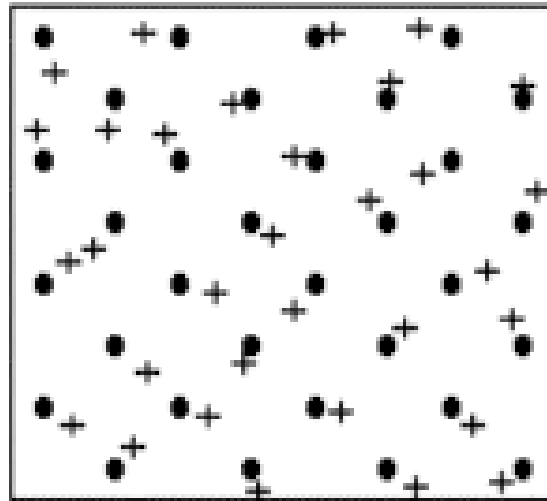
STAGGERED START



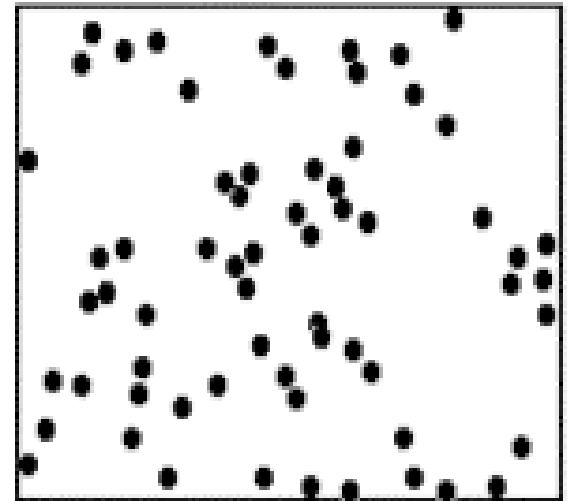
RANDOM START



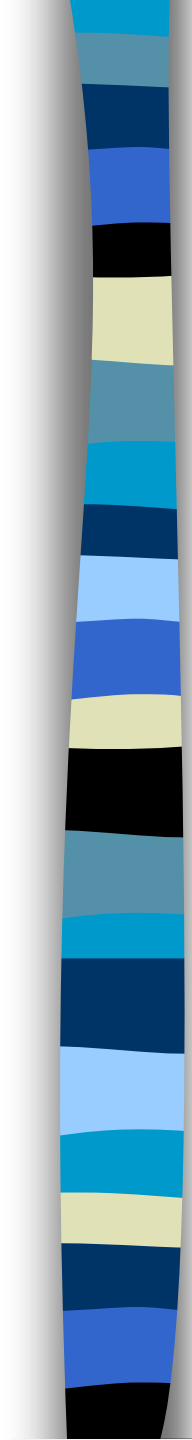
SYSTEMATIC UNALIGNED



RANDOM CLUSTER



SIMPLE RANDOM

- 
- Note: Using Box-Muller method with congruential generators must be careful. It is found by several researchers that

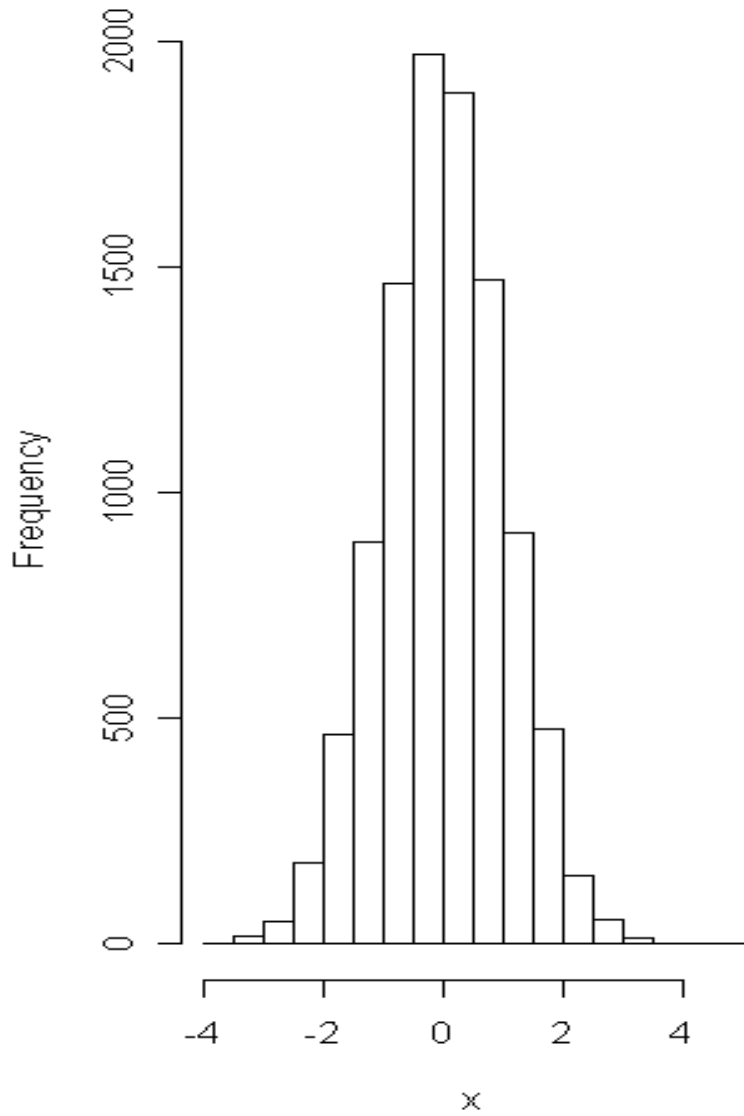
$$a \text{ (乘數)} = 131$$

$$c \text{ (增量)} = 0$$

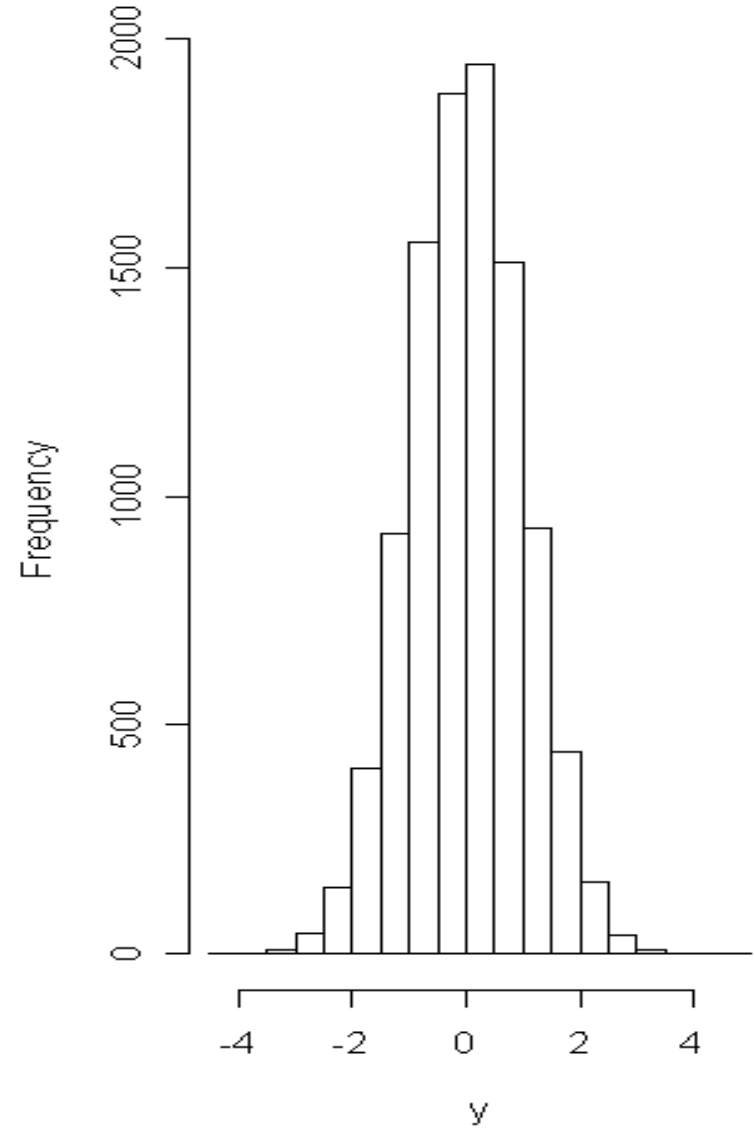
$$m \text{ (除數)} = 2^{35}$$

would have $X \in (-3.3, 3.6)$. See Neave (1973) and Ripley (1987, p.55) for further information.

a=131, c=0, m=2³⁵



Box-Muller



I use 123,456 and 3,456 as seeds but did not find problems.



- Polar Method (recommended!)

→ Rejection method for generating two independent normal variables.

- Algorithm

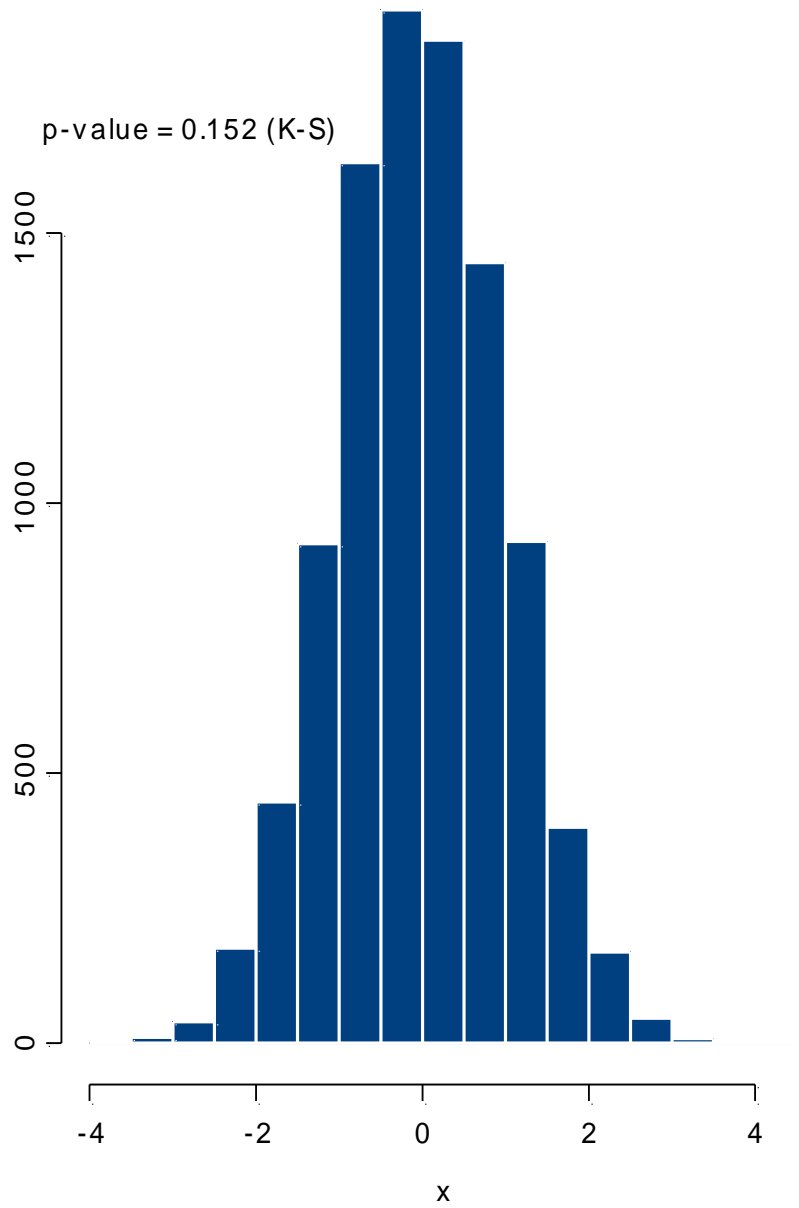
1. Generate $V_1, V_2 \sim U(-1, 1)$

retain if $W = V_1^2 + V_2^2 < 1$

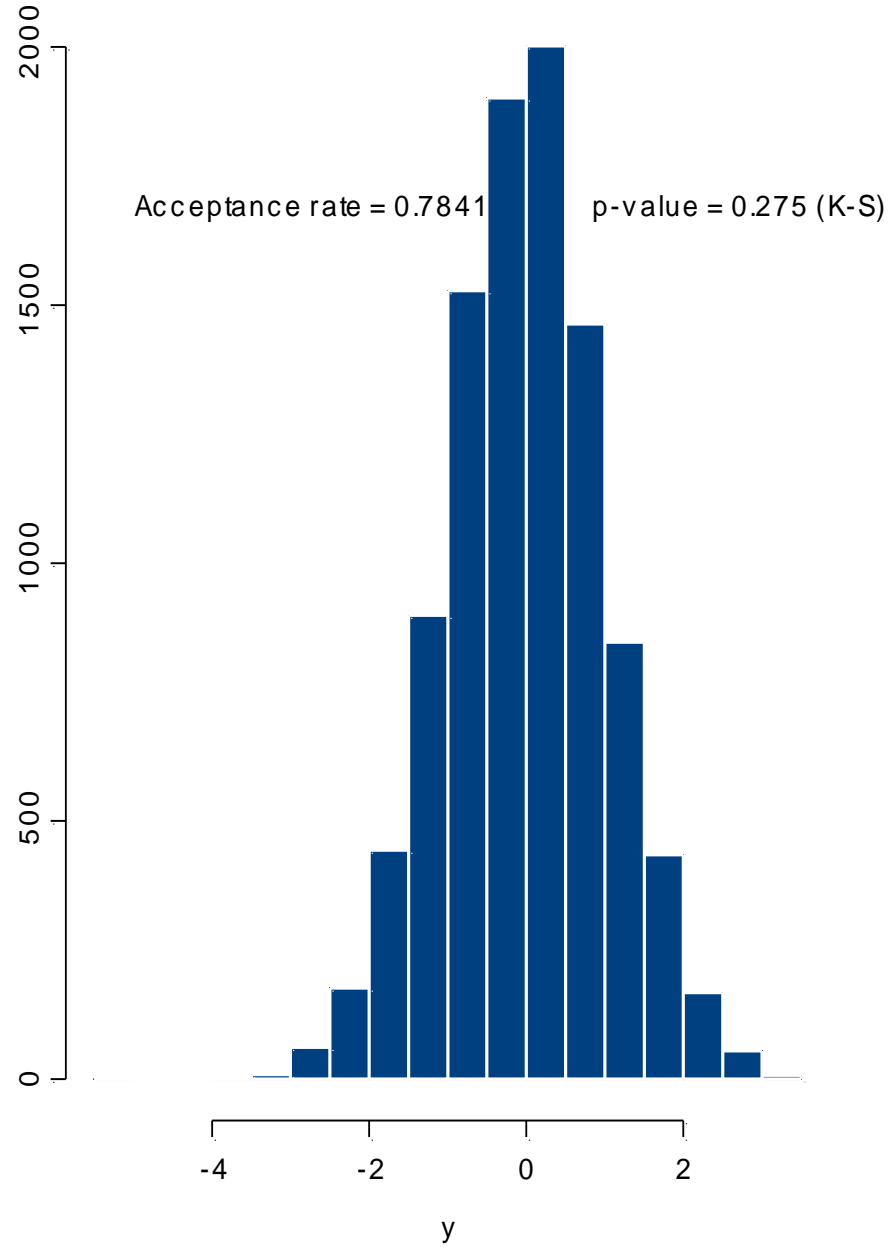
2. Let $C = \sqrt{-2W^{-1} \log W}$

3. Then $X = CV_1$ and $Y = CV_2$ are independent standard normal variables.

Polar method (10,000 runs)



Correlation(X,Y)=0.0087





- Ratio-of-uniforms (recommended!)

→ Similar to Polar method, Ratio-of-uniforms is a rejection method.

- Algorithm

1. Generate $U_1, U_2 \sim U(0, 1)$,

and let $V = \sqrt{2/e} (2U_2 - 1)$

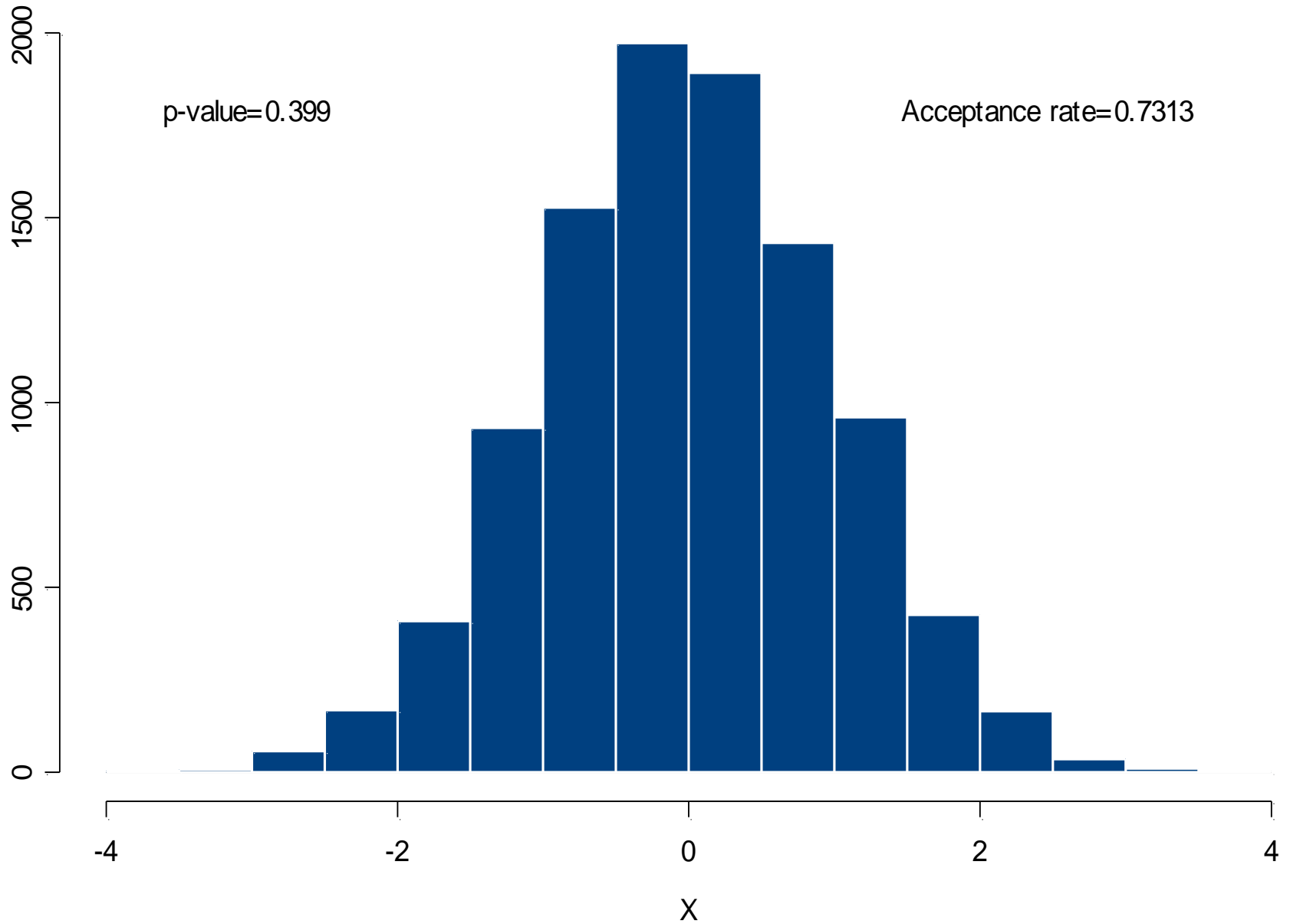
2. Let $X = V / U_1$, $Z = X^2/4$

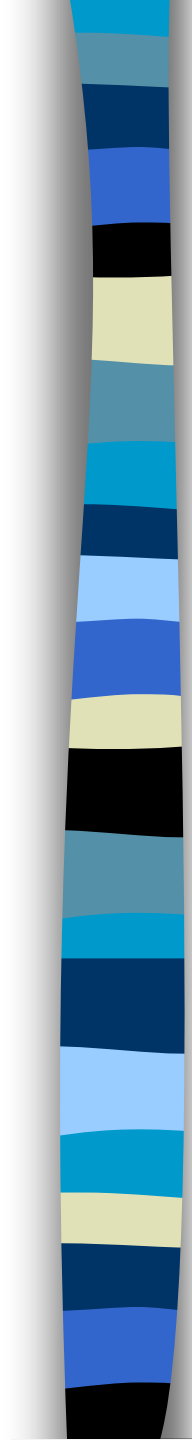
3. Retain if $Z < 1 - U_1$ → Suggest deleting this step!

4. Retain if $Z \leq 0.259 / U_1 + 0.35$ & $Z \leq -\log U_1$

5. Then X is normally distributed.

Ratio-of-uniforms (10,000 runs)





■ 問題：隨機變數有不同產生方法時，你/妳會選擇哪一種？(Choices of Generation)

(有哪些判斷標準可供參考？)

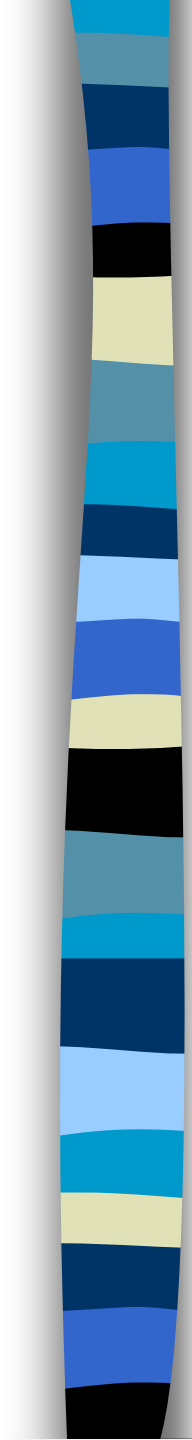
→ 產生效率(e.g.成功接受率)？

→ 方法的複雜/方便程度？

→ 方法是否有瑕疵？(例如：與線性同餘法配合時是否有瑕疵？)

→ 取得的方便/廣為接受的方法？

→ 如何綜合判斷及考量？



■ 是否有需要開發新的隨機變數產生方法？

→ 除非有特別需求(例如：學術研究、軟體配合等)，或是目標的隨機變數較為特殊，建議採用已經廣為大家認可的方法，可省卻驗證方法是否有效，也較不易遭受質疑。

註：如果其他軟體可以產生需要的變數，或者直接由該軟體輸出亂數，或者參考該軟體產生亂數的語法。(但可能會遭遇問題！)



- Ratio of Uniform (Cauchy Distribution)

→ Ratio-of-uniforms can also be used to create random variables from Cauchy Distribution.

- Algorithm

1. Generate $U_1, U_2 \sim U(0,1)$, and $V = 2U_2 - 1$
retain if $U_1^2 + V^2 < 1$.

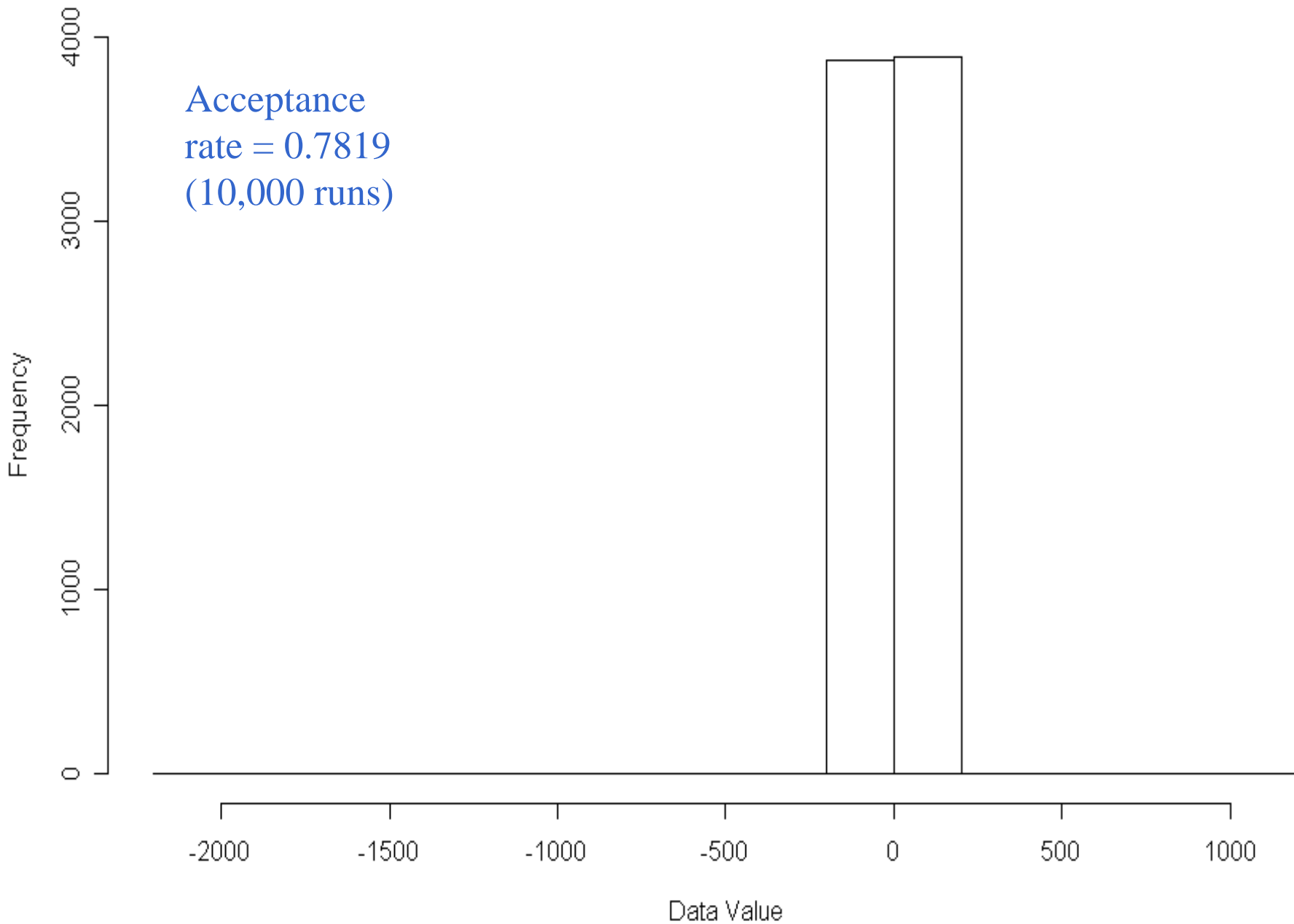
2. Then $X = V / U_1 \sim \text{Cauchy}(0,1)$, i.e.

$$f(x) = \frac{1}{\pi} \frac{1}{1+x^2}.$$

e.g. 10,000 runs → p-value=0.9559

(Acceptance rate = 0.7819)

Histogram of Ratio-of-Uniform (Cauchy)



Acceptance
rate = 0.7819
(10,000 runs)

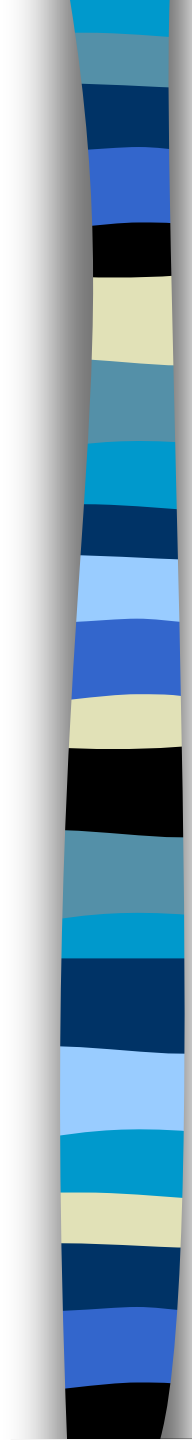


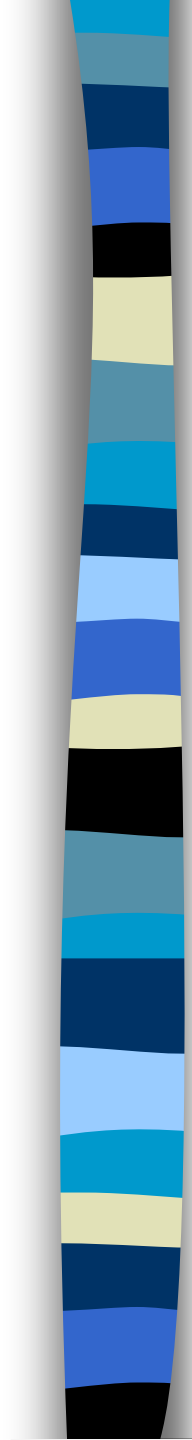
Inverse Transformation Method

Generates a random number from a probability density function by solving the probability.

Density function's variable in terms of randomly generated numbers. This is achieved as follows:

- We solve the inverse of the integral of our probability density function at an arbitrary point $F(a)$, in terms of a random number r .
- We generate a unique random variable a , as follows: $a = F^{-1}(r)$. The foundation of this method is $F(X) \sim U(0,1)$ for all X .

- 
- Note: Usually, we only use Inversion to create simpler r.v.'s, such as exponential distribution (i.e. $Exp(\lambda) \equiv -\lambda \log(U(0,1))$). Although Inversion is a universal method, it may be too slow (unless subprograms to calculate F^{-1} are available).
 - In other words, although theoretically it is possible to create any r.v.'s, usually there are simpler methods.



■ Example 1. $F(x) = x^2, 0 < x < 1 \rightarrow X = U^{1/2}$.

■ Example 2. Let $X_1, X_2, \dots, X_n \stackrel{i.i.d.}{\sim} F(x)$

and we want to generate the minimum and maximum of X 's.

\rightarrow Since $Y_n = \max(X_1, \dots, X_n)$ & $Y_1 = \min(X_1, \dots, X_n)$
which means $F_{y_n}(y) = [F(y)]^n$ & $F_{y_1}(y) = 1 - [1 - F(y)]^n$,
we can generate these two r.v.'s by

$$Y_n = F^{-1}(U^{1/n}) \text{ \& } Y_1 = F^{-1}(1 - U^{1/n}).$$

Or, $Y_n = U^{1/n}$ & $Y_1 = 1 - U^{1/n}$ if $X \sim U(0,1)$.

- 
- Example 3. Generate $X \sim \text{Poisson}(\lambda)$, i.e.

$$F(i-1) = P(X \leq i-1) < u \leq P(X \leq i) = F(i),$$

where $i \in \{0, 1, 2, \dots\}$.

- Algorithm:

1. Generate $U_1 \sim U(0,1)$ and let $i = 0$.

2. If $U_1 \geq F(i)$, let $i = i + 1$;

Otherwise $X = i$.

Note: This method can be used to generate any discrete distributions.



Notes:

- (1) If total number of classes ≥ 30 , we start from the middle (or mode).
- (2) The expected number of trials is $E(X)+1$.
- (3) We can use “*Indexed Search*” to increase the efficiency:

→ Fix m , let $q_j = \min\{i \mid F(i) \geq \frac{j}{m}\}$, $j = 0, \dots, m-1$

Step 1. Generate $U \sim U(0,1)$, let $k = [mU]$ & $i = q_k$

Step 2. If $U \geq F(i)$, let $i = i + 1$;

Otherwise $X = i$.



■ Example 4. $X \sim \text{Poisson}(10)$

- (1) Usual method: 11 comparisons on average
- (2) Mode: Reduced to about 3.54 comparisons
- (3) Indexed search: we choose $m = 5$, i.e.

$$q_0 = 0, q_1 = 7, q_2 = 9, q_3 = 11, q_4 = 13.$$

Under 10,000 simulation runs (S-Plus), I found that one check on the table plus 2.346 comparisons \rightarrow 3.346

(Comparing to 3.3 in Ripley's book)



Composition Method

- We can generate complex distribution from simpler distributions, i.e.

$$F(x) = \sum_{i=1}^m \alpha_i F_i(x),$$

where $F_i(x)$ are d.f. of other variables.

→ Or, from a conditional distribution,

$$f(x) = \sum_i p_i g(x | y = i)$$

$$f(x) = \int g(x | y) dF_Y(y).$$

- 
- Example 1. To simulate x , where

$$P(x = i) = \begin{cases} 0.05, & i = 1, 2, 3, 4, 5 \\ 0.15, & i = 6, 7, 8, 9, 10 \end{cases}$$

We independently generate $x_1 \in U\{1, 2, \dots, 10\}$ and $x_2 \in U\{6, 7, \dots, 10\}$. Let $X = X_1$ or X_2 with probability 0.5.

- Example 2. $X \sim B(5, 0.2)$

→ Sampling on each digit:

$$P(X = i) = \begin{cases} 0.3277, & i = 0 \\ 0.4096, & i = 1 \\ 0.2048, & i = 2 \\ 0.0512, & i = 3 \\ 0.0064, & i = 4 \\ 0.0003, & i = 5 \end{cases}$$



- Table method: (Composition)

Example 1. $X \sim B(3, 1/3)$

	位置	10^{-1}	10^{-2}	10^{-3}
$P(X=0)=0.296$		2	9	6
$P(X=1)=0.445$		4	4	5
$P(X=2)=0.222$		2	2	2
$P(X=3)=0.037$		0	3	7
	總數	8	18	20



■ Algorithm:

1. Generate $U \sim U(0,1)$

2. If $0 \leq U < 0.8$, let $I = [10U] + 1$, $X = a_1[I]$

$0.8 \leq U < 0.98$, let $I = [100U] - 80 + 1$, $X = a_2[I]$

$0.98 \leq U$, let $I = [1000U] - 980 + 1$, $X = a_3[I]$

其中

$$a_1[.] = 00 \ 1111 \ 22$$

$$a_2[.] = 0000000000 \ 1111 \ 22 \ 333$$

$$a_3[.] = 00000 \ 11111 \ 22 \ 33333333$$

- Example 3. Generate an r.v. X from

$$f(x) = n \int_1^{\infty} y^{-n} e^{-xy} dy, \quad 0 < x < \infty,$$

where $dF_Y(y) = \frac{n dy}{y^{n+1}}, 1 < y < \infty, n \geq 1.$

- Algorithm:

1. Generate U_1, U_2 from $U(0,1)$
2. Let $Y \leftarrow (U_1)^{-1/n}$
3. Return $X \leftarrow -\log(U_2)/y$

Note: $dF_Y(y) = \frac{n dy}{y^{n+1}} \Rightarrow F_Y(y) = \frac{1}{y^n} \sim U(0,1).$

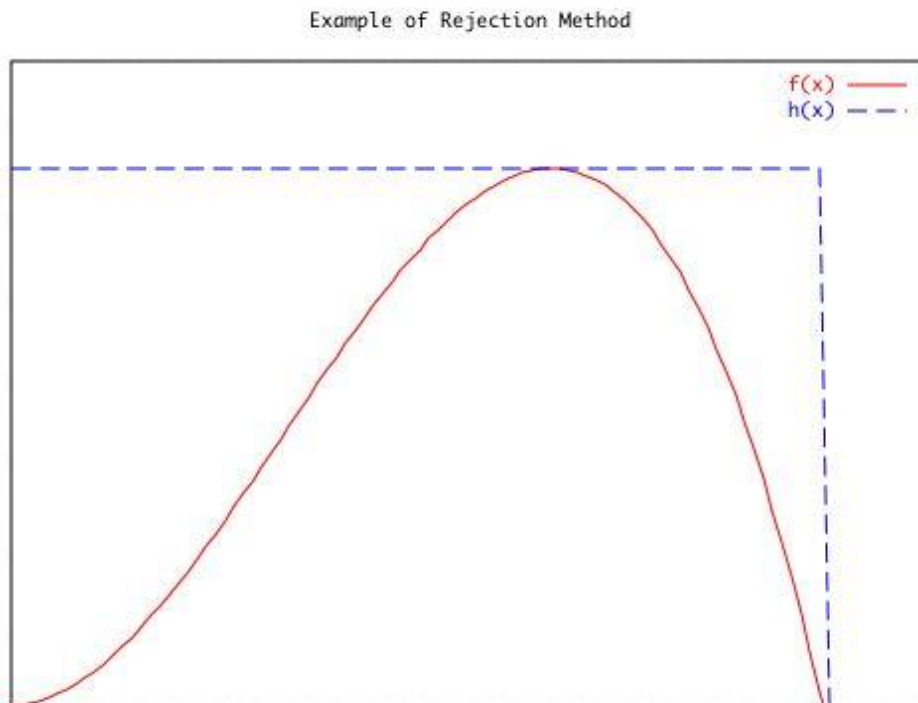


Rejection Method

Generates random numbers for a distribution function $f(x)$. This is achieved as follows:

- Define a comparison function $h(x)$ such that it encloses the desired function $f(x)$.
- Choose uniformly distributed random points under $h(x)$.
- If a point lies outside the area under $f(x)$ reject it and choose another point.

Illustration of the Rejection Method



The following is an illustration of the rejection method using a square function for the comparison function.

- Example 1. $X \sim \text{Beta}(2,4)$, i.e. $E(X)=1/3$,

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

Then we use $g(x)=1$, $0 < x < 1$ as “envelop” to create $f(x)$.

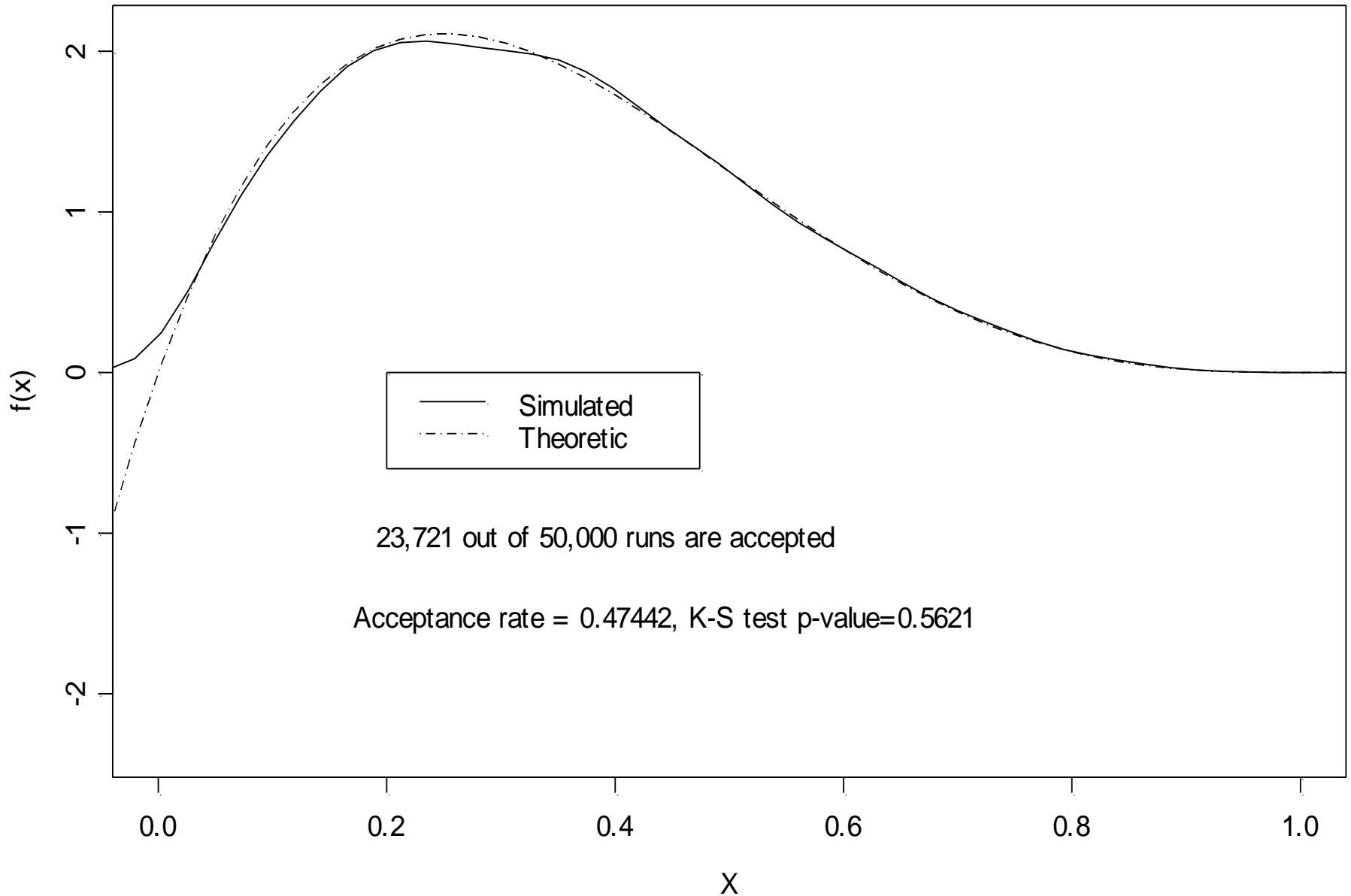
Note: $\frac{f(x)}{g(x)} = 20x(1-x)^3 \leq \frac{135}{64} = C \approx (0.4741)^{-1}$.

- Algorithm:

1. Generate $X, U_1 \sim U(0,1)$.

2. If $U_1 \leq \frac{f(x)}{C \cdot g(x)}$ return $Y = X$. (Q: Rejection rate?)

Theoretic and simulated $f(x)$'s for Beta(2,4)



- Example 2. Generate $\text{Gamma}(3/2, 1)$, i.e.

$$f(x) = \frac{2}{\sqrt{\pi}} x^{\frac{1}{2}} e^{-x}, x > 0.$$

We want to generate X from $g(x) = \frac{2}{3} e^{-2x/3}$.

The max. of $f(x)/g(x)$ is obtained when

$$\frac{1}{2} x^{-1/2} e^{-x/3} = \frac{1}{3} x^{1/2} e^{-x/3} \Rightarrow x = \frac{3}{2},$$

since $\frac{f(x)}{g(x)} = \frac{3}{\sqrt{\pi}} x^{1/2} e^{-x/3}$.

$$\therefore C = \frac{3}{\sqrt{\pi}} \left(\frac{3}{2}\right)^{1/2} e^{-1/2} = \frac{3\sqrt{3}}{\sqrt{2\pi e}} \cong 1.257317.$$



■ Algorithm:

1. Generate $U, U_1 \sim U(0,1)$

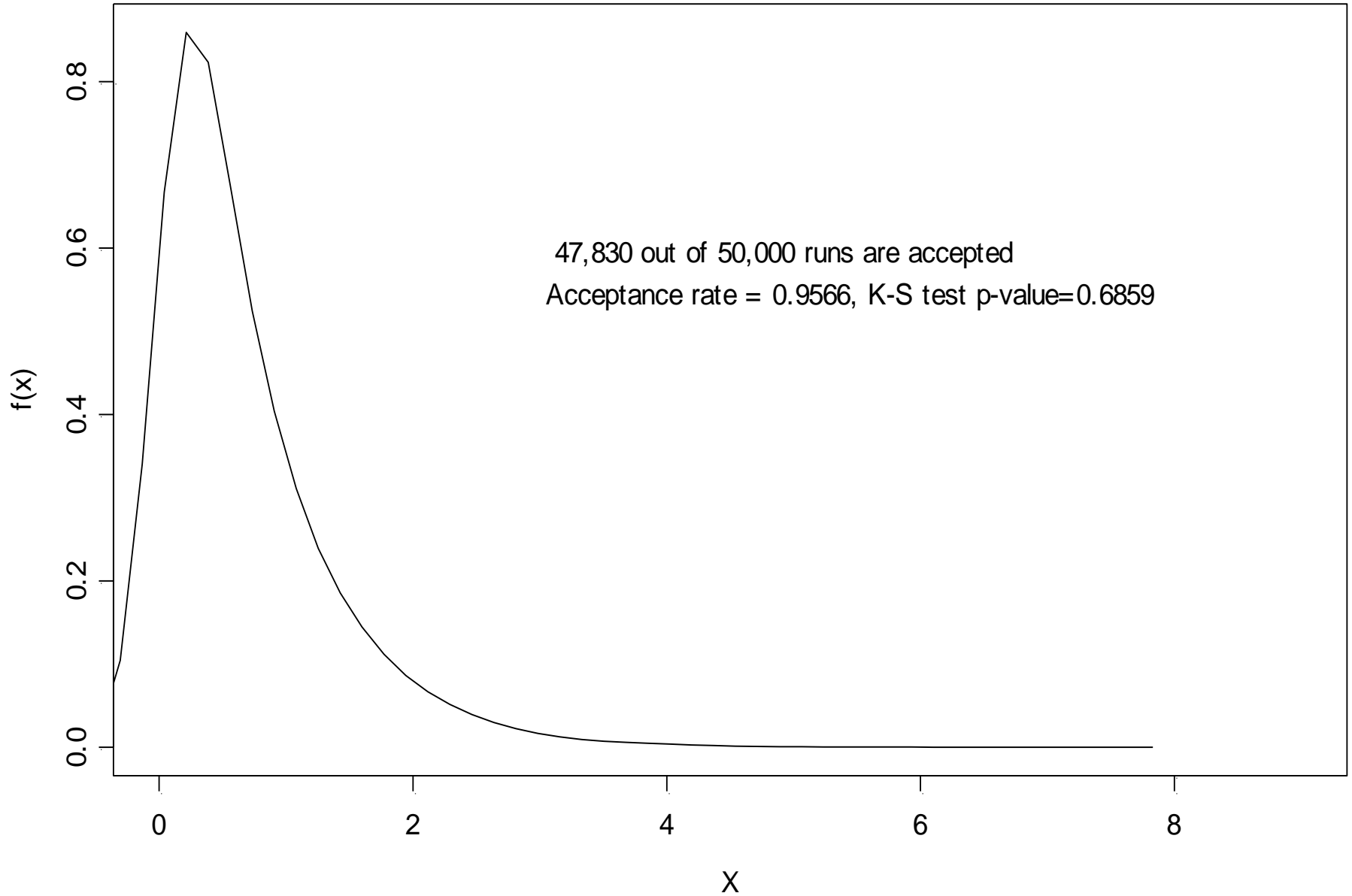
Let $X = -3 \log U / 2$.

2. Return $Y = X$ if $U_1 \leq \frac{f(y)}{C \cdot g(y)}$.

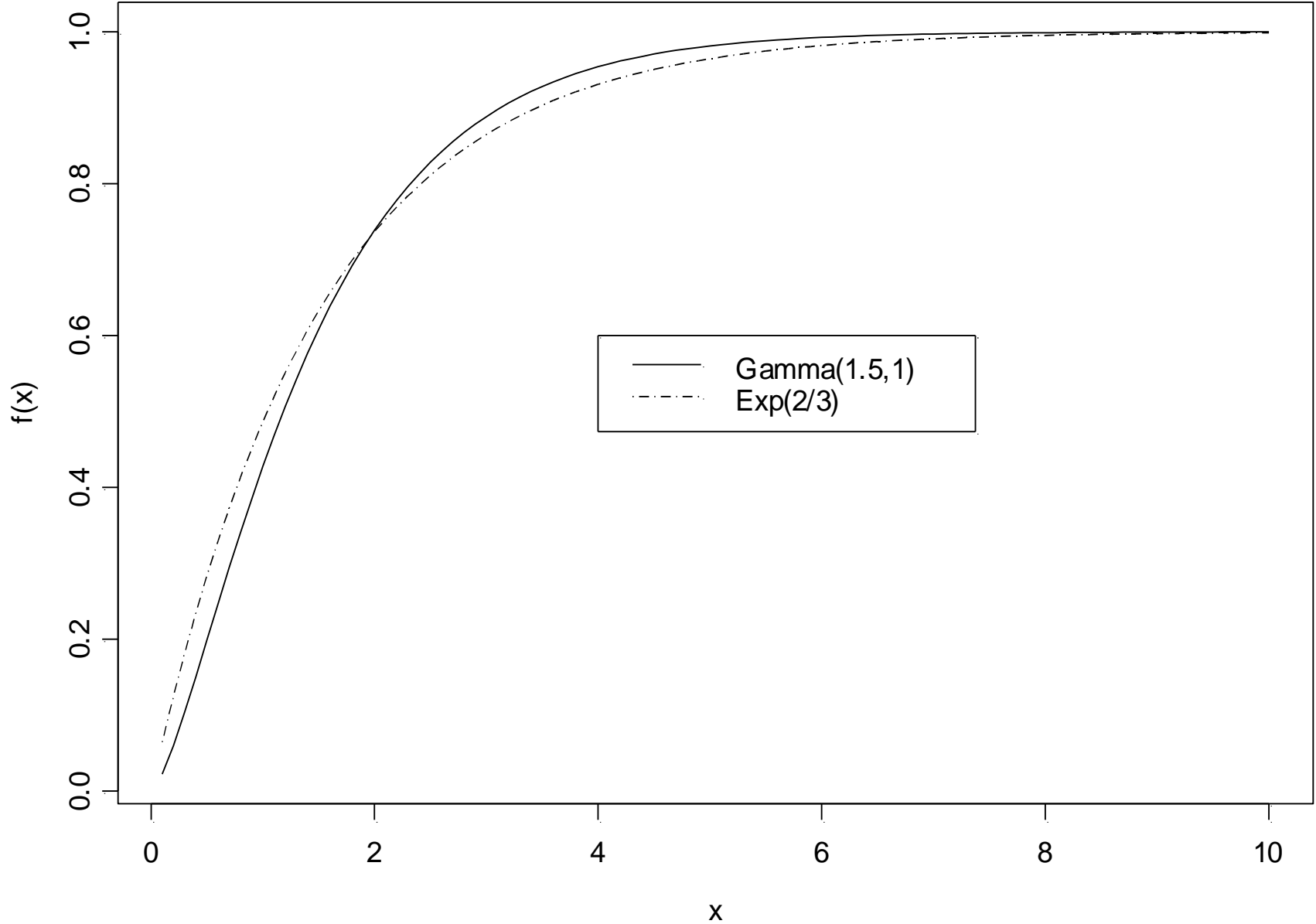
■ Question: Why do we choose $Y \sim \text{Exp}(2/3)$?

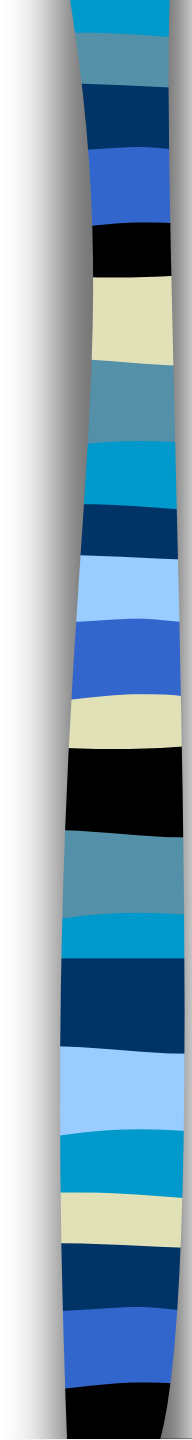
→ $\text{Gamma}(3/2, 1)$ and $\text{Exp}(2/3)$ have the same mean!

Simulated $f(x)$'s for Gamma(3/2, 1)



Density functions of Gamma(1.5,1) and Exp(2/3)



- 
- Alias method: Looks like “rejection” but it is indeed “composition”.
 - Example 1. $X \sim B(3, 1/3)$, i.e.

$$P(X = i) = \frac{8}{27}, \frac{12}{27}, \frac{6}{27}, \frac{1}{27} \text{ for } i = 0, 1, 2, 3.$$

$$P(X = 0) = \frac{1}{4} + \left[\frac{2/27}{4} + \frac{3/27}{4} \right] = \frac{32}{108};$$

$$P(X = 1) = \frac{25}{108} + \left[\frac{23/27}{4} \right] = \frac{48}{108};$$

$$P(X = 2) = \frac{24}{108};$$

$$P(X = 3) = \frac{4}{108}.$$

	<u>0</u> <u>1</u> <u>2</u> <u>3</u>		<u>0</u> <u>1</u> <u>2</u> <u>3</u>
108a	32 48 24 4		32 25 24 4
A	- - - -		- - - 1
27Q	27 27 27 27	→	27 27 27 27
Ind.	T T T T		T T T F
	Move 1-4/27=23/27		Move 1-24/27=3/27

	<u>0</u> <u>1</u> <u>2</u> <u>3</u>		<u>0</u> <u>1</u> <u>2</u> <u>3</u>
	29 25 24 4		27 25 24 4
	- - 0 1		- 0 0 1
→	27 27 27 27	→	27 27 27 27
	T T F F		T F F F

Move 1-25/27=2/27