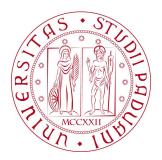
Random Numbers and Variable Generation

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Why Random Numbers?

- random numbers are commonly used for
- simulation of physical systems involving stochastic variables. Several simulations of physical or real systems (e.g. passage of ionizing particles through matter, hospital acceptance system simulation) need random variables
- > sampling: to study and/or use different probability distributions
- numerical analysis: different techniques involving random numbers are employed to solve problems with numerical techniques (from simple to complex ones)
- computer programming : random numbers are often used in current computer programs
- decision making
- games theory

Random Number Generation

Historical excursus

- ▶ early times: manual techniques used. Es. coin flipping, dice rolling, card shuffling.
- → in 1995, RAND Corporation published a list of 1 Million random numbers obtained with mechanical methods
- ▶ later on : physical devices: noise diodes, Geiger counters
- computer era : simple algorithms on a computing element.
- → They are not based on a specific physical device. Run fast, require little storage, and they can reproduce a given sequence of random numbers

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The Middle-Square Method

 the first to suggest an algorithm for random number generation was John von Neumann back in 1946

Algorithm

- 1 take a number with a large number of digits, for instance 10, and square it
- 2 extract the 10 central digits
- 3 repeat the sequence from 1

Q&A

- Q: the generated sequence is not randomly generated, since each number is determined by its predecessor. Why it is called random?
- A: Yes, but it seems random, Therefore it is called *pseudo-random*

The Linear Congruential Generator (LCG)

- it was the most popular. Introduced by D. H. Lehmer in 1949
- it allows to generate a random sequence $\{X_n\}$ using

$$X_{n+1} = (aX_n + C) \mod m$$

- where

0 < a < m : multiplier 0 < C < m : increment

 $0 < X_{\circ} < m$: seed. i.e. starting point m > 0 : modulus

Example

let's consider the following generator

$$X_{n+1} = (7 \cdot X_n + 7)$$
 modulus 10

• starting with $X_{\circ} = 7$, we get

$${X_n} = {7,6,9,0,7,6,9,0,\ldots}$$

the sequence repeats, with a 4 elements cycle

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LCG parameters and examples

- to get an useful sequence we need a large cycle
- several parameters have been studied (many papers in literature)
- from a Theorem (see D. Knuth, The Art of Computer Programming, vol 2, semi-numerical algorithms, Addison Wesley 1981, ISBN 0-201-03822-6)
- the LCG period is at most *m* if and only if
- i) c is relatively prime to m
- ii) a 1 is multiple of p, for every prime p dividing m
- iii) a-1 is a multiple of 4, if m is a multiple of 4

Source	m	а	С
Numerical Recipes	2 ³²	1664525	1013904223
Borland C/C++	2 ³²	22695477	1
glibc	2 ³²	1103515245	12345
ANSI C	2 ³²	1103515245	12345
Borland Delphi, Virtual Pascal	2 ³²	134775813	1
Microsoft Visual/Quick C/C++	2 ³²	214013	2531011
Apple CarbonLib	$2^{31} - 1$	16807	0
MMIX (D. Knuth)	2 ⁶⁴	6364136223846793005	1442695040888963407

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LCG in R

- let's consider the LCG: $X_{n+1} = (137 \cdot X_n + 187) \mod 2^8 = 256$
- when we plot the points (X_{i+1}, X_i)
- we find out that the points do not fill up the whole space, but they lay on selected lines
- the distance between the lines is $\sqrt{m}/m = 16/256 = 1/16 = 0.625$

```
lcg.user <- function(nsample=100, seed=1) {</pre>
                                                       0
    rand <- vector(length = nsample)</pre>
    m <- 256; a <- 137; c <- 187
    d <- seed
                                                       ω
    for (i in 1:nsample) {
       d < - (a * d + c) \% m
       rand[i] \leftarrow d / m
    return(rand)
  }
  u \leftarrow lcg.user(257)
  points( u[-1], u[-257],
            col='firebrick4', pch=20)

    this problem was discovered on the RANDU

  generator, available on the IBM in 1950-1960
                                                                0.2
                                                                           0.6
                                                                                      1.0
                                                                                 8.0
```

G. Marsaglia, Random Numbers Fall Mainly in the Planes, Proc. Natl. Acad. Sci. USA. 6 (1968)

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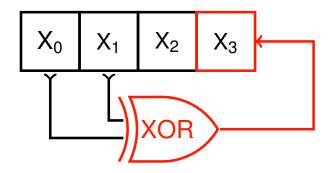
Shift Register generators

- each bit of the number is seen as an element of a binary vector
- logical linear functions are applied on each bit
- one set of generators is based on the XOR logical function

Example

- let's assume a 4-bit number: {X₀X₁X₂X₃}
- XOR is applied on bits X_0 , X_1 and the result is inserted on the most significant bit (with shift towards less significant bits)

0	1101	8	1000
1	1010	9	0001
2	0101	10	0010
3	1011	11	0100
4	0111	12	1001
5	1111	13	0011
6	1110	14	0110
7	1100	15	1101



The number 0000 is excluded from the sequence

The 64bit XOR Shift generators

Algorithm

- i) init the seed with a number \neq 0 on 64-bits
- ii) apply the following operations in sequence:

$$x = x \oplus (x >> a_1)$$

$$x = x \oplus (x << a_2)$$

$$x = x \oplus (x >> a_3)$$

- iii) release *x*
- the generator period is 2⁶⁴ − 1

a ₁	a ₂	a 3
21	35	4

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Lagged Fibonacci generators

- they are to be considered an extension to the LCGs
- they use a recurring formula

$$X_{n+1} = (X_{n-r} \square X_{n-s}) \mod m$$

- where \square indicates a generic binary operator, $\square = +, -, *, \oplus, \otimes, \mathit{Idots}$
- They are indicated as $F(r, s, \Box)$ generators

Examples

• F(0,1,+): generates the standard Fibonacci sequence:

$$X_{n+1} = (X_n + X_{n-1}) \bmod m$$

• the Knuth-TAOCP-2002 generator:

$$F(37,100,+): X_{n+1} = (X_{n-37} + X_{n-100}) \mod m = 2^{30}$$

• the period is around 2²¹⁹

D. Knuth, *The Art of Computer Programming*, Vol 2, semi-numerical algorithms, Addison Wesley 2002

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Random number generation in R

- random numbers, in a specific interval, can be generated using the runif(n, lower, upper) function
- the underlying random number generator can be set/retrieved using the RNGkind(kind = NULL, normal.kind = NULL, sample.kind = NULL) function
- set.seed uses a single integer argument to set as many seeds as are required

```
RNGkind()
# [1] "Mersenne-Twister" "Inversion"

RNGkind()
# [1] "Wichmann-Hill" "Inversion"

.Random.seed
# [1] 400 24434 13963 16439

RNGkind("Super") # matches "Super-Duper"
RNGkind()
# [1] "Super-Duper" "Inversion"

.Random.seed # new, corresponding to Super-Duper
# [1] 402 -1462836548 -1846862707
```

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Random number generators in R

- Wichmann-Hill: the Wichmann-Hill generator has a cycle length of 6.9536e12
 B. A. Wichmann and I. D. Hill, n Efficient and Portable Pseudo-Random NumberGenerator,
 Applied Stat. 33 (1984), 123
- Marsaglia-Multicarry: a multiply-with-carry RNG. It has a period of more than 2⁶⁰ and passed all Marsaglia Diehard battery tests
- Super-Duper: this is Marsaglia's famous Super-Duper from the 70's. It has a period of about 4.6 * 10¹⁸ for most initial seeds. R uses the implementation due to Reeds et al (1982–84)
- Mersenne-Twister: it is a twisted GFSR with period 2¹⁹⁹³⁷ − 1. In R, the initialization method due to B. D. Ripley is used.
- Knuth-TAOCP-2002: a 32-bit integer GFSR using lagged Fibonacci sequences with subtraction. The period is roughly 2¹²⁹
- Knuth-TAOCP: an earlier version of the algorithm due to Knuth (1997). This generator is written in interpreted R code
- L'Ecuyer-CMRG: a combined multiple-recursive generator from L'Ecuyer (1999). The period is around 2¹⁹¹
- user-supplied : use a user-supplied generator

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Diehard Battery of Test of Randomness

- a collection of complete statistical tests for random number generators
- initiated by G. Marsaglia
- original version in https://web.archive.org/web/20160125103112/http://stat.fsu.edu/pub/diehard/
- updated version: https://webhome.phy.duke.edu/~rgb/General/dieharder.php
- an R package exists: RDieHarder: An R interface to the DieHardersuite of RandomNumber Generator Tests

Some of the tests

- Birthday spacing
- Overlapping Permutations
- Ranks of matrices
- Monkey tests
- Count the 1s
- Parking lot test

- Minimum distance test
- Random spheres test
- The squeeze test
- Overlapping sums test
- Runs test
- The craps test

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Generating from a probability distribution

- this is a fundamental aspect of all Monte Carlo methods
- given a sequence $\{X_n\}$ of pseudo-random numbers between 0 and X_{max} , it is always possible to re-scale them between 0 and 1 as follows: $u_i = X_i/X_{max}$
- four basic methods are used:
- i) inverse transform method
- ii) composition method
- iii) acceptance/rejection method
- iv) ratio-of-uniforms method

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The inverse transform sampling method

- it's a direct method and it is based on the following facts:
- 1) all cumulative distributions are monotone increasing functions in the interval [0, 1]
- 2) if the analytical form of F(X) is known, it is also invertible:

$$F^{-1}(y) = \inf\{x : F(x) \ge y\} \quad u \in [0, 1]$$

- 3) there is a 1:1 correspondence between CDFs, since they have the same image
- given X and Y with CDFs F(X) and G(Y)
- we ask for the same probability, and search for x_i and y_i such that

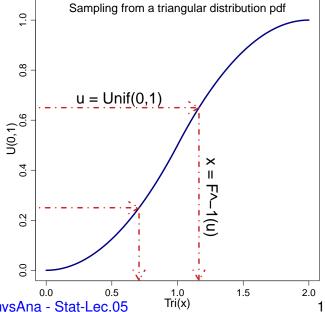
$$F(x_i) \equiv P(X \le x_i) = G(y_i) \equiv P(Y \le y_i)$$

assuming

$$G(y) = \mathcal{U}(0,1) = u$$

$$\to F(x_i) = u$$

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



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The inverse transform sampling method - ex 1

Algorithm

- 1) generate $u \in \mathcal{U}(0,1)$
- 2) compute $X = F^{-1}(u)$
- 3) release X, as it follows $X \sim F(x)$

Exercise 1

- generate random numbers from $\mathcal{U}(a,b)$
- the probability density and cumulative functions are

$$f(x) = \frac{1}{b-a}$$
 $a \le x \le b$ $F(x) = \frac{x-a}{b-a}$

▶ we generate $u \in \mathcal{U}(0,1)$

$$u = \frac{x-a}{b-a}$$
 \Rightarrow $x = a + u(b-a)$

The inverse transform sampling method - ex 2-3

Exercise 2

- generate random numbers from f(x) = 2x with domain [0, 1]
- we evaluate the cumulative density function as

$$F(x) = \int_{0}^{x} 2 y \, dy = x^2 \text{ for } 0 \le x \le 2$$

▶ we generate $u \in \mathcal{U}(0,1)$

$$u = x^2 \implies x = \sqrt{u}$$

Exercise 3

generate random numbers from Exp(λ)

$$f(x) = \lambda e^{-\lambda x}$$
 $F(x) = 1 - e^{-\lambda x}$

▶ we generate $u \in \mathcal{U}(0,1)$

$$\begin{array}{rcl} u & = & 1 - \mathrm{e}^{-\lambda \; x} \\ \mathrm{e}^{-\lambda \; x} & = & 1 - u = u \\ -\lambda \; x & = & \ln u \\ x & = & -\frac{1}{\lambda} \ln u \end{array} \qquad \begin{array}{rcl} u \; \mathrm{and} \; 1 - u \; \mathrm{have \; the \; same} \\ \mathrm{probability \; distributions} \end{array}$$

probability distributions

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Example: generating from a discrete distribution

let's assume the probabilities assume discrete values:

$$f(X) = \begin{cases} C_j & x_{j-1} < x < x_j \\ 0 & \text{otherwise} \end{cases}$$

we set

$$P_{j} = \int_{x_{j-1}}^{x_{j}} f(x) dx = \int_{x_{j-1}}^{x_{j}} C_{j} dx = C_{j}(x_{j} - x_{j-1})$$

and

$$F_j = \sum_{k=1}^j P_k$$

$$F(x) = \sum_{j=1}^{i-1} + \int_{x_{i-1}}^{x} C_j dx = F_{j-1} + C_i(x - x_{i-1})$$

• generating $u \in \mathcal{U}(0,1)$, by inversion

$$u = F_{i-1} + C_i(x - x_{i-1})$$

$$x = x_{i-1} + \frac{u - F_{i-1}}{C_i}$$

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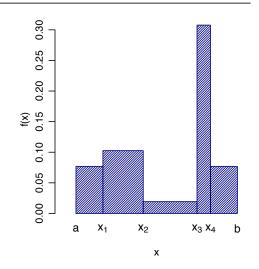
Generating from a discrete distributionin R

Algorithm

- generate random numbers from $\mathcal{U}(0,1)$
- find i such that

$$\sum_{j=1}^{i-1} P_j \le u < \sum_{j=1}^{i-1} P_j$$

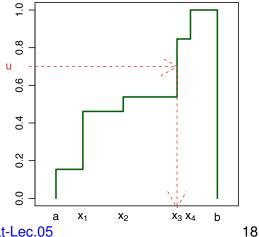
• deliver $x = x_{i-1} + (u - F_{i-1})/C_i$



Example

- from u we find i = 3
- $x = x_2 + (u F_2)/C_3 = x_2 + (u 6)/1 \implies u = 9/13$

$$C_1 = 2$$
 $C_2 = 4$ $C_3 = 1$ $C_4 = 4$ $C_5 = 2$ $F_1 = 2$ $F_2 = 6$ $F_3 = 7$ $F_4 = 11$ $F_5 = 13$



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The Composition sampling method

 it is based on the fact that our pdf can be written as linear combination of other pdfs

$$F(x) = \sum_{j=1}^{r} \omega_j F_j(x)$$

with

$$0 < \omega_i < 1$$
 and $\sum \omega_i = 1$

Algorithm

- 1) generate $u \in \mathcal{U}(0,1)$
- 2) according to the weights, ω_i , extract the correct index j
- 3) generate x from $F_j(x)$

Example with the Composition sampling method

• we want to sample from the pdf

$$f(x) = \frac{5}{12} [1 + (x-1)^4]$$
 with $0 \le x \le 2$

we can rewrite it as follows

$$f(x) = \frac{5}{6}f_1(x) + \frac{1}{6}f_2(x)$$

• therefore, $\omega_1 = 5/6$ and $\omega_2 = 1/6$ with $\omega_1 + \omega_2 = 1$

$$f_1(x) = \frac{1}{2} \quad \Rightarrow \quad F_1(x) = \int_1^x \frac{dx}{2} = \frac{x}{2}$$

$$f_2(x) = \frac{5}{2}(x-1)^4 \quad \Rightarrow \quad F_2(x) = \int_1^x \frac{5}{2}(x-1)^4 \, dx = \frac{(x-1)^5}{2} + \frac{1}{2}$$

Algorithm

- generate $u_1, u_2 \in \mathcal{U}(0,1)$
- if $u_1 < 5/6$, $\Rightarrow x = 2 u_2$
- else $\Rightarrow 2u_2 1 = (x 1)^5 \Rightarrow x = (2 u_2 1)^{1/5} + 1$

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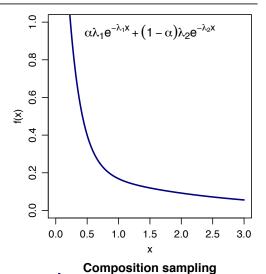
Example with the Composition sampling method

we want to sample from two exponential distributions

$$f(x) = \alpha \lambda_1 e^{-\lambda_1 x} + (1 - \alpha) \lambda_2 e^{-\lambda_2 x}$$

• the weights are: $\omega_1 = \alpha$ and $\omega_2 = 1 - \alpha$, with $\omega_1 + \omega_2 = 1$

$$F_1(x) = 1 - e^{-\lambda_1 x}$$
 and $F_2(x) = 1 - e^{-\lambda_2 x}$





1.0

1.5

2.0

2.5

0.0

0.5

Algorithm

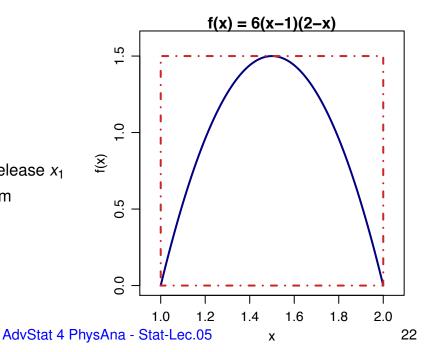
- generate $u_1, u_2 \in \mathcal{U}(0,1)$
- if $u_1 < \alpha$, $\Rightarrow x = \ln u_2/\lambda_1$
- else $x = \ln u_2/\lambda_2$

The acceptance/rejection method

- this is very useful when we are not able to compute the analytical form of the CDF
- or when the CDF is not easily invertible
- the method, due to von Neumann in 1951, is based on the hypothesis that our pdf is defined analytically in the interval [a,b] and that $\forall x \in [a,b] \rightarrow f(x) < M$

Algorithm

- generate $u_1 \in \mathcal{U}(0,1)$
- compute $x_1 = a + (b a) \cdot u_1$
- generate $u_2 \in \mathcal{U}(0,1)$
- if $u_2 \cdot M < f(x_1)$ we accept and release x_1
- otherwise we restart the algorithm

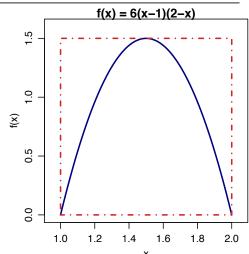


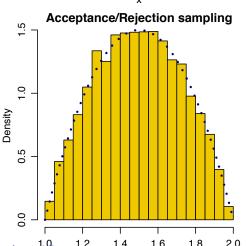
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The acceptance/rejection method

 the efficiency of the method is given by the ratio of the two areas

$$\epsilon = \frac{\int_{a}^{b} f(x) dx}{M(b-a)} = \frac{1}{M(b-a)}$$





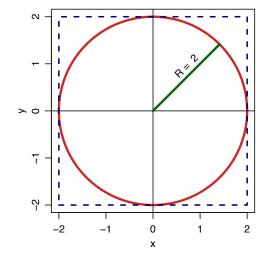
Example: sampling from a disc 1

- we want to sample, uniformly, inside a disc of radius R
- i.e. sample points (x_j, y_j) such that $x_i^2 + y_i^2 \le R$

Acceptance/Rejection sampling algorithm

- generate $u_1, u_2 \in \mathcal{U}(0,1)$
- compute $x_i = R(1 2u_1)$ and $y_i = R(1 2u_2)$
- if $x_i^2 + y_i^2 \le R$, accept and release (x_j, y_j)
- otherwise we restart the algorithm
- the efficiency of the method is given by the ratio

$$\epsilon = \frac{A_{disc}}{A_{square}} = \frac{\pi R^2}{4R^2} = \frac{\pi}{4}$$



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Example: sampling from a disc 2

 the alternative is to change from Cartesian to polar coordinates

$$\begin{cases} x_j = R \cos \theta_j \\ y_j = R \sin \theta_j \end{cases}$$

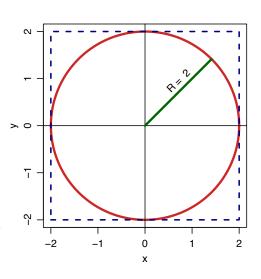
• the probability for a point (x_j, y_j) to be at a distance r + dr from the disc center is

$$F(r) = \int_0^r f(\rho) d\rho = \int_0^r \frac{2\pi \rho d\rho}{\pi R^2} = \frac{r^2}{R^2}$$

Algorithm

- generate $u_1 \in \mathcal{U}(0,1)$
- using the inverse transform, $u_1 = r^2/R^2 \Rightarrow \hat{r} = R\sqrt{u_1}$
- generate $u_2 \in \mathcal{U}(0,1)$
- compute $\hat{\theta} = 2\pi u_2$
- evaluate

$$\begin{cases} x_j &= \hat{r}\cos\hat{\theta} \\ y_i &= \hat{r}\sin\hat{\theta} \end{cases}$$



this method has 100% efficiency, but computations are heavier since trigonometric functions are required

Normal distribution - Box-Müller

• if $X \sim \text{Norm}(\mu, \sigma^2)$, the pdf is

$$f(x) = \frac{1}{\sigma \sqrt{2\pi}} \exp{-\frac{(x-\mu)^2}{2\sigma^2}}$$

- the inverse-transform method is inefficient (we do not have an analytical CDF)
- to simplify we can sample $X \sim \text{Norm}(0,1)$ and then transform $Z = \mu + \sigma X$

The Box-Müller algorithm

- let's consider the pdf of two independent normal distributed random variables \Rightarrow (X, Y) is a random point in the plane
- let's move to polar coordinates (r, θ)
- the joint pdf becomes

$$f(r,\theta) = \frac{1}{2\pi}r \cdot \exp{-\frac{r^2}{2}}$$

• since $x = r \cos \theta$ and $y = r \sin \theta$

$$f(x,y) = \frac{1}{2\pi}r \cdot \exp \frac{-(x^2 + y^2)}{2}$$

- 1 generate two independend random variables, $U_1, U_2 \in \mathcal{U}(0,1)$
- 2 release

$$X = \sqrt{-2 \ln U_1} \cos 2\pi U_2$$
 and $Y = \sqrt{-2 \ln U_1} \sin 2\pi U_2$

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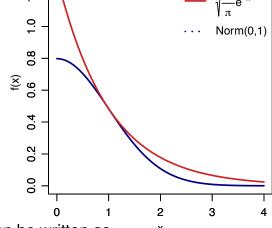
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Normal distribution - Acceptance/Rejection

- an alternative method to generate from X ~ Norm(0, 1) is based on the acceptance/rejection method
- let's generate from the pdf

$$f(x) = \sqrt{\frac{2}{\pi}} \exp{-x^2/2}$$
 with $x \ge 0$

- (the sign can be generated with another $\mathcal{U}(0,1)$)
- we bind f(x) by $C \cdot g(x)$ where $g(x) = \exp(-x)$
- the smallest constant such that $f(x) \le C \cdot g(x)$ is $C = \sqrt{2e/\pi}$



• the acceptance condition $U \le f(X)/(C \exp -X)$ can be written as

$$U \le \exp\left[-(X-1)^2/2\right]$$

which is equivalent to

$$-\ln U \ge \frac{(X-1)^2}{2} \quad \text{with} \quad X \sim \text{Exp}(1)$$

• but $- \ln U$ follows from Exp(1), therefore the inequality can be rewritten as

$$V_1 \ge \frac{(V_2 - 1)^2}{2}$$
 with $V_1 = -\ln U$ and $V_2 = X$

• both V_1 and V_2 are independent and Exp(1) distributed

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