Numerical methods in Fortran: Lec. I & II

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Topics to be covered

- Random numbers generators, middle square method, linear congruent method, in-built FORTRAN random number generators.

- Non-uniform random number generators: Transformation method, exponential and Gaussian random number generator.

- Rejection method and Monte-Carlo integration.

- Non parametric density estimation.

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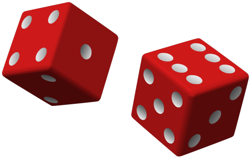
Random number generators and their uses

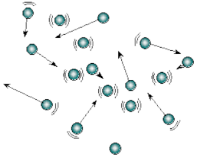
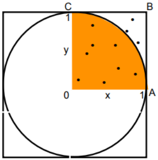
- Generates a sequence of numbers that can not be predicted.

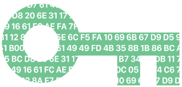
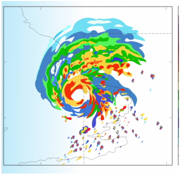


◇ Physical process that contains randomness: radioactive decay, thermal motion.

◇ Monte Carlo integration: multi-dimensional integrals.

◇ Simulation in Classical Statistical and Quantum Mechanics.

True random number generators

◇ Computer must use some external physical variable that is unpredictable, such as radioactive decay of isotopes and atmospheric noise.

◇ Truly random numbers are difficult to generate because they are not cost-efficient.

◇ Slow to generate, no reproducibility.

◇ Required for cryptography.

Pseudo random number generators

◇ Long sequences of numbers $(x_1, x_2, x_3, ...)$ generated by an algorithm on a computer. Look "nearly random" but completely deterministic!

◇ They have statistical properties similar to true random numbers and usually distributed uniformly in range $[0,1]$: uniform distribution:

$$P(x) = \begin{cases} 1 & \text{if } 0 \le x \le 1, \\ 0 & \text{otherwise.} \end{cases} \qquad P(x) = \begin{cases} \frac{1}{(b-a)} & \text{if } a \le x \le b, \\ 0 & \text{otherwise.} \end{cases}$$

◇ To be precise, the algorithm generates integers I_n between 0 and M, and returns a real value. The real value is : $x_n = \frac{\text{float}(I_n)}{M}$.

◇ **Correlations**: $\begin{cases} P(x_n, x_{n+j}) \simeq P(x_n)P(x_{n+j}) \\ P(x_n, x_{n+j}, x_{n+k}) \simeq P(x_n)P(x_{n+j})P(x_{n+k}). \end{cases}$

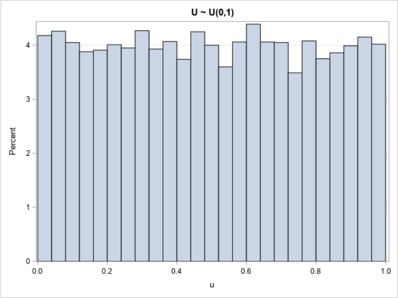
Ideally (no correlations) we have equalities!

Pseudo random numbers generation - Algorithms

Two among the simplest (and oldest) algorithms:

- ◇ The von Neumann method (Middle square algorithm)
- ◇ The Linear Congruential Method (LCM)

We will eventually use the in-built FORTRAN function to generate random numbers!



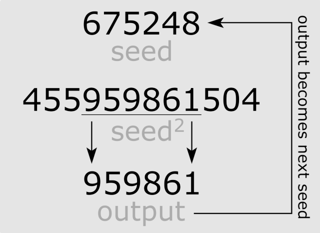
von Neumann (Middle square) algorithm

To generate a d-digit integer sequence:

- take any d digit number
- square it
- take the middle d digits of the result

loop it.

Limitation:
depending on the initial choice, you can be trapped into short loops.



Algorithm

Data: Seed X_0
Result: Random numbers
while *true* **do**
    $X_0 \leftarrow X_0^2$;
    Extract the middle digits as the random number;
    Output the random number;
end

Hint: To get the middle d digits: $M_1 = \frac{M}{10^{d/2}}$ and then $\mathrm{mod}(M_1, 10^{2d})$.

Linear Congruential Method (LCM)

The Linear Congruential Method is defined by the recurrence relation:

$$X_{n+1} = (a \cdot X_n + c) \mod m$$

Where:

X_n is the current pseudorandom number. X_0 - initial value (seed)

a is the multiplier. c is the increment.

m is the modulus.

$m - 1$ is the largest number.

Algorithm

Data: Seed X_0, Multiplier a, Increment c, Modulus m

Result: Random numbers

while *true* **do**

  $X_{n+1} = (a \cdot X_n + c) \mod m$;

  Output X_{n+1} as the random number;

end

Limitation of LCG

• A poor choice for the constants can lead to very poor sequences. Finite period, then sequence repeats itself.

Example:

$$a = c = I_0 = 7 \text{ and } m = 10, \qquad \text{Sequence} : 7, 6, 9, 0, 7, 6, 9, 0, ...$$

• Overflow issue - multiplication of large numbers will be out of bound. Resolution: Schrage's trick (Schrage, 1979)

• m should be as large as possible since the period can never be longer than m

• Typically, one usually chooses m to be near the largest integer than that can be represented. On a 32 bit machine, that is $2^{31} \approx 2 \times 10^9$

• Good choice (a and m are coprime): $c = 0, m = 2^{31} - 1, a = 16807$

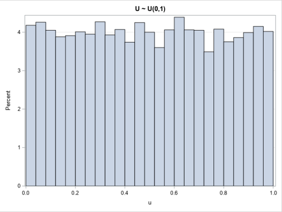
Using in-built FORTRAN function

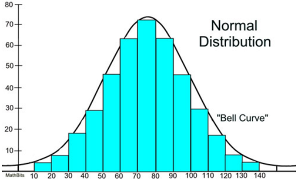
```
program testrand
  implicit none
  integer, parameter :: seed = 12345
  integer :: i, N, M
  real(8), allocatable :: random_array_1d(:), random_array_2d(:,:)
  call srand(seed)
  N = 100
  M = 200
  allocate(random_array_1d(N))
  do i = 1, N
    random_array_1d(i)=rand()
  end do
  allocate(random_array_2d(N,M))
  call random_number(random_array_2d)
  deallocate(random_array_1d)
  deallocate(random_array_2d)
end program testrand
```

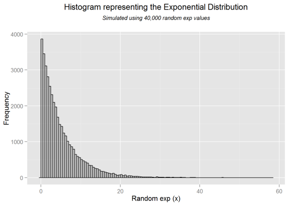
• Other uniform distributions, uniform x in $[a, b]$: $x = a + (b - a)u$, where u is a random number in $[0, 1]$

Non-uniform random number generators

How can we get a random number x distributed with a probability distribution $f(x)$ in the interval $[x_{min}, x_{max}]$ from a uniform random number u?







Methods:

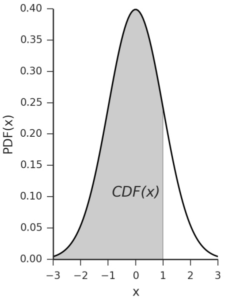
- Transformation method: need a transformation function- $T(u) = X$
- Rejection method

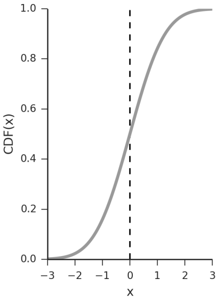
Cumulative Density Function (CDF)

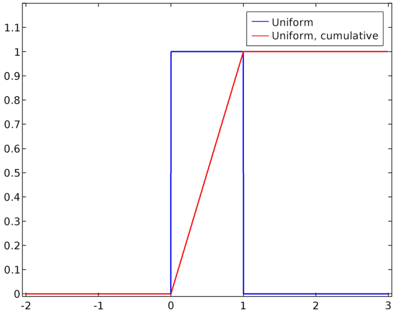
The Cumulative Density Function, denoted as $G_X(x)$, gives the probability that a continuous random variable is less than or equal to x. It is defined as the integral of the PDF from $-\infty$ to x.

$$G_X(x) = \Pr(X \leq x) = \int_{-\infty}^{x} f(t)dt$$

For example, for uniform distribution: $G_X(x) = x$







Transformation method

Desire: Random numbers from a probability density function $f(x)$ using the transformation: $T(u) = X$

Statement: Given a probability density function (PDF) $f(x)$, its corresponding cumulative density function (CDF) G_X, and a uniform variable $u \in [0, 1]$, the random numbers from the distribution $f(x)$ can be generated by $G_X^{-1}(u)$ or the transformation function is $T = F_X^{-1}$.

$$G_X(x) = \Pr(X \leq x) = \Pr(T(u) \leq x) = \Pr(u \leq T^{-1}(x)) = T^{-1}(x)$$

Algorithm

Data: Uniform random number u in the range $[0, 1]$
Data: Desired PDF and its CDF $G_X(x)$ and its inverse $G_X^{-1}(u)$
Result: Non-uniform random number X with the desired distribution

Generate u in the range $[0, 1]$;
Use $X = G^{-1}(u)$ to transform u into X with desired distribution;

Transformation method: exponential distribution

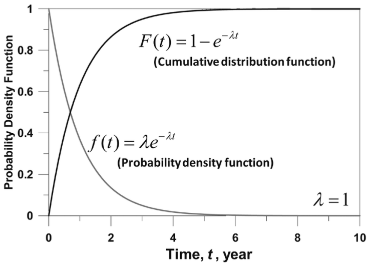
Algorithm

Data: Uniform random number u in the range $[0, 1]$
Data: Desired PDF and its CDF $G_X(x)$ and its inverse $G_X^{-1}(u)$
Result: Non-uniform random number X with the desired distribution

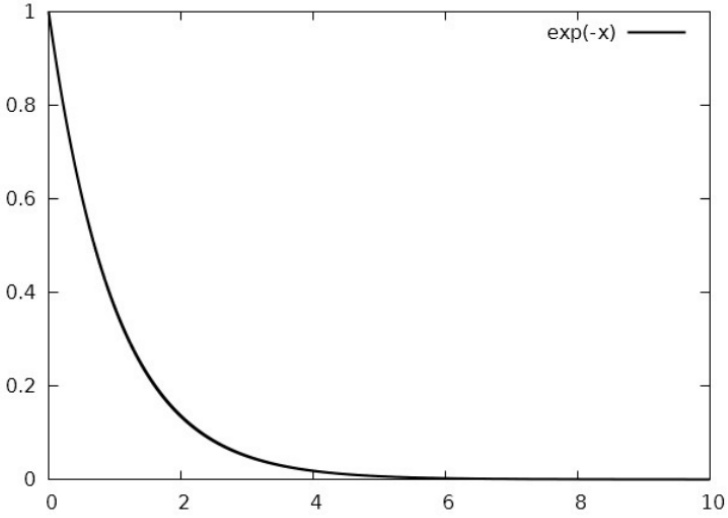
Generate u in the range $[0, 1]$;
Use $X = G^{-1}(u)$ to transform u into X with desired distribution;

- **PDF:** $f(x) = \lambda e^{-\lambda x}$
- **CDF:** $G_X(x) = \int_0^x f(x')dx' = 1 - e^{-\lambda x}$
- **Inverse CDF:**

$$X = G^{-1}(u) = -\frac{1}{\lambda}\ln(1-u)$$

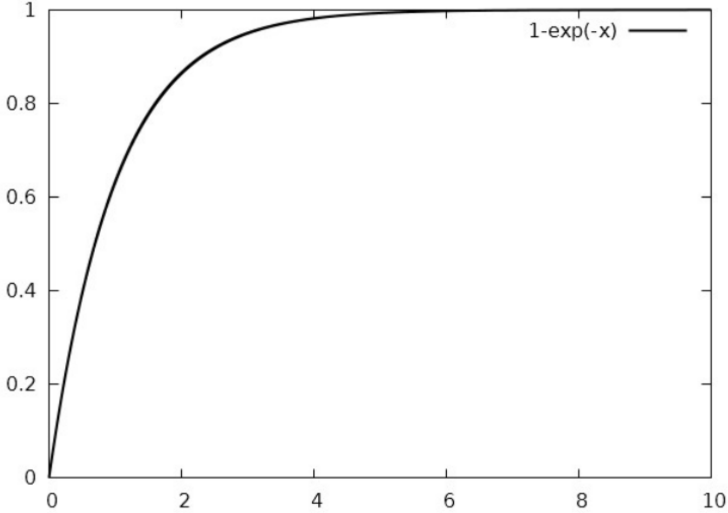


Understanding the transformation method



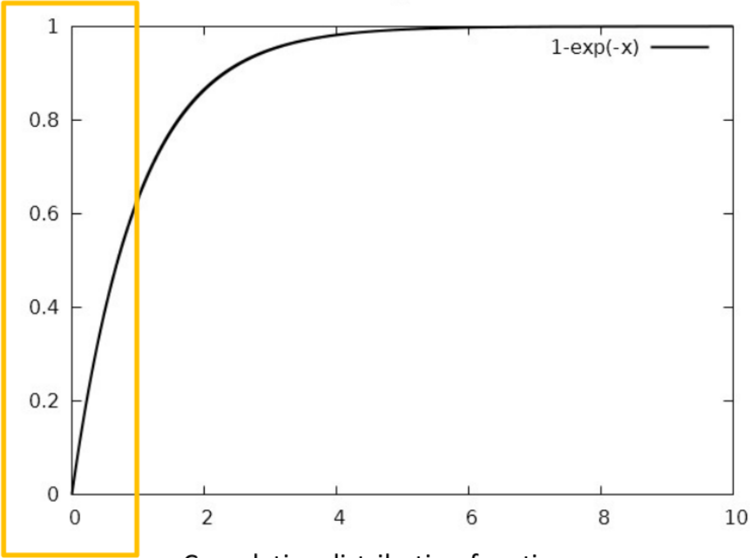
Probability distribution function

Understanding the transformation method



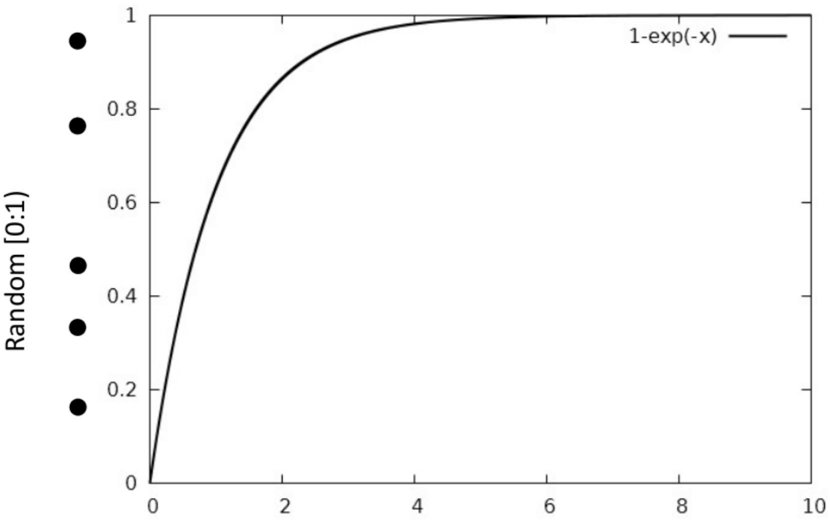
Cumulative distribution function

Understanding the transformation method



Cumulative distribution function

Understanding the transformation method



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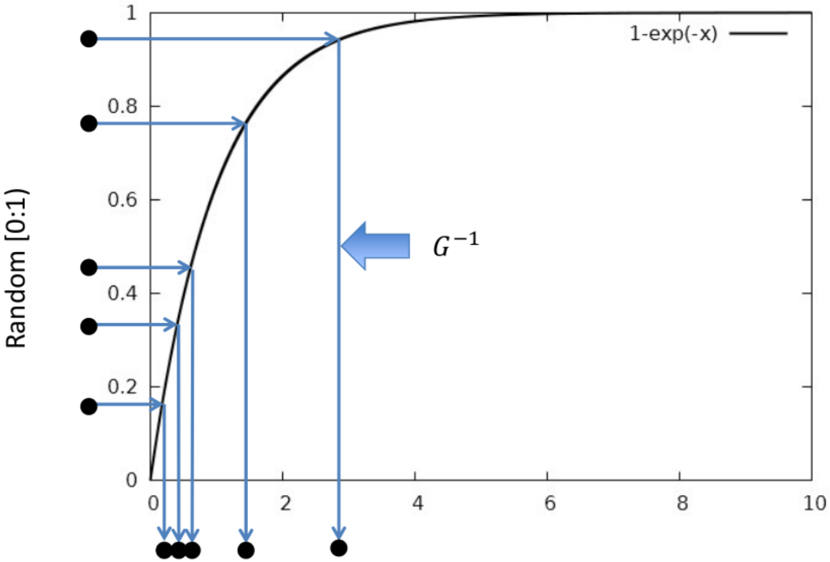

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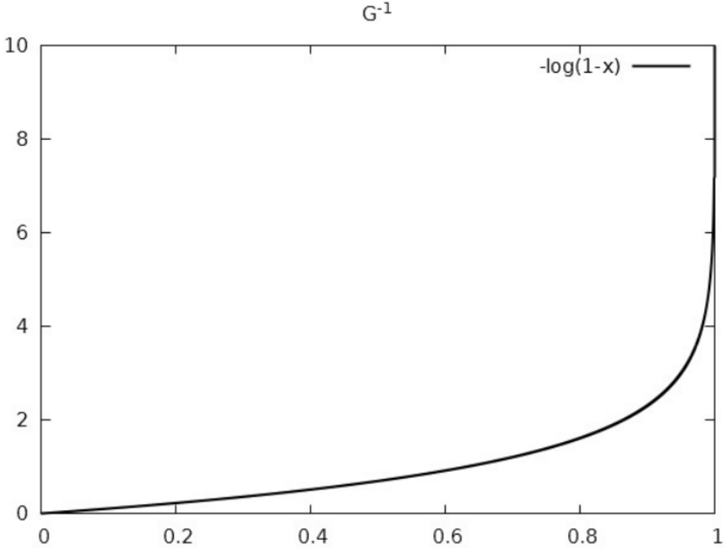
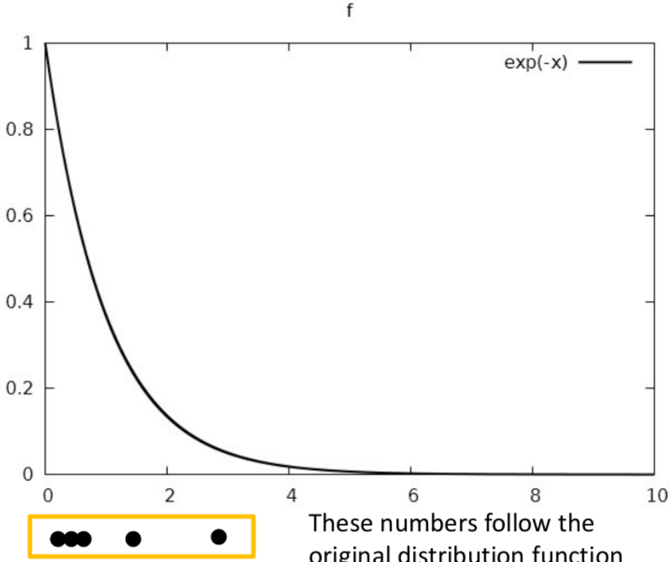


Understanding the transformation method



These numbers follow the original distribution function

Gaussian distribution: Box-Muller Method

For Gaussian PDF, it is impossible to invert $u = T^{-1}(x)$ in $1d$ but possible in $2d$. $f(x,y) = \frac{1}{2\pi} \exp\left(-\frac{x^2+y^2}{2}\right)$ and use polar coordinates.

Step 1: Generate Uniform Random Numbers

Generate two uniform random numbers U_1 and U_2 in the range $[0,1]$.

Step 2: Transform Uniforms into Normals

Use the inverse transformation to convert the uniform random numbers into two independent standard normal random numbers Z_1 and Z_2:

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

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

The generated Z_1 and Z_2 are independent standard normal random numbers $(N(0,1))$.

Assignment-12 & 13

1) Write subroutines for the middle square and the linear congruent method. Use these subroutine to generate N random numbers, use allocatable array to store them. Finally save them in a file. Use "Good choice" of a, m, c.

2) Generate 1000 couples (x, y) of random numbers using Linear Congruential Method (LCM). Plot the generated data on a 2D graph. (use the couples as x, y coordinates of the points)

4) Repeat **(2)** but with the inbuilt FORTRAN function.

3) Use inbuilt function generates 100000 points in the interval $[0, 1]$ from the distribution $f(x) = 3x^2$ using the transformation method.

4) Make a subroutine implementing the Box-Muller method. Generate 10000 random numbers from this distribution and plot the histogram.

Submit your code as ***surname_assignment_12.f90*** to ***dbhakuni@ictp.it*** before the next lesson. Use "gnuplot script.p" to plot histogram.