993SM - Laboratory of Computational Physics week V October 21, 2024

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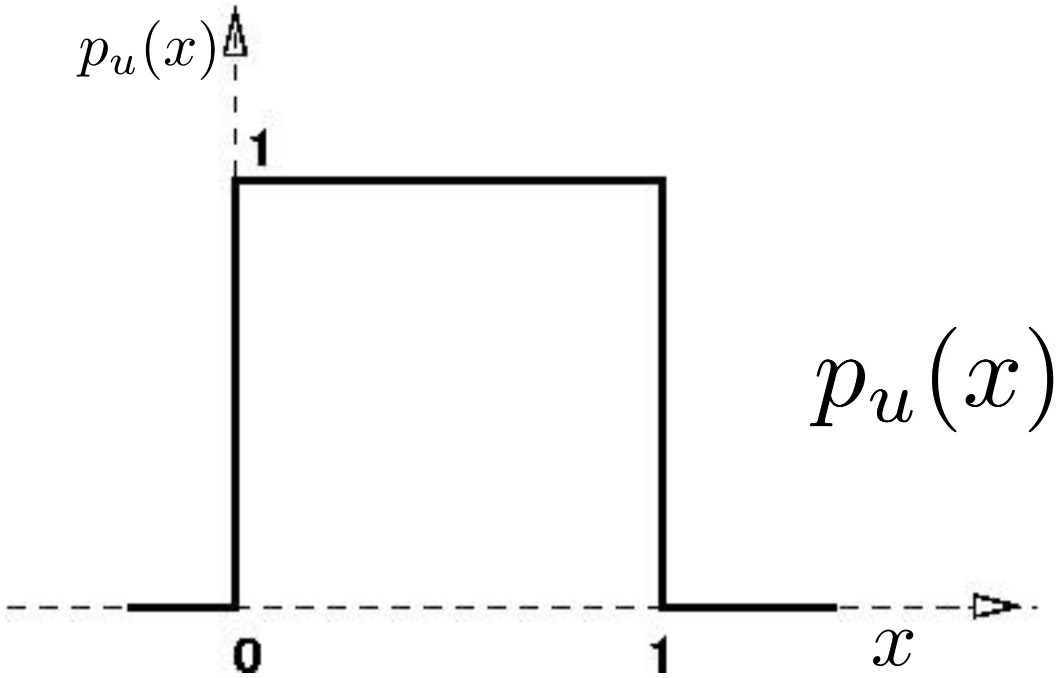
Part I - Random numbers with non uniform distributions

M. Peressi - UniTS - Laurea Magistrale in Physics
Laboratory of Computational Physics - week V

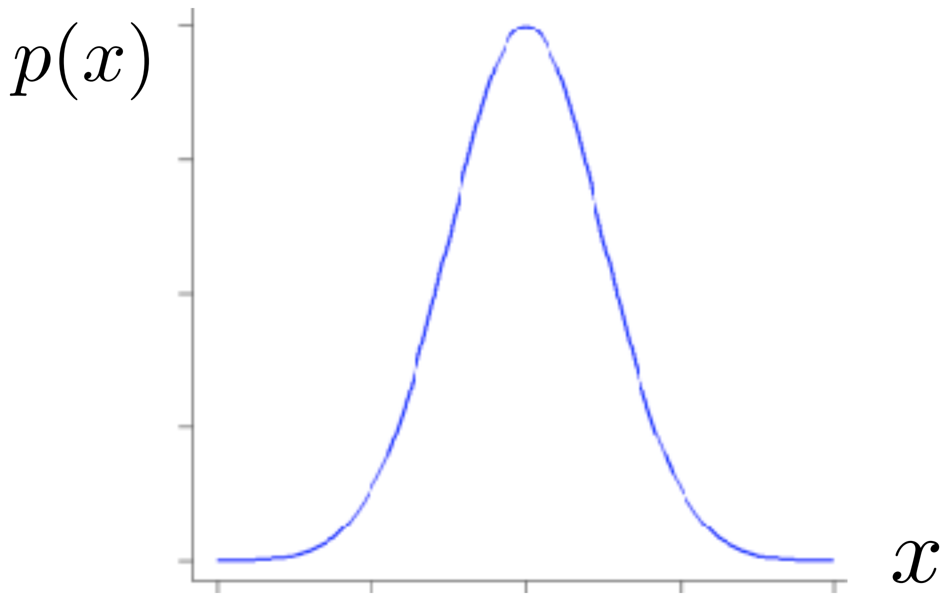
last lecture:

generation of real (pseudo)random numbers with uniform distribution in [0;1[



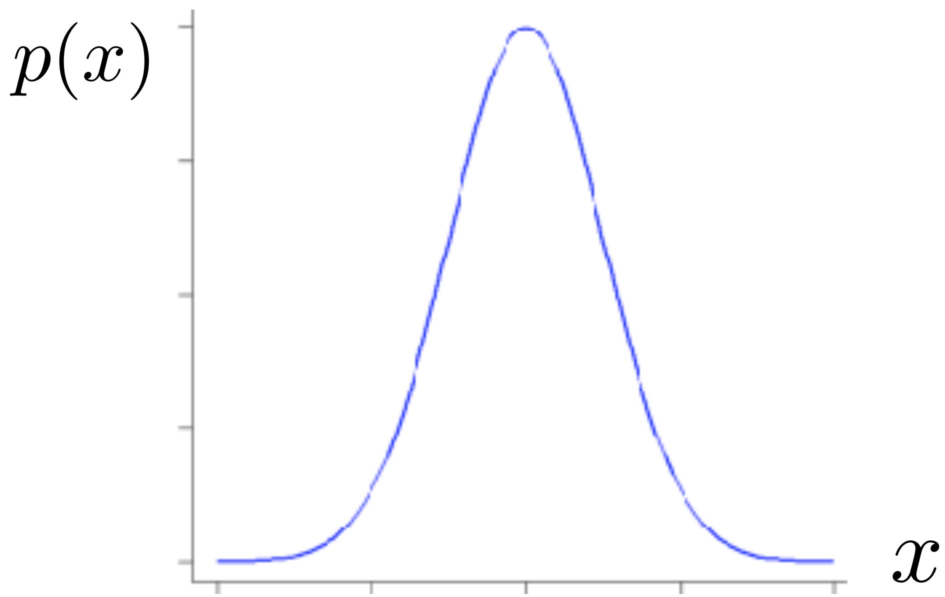
$$p_u(x) = \begin{cases} 1 & 0 \leq x < 1 \\ 0 & \text{otherwise} \end{cases}$$

Random numbers with non uniform distributions:



How can we generate random numbers with a given distribution p(x) ?

Random numbers with non uniform distributions:



1) inverse transformation method (general)
2) rejection method (even more general)
3) some "ad hoc" methods: e.g. for the gaussian distribution: the Box-Muller algorithm, the central limit theorem

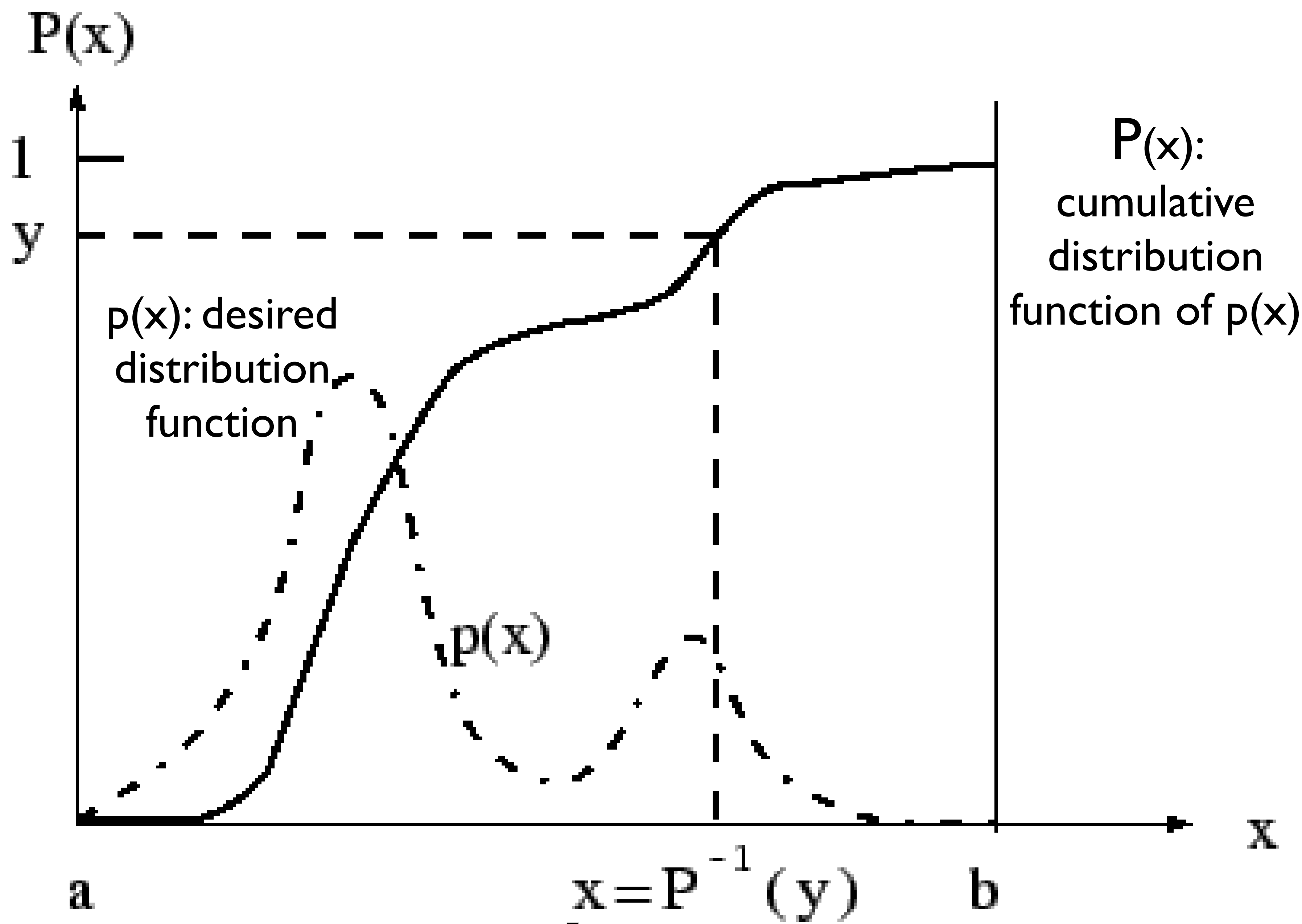
1) inverse transformation method (general)

Problem: Generate sample of a random variable (or *variate*) x with a given distribution p.

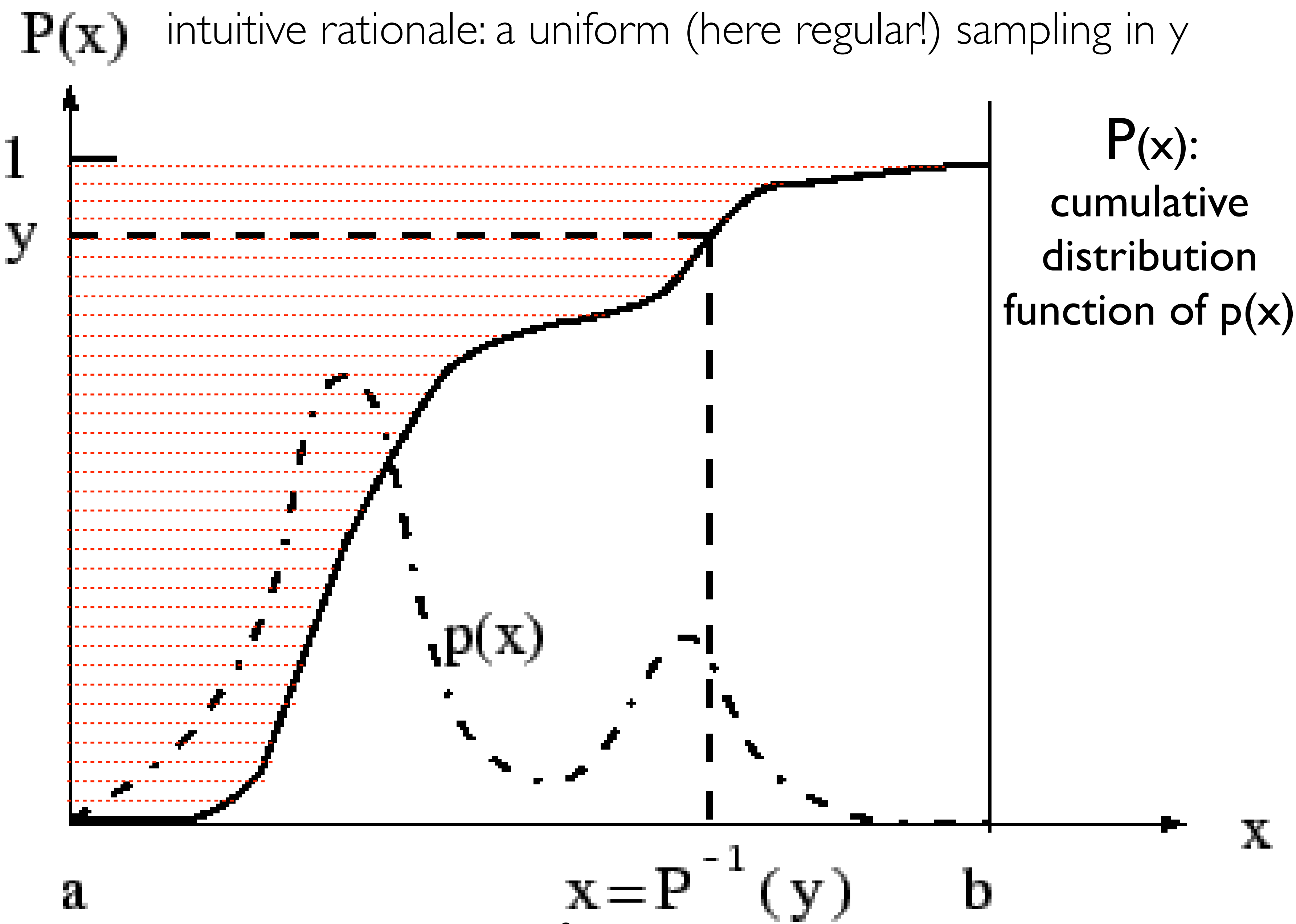
Solution: 2-step process

- Generate a random variate uniformly distributed in $[0,1]$ .. also called a *random number*
- Use an appropriate transformation to convert the random number to a random variate of the correct distribution

1) inverse transformation method - the idea

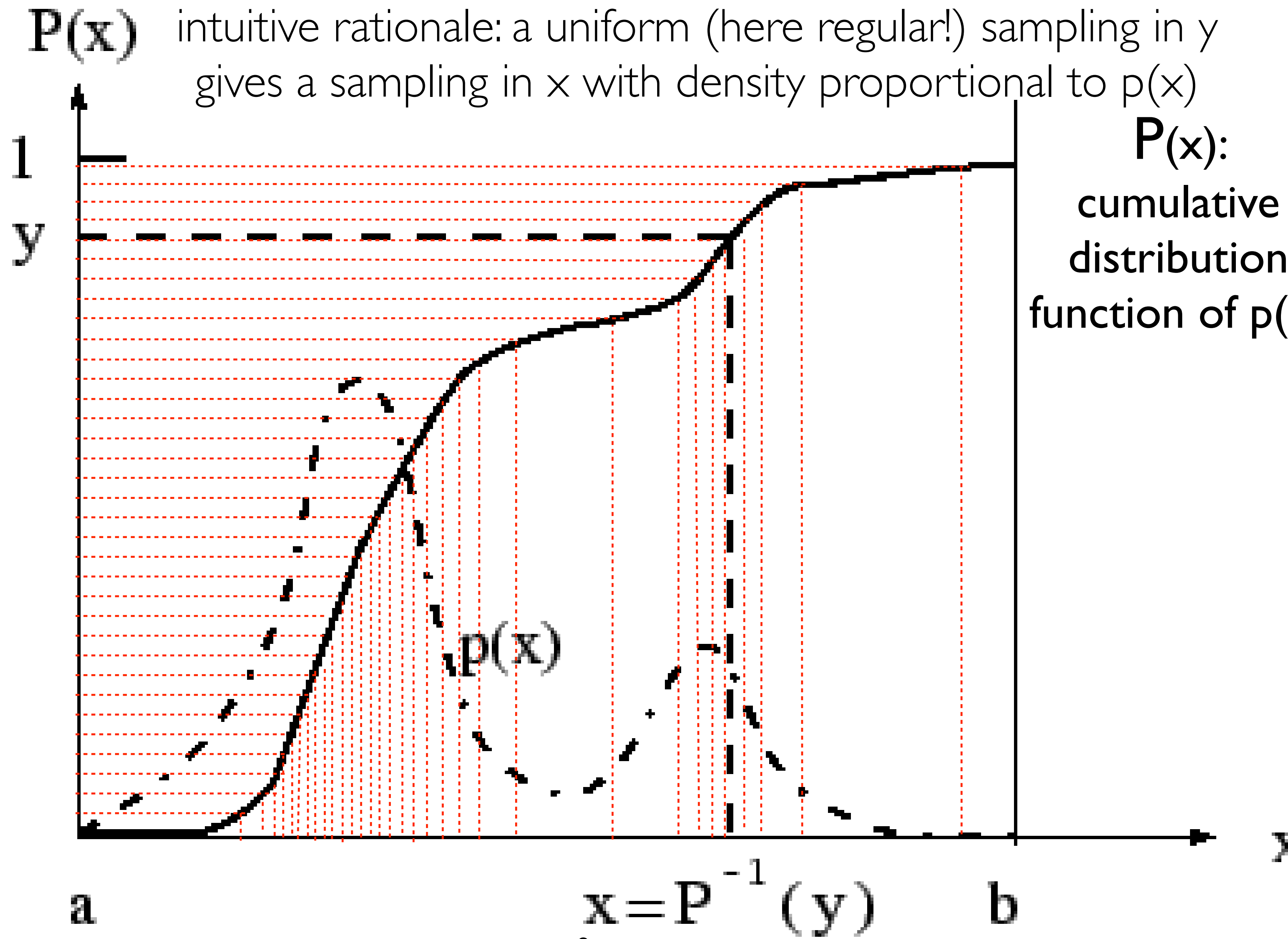


1) inverse transformation method - the idea



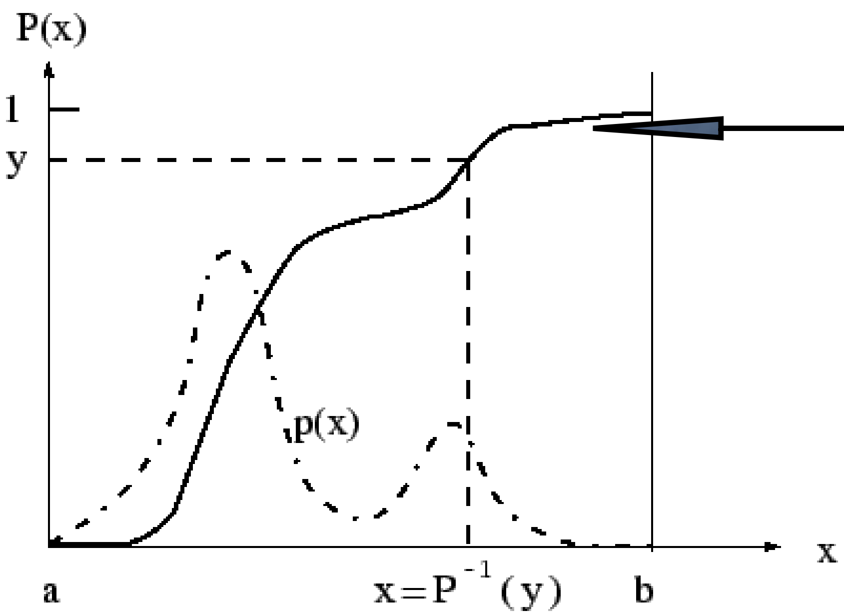
1) inverse transformation method - the idea

intuitive rationale: a uniform (here regular!) sampling in y gives a sampling in x with density proportional to p(x)



P(x): cumulative distribution function of p(x)

1) inverse transformation method - algorithm



cumulative distribution function P(x)

$$\int_{-\infty}^{+\infty} p(x)dx = 1$$

Let $p(x)$ be a desired distribution, and $y = P(x) = \int_{-\infty}^{x} p(x')dx'$ the corresponding *cumulative distribution*. Assume that $P^{-1}(y)$ is known.

- Sample y from an equidistribution in the interval (0,1). (i.e., use $p_u(y)$)
- Compute $x = P^{-1}(y)$.

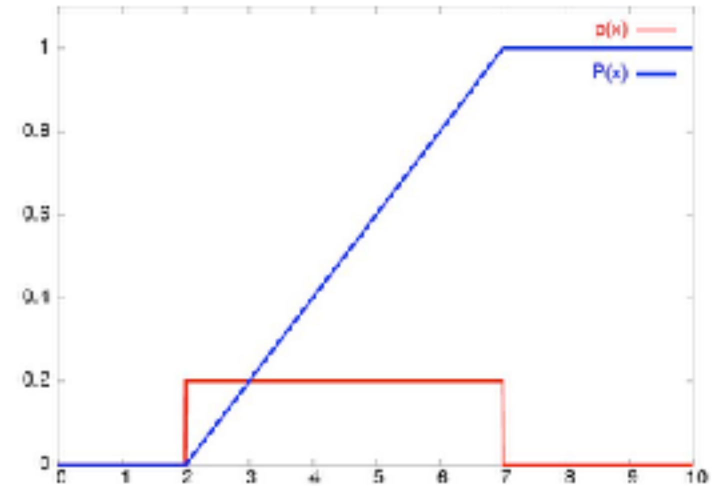
The variable x then has the desired probability density $p(x)$.

$$y = P(x) \Longrightarrow dy = dP(x) \Longrightarrow p_u(y)dy = dP(x) \;\; (\text{since } p_u(y) = 1 \text{ for } 0 \leq y \leq 1)$$

$$\text{But :} \quad dP(x) = p(x)dx, \quad \text{therefore} \;\; p(x)dx = p_u(y)dy$$

1) inverse transformation method - examples

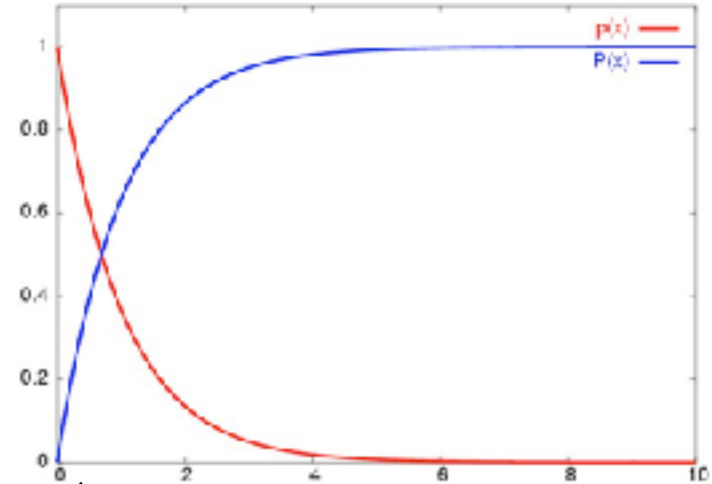
1) $$p(x) = \begin{cases} \frac{1}{b-a} & a \leq x \leq b \\ 0 & \text{otherwise} \end{cases}$$



$$y = \quad P(x) = \begin{cases} 0 & x \leq a \\ \int_a^x \frac{1}{b-a} dx' = \frac{x-a}{b-a} & a \leq x \leq b \\ 1 & x > b \end{cases}$$

$$x = y(b-a) + a$$

2) $$p(x) = \begin{cases} 0 & x \leq 0 \\ ae^{-ax} & x \geq 0 \end{cases}$$



$$y = \quad P(x) = \begin{cases} 0 & x \leq 0 \\ 1 - e^{-ax} & x \geq 0 \end{cases}$$

$$x = -\frac{1}{a} \ln(1-y) \quad \text{or (same distribution!)} \quad x = -\frac{1}{a} \ln y$$

1) inverse transformation method - examples

1) $$p(x) = \begin{cases} \frac{1}{b-a} & a \le x \le b \\ 0 & \text{otherwise} \end{cases}$$

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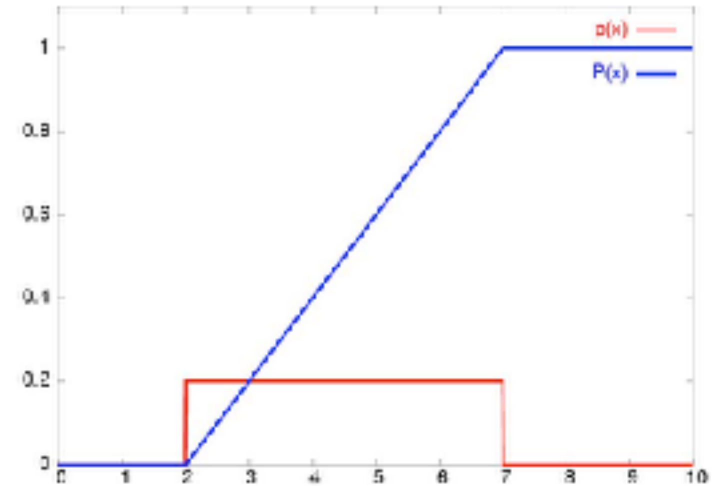

2) $$p(x) = \begin{cases} 0 & x \le 0 \\ ae^{-ax} & x \ge 0 \end{cases}$$

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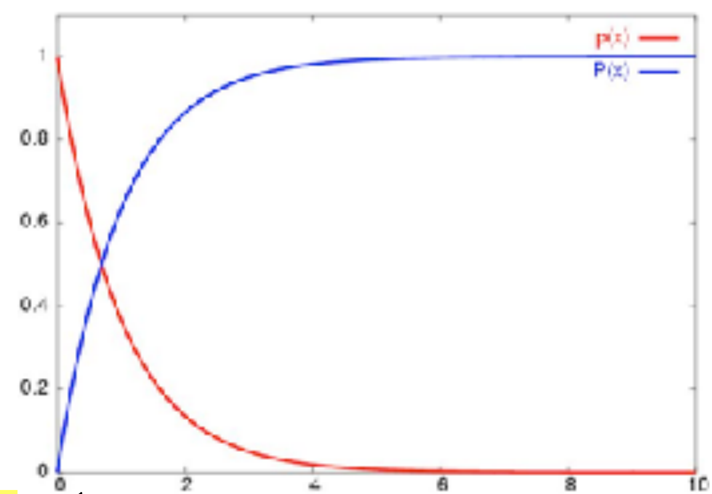


$$x = -\frac{1}{a} \ln(1-y) \quad \text{or (same distribution!)} \quad x = -\frac{1}{a} \ln y$$

Codes available on moodle

expdev.f90

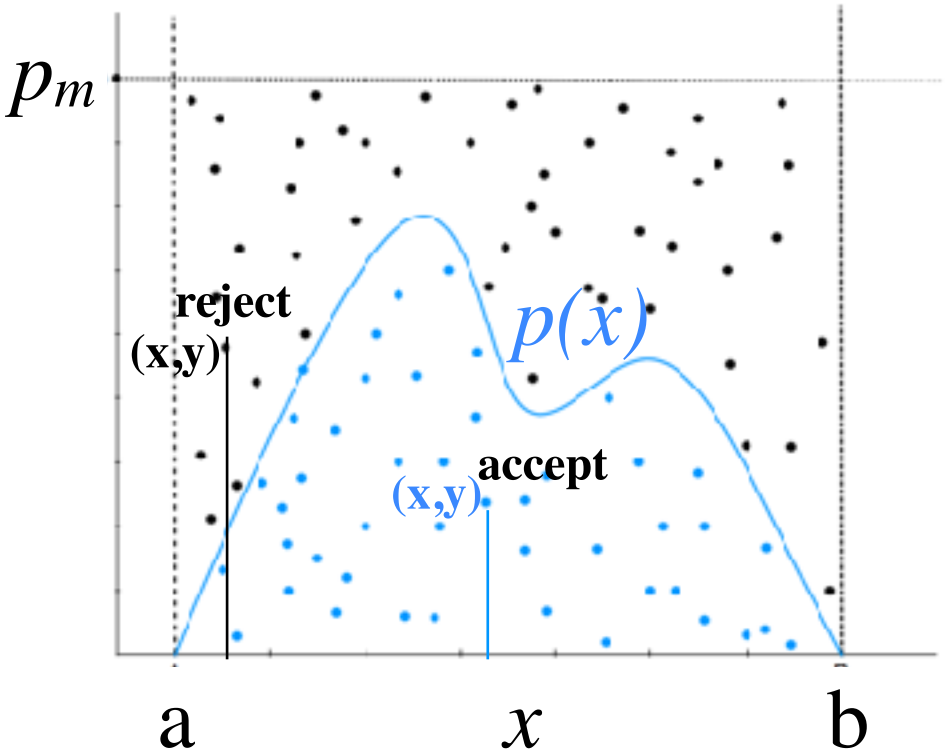
```
subroutine expdev(x)
   REAL, intent (out) :: x
   REAL :: r
   do
      call random_number(r)
      if(r > 0) exit
   end do
   x = -log(r)
 END subroutine expdev
```

r is generated in [0,1[;
but r=0 has to be discarded;
if r=0, generate another random number;
if not, exit from the **unbounded** loop
and calculate its log

2) rejection method (general)

Let $[a, b]$ be the allowed range of values of the variate x, and p_m the maximum of the distribution $p(x)$.

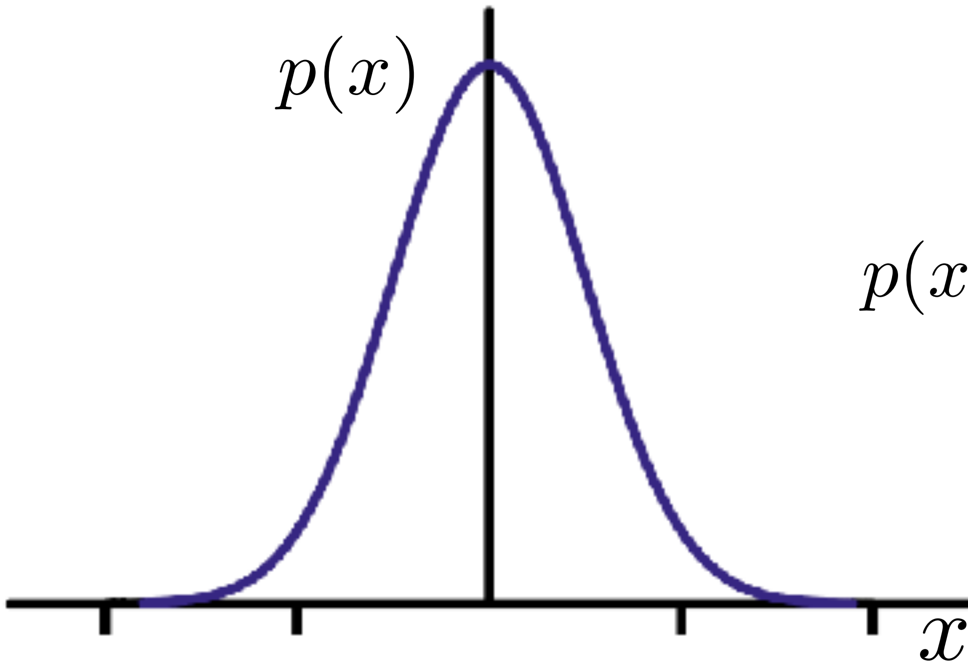
1. Sample a pair of equidistributed random numbers, $x \in [a, b]$ and $y \in [0, p_m]$.
2. If $y \leq p(x)$, accept x as the next random number, otherwise return to step 1.



Due to Von Newmann (1947).
Applicable to almost all distributions.
Can be inefficient if the area of the rectangle $[a, b] \otimes [0, p_m]$ is large compared to the area below the curve p(x)

[no exercises on that]

3) gaussian distribution



$$p(x) = \frac{1}{\sigma} \frac{1}{\sqrt{2\pi}} \; e^{-x^2/(2\sigma^2)}$$

How to produce numbers with gaussian distribution?

- Inverse transformation method: impossible

The cumulative distribution function P(x) cannot be analytically calculated!

- Rejection method: inefficient

3) gaussian distribution - Box-Muller technique

$$p(x) = \frac{1}{\sigma}\frac{1}{\sqrt{2\pi}}\ e^{-x^2/(2\sigma^2)}$$

Hint: consider the distribution in 2D instead of 1D (here $\sigma = 1$):

$$p(x)p(y)dxdy = (2\pi)^{-1}\ e^{-(x^2+y^2)/2}\ dxdy$$

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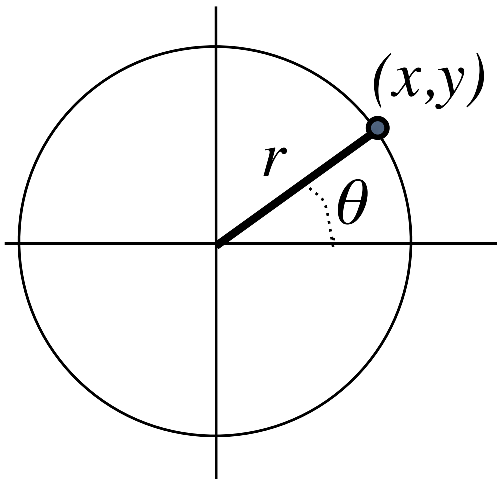
Use polar coordinates: $r = \sqrt{x^2+y^2}$, $\theta = \arctan\,(y/x)$; def.: $\rho \equiv r^2/2$



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$$\rightarrow\ dxdy = r\ dr\ d\theta = d\rho\ d\theta$$

and therefore:

$$p(x)p(y)\ dx\ dy = p(\rho,\theta)\ d\rho\ d\theta = (2\pi)^{-1}\ e^{-\rho}\ d\rho\ d\theta$$

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$$\rightarrow dxdy = r\; dr\; d\theta = d\rho\; d\theta$$

and therefore:

$$p(x)p(y)\; dx\; dy = p(\rho, \theta)\; d\rho\; d\theta = (2\pi)^{-1}\; e^{-\rho}\; d\rho\; d\theta$$

If $\begin{cases} \rho \text{ exponentially distributed} \\ \theta \text{ uniformly distributed in} [0, 2\pi] \end{cases}$ $\rightarrow$ $\begin{cases} x = r\cos\theta = \sqrt{2\rho}\cos\theta \\ y = r\sin\theta = \sqrt{2\rho}\sin\theta \\ x, y \text{ have gaussian distribution} \\ \text{with } \langle x \rangle = \langle y \rangle = 0 \text{ and } \sigma = 1 \end{cases}$

3) gaussian distribution - Box-Muller recipe #1

If $\begin{cases} \rho \text{ exponentially distributed} \\ \theta \text{ uniformly distributed in}[0, 2\pi] \end{cases} \rightarrow \begin{cases} x = r\cos\theta = \sqrt{2\rho}\cos\theta \\ y = r\sin\theta = \sqrt{2\rho}\sin\theta \\ x, y \text{ have gaussian distribution} \\ \text{with } \langle x \rangle = \langle y \rangle = 0 \text{ and } \sigma = 1 \end{cases}$

Recipe #1 (BASIC FORM):

$$\begin{cases} X, Y \ unif.\ distrib.\ in\ [0, 1[\\ \rho = -\ln(X)\ distributed\ with\ p(\rho) = e^{-\rho} \\ \theta = 2\pi Y\ distributed\ with\ (2\pi)^{-1} p_u \end{cases} \rightarrow \begin{cases} x = r\cos\theta = \sqrt{-2\ln X}\cos(2\pi Y) \\ y = r\sin\theta = \sqrt{-2\ln X}\sin(2\pi Y) \end{cases}$$

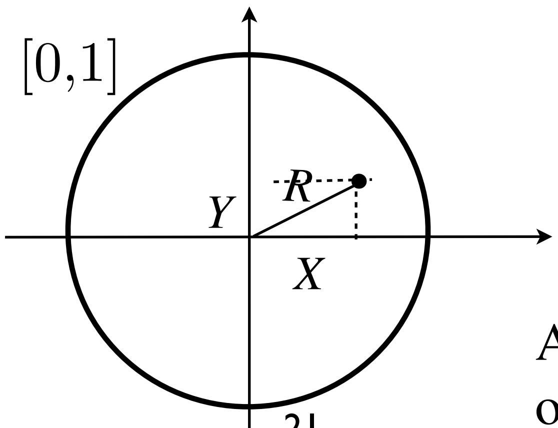
NOTE:
x, y are normally distributed and statistically independent. Gaussian variates with given variances σ_x, σ_y are obtained by multiplying x and y by σ_x and σ_y respectively

3) gaussian distribution - Box-Muller recipe #2

If $\begin{cases} \rho \text{ exponentially distributed} \\ \theta \text{ uniformly distributed in} [0, 2\pi] \end{cases}$ $\rightarrow$ $\begin{cases} x = r\cos\theta = \sqrt{2\rho}\cos\theta \\ y = r\sin\theta = \sqrt{2\rho}\sin\theta \\ x, y \text{ have gaussian distribution} \\ \text{with } \langle x \rangle = \langle y \rangle = 0 \text{ and } \sigma = 1 \end{cases}$

Recipe #2 (POLAR FORM) (implemented in **boxmuller.f90**) :

$\begin{cases} X,\ Y \text{ uniformly distributed in } [-1,1]; \\ \text{take } (X, Y) \text{ only within the unitary circle;} \\ \Rightarrow R^2 = X^2 + Y^2 \text{ is} \\ \textbf{uniformly} \text{ distributed in } [0,1] \end{cases}$ $\rightarrow$ $\begin{cases} x = \sqrt{-2\ln R^2}\ \dfrac{X}{R} \\ y = \sqrt{-2\ln R^2}\ \dfrac{Y}{R} \\ \text{since:} \\ \cos\theta = \dfrac{X}{R}, \quad \sin\theta = \dfrac{Y}{R} \end{cases}$



Advantages: avoids the calculations of sin and cos functions

Codes available on moodle

boxmuller.f90

A look at the boxmuller.f90 code

```
SUBROUTINE gasdev(rnd)
   IMPLICIT NONE
   REAL, INTENT(OUT) :: rnd
   REAL :: r2, x, y
   REAL, SAVE :: g
   LOGICAL, SAVE :: gaus_stored=.false.
   if (gaus_stored) then
      rnd=g
      gaus_stored=.false.
   else
      do
         call random_number(x)
         call random_number(y)
         x=2.*x-1.
         y=2.*y-1.
         r2=x**2+y**2
         if (r2 > 0. .and. r2 < 1.) exit
      end do
      r2=sqrt(-2.*log(r2)/r2)
      rnd=x*r2
      g=y*r2
      gaus_stored=.true.
   end if
END SUBROUTINE gasdev
```

Every two calls
uses the random number
already generated in the previous call

2 examples of optimization!

→ since: $x = \sqrt{-2\ln R^2}\,\frac{X}{R} = X\sqrt{-2\ln R^2/R^2}$

(thus avoiding the calculation of another √ to calculate R separately)

A look at the gasdev.c code

```c
#include <math.h>

float gasdev(long *idum)
{
    float ran1(long *idum);
    static int iset=0;
    static double gset;
    double fac,rsq,v1,v2;

    if (iset == 0) {
        do {
            v1=2.0*ran1(idum)-1.0;
            v2=2.0*ran1(idum)-1.0;
            rsq=v1*v1+v2*v2;
        } while (rsq >= 1.0 || rsq == 0.0);
        fac=sqrt(-2.0*log(rsq)/rsq);
        gset=v1*fac;
        iset=1;
        return (float)(v2*fac);
    } else {
        iset=0;
        return (float)gset;
    }
}
```

Every two calls
uses the random number
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2 examples of optimization!

→ since: $x = \sqrt{-2 \ln R^2} \, \frac{X}{R} = X \sqrt{-2 \ln R^2 / R^2}$

(thus avoiding the calculation of another √ to calculate R separately)

3) gaussian distribution: the central limit theorem

Consider a continuous random variable x with probability density $f(x)$.

characterized by $\langle x^m \rangle = \int x^m f(x)\, dx$ and $\sigma_x{}^2 = \langle x^2 \rangle - \langle x \rangle^2$.

Consider y s.t. y_n corresponding to the average of n values of x:

$$y = \quad y_n = \frac{1}{n}(x_1 + x_2 + \ldots + x_n)$$

Suppose that we make many measurements of y. The variable y is distributed according to a probability density $P(y) \neq f(x)$

quantities of interest are the mean $\langle y \rangle$, the variance $\sigma_y{}^2 = \langle y^2 \rangle - \langle y \rangle^2$, and $P(y)$ itself.

3) gaussian distribution: the central limit theorem

The random variable:

$$y = \quad y_n = \frac{1}{n}(x_1 + x_2 + \ldots + x_n)$$

is distributed according to:

$$P(y): \ \text{gaussian distribution}$$

with:

$$<y> = <x> \qquad\qquad \sigma_y \approx \sigma_x / \sqrt{n}$$

(Therefore, the sample mean of a random sample is better than a single observation)

$$provided\ \langle x \rangle\ and\ \langle x^2 \rangle\ exist\ (finite)\ and\ n\ is\ large!$$

3) gaussian distribution: the central limit theorem

Analogously, is instead of considering the new random variable as the **average** we consider just the **sum:**

$$y = x_1 + x_2 + \ldots + x_n$$

it also has a gaussian distribution but with:

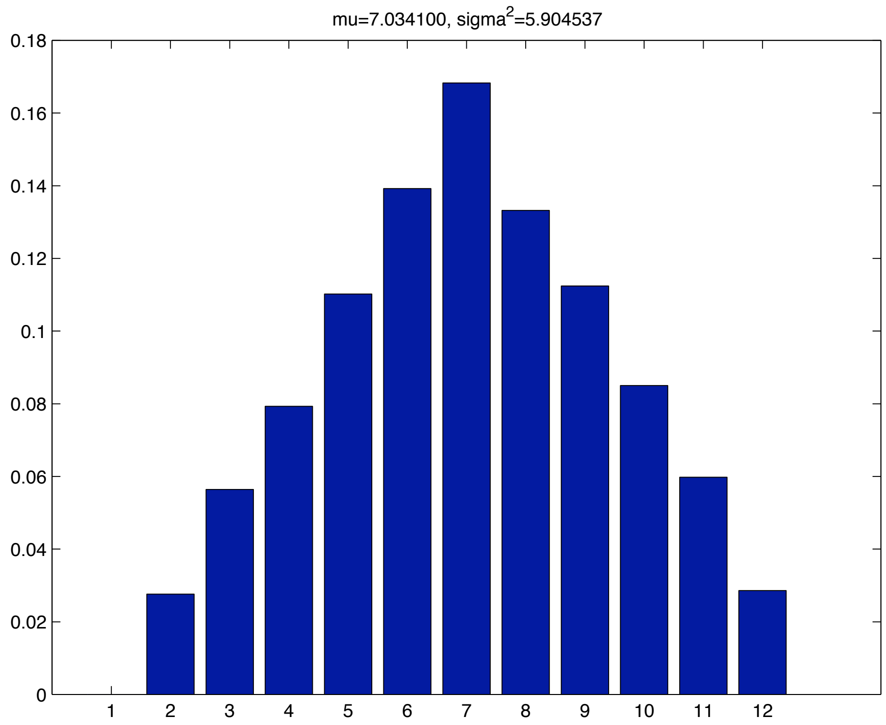
$$< y > = n < x > \quad \text{and} \quad \sigma_y \approx \sqrt{n}\ \sigma_x$$

$$provided\ \langle x \rangle\ and\ \langle x^2 \rangle\ exist\ (finite)\ and\ n\ is\ large!$$

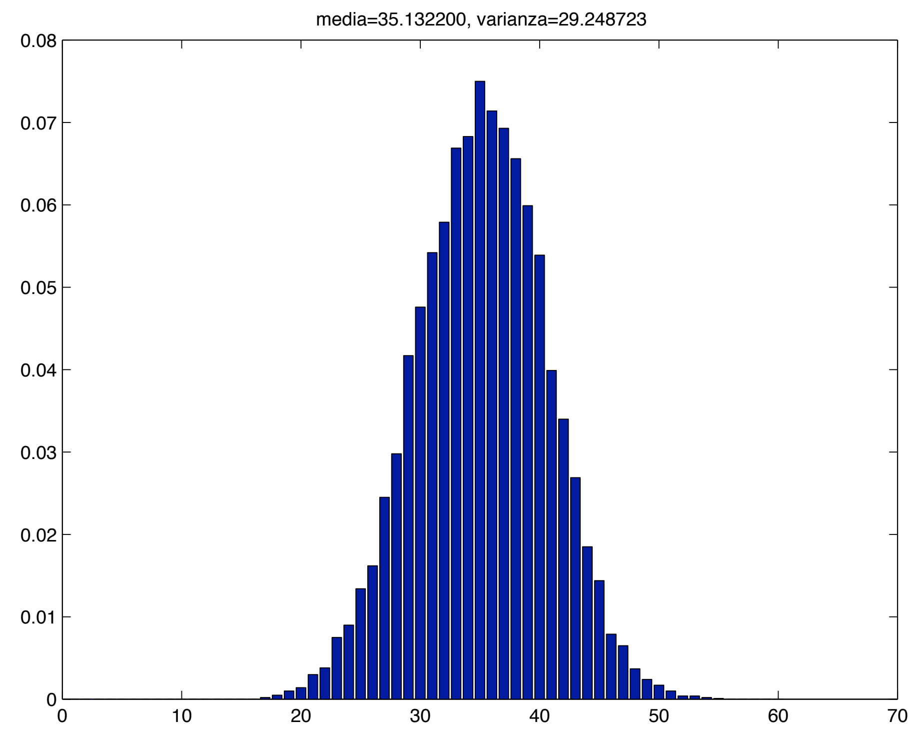
3) gaussian distribution: the central limit theorem

Note: large enough n needed to obtain the gaussian distribution.
Suppose that f(x) is uniform: e.g., playing dice:

n=2 not enough



n=100 OK



3) gaussian distribution: the central limit theorem

The previous example was for UNIFORM distribution (dice)
but the central limit theorem work also with random deviates x
with NON UNIFORM distribution; e.g. with exponential distribution:

$$f(x) = \begin{cases} e^{-x}, & \text{if } x \geq 0 \\ 0, if & x < 0\ . \end{cases}$$

???

the central limit theorem

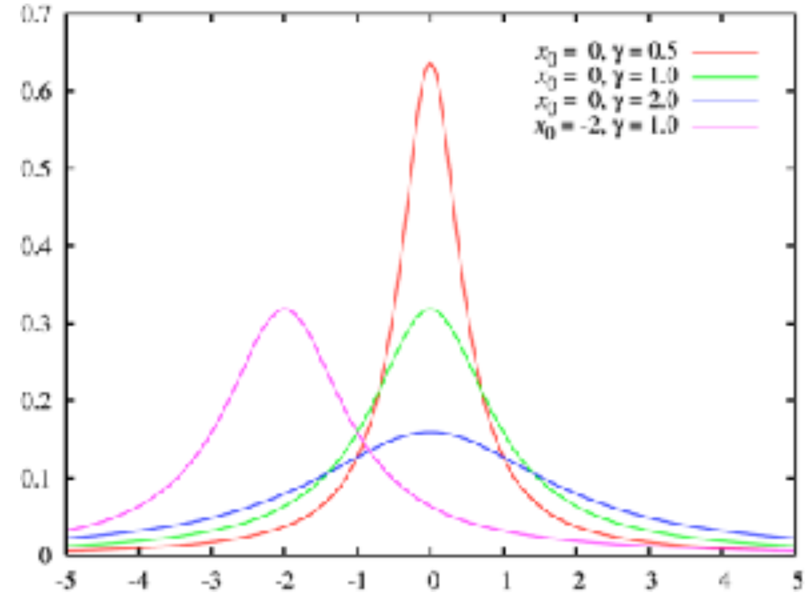
...but sometimes it doesn't work:

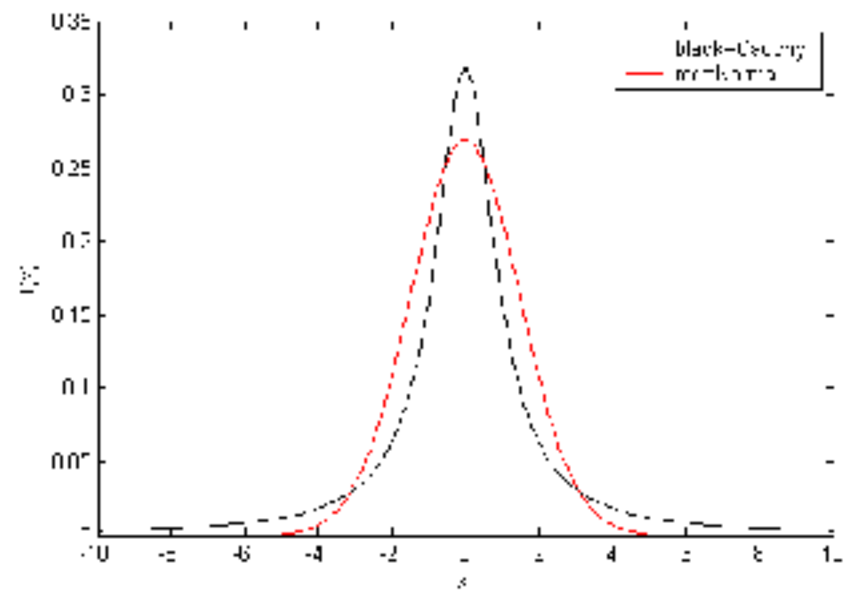
Cauchy-Lorentz

probability density function

$$f(x; x_0, \gamma) = \frac{1}{\pi\gamma\left[1 + \left(\frac{x - x_0}{\gamma}\right)^2\right]}$$

$$= \frac{1}{\pi}\left[\frac{\gamma}{(x - x_0)^2 + \gamma^2}\right]$$





The Cauchy-Lorentz distribution is an example of "fat-tailed" distribution.

Fat-tailed distributions decay to infinity slower than exponentially.

For instance, they can decay with a power law: $f(x) \sim x^{-(1+\alpha)}$ as $x \longrightarrow +\infty$

In some cases the expression "fat-tailed" indicates distributions where $0 < \alpha < 2$.

???

the central limit theorem

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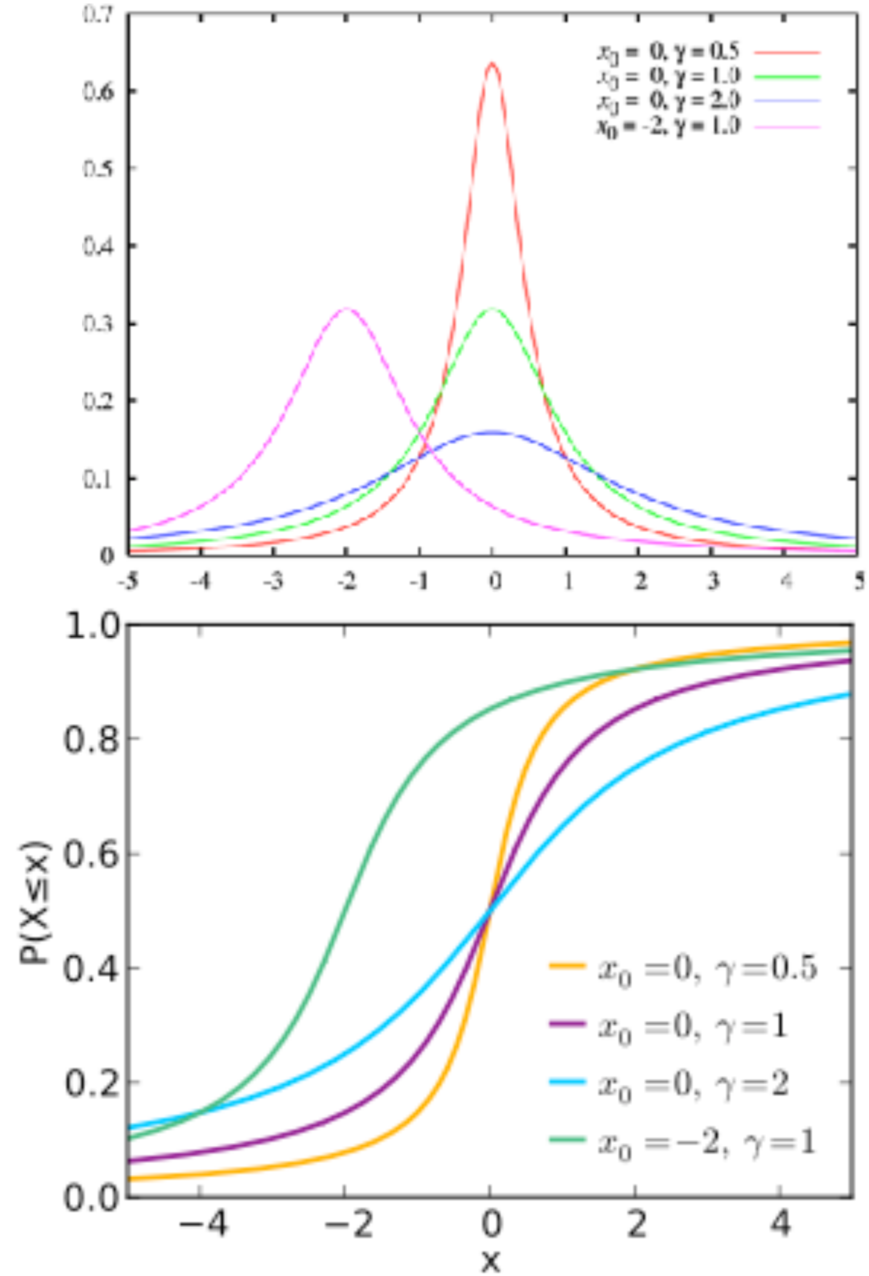
Cauchy-Lorentz

probability density function

$$f(x; x_0, \gamma) = \frac{1}{\pi\gamma\left[1 + \left(\frac{x-x_0}{\gamma}\right)^2\right]}$$

$$= \frac{1}{\pi}\left[\frac{\gamma}{(x-x_0)^2 + \gamma^2}\right]$$

Cumulative distribution : $\frac{1}{\pi}\arctan\left(\frac{x-x_0}{\gamma}\right) + \frac{1}{2}$



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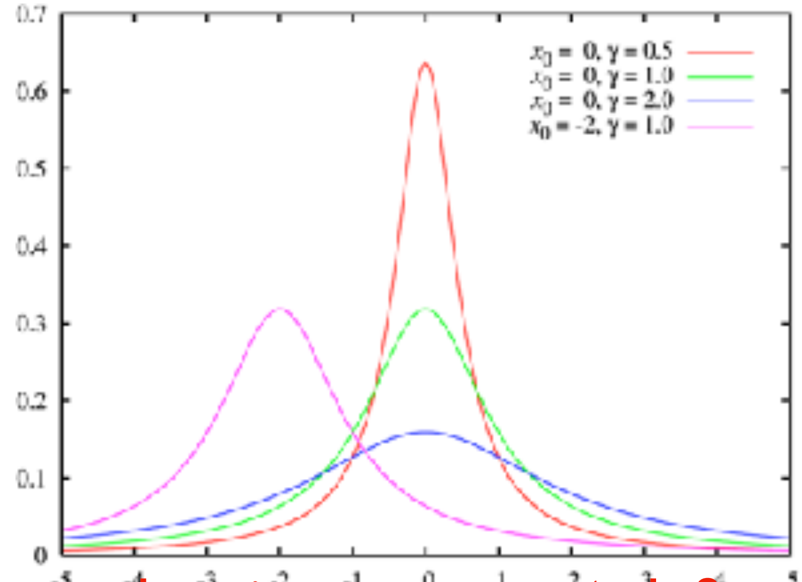


Mean and variance are **not** defined

The mean: $\int_{-\infty}^{\infty} x f(x)\, dx$ which can be rewritten as: $\int_{0}^{\infty} x f(x)\, dx - \int_{-\infty}^{0} |x| f(x)\, dx$

$(here\ for\ x_0 = 0)$

is not defined since both terms are infinite; only the Cauchy principal value is defined:

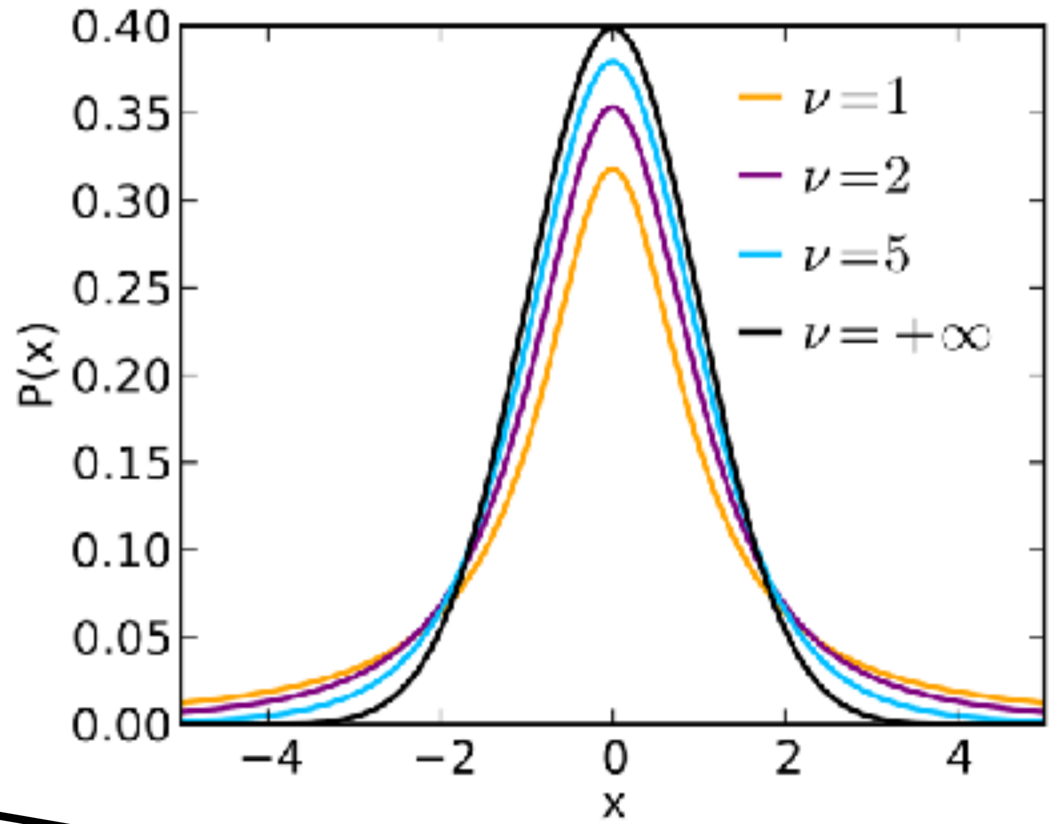
$$\lim_{a \to \infty} \int_{-a}^{a} x f(x)\, dx$$

Without a defined mean, it is impossible to define the variance (but the second moment is defined and it is infinite). Some results in probability theory about expected values, such as the law of large numbers, do not work in such cases.

Also, the mean of a set of random variates drawn from a Cauchy distribution is no better than a single observation, because the chance of including extreme values is high.

Student's *t*-distribution

(più generale)



$$f(t_n) = \frac{\Gamma\left(\frac{n+1}{2}\right)}{\sqrt{\pi n}\,\Gamma\left(\frac{n}{2}\right)} \cdot \left(1 + \frac{t^2}{n}\right)^{-\frac{n-1}{2}}$$

$$\lim_{n\to\infty}\left(1+\frac{t^2}{n}\right)^{-\frac{n+1}{2}} \sim \frac{1}{t^{-(n+1)}}$$

Notiamo che il limite di questa successione di funzioni per $n \to \infty$ è

$$\lim_{n\to\infty} f(t_n) = \frac{1}{\sqrt{\pi}} \lim_{n\to\infty} \frac{\Gamma\left(\frac{n+1}{2}\right)}{\sqrt{n}\,\Gamma\left(\frac{n}{2}\right)} \lim_{n\to\infty}\left(1+\frac{t^2}{n}\right)^{-\frac{n+1}{2}} = \frac{1}{\sqrt{2\pi}} e^{-\frac{t^2}{2}}.$$

Varianza	$\frac{n}{n-2}$ se $n > 2$ infinita altrimenti

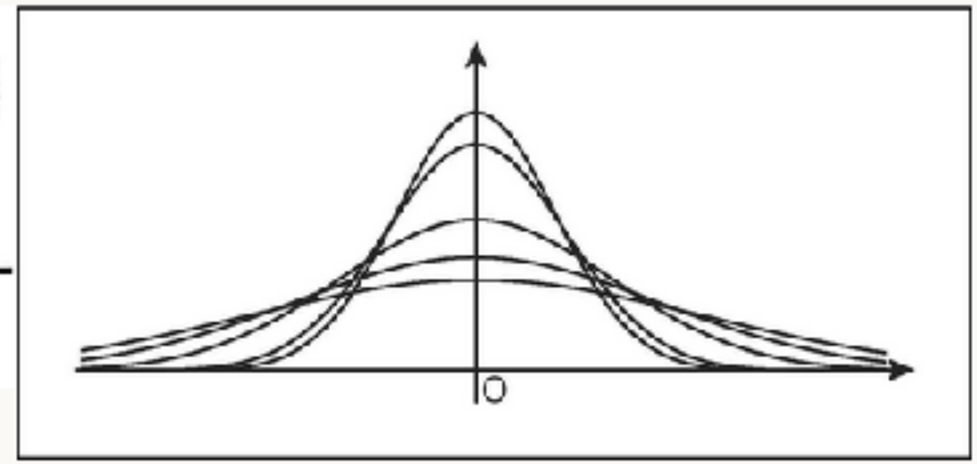
Sapendo che il primo limite ha come risultato $\frac{1}{\sqrt{2}}$ e il secondo tende a $e^{-\frac{t^2}{2}}$.

In pratica, prendendo una popolazione di numerosità N molto grande, la variabile aleatoria t tende ad essere una normale standard.

Curtosi (dal greco *kurtós*, gobba) in statistica, termine che indica quanto una distribuzione di dati si allontani da una curva normale standardizzata (cioè se è, rispetto a questa, per la quale l'indice è 0, più "schiacciata" o meno "schiacciata"). L'*indice di curtosi* per una distribuzione discreta X di n elementi è dato da:

$$Curt(x) = \frac{\sum_{1}^{n} (x_i - \mu)^4}{n\sigma^4}$$

formula

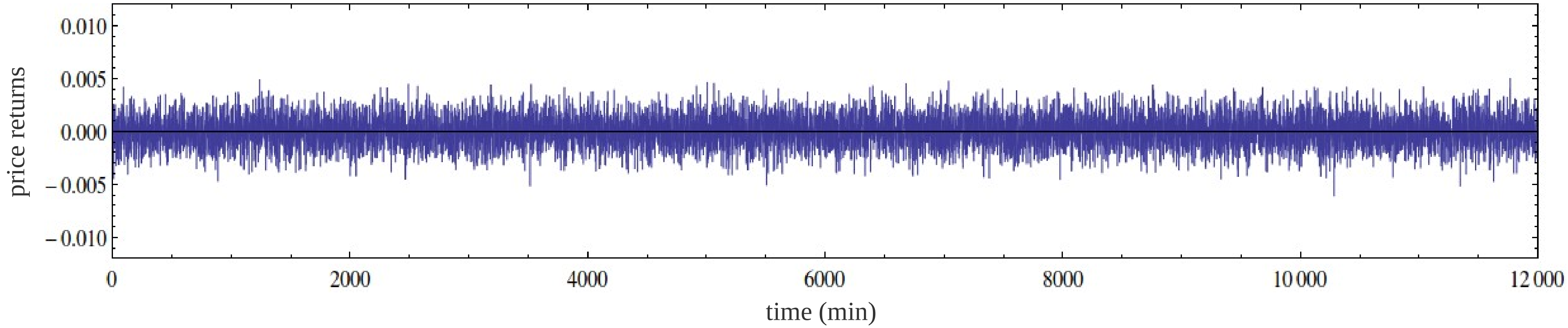


CURTOSI

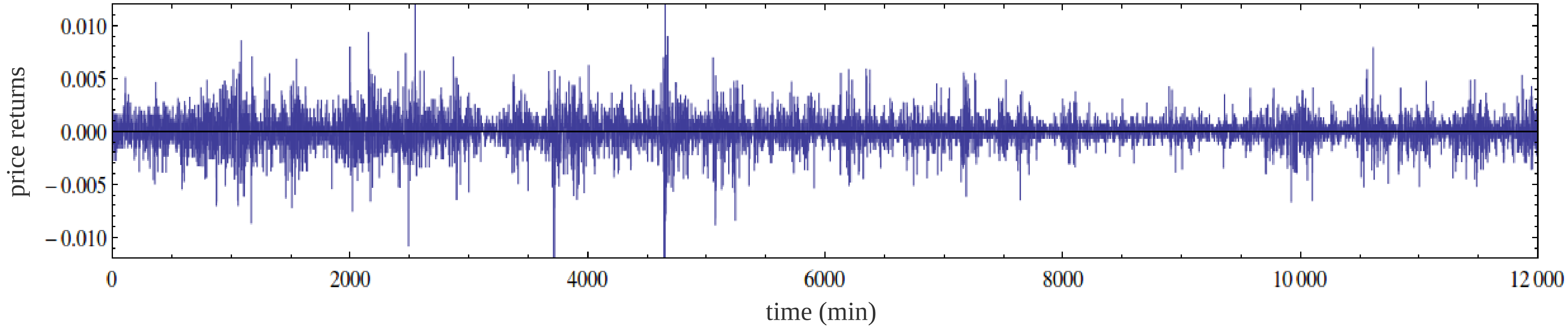
… a short digression …

Statistical Properties of Price Returns

Simulated Returns (Geometric Brownian Motion)



Real Returns (Financial Time-Series)



Cont, *Empirical properties of asset returns, stylized facts and statistical issues*, 2001

Statistical Properties of Price Returns

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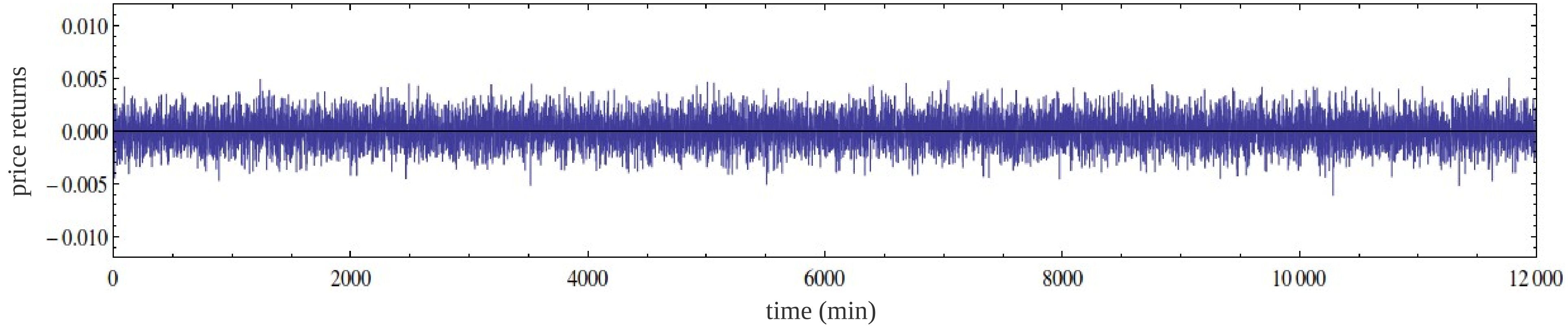
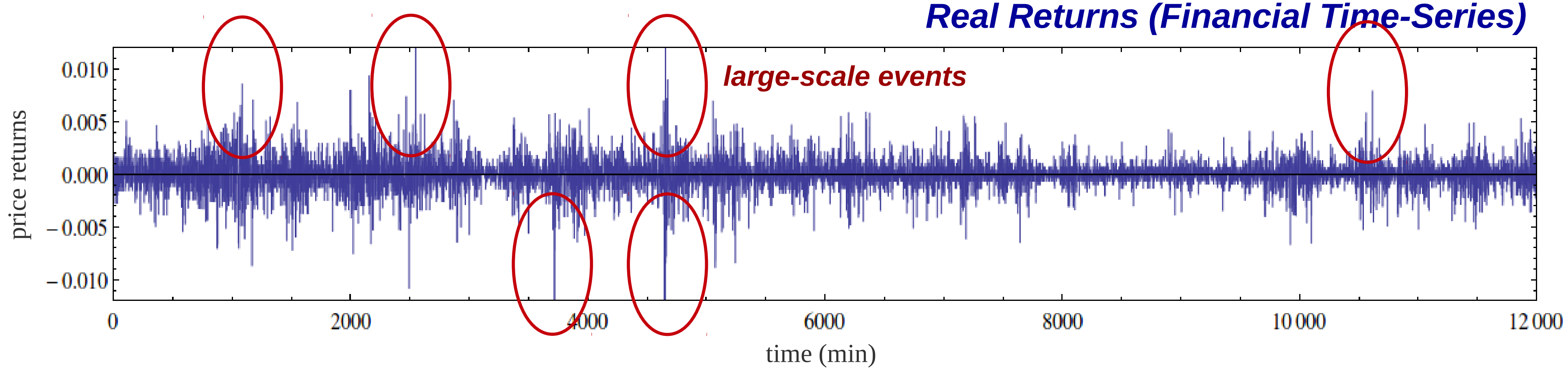


Real Returns (Financial Time-Series)



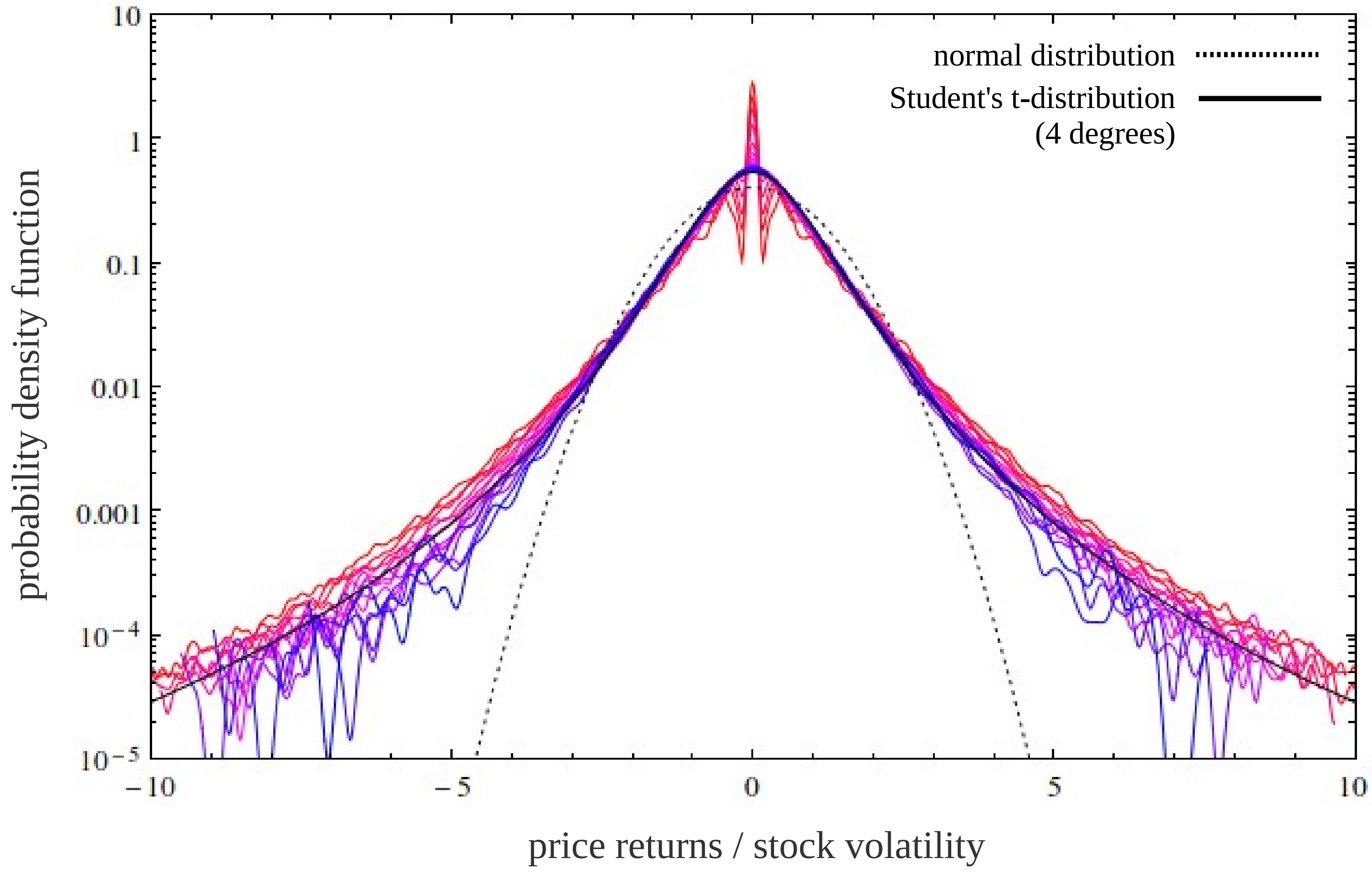
1st issue

Price returns are not normal

Cont, *Empirical properties of asset returns, stylized facts and statistical issues*, 2001

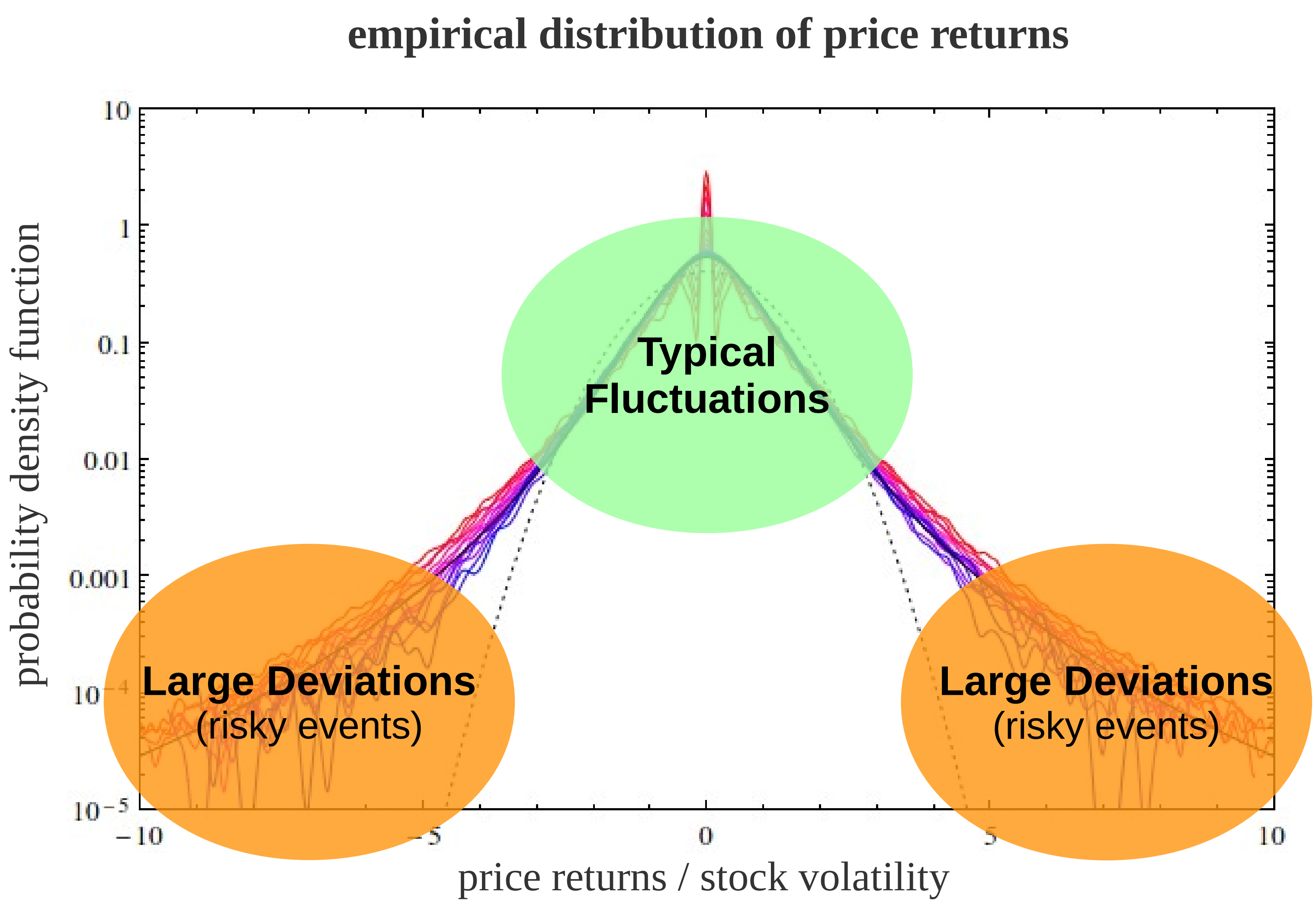
Empirical Distribution of Price Returns

Empirical Distribution of Returns (superposition of all stocks)
different time-scales – from **1 minute** to **2 hours**



Filiasi, *PhD Thesis*
Cont, Empirical properties of asset returns, stylized facts and statistical issues, 2001

Empirical Distribution of Price Returns



Filiasi, *PhD Thesis*
Cont, Empirical properties of asset returns, stylized facts and statistical issues, 2001

Part II - Using random numbers to simulate random processes

Random processes: radioactive decay

$N(t)$ Atoms present at time t

λ Probability for each atom to decay in Δt

$\Delta N(t)$ Atoms which decay between t and $t + \Delta t$

$$\Delta N(t) = -\lambda N(t) \Delta t$$

we use the probability λ of decay of each atom to simulate the behavior of the number of atoms left; we should be able to obtain (on average):

$$N(t) = N(t = 0) e^{-\lambda t}$$

Radioactive decay: numerical simulation

A scheme for the simulation

1. Assign a value to the decay constant $\lambda \leq 1$ (the probability for each nucleus to decay in a given interval of time Δt)
   λ establishes the time scale; one iteration in the "do loop" corresponds to one time step Δt

2. Start with **Nleft** = **Nstart**= total number of nuclei at time $t = 0$

3. Basic algorithm: **for each nucleus** left (not yet decayed):
   - Generates a random number $0 \leq x \leq 1$
   - if $x \leq \lambda$, the nucleus decays and **Nleft** = **Nleft - 1**, otherwise it remains and **Nleft** is unchanged.

4. Repeat for each nucleus

5. Repeat the cycle for the next time step

Note: unbounded loop

```
DO                                        ! loop on time
  DO  i = 1, nleft                        ! loop on all the nuclei left
    call random_number(r)
    IF (r <= lambda) THEN                 ! BASIC   ALGORITHM
      nleft = nleft - 1                   !  update the nuclei left (*)
    ENDIF
  END DO
WRITE (unit=7,fmt=*) t , nleft
  if (nleft == 0) exit
  t = t + 1
END DO
```

Note: "exit" ≠ "cycle"

(*) Notice that the upper bound of the inner loop (nleft) is changed within the execution of the loop; but with most compilers, in the execution the **loop** goes on up to the **initial value of the upper bound** (nleft); this ensures that the implementation of the algorithm is correct. The program checkloop.f90 is a test for the behavior of the loop. Look also at decay_checkloop.f90. If nleft would be changed (decreased) during the execution, the effect would be an overestimate of the decay rate. CHECK with your compiler!

Programs:

decay.f90
decay_checkloop.f90

checkloop.f90

Details on Fortran: unbounded loops

```
[name:] DO
        exit [name]

or [name:] DO
        END DO [name]
```

(name is useful in case of nested loops for explicitly indicating which loop we exit from)

Alternative form: "do while" loop

Always set a condition to exit from a loop! E.g.:

```
DO
 if (condition)exit
END DO
```

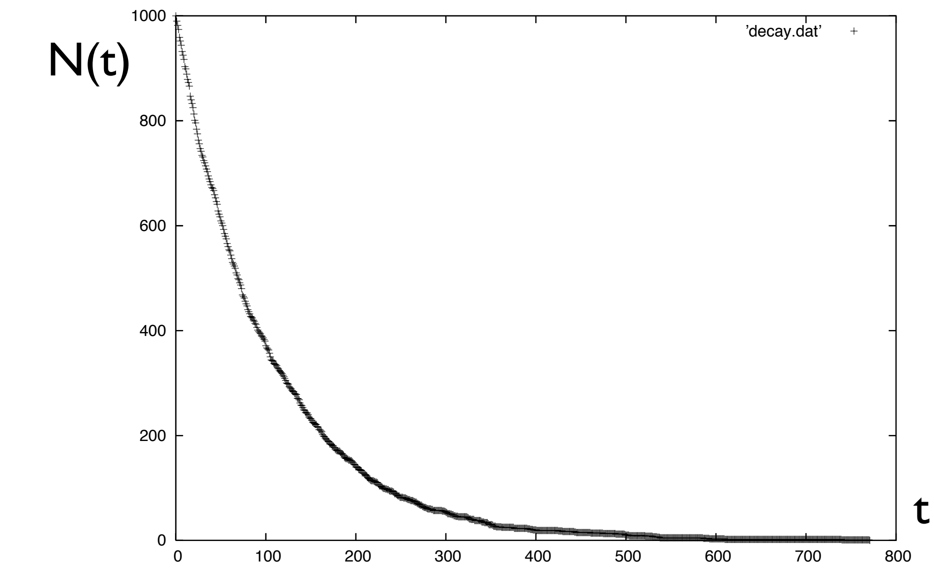
or:

```
DO WHILE (.not. condition)
 ...
END DO
```

NOTE: first is better ("if () ..exit" can be placed everywhere in the loop, whereas DO WHILE must execute the loop up to the end)

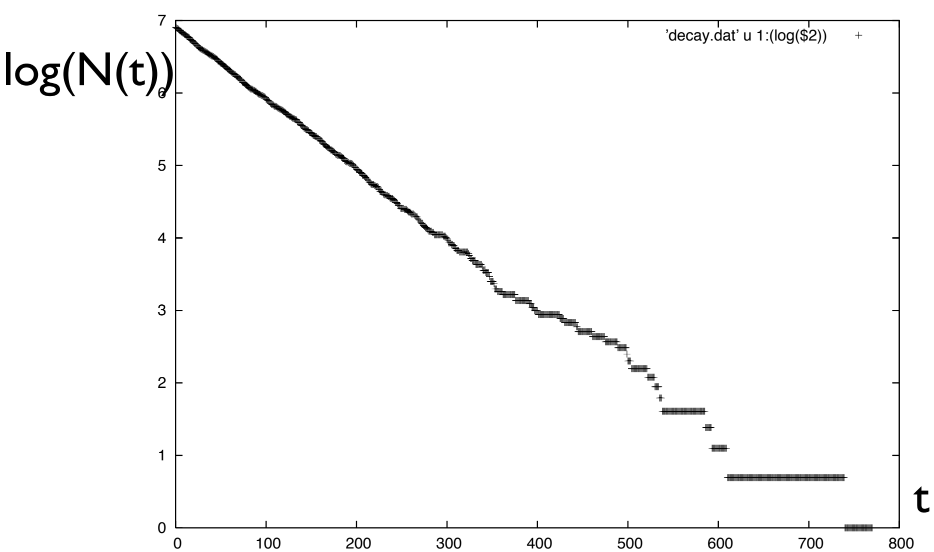
- Additional note:
Difference between EXIT and CYCLE

Radioactive decay:
results of numerical simulation



results of decay simulation (N vs t) with N=1000

$N(t) \sim N_0 \exp(- a\ t)$

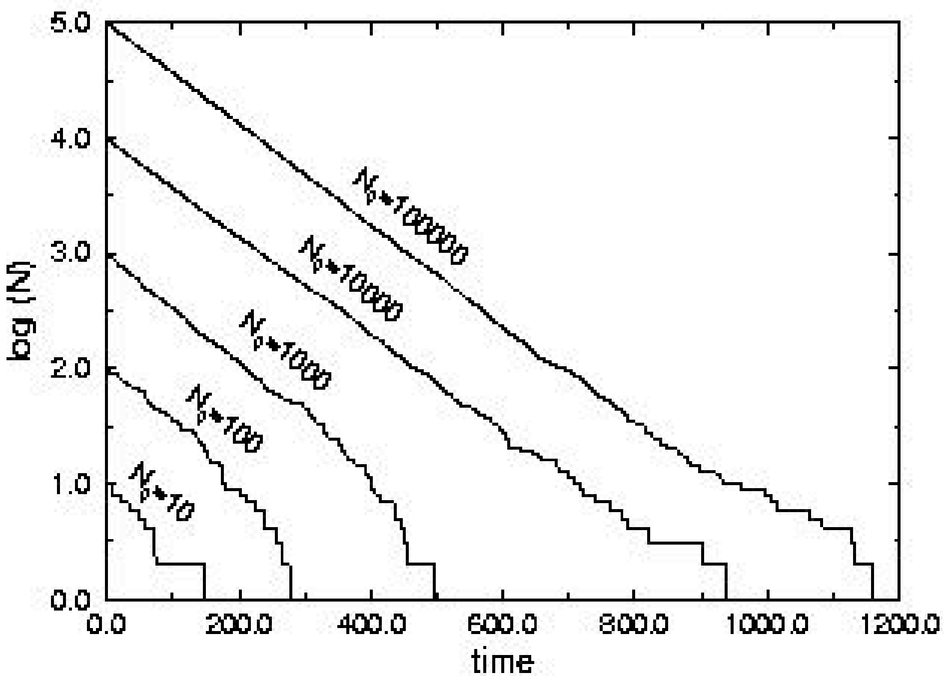


semilog plot (log(N) vs t)

=> $\log(N(t)) = \log N_0 - a\ t$

=> slope is $-a$

Radioactive decay:
results of numerical simulation



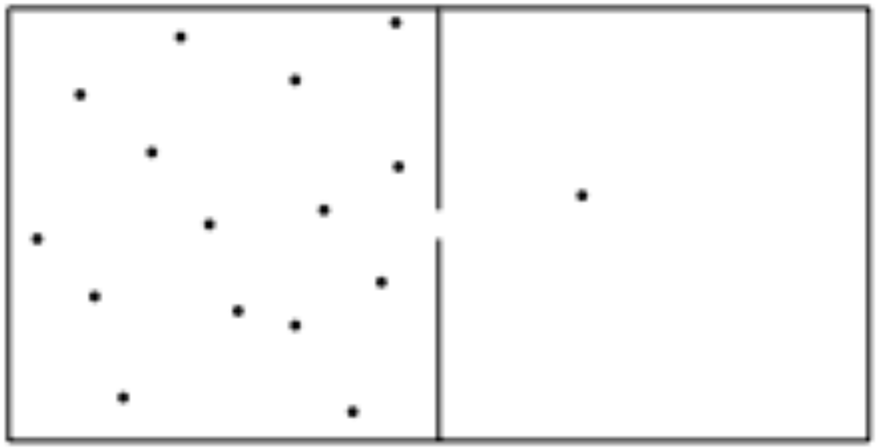
Semilog plots of the results of simulations for the same decay rate and different initial number of atoms: almost a straight line, but with important deviations (stochastic) for small N

Stochastic simulations give reliable results when obtained:

- on average and for large numbers
- fine discretisation of time evolution

(in the exercise: change λ; compare the value obtained from the simulation with the one inserted; does the "quality" of the results change with λ?)

Other random processes: order and disorder

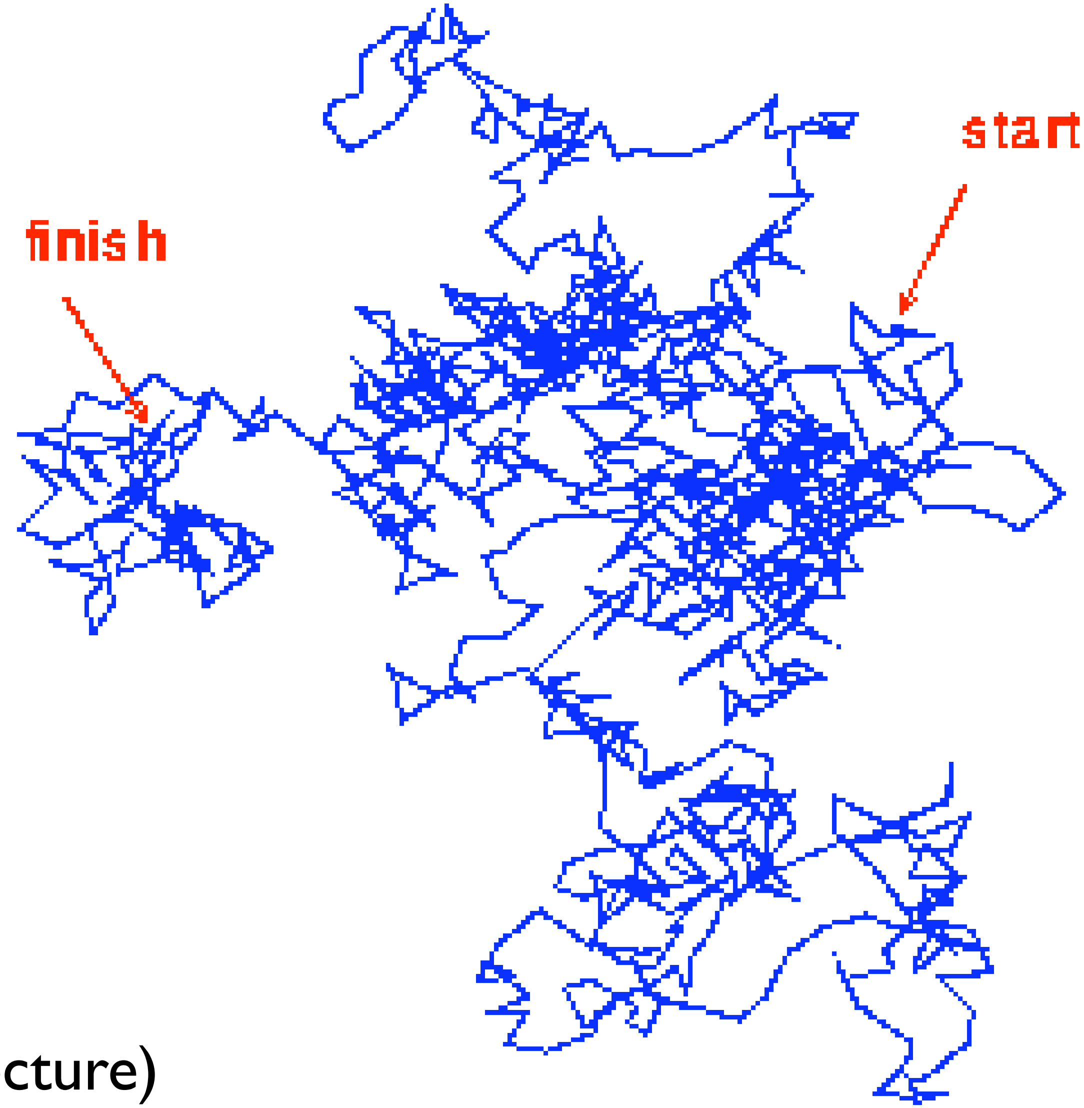


A box is divided into two parts communicating through a small hole. One particle randomly can pass through the hole per unit time, from the left to the right or viceversa.

$N_{left}(t)$: number of particles present at time t in the left side
Given $N_{left}(0)$, what is $N_{left}(t)$?

(more on that in a future Lecture)

Other random processes: random walks



(see next lecture)

miscellanea

list of EXERCISES;
more on fortran90,
fit, gnuplot…

LIST OF EXERCISES V week

Random numbers with non uniform distributions

1) exponential distribution generated with Inverse Transformation Method

2) another distribution generated with ad-hoc algorithms (compare!), including Inverse Transformation Method

3) gaussian distribution generated with Box-Muller algorithm

4) gaussian distribution generated with the central limit theorem

5) other random distributions (different algorithms, subroutines from the web…). [optional]

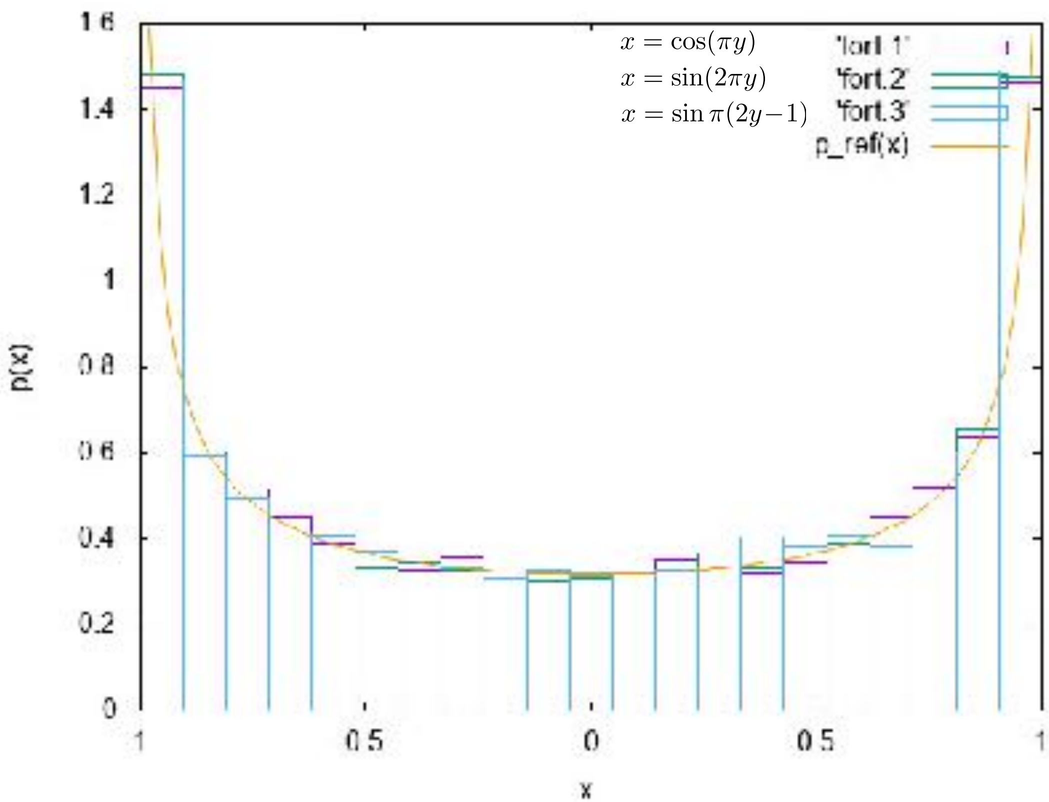
To do: implementation of the algorithms (or understanding…), histogram, fit…

Making histograms: use int() or similar intrinsic functions?

e.g. Ex. 2:

Suppose you want to generate a random variate x in (-1,1) with distribution

$$p(x) = \frac{1}{\pi}(1-x^2)^{-1/2}.$$



$$y = P(x) = \int_{-1}^{x} \frac{1}{\pi}(1-x^2)^{-1/2}\, dx$$

$$= \frac{1}{\pi}\arcsin(x)\,|_{-1}^{x} = \frac{1}{\pi}\arcsin(x) + \frac{1}{2}$$

and invert…

Here:
different histograms, from distributions generated with different algorithms

=> how to do these histograms?

Making histograms: use int() or similar intrinsic functions?

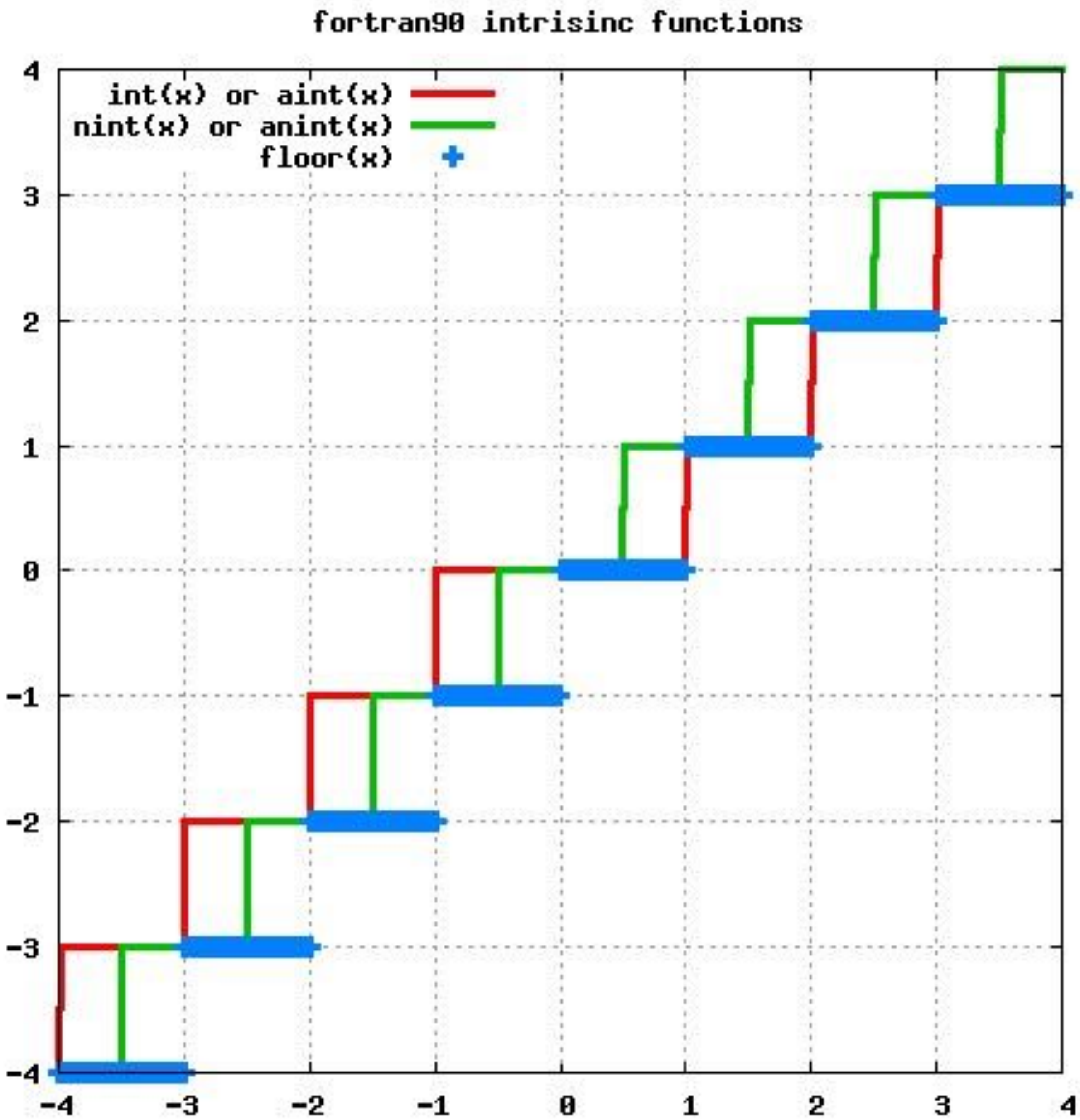
AINT(A[,KIND])
· Real elemental function
· Returns A truncated to a whole number. AINT(A) is the largest integer which is smaller than |A|, with the sign of A. For example, AINT(3.7) is 3.0, and AINT(-3.7) is -3.0.
· Argument A is Real; optional argument KIND is Integer

ANINT(A[,KIND])
· Real elemental function
· Returns the nearest whole number to A. For example, ANINT(3.7) is 4.0, and AINT(-3.7) is -4.0.
· Argument A is Real; optional argument KIND is Integer

FLOOR(A,KIND)
· Integer elemental function
· Returns the largest integer $\leq$ A. For example, FLOOR(3.7) is 3, and FLOOR(-3.7) is -4.
· Argument A is Real of any kind; optional argument KIND is Integer
· Argument KIND is only available in Fortran 95

INT(A[,KIND])
· Integer elemental function
· This function truncates A and converts it into an integer. If A is complex, only the real part is converted. If A is integer, this function changes the kind only.
· A is numeric; optional argument KIND is Integer.

NINT(A[,KIND])
· Integer elemental function
· Returns the nearest integer to the real value A.
· A is Real


fortran90 intrisinc functions
int(x) or aint(x)
nint(x) or anint(x)
floor(x)
4
3
2
1
0
-1
-2
-3
-4
-4
-3
-2
-1
0
1
2
3
4

Example: fit using gnuplot - I

Suppose you want to fit your data (say, ‘data.dat’) with an exponential function.
You have to give: 1) the functional form ; 2) the name of the parameters

gnuplot> f(x) = a * exp (-x*b)

Then we have to recall these informations together with the data we want to fit:
it can be convenient to inizialize the parameters:
gnuplot> a=0. ; b=1. (for example)

gnuplot> fit f(x) 'data.dat' via a,b

On the screen you will have something like:

```
Final set of parameters Asymptotic Standard Error
======================= ===========================

a = 1 +/- 8.276e-08 (8.276e-06%)
b = 10 +/- 1.23e-06 (1.23e-05%)

correlation matrix of the fit parameters:

a b
a 1.000
b 0.671 1.000
```

It’s convenient to plot together the original data and the fit:

gnuplot> plot f(x), 'data.dat'

Example: fit using gnuplot - II

If you prefer to use linear regression, **use logarithmic data in the data file**, **or** directly fit the log of the original data using **gnuplot:**

gnuplot> f(x) = a + b*x

Then we have to recall these informations together with the data we want to fit (in the following example: x=log of the first column; y=log of the second column):

gnuplot> fit f(x) 'data.dat' u (log($1)):(log($2)) via a,b

```
...
 Final set of parameters Asymptotic Standard Error
 ======================= ==========================  (...gnuplot will work for you....)
...
```

Also in this case it will be convenient to plot together the original data and the fit:

gnuplot> plot f(x), 'data.dat' u (log($1)):(log($2))

In case of needs, we can limit the set of data to fit in a certain range **[x_min:x_max]**:

gnuplot> fit [x_min:x_max] f(x) 'data.dat' u ... via ...

A few notes on Fortran

related to the exercises

Intrinsic functions:

LOGARITHM

log returns the natural logarithm

log10 returns the common (base 10) logarithm

(NOTE: also in **gnuplot, log** and **log10** are defined with the same meaning)

INTEGER PART

nint(x) and the others, similar but different (see Lect. II) => ex. II requires histogram for negative and positive data values

Arrays:

possible to label the elements from a negative number or 0:

dimension array(-n:m) (e.g., useful for making histograms)

[default in Fortran: n=1; in c and c++: n=0]

Array dimension:

default : dimension array([1:]n)
but also using other dimensions e.g.:   dimension array(-n:m)

Important to **check dimensions** of the array when compiling or during execution !
If not done, it is difficult to interpret error messages (typically: "segmentation fault"),   or even possible to obtain unpredictable results!

Default in gfortran:
boundaries not checked; use **compiler option**:

gfortran -fcheck=bounds myprogram.f90
(obsolete but still active alternative: -fbounds-check)

Typing (Unix line command):
man gfortran
you can scroll the manual pages and see the possible compilation options

Some Fortran compiler options

-fcheck=bounds enables checking for array subscript expressions

-fbacktrace generate extra information to provide source file traceback at run time
Specify that, when a runtime error is encountered or a deadly signal is emitted (segmentation fault, illegal instruction, bus error or floating-point exception), the Fortran runtime library should output a backtrace of the error. This option only has influence for compilation of the Fortran main program.

-Wall Enables commonly used warning options

…

Structure of a main program with one function or subr.

```
program name_program            (see: expdev.f90 or boxmuller.f90)
  implicit none  (*)
 <declaration of variables>
 <executable statements>

contains
   subroutine ...  (or function)
    ...
    end subroutine

end program
```

(*) General suggestion for variable declaration:

Use “implicit none” + explicit declaration of variables

See also the use of **module**

Other programs:

(optional, but useful!)

random.f90 (is a module - generation of rnd with different distributions)

t_random.f90 (main test program)

to compile:

$gfortran random.f90 t_random.f90
(the module first!)

or in more than one step:
Compile the module with the option -c: this produces .mod and .o (the objects):
gfortran -c *random.f90*

Compile the main program:

gfortran -c *t_random.f90*

*Finally you link all the files *.o and produce the executable:*

gfortran -o a.out *random.o t_random.o*