993SM - Laboratory of Computational Physics lecture 3 - part 1 March 25, 2020

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past week:

3. Intrinsic generators

(b) For a quantitative test of *uniformity* consider the moment of order k:

$$\langle x^k \rangle^{calc} = \frac{1}{N} \sum_{i=1}^{N} x_i^k; \qquad \langle x^k \rangle^{th} = \int_0^1 dx\ x^k\ P(x)$$

For the uniform distribution $p_u(x)$ in [0,1[, i.e. for

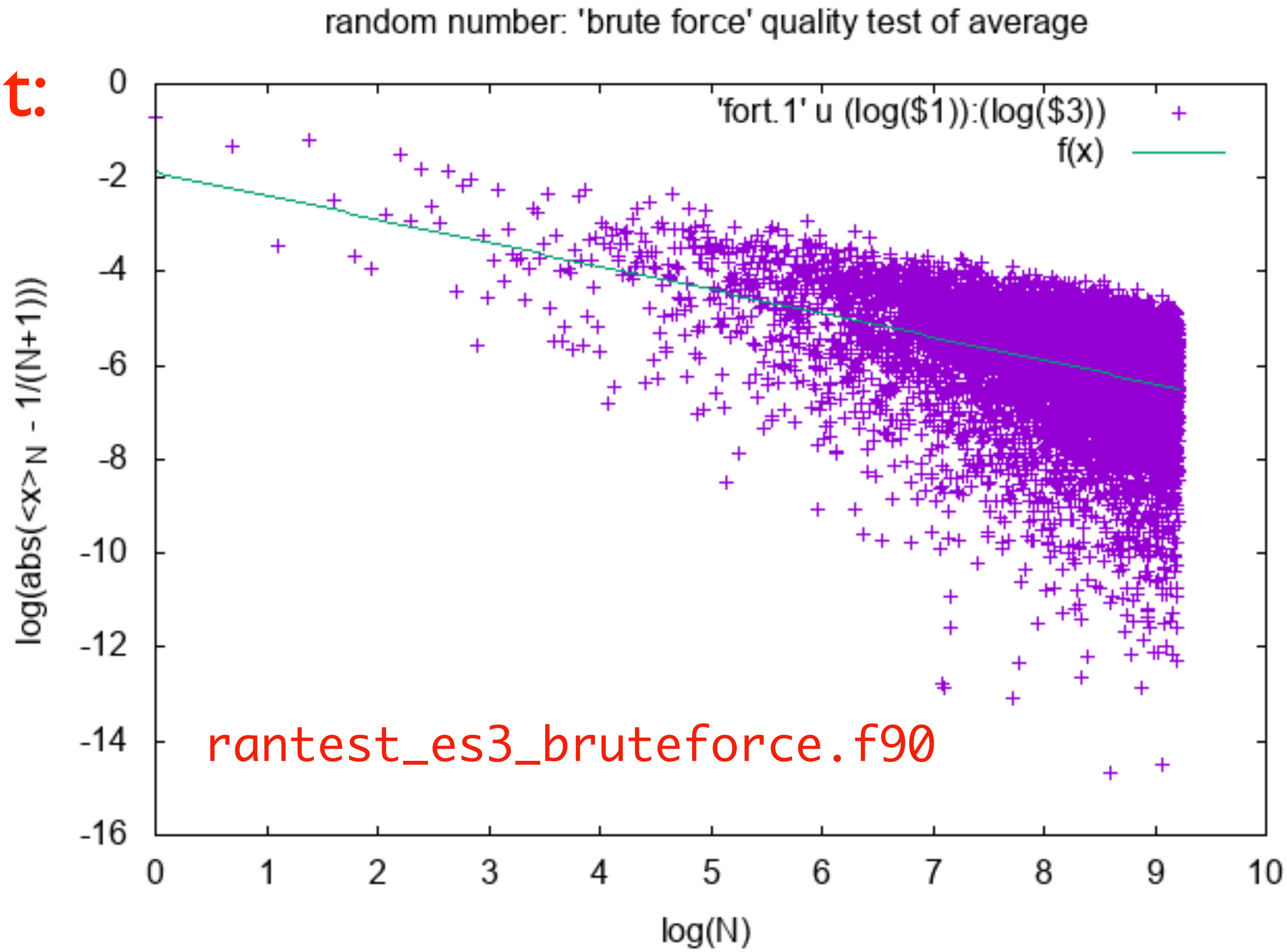
$$p_u(x) = \begin{cases} 1\ for\ 0 \leq x \leq 1 \\ 0\ outside \end{cases}$$

we have $\langle x^k \rangle^{th} = 1/(k+1)$. Consider the error

$$\Delta_N(k) = \left| \langle x^k \rangle^{calc} - \langle x^k \rangle^{th} \right| = \left| \frac{1}{N} \sum_{i=1}^{N} x_i^k - \frac{1}{k+1} \right|$$

for the expected moment of order k and study its asymptotic behaviour for large N. If the behaviour is $\sim 1/\sqrt{N}$, then the distribution is random and uniform. Do the test for k=1, 3, 7, and N=100, 10.000, 100.000.

A “brute force” test: Do several sequences of different length



rantest_es3_bruteforce.f90

```
…
do i=1,N
allocate (rnd(i))

call random_number(rnd)  ! generate a new sequence of "i" random numbers
                         ! (seed changes automatically)
somma = sum(rnd**k)  <= this sum() corresponds to an internal loop (nested loops)
write(1,*)i,somma/i, abs(somma/i - 1./(k+1))
! somma/i is the PARTIAL sum of the sequence for the momentum k
deallocate(rnd)

end do
```

ok, but time consuming…

how to calculate the sum of the series for increasing N?

no need of recalculating again the sum from scratch; print out **partial** sums:

rantest_es3_simplest.f90

```
implicit none
integer :: N, i, k
real :: sum
real, dimension (:), allocatable :: rnd

print*,' Insert how many random numbers >'
read(*,*)N
allocate (rnd(N))
call random_number(rnd)

print*,' Insert the order of momentum >'
read(*,*)k

sum = 0.

open (unit=1,file='momentumk.dat')

do i=1,N
sum = sum + rnd(i)**k
write(1,*)i,sum/i, abs(sum/i - 1./(k+1))
! sum/i is the PARTIAL sum of the sequence for the momentum k
end do
```

print out the result as a function of "i"

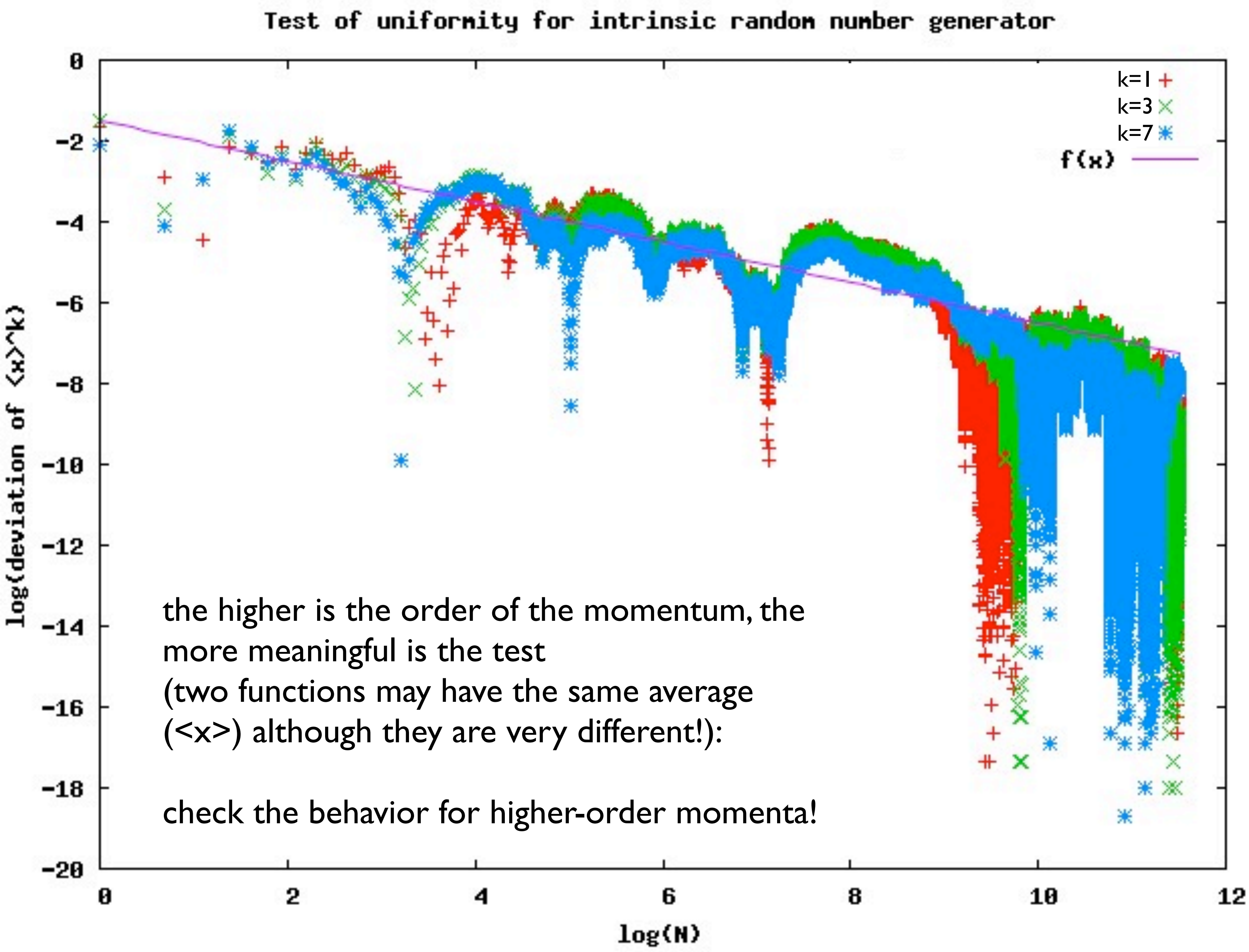
Test on one sequence, several momenta

rantest_es3_simple.f90

```
…
allocate (rnd(N))
call random_number(rnd)
…
allocate(sum(kmax))
..
sum = 0.

do k = 1, kmax  ! Loop for the different momenta

do i=1,N
sum(k) = sum(k) + rnd(i)**k
write(klabel,*)i, sum(k)/i, abs(sum(k)/i - 1./(k+1))
! sum(k)/i is the PARTIAL sum of the sequence for the momentum k
end do ! I

close(klabel)
end do ! k
```

also here print the results as a function of “i”

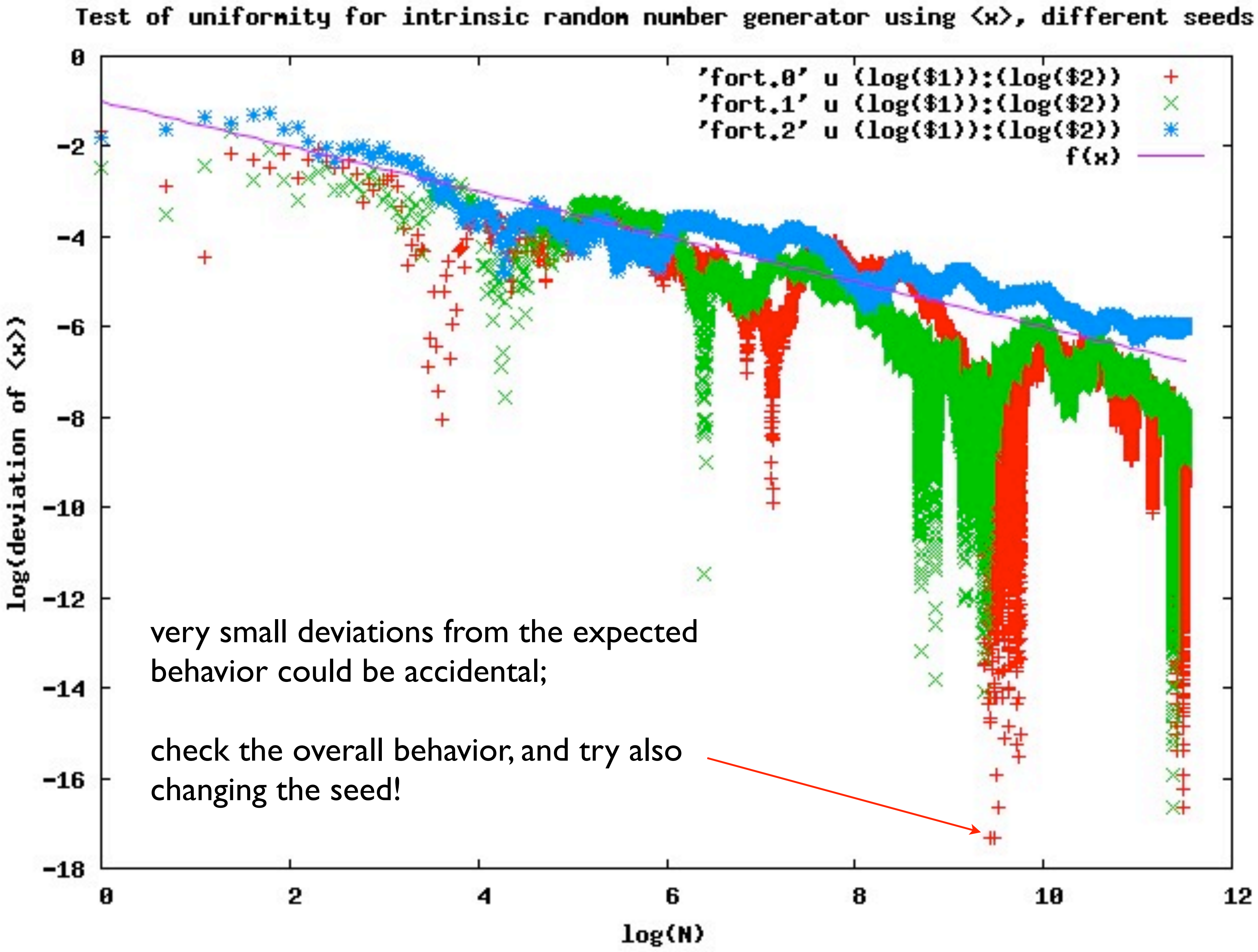
Test on one sequence, several momenta



the higher is the order of the momentum, the more meaningful is the test (two functions may have the same average (<x>) although they are very different!):

check the behavior for higher-order momenta!

Test on different sequences, a single momentum



very small deviations from the expected behavior could be accidental;

check the overall behavior, and try also changing the seed!

A general suggestion:

do you want to check a power law?

deviation of $\langle x \rangle^k$ = $\left|\frac{1}{N}\sum_{i=1}^{N} x_i^k - \frac{1}{k+1}\right| \sim 1/\sqrt{N} + \text{cost.}$

numerically calculated

from the sequence

expected if the sequence

was

truly uniform

linear regression: much better

$$\log(\text{deviation of } \langle x \rangle^k) \sim -1/2 \; \log(N) + \text{cost.'}$$

check the slope of the log-log !!!

do you want to fit with gnuplot?

Suppose you have the data in two columns, x and y, and you suspect a power low y = x^a + const

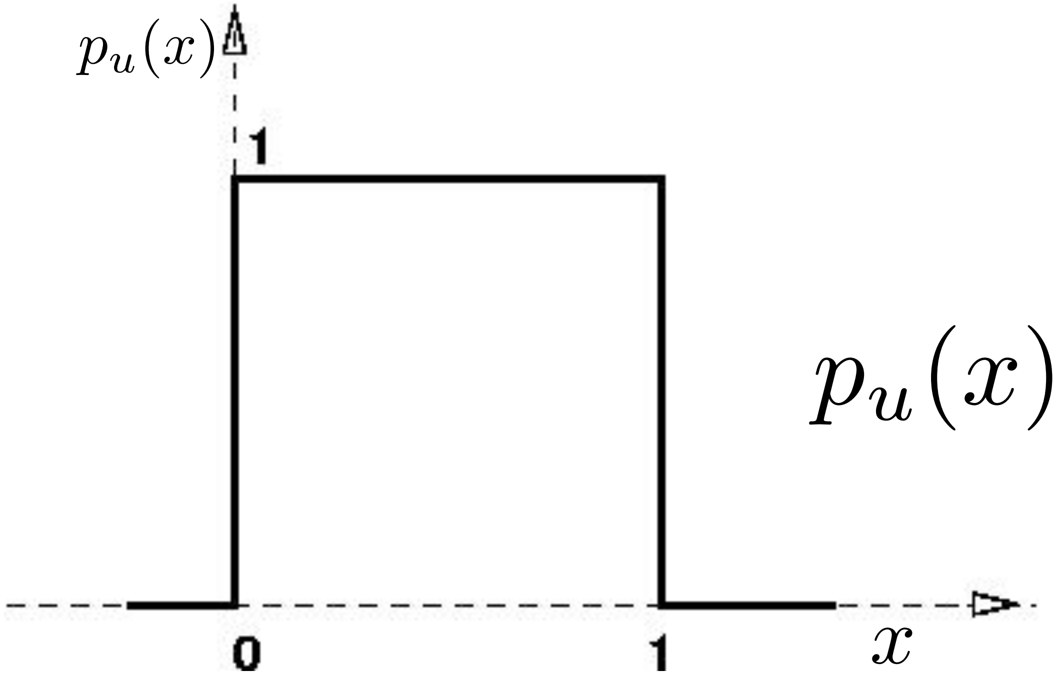
Consider that: log(y) = a * log(x) + b

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

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

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

I) Random numbers with non uniform distributions and II) random processes

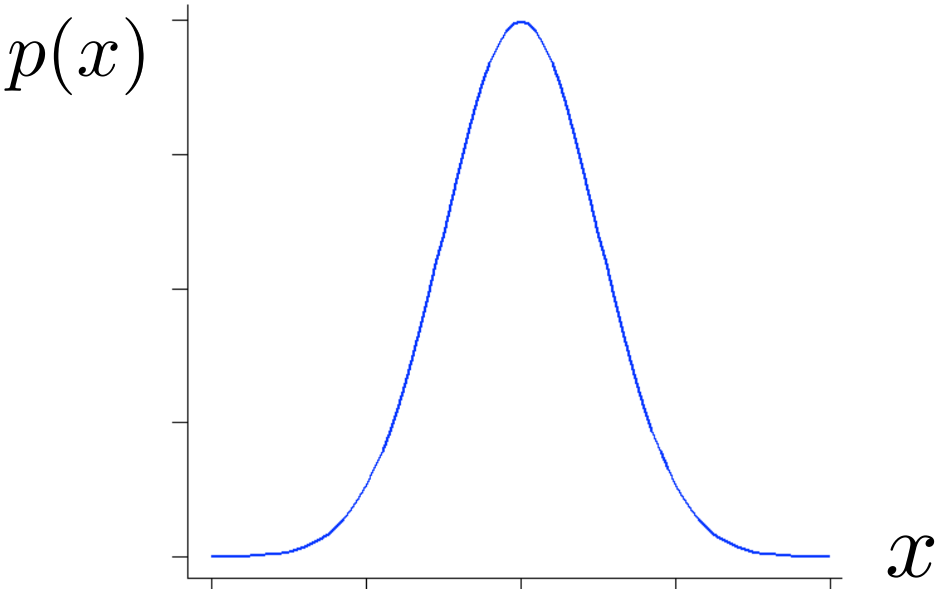
last lecture:

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



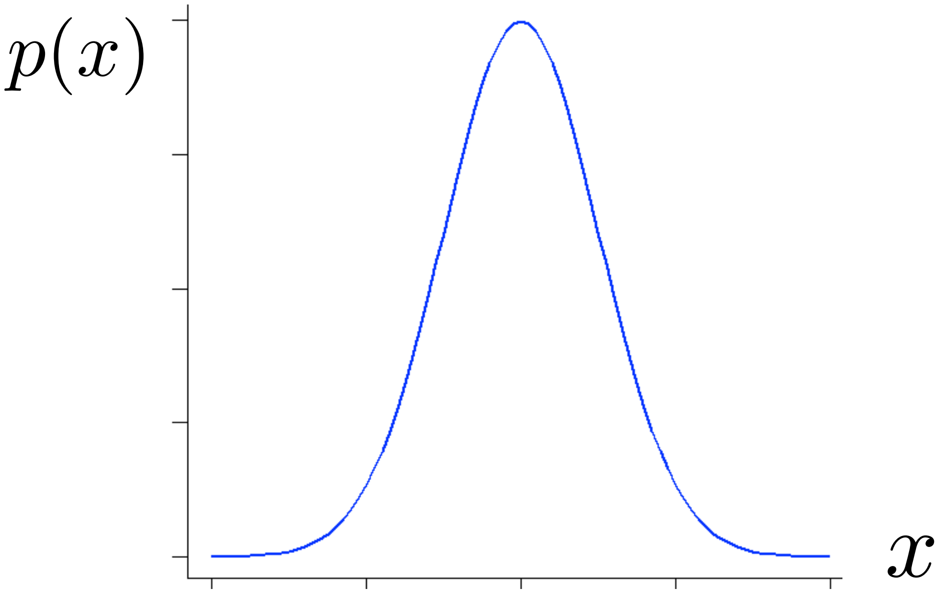
$$p_u(x) = \begin{cases} 1 & 0 \leq x < 1 \\ 0 & \text{otherwise} \end{cases}$$

Part I - Random numbers with non uniform distributions:



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

Part I - Random numbers with non uniform distributions:



1) inverse transformation method (general)
2) rejection method (even more general)
3) some “ad hoc” methods: the Box-Muller algorithm for the gaussian distribution

Non uniform random numbers distribution:
1) inverse transformation method (general)

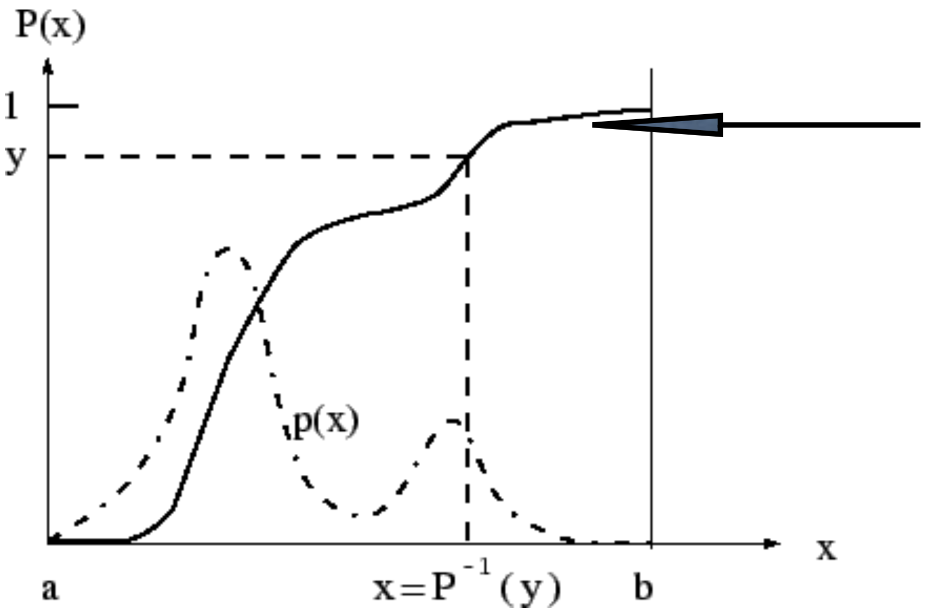
Problem: Generate sample of a random variable (or *variate*) x with a given distribution p .

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

Non uniform random numbers distribution: 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.

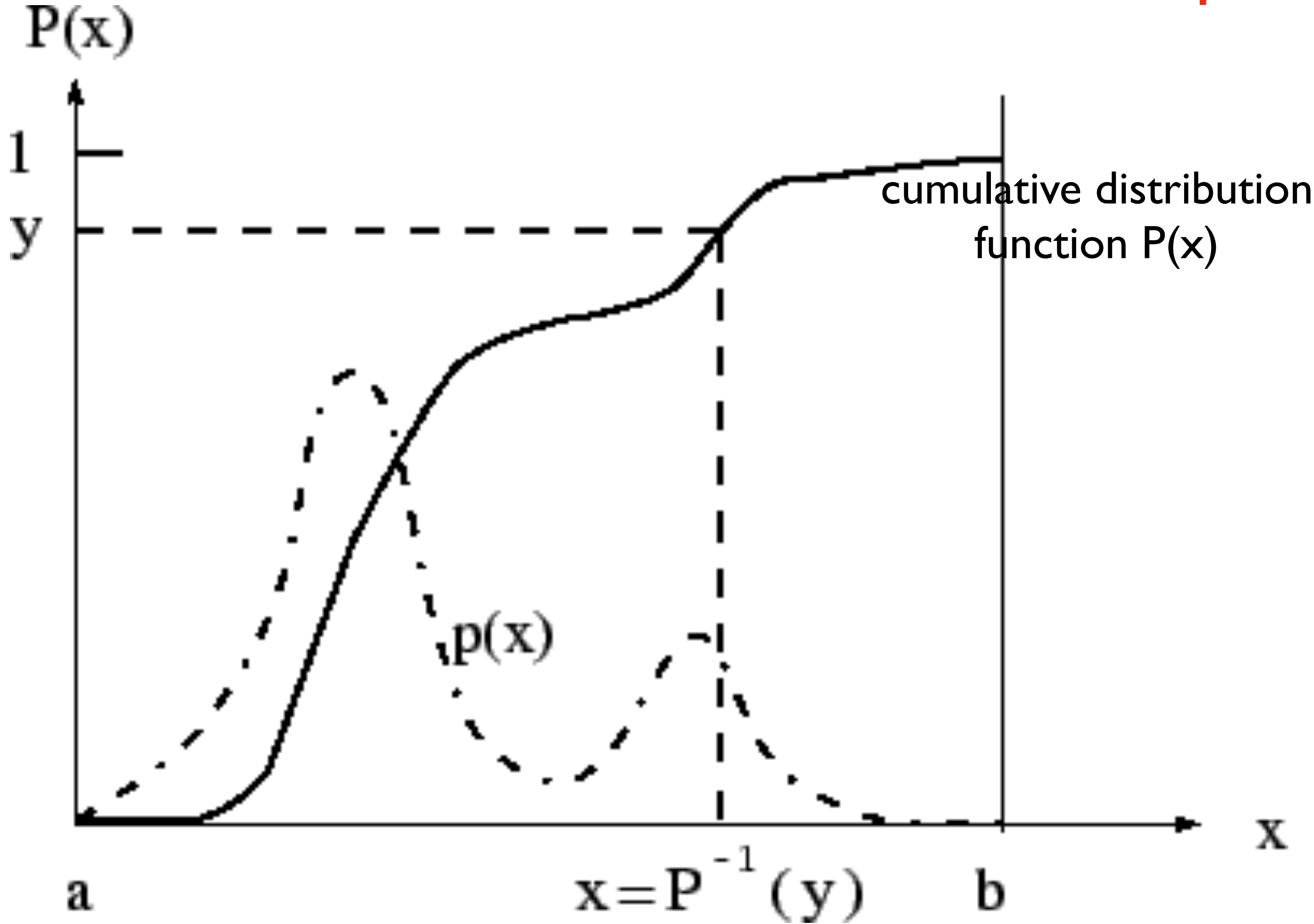
- Sample y from an equidistribution in the interval (0,1). (i.e., use $p_u(y)$)
- Compute $x = P^{-1}(y)$.

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

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

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

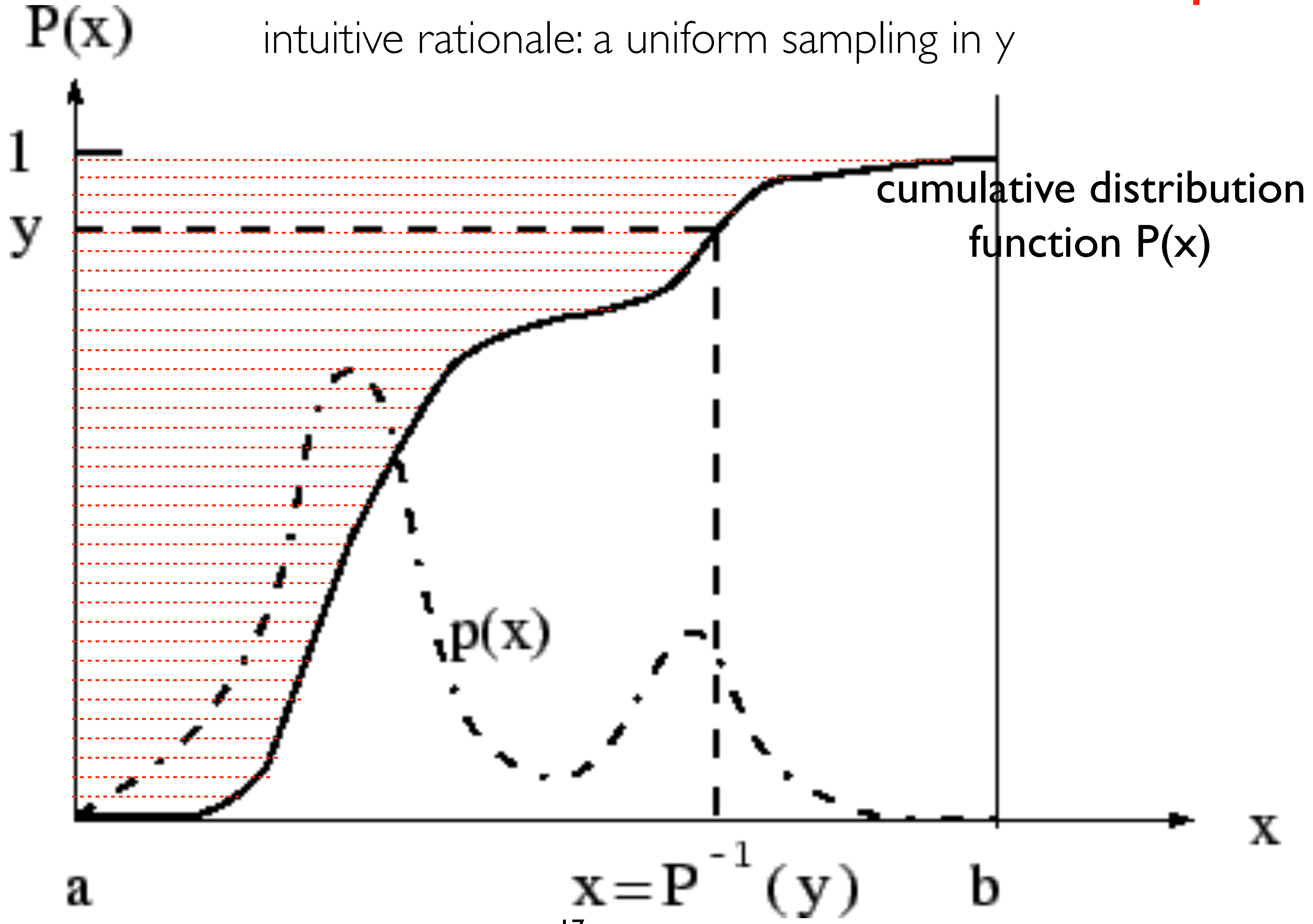
Non uniform random numbers distribution:
1) inverse transformation method - the concept



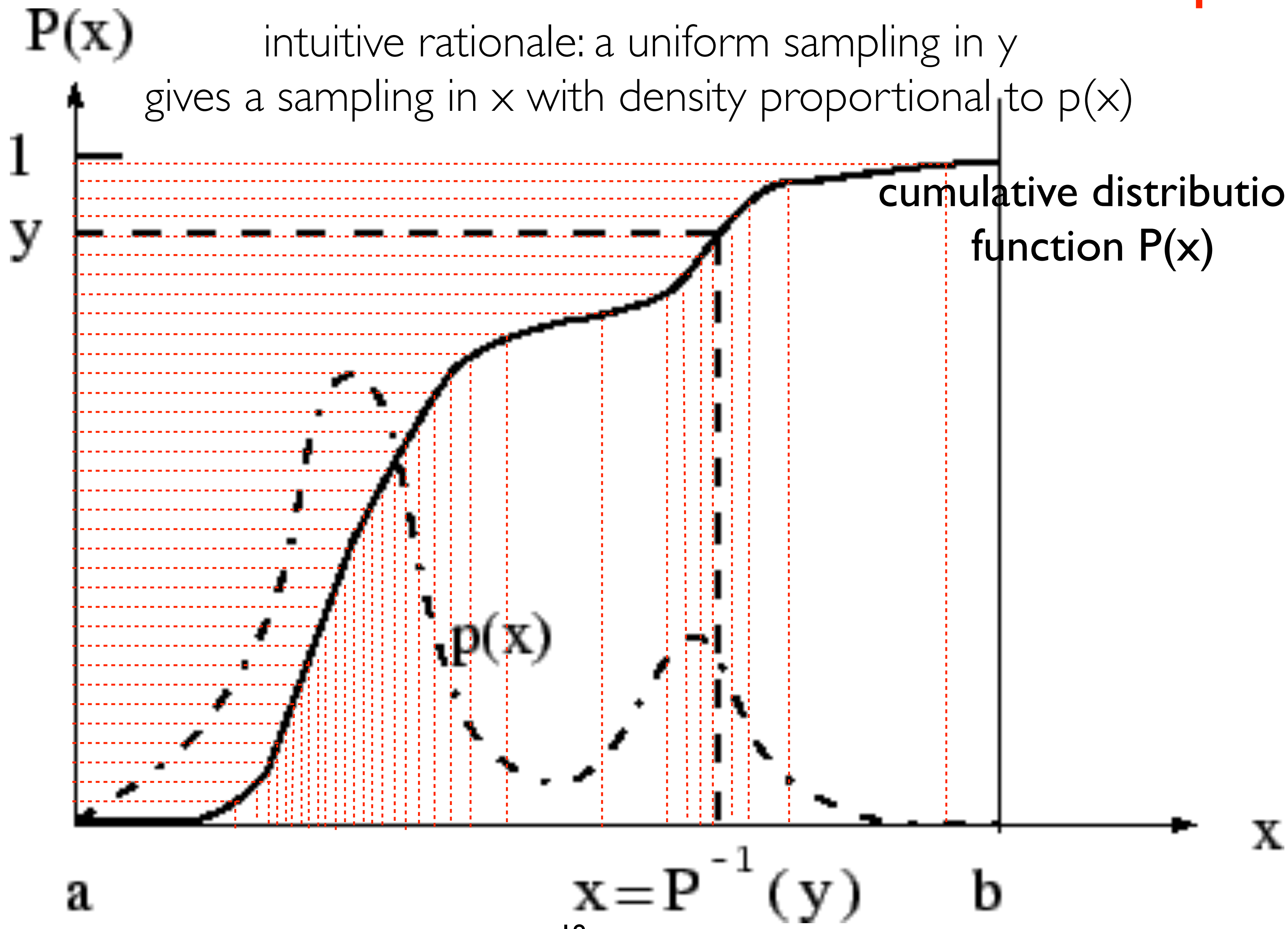
cumulative distribution function P(x)

Non uniform random numbers distribution: 1) inverse transformation method - the concept

intuitive rationale: a uniform sampling in y



Non uniform random numbers distribution: 1) inverse transformation method - the concept

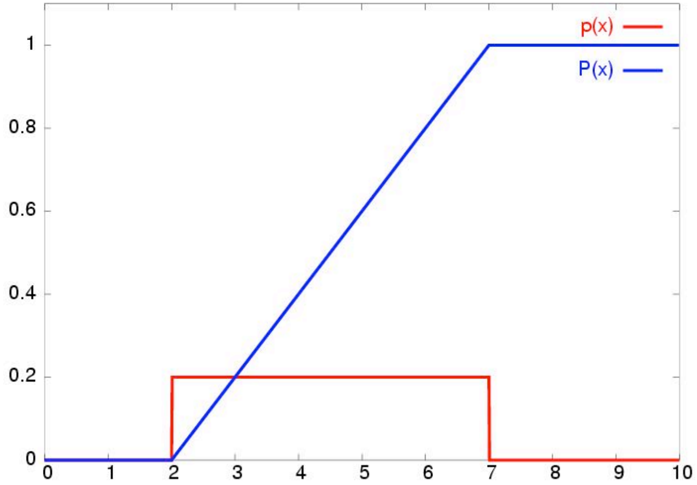


intuitive rationale: a uniform sampling in y gives a sampling in x with density proportional to p(x)

cumulative distribution function P(x)

Non uniform random numbers distribution: 1) inverse transformation method - examples

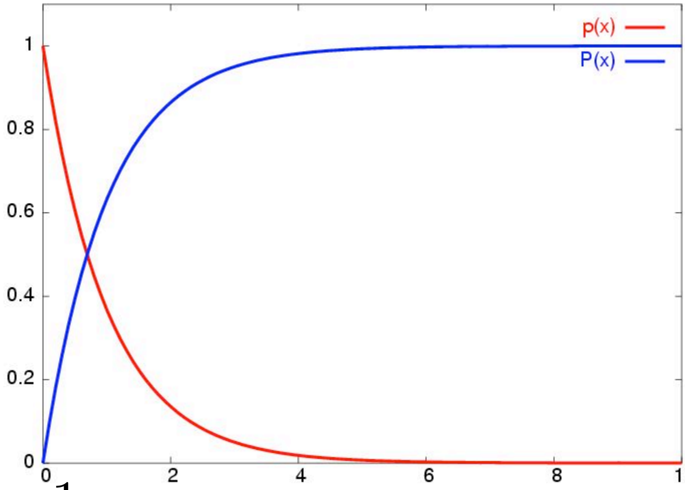
1) $$p(x) = \begin{cases} \frac{1}{b-a} & a \le x \le b \\ 0 & \text{otherwise} \end{cases}$$



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

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

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



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

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

Non uniform random numbers distribution: 1) inverse transformation method - examples

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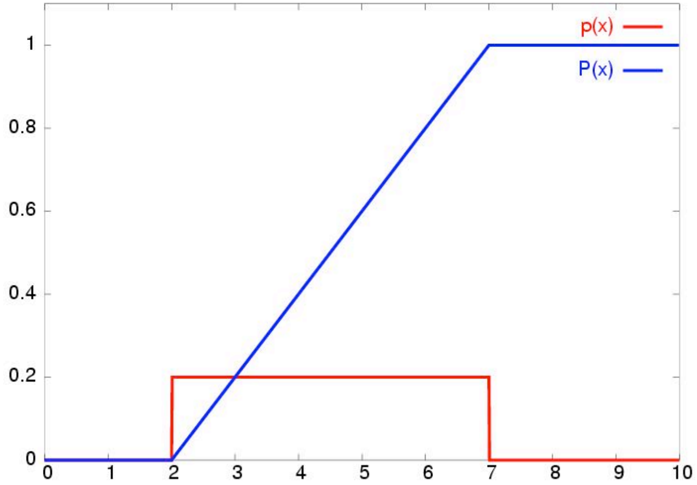

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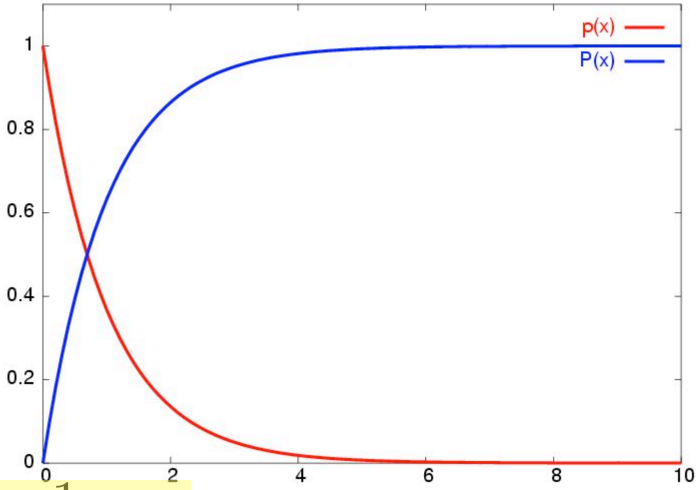

2) $$p(x) = \begin{cases} 0 & x \leq 0 \\ ae^{-ax} & x \geq 0 \end{cases}$$

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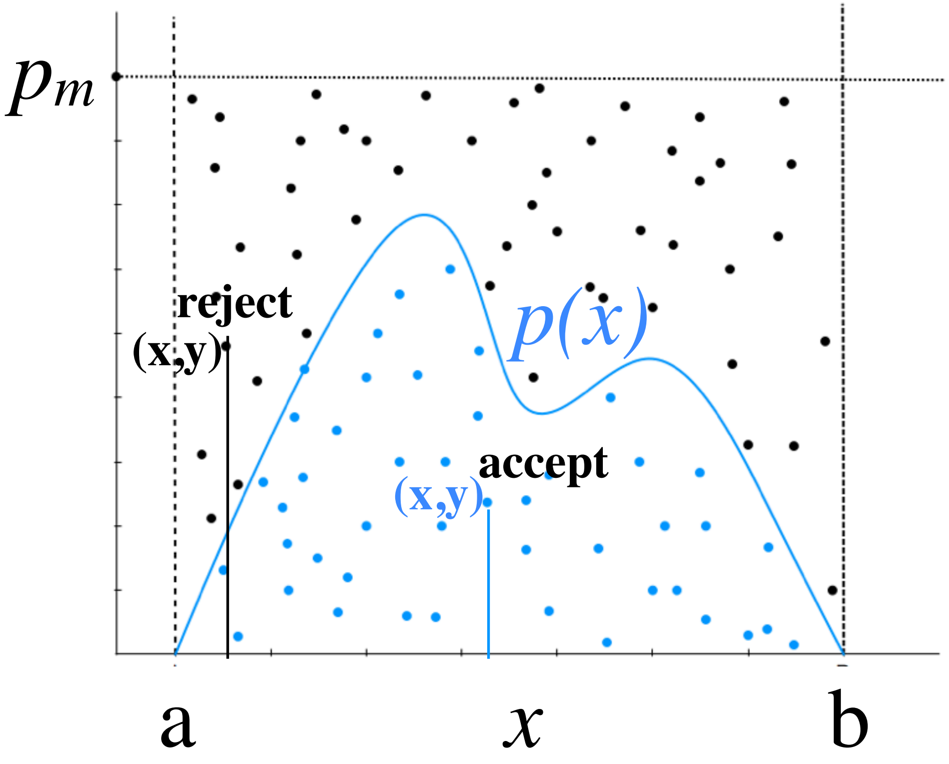
$$x = -\frac{1}{a}\ln(1-y) \quad \text{or (same distribution!)} \quad x = -\frac{1}{a}\ln y$$

Non uniform random numbers distribution: 2) rejection method (general)

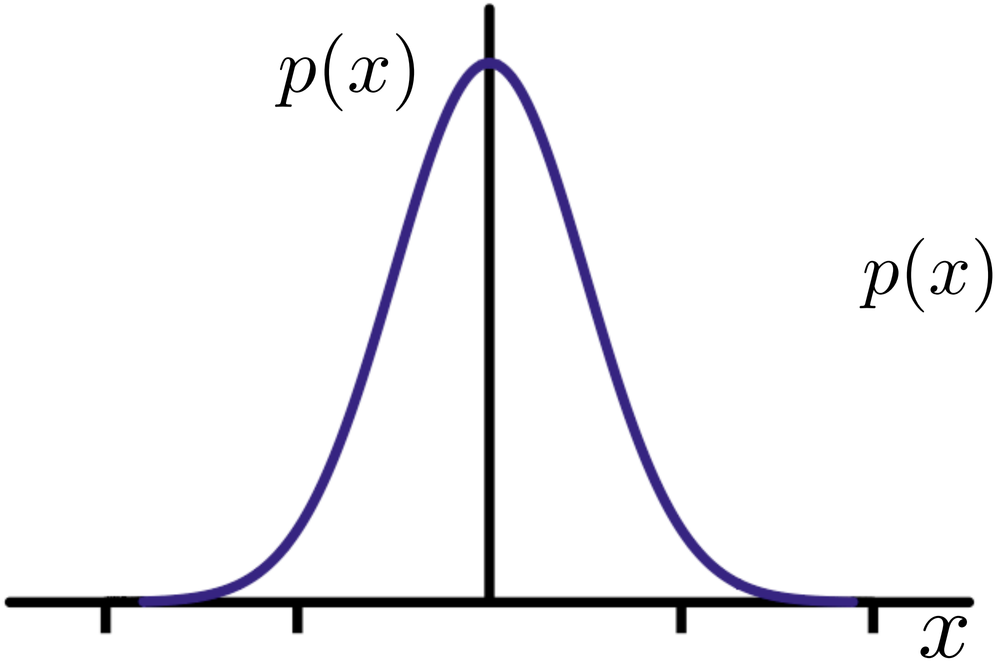
Let $[a, b]$ be the allowed range of values of the variate x, and p_m the maximum of the distribution $p(x)$.

1. Sample a pair of equidistributed random numbers, $x \in [a, b]$ and $y \in [0, p_m]$.
2. If $\boxed{y \leq p(x)}$, 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)

Non uniform random numbers distribution:
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

Non uniform random numbers distribution:

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 σ =1):

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

Non uniform random numbers distribution: 3) gaussian distribution - Box-Muller technique

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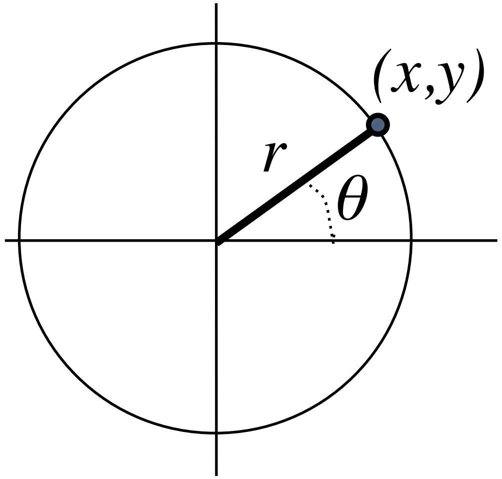
Use polar coordinates: $r = \sqrt{x^2+y^2}$, $\theta = \arctan(y/x)$; def.: $\rho \equiv r^2/2$



Non uniform random numbers distribution:
3) gaussian distribution - Box-Muller technique

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

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

and therefore:

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

Non uniform random numbers distribution:
3) gaussian distribution - Box-Muller technique

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

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

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

and therefore:

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

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

Non uniform random numbers distribution:

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):

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

NOTE:

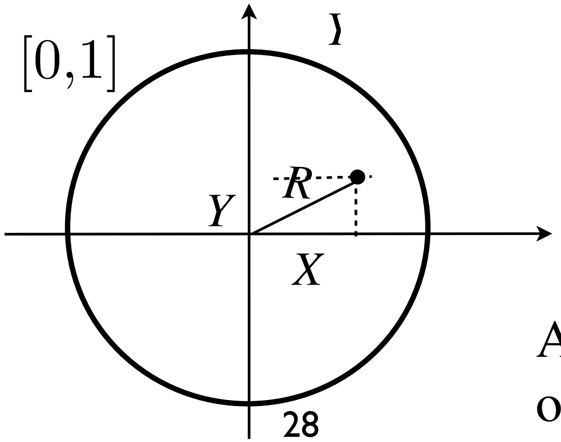
x, y are normally distributed and statistically independent. Gaussian variates with given variances σ_x, σ_y are obtained by multiplying x and y by σ_x and σ_y respectively

Non uniform random numbers distribution:
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

Some programs:

on moodle2 or on INFIS account:
$/home/peressi/comp-phys/III-random-non-uniform-and-processes/f90
[do: $cp /home/peressi/... .../f90/* .]

expdev.f90   boxmuller.f90

993SM - Laboratory of Computational Physics lecture 3 - part 1 March 25, 2020

Maria Peressi

END OF THE FIRST PART

993SM - Laboratory of Computational Physics lecture 3 - part 2 March 25, 2020

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A look at the expdev.f90 code

```
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

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 $\sqrt{}$ to calculate R separately)

A look at the gasdev.c code

```
#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
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 $\sqrt{\ }$ to calculate R separately)

Other programs:

in the same directories indicated before:

(optional, but useful!)

random.f90 (is a module)
t_random.f90

to compile:

```
$gfortran random.f90 t_random.f90
```

(the module first!)

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 $t = 0$

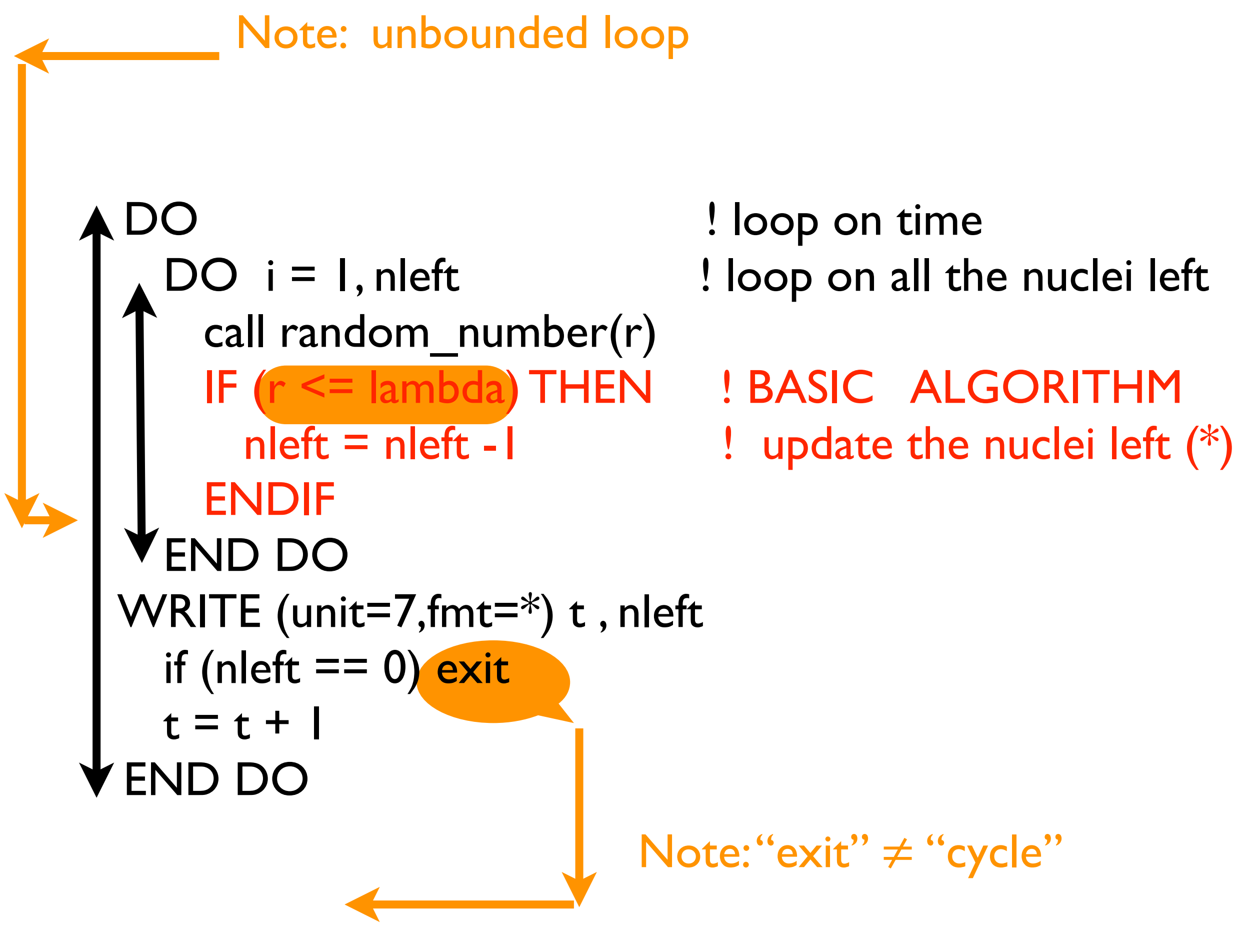
3. Basic algorithm: **for each nucleus** left (not yet decayed):

   - 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 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:

in the same directory indicated before:

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 from which loop to exit)

possible forms of "do while":

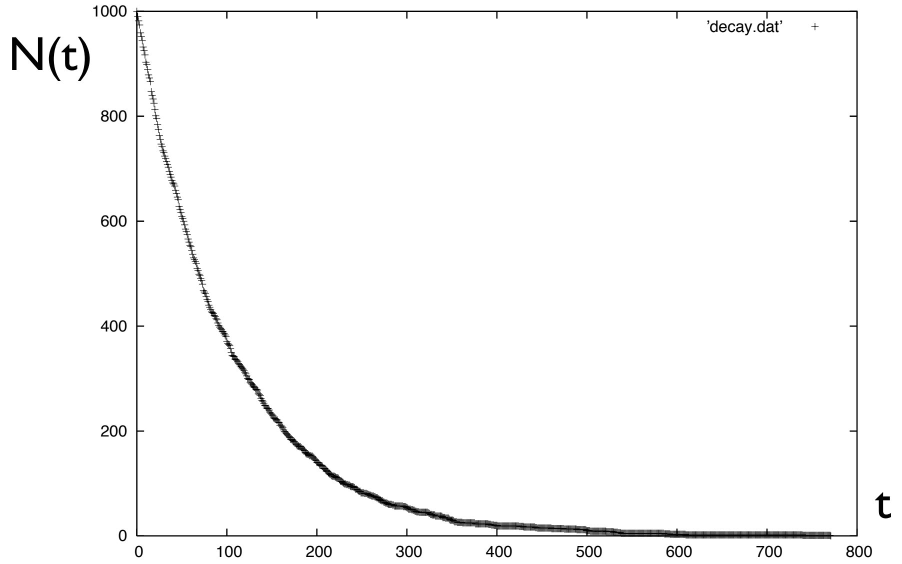
```
     DO
      if (condition)exit
     END DO
or:
     DO WHILE (.not. condition)
      ...
     END DO
```

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

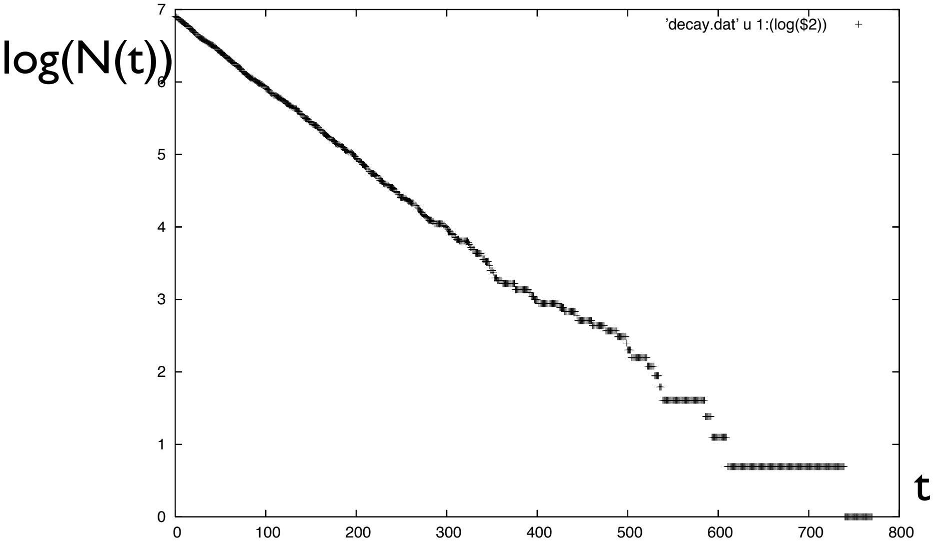
Radioactive decay:

results of numerical simulation



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

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

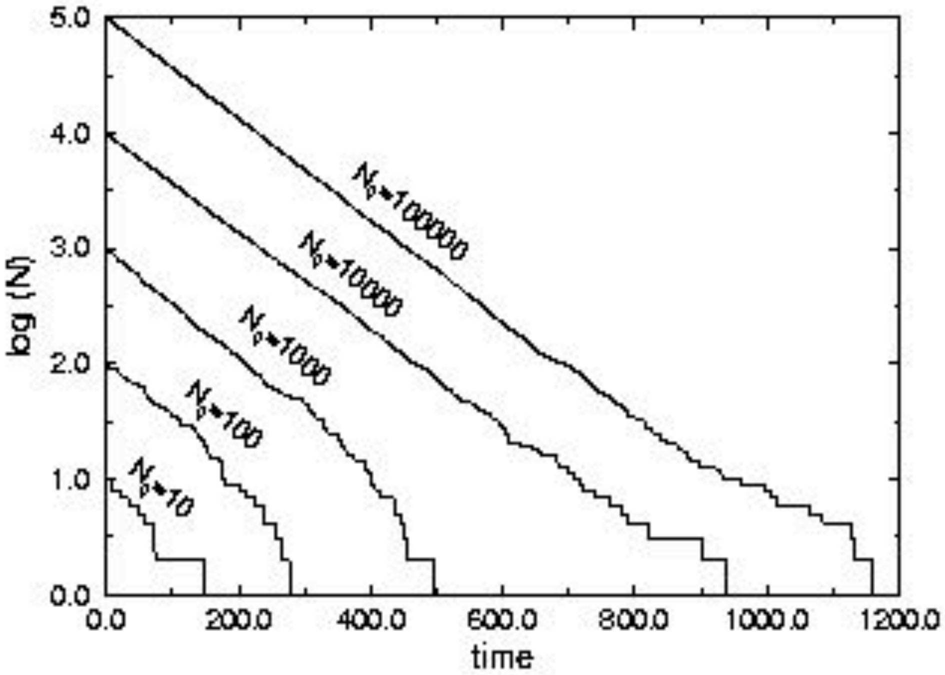


semilog plot (log(N) vs t)

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

=> slope is $-a$

Radioactive decay:
results of numerical simulation



Semilog plot of the results of decay simulation for the same decay rate and different initial number of atoms:

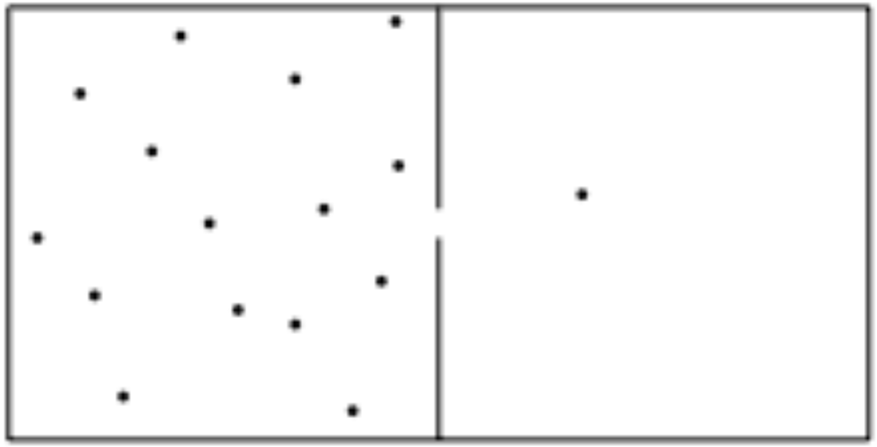
almost a straight line, but with important deviations (stochastic) for small N

Stochastic simulations give reliable results when obtained:

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

(homework: 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



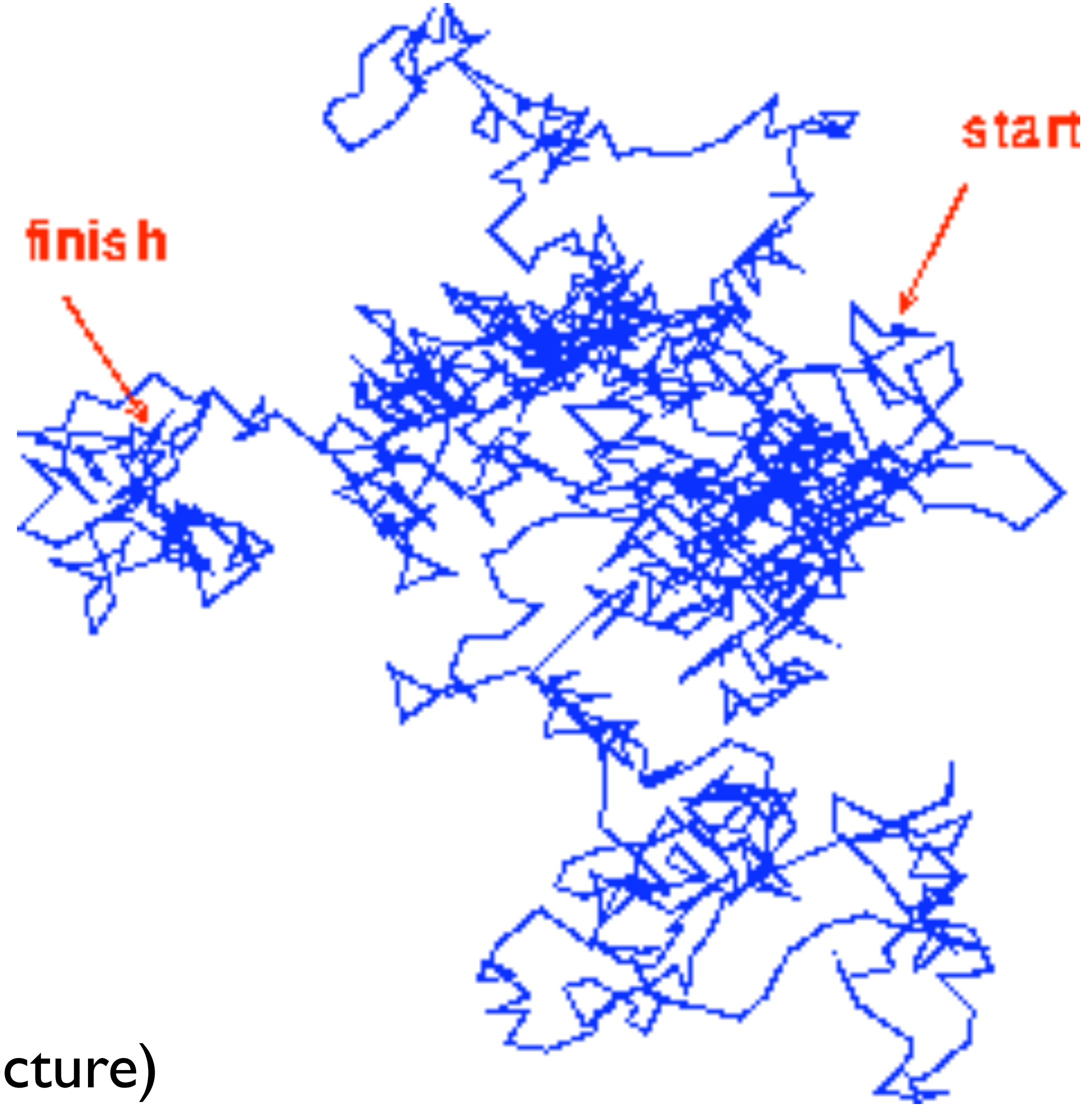
A box is divided into two parts communicating through a small hole. One particle randomly can pass through the hole per unit time, from the left to the right or viceversa.

$N_{left}(t)$: 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)

Part III - Fitting data

Least-square method

- Suppose to have N_D data (independent measurements of the variable y which is function of the variable x):

$$(x_i, y_i \pm \sigma_i), \qquad i = 1, N_D$$

with $\pm\sigma_i$ error associated to the i value of y.

- Purpose: determine the function $y = f(x)$ which better described these data. If the analytic form of the function is known, a part from a set M_P of parameters $\{a_1, a_2 \ldots, a_{M_P}\}$, i.e., $f(x) = f(x; \{a_m\})$, the goal is to find the best set of parameters.

- To test whether the data *fit* via $f(x)$ is good or not calculate the quantity

  $$\chi^2 := \sum_{i=1}^{N_D} \left(\frac{y_i - f(x_i; \{a_m\})}{\sigma_i} \right)^2$$

  Note that by dividing by σ_i, data with larger errors have smaller weight in this weighted average.

- The smallest χ^2, the better the fit is.

- **Least-squares fitting**: The parameters M_P that minimize χ^2 are found by:

$$\frac{\partial \chi^2}{\partial a_m} = 0 \quad (m = 1, M_P)$$

$$\Longrightarrow \sum_{i=1}^{N_D} \frac{y_i - f(x_i)}{\sigma_i^2} \, \frac{\partial f(x; \{a_m\})}{\partial a_m} = 0 \qquad (1)$$

example: see program **fit.f90**

- If $f(x;a,b) = ax+b$ **(linear regression)**, the equations giving χ^2 minimum reduce to:

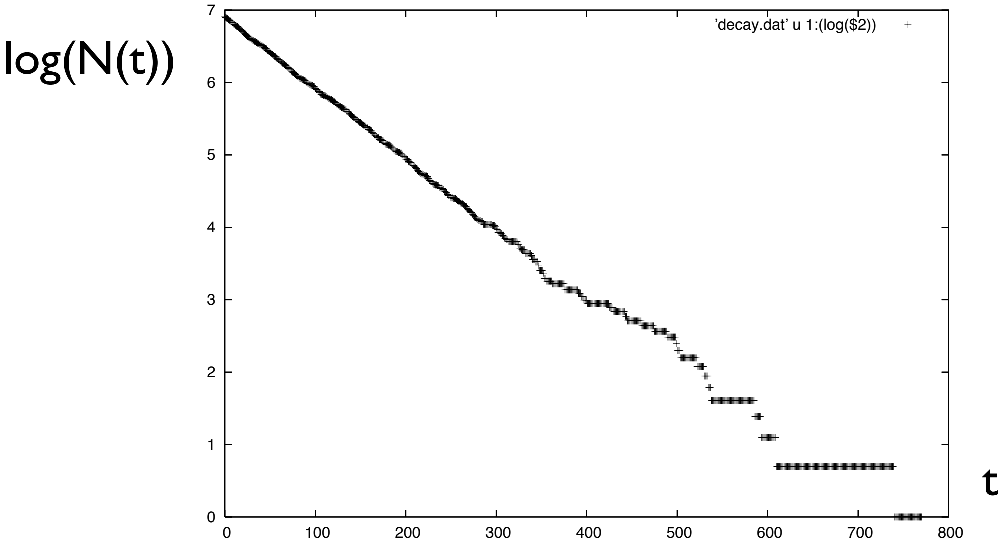
$$a = \frac{SS_{xy} - S_xS_y}{\Delta}, \quad b = \frac{S_{xx}S_y - S_xS_{xy}}{\Delta}$$

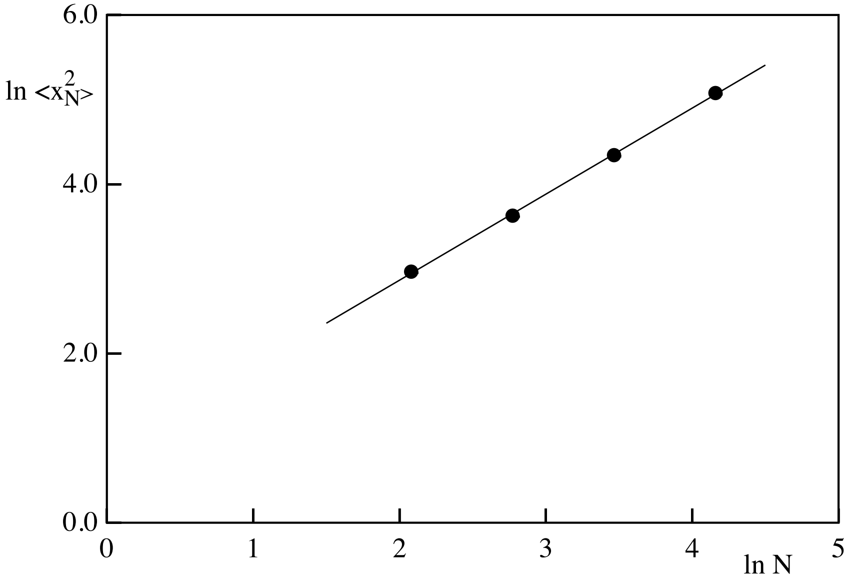
$$S = \sum_{i=1}^{N_D} \frac{1}{\sigma_i^2}, \quad S_x = \sum_{i=1}^{N_D} \frac{x_i}{\sigma_i^2}$$

$$S_y = \sum_{i=1}^{N_D} \frac{y_i}{\sigma_i^2}, \quad S_{xx} = \sum_{i=1}^{N_D} \frac{x_i^2}{\sigma_i^2}$$

$$S_{xy} = \sum_{i=1}^{N_D} \frac{x_iy_i}{\sigma_i^2}, \quad \Delta = SS_{xx} - S_x^2 \tag{2}$$

Examples - linear regression





radioactive decay:
$N(t) \sim N_0 \exp(- a\ t)$

we can fit with the exp.
but it is better to fit:

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

Random walk:
$<x^2_N> \sim N^a$

but it is better to fit:

$\log <x^2_N> = a \log N$

Example: fit using gnuplot - 1

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 ...
```

Part IV -
more on fortran

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 g95 and gfortran:
boundaries not checked; use compiler option:

```
gfortran -fbounds-check myprogram.f90
```

Print:

```
man gfortran
```

and scroll the pages to see the possible options of compilation

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)

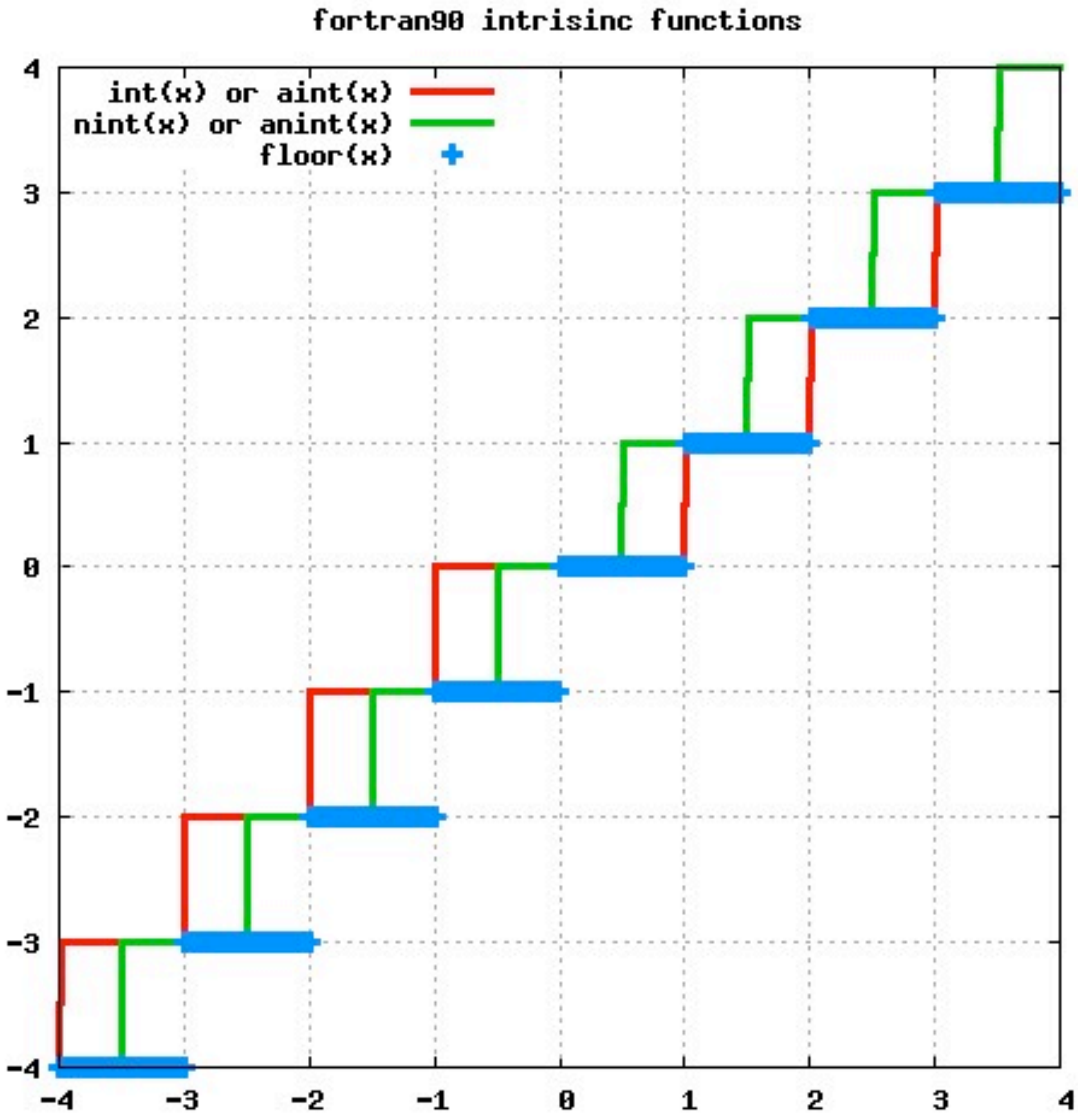
- Integer elemental function
- Returns the largest integer ≤ A. For example, FLOOR(3.7) is 3, and FLOOR(-3.7) is -4.
- Argument A is Real of any kind; optional argument KIND is Integer
- Argument KIND is only available in Fortran 95

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

INTEL Fortran compiler

The following flags are useful (in addition to "-O0 -g") for debugging your code:

-traceback   generate extra information to provide source file traceback at run time
-fp-stack-check   generate extra code to ensure that the floating-point stack is in the expected state
-check bounds   enables checking for array subscript expressions
-fpe0   allows some control over floating-point exception handling at run-time

GNU Fortran compilers

The following flags are usefull (in addition to "-O0 -g")for debugging your code:

-Wall   Enables warnings pertaining to usage that should be avoided
-fbounds-check   Checks for array subscripts.

GNU: gdb (serial debugger)

GDB is the GNU Project debugger and allows you to see what is going on 'inside' your program while it executes -- or what the program was doing at the moment it crashed.

GDB can do four main kinds of things (plus other things in support of these) to help you catch bugs in the act:

- Start your program, specifying anything that might affect its behavior.
- Make your program stop on specified conditions.
- Examine what has happened, when your program has stopped.
- Change things in your program, so you can experiment with correcting the effects of one bug and go on to learn about another.

More details in the on line documentation, using the "man gdb" command.

To use this debugger, you should compile your code with one of the gnu compilers and the debugging command-line options described above, then you run your executable inside the "gdb" environment:

```
> gfortran -O0 -g -Wall -fbounds-check -o myexec myprog.f90
> ulimit -c unlimited  (number of processes an existing user on the server may be authorized to have - use it in the same window!)
> ./myexec
> gdb ./myexec
```

Structure of a main program with one function

```
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** in previous Lectures

993SM - Laboratory of Computational Physics lecture 3 - part 2 March 25, 2020

Maria Peressi

END OF THE LECTURE