The Monte Carlo Method

Basics and (simple) applications

Thanks to H. Jung for a lot of material !!!

Thomas Schörner-Sadenius

GEANT4 Training Event
DESY Hamburg, 28 January 2010

OUTLINE

- The Monte Carlo method
  - Monte Carlo: What, why, and where?
- Random numbers
  - True random versus pseudo-random …
- Some mathematical basics
- Generating arbitrary distributions
  - Hit&miss, inversion of cumulative distribution, …
- MC integration
  - Hit&Miss, importance sampling, …
- Applications in HEP

MONTE CARLO METHOD: DEFINITION

> Monte Carlo methods

… a class of computational algorithms that rely on repeated random sampling to compute their results. Monte Carlo methods are often used when simulating physical and mathematical systems. Because of their reliance on repeated computation of random or pseudo-random numbers, these methods are most suited to calculation by a computer and tend to be used when it is infeasible or impossible to compute an exact result with a deterministic algorithm.

> So use MC when there is **no (known) analytical solution** to a (mathematical or physical) problem:

- Difficult integrals, numerical analysis
- Complex systems with many degrees of freedom, natural phenomena
- Social or economical systems
- Higher-order processes in particle physics

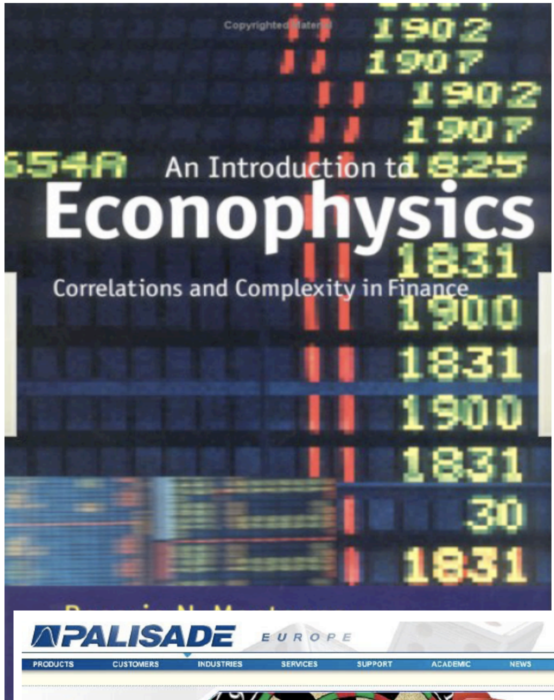
> In the following, "MC method" denotes any algorithm that arrives, by the use of "random" numbers, at the solution of a problem.

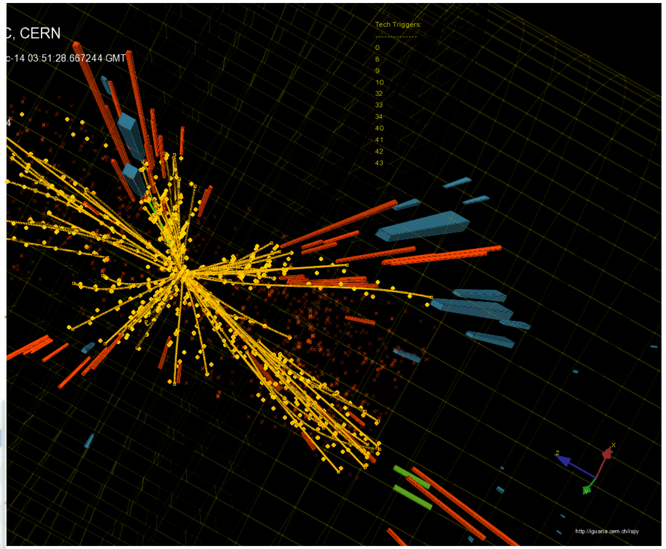
MONTE CARLO METHOD: DEFINITION

> Monte Carlo methods:

- " … their methods (v. Neumann et al.) … were aptly named after the international gaming destination …"
- " … after the War a wide range of sticky problems yielded to the new techniques …"
- " … virtually impossible to find a succint definition of `Monte Carlo' method …"
- " … some authors prefer the term `stochastic simulation' …"
- "Monte Carlo is the art (sic!) of approximating an expectation by the **sample mean of a function of simulated random variables**."
- "Monte Carlo is about **invoking laws of large numbers** to approximate expectations."

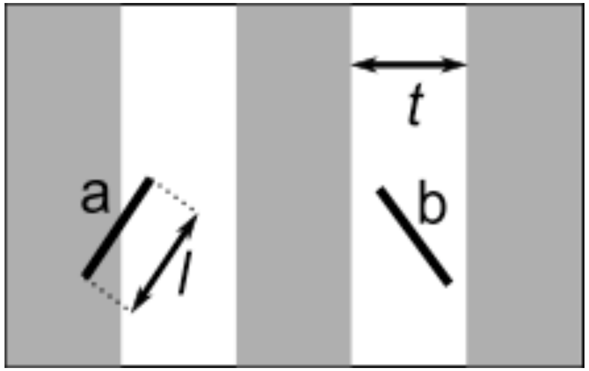
MONTE CARLO METHOD: APPLICATIONS





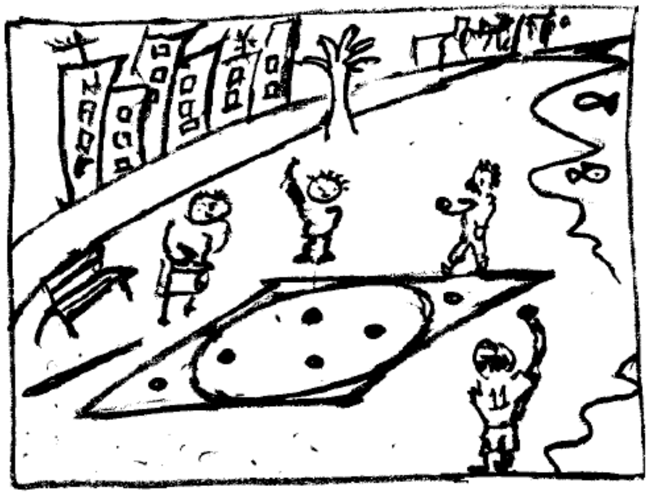
PARADIGMATIC EXAMPLES

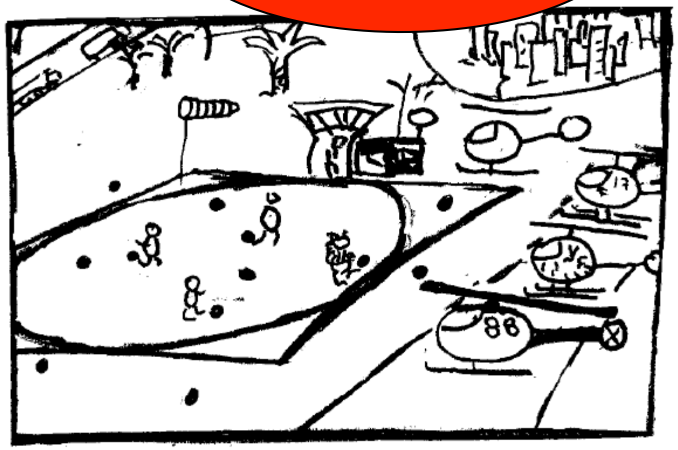
- Buffon's needle: a question first posed in the 18th century by Georges-Louis Leclerc, Comte de Buffon:
  - Suppose we have a floor made of parallel strips of wood, each of the same width t, and we drop a needle of length l onto the floor. What is the probability that the needle will lie across a line between two strips?



- Calculating pi
  - Very amusing description in W. Krauth, "Introduction To Monte Carlo Algorithms" (arXiv:cond-mat/9612186v2)

See example later today





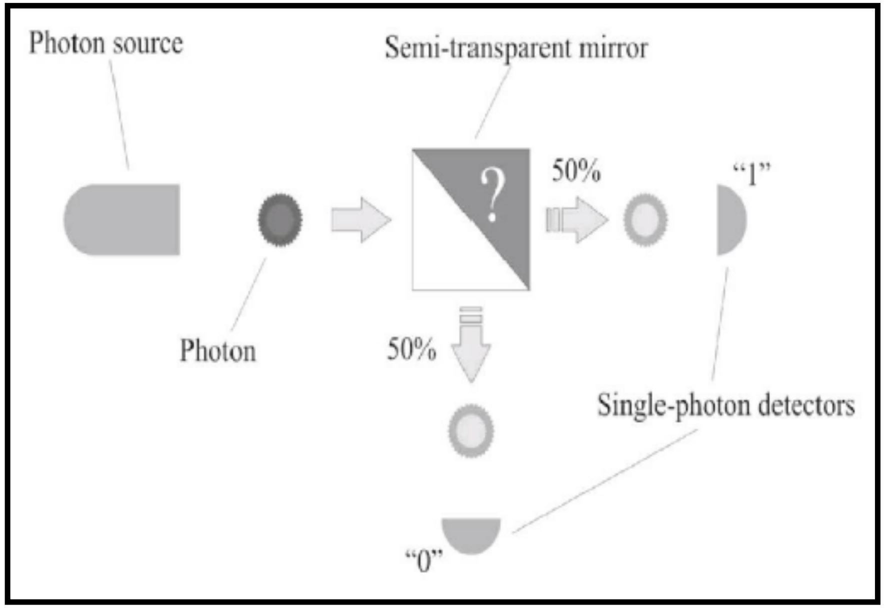
(PSEUDO)RANDOM NUMBERS

- “Random” numbers are at the heart of the MC method.
- A **sequence of random numbers** is a set of numbers that have nothing to do with the other numbers in the sequence.
- There is no unique random number (sequence)!
- So … how to get random numbers usable for our purposes?
- One (very attractive) option: Gambling in Monaco!

Tiresome and
potentially
expensive!

(TRUE) RANDOM NUMBERS

- To obtain true random numbers …
- … use some **classical chaotic system** like roulette, lotto, dices, coin tossing…
  - In principle, knowing all initial conditions, such a system is predictable – however, it is extremely sensitive → true random …
- … or **use "modern physics" random processes** like
  - radioactive decay, …
  - … or other quantum mechanical process. Nice example: Photons on semi-transparent mirror!
    ➔ available and tested by DESY summer student!



- However, for typical nowadays applications (implementation in computer programs) all these true random number principles are too, slow, to cumbersome, not easily automatised, etc.
  ➔ go for "second-best": **pseudo-random numbers**!

(TRUE) RANDOM NUMBERS

- Another nice example: random.org
  - Making use of atmospheric noise which ican be picked up with a normal radio!

PSEUDO-RANDOM NUMBERS

- … are a sequence of numbers that … well, APPEAR to be random,
  - but where in fact each number is derived from the previous N numbers by a well-defined algorithm.
- More precisely, you want to generate integers **I_n** in the interval **[0;M]** and from that derive **$R_i = I_n/M$**.
- Numerous algorithms developed, for example “Middle Square Algorithm” (J. v. Neumann, 1946):
  - Start with a number of 10 digits, square it, take the middle 10 digits as the next number etc.
  - More complex algos don’t necessarily lead to better results. Best to use algorithms that are well understood in their degree of “randomness”.
- Nice example: “Linear congruential generator”:

$$I_{n+1} = \mathrm{mod}\left(a \cdot I_n + c, m\right)$$

$$R_{n+1} = I_{n+1}/m$$

Seed I_0 modulus m
Multiplicative constant a
Additive constant c

PSEUDO-RANDOM NUMBERS

Example for linear congruential generator: $I_0 = 10$, $a = 2$, $c = 5$, $m = 20$:

$I_1 = \mathrm{mod}(2*10 + 5, 19) =$	6
$I_2 = \mathrm{mod}(2*6 + 5, 19) =$	17
$I_3 = \mathrm{mod}(2*17 + 5, 19) =$	1
$I_4 = \mathrm{mod}(2*1 + 5, 19) =$	7
$I_5 = \mathrm{mod}(2*7 + 5, 19) =$	0
$I_6 = \ldots$	5, 15, 16, 18, 3, 11, 8, 2, 9, 4, 13, 12, 10, **6, …**

➔After m steps, the sequence repeats!

Note: Criteria for randomness:

- uniformity
- correlation tests
- sequence-up / sequence-down tests
- gap tests
- random walk tests
- …

LINEAR CONGRUENTIAL GENERATOR

> By definition, the LCG generator has a maximum “random” sequence of length m.

$$I_{n+1} = \mathrm{mod}\left(a \cdot I_n + c, m\right)$$
$$R_{n+1} = I_{n+1} / m$$

- After that, repetition → strong correlation of generated numbers:

> Example for demonstration (I_0 = 4711, a = 205, c = 29573, m = 139968).

- Shown is the correlation between pairs of numbers (R_n;R_{n+1}):

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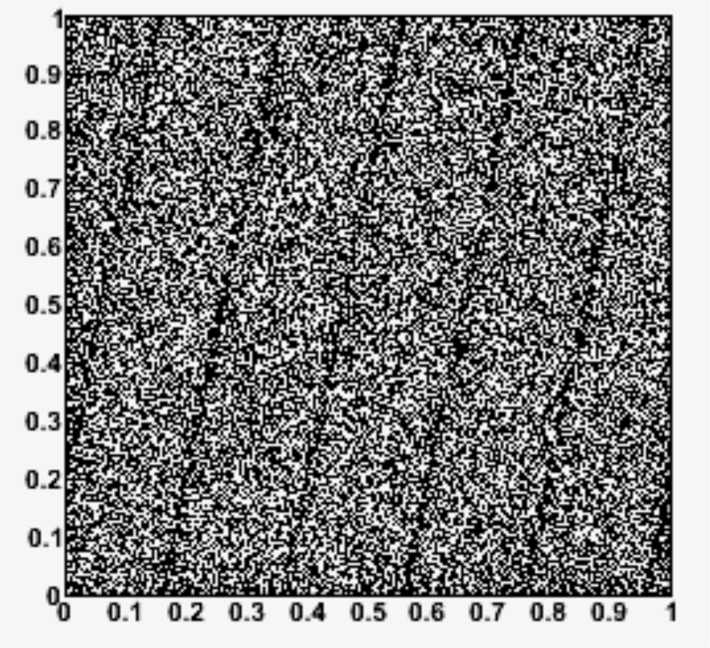

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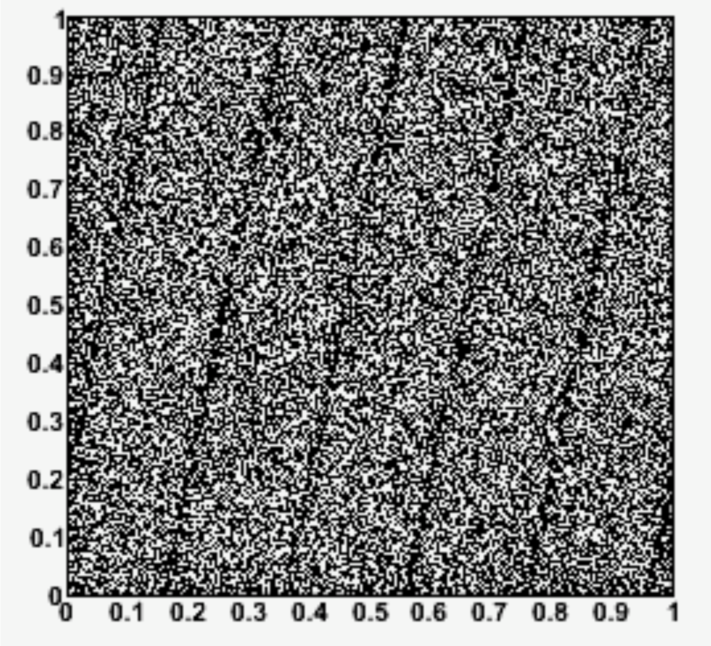
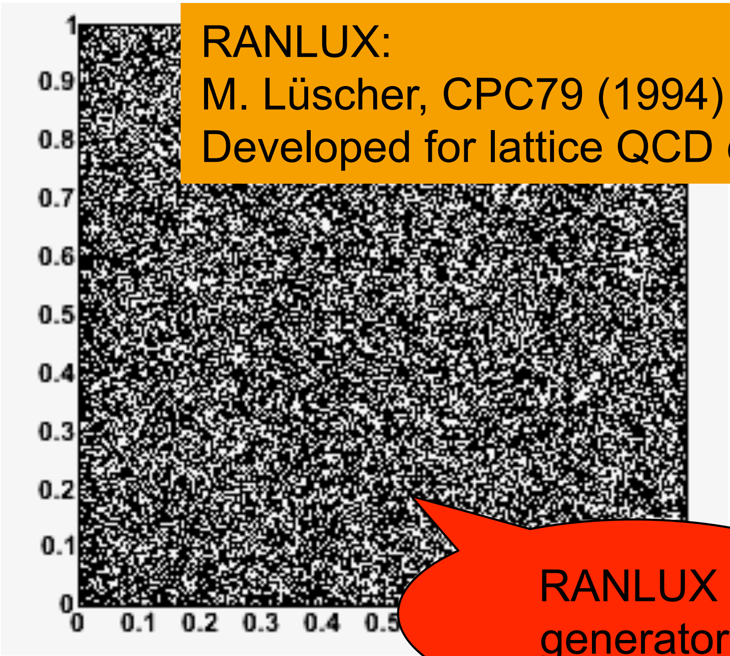




RANLUX:
M. Lüscher, CPC79 (1994) 100.
Developed for lattice QCD calc.

RANLUX generator

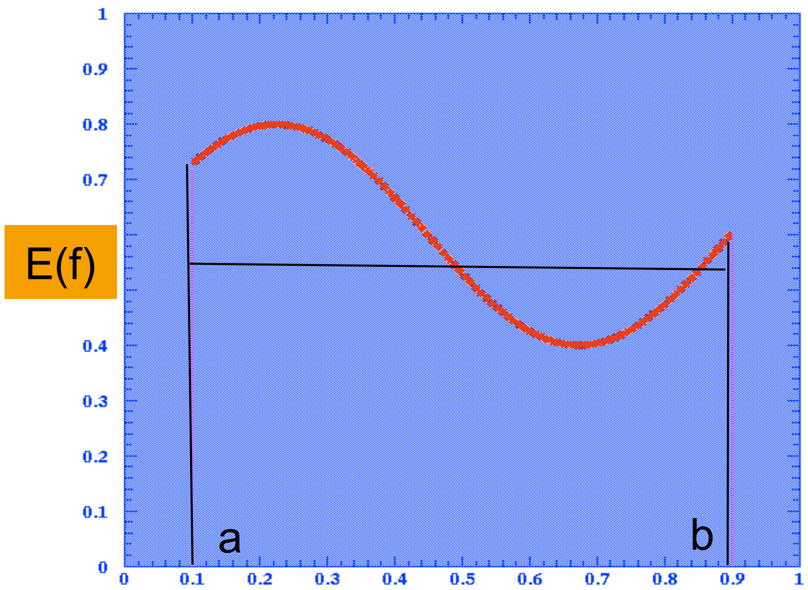
- … let's now assume we have random numbers …

(MATHEMATICAL) BASICS

> Expectation value E(f) or μ: defined as the average/mean value of function f:
(“mean value theorem”)

$$E(f) = \int f(u)dG(u) \underset{uniformPDF}{=} \left(\frac{1}{b-a}\int_a^b f(u)du\right)$$

$$E(cx+y) = cE(x) + E(y)$$



➔ close connection to integration (later) etc.!

> Variance V(f) (~standard deviation σ^2):

$$V(f) = \int (f - E(f))^2 dG = \left(\frac{1}{b-a}\int_a^b (f - E(f))^2 du\right)$$

➔ relevance: want small uncertainties on MC predictions / results
➔ aim to reduce variance (not really covered here).

(MATHEMATICAL) BASICS

- Law of large numbers: For large enough statistics, relative frequency of an outcome approaches probability.
  - For MC relevant (integration!): Choose N numbers u_i randomly with uniform probability density in interval [a;b], evaluate $f(u_i)$ for each u_i:

$$\frac{1}{N}\sum_{i=1}^{N} f(u_i) \rightarrow \frac{1}{b-a}\int_a^b f(u)\,du$$

For large enough N, the Monte Carlo estimate of the integral converges to the correct answer.

- Central limit theorem: For large N, the sum of N independent random variables is **ALWAYS** normally (Gaussian) distributed!

$$Z_n \equiv \sum_{i=1}^{N} x_i$$ is Gaussian (for n→infty)!!! :

$$f(Z_n) \overset{n\to\infty}{=} \frac{1}{\sigma\sqrt{2\pi}}\exp\left[-\frac{(Z_n-\mu)^2}{2\sigma^2}\right]$$

➔ This outcome is independent of the original distributions of the x_i!

(MATHEMATICAL) BASICS

> Simple example: sum of n random numbers x_i from [0;1] :

$$R_n = \sum_{i=1}^{n} R_i$$

$$E(R_1) = \int_0^1 u\,du = 1/2$$

$$V(R_1) = \int_0^1 (u-1/2)^2\,du = 1/12$$

$$E(R_n) = n/2$$

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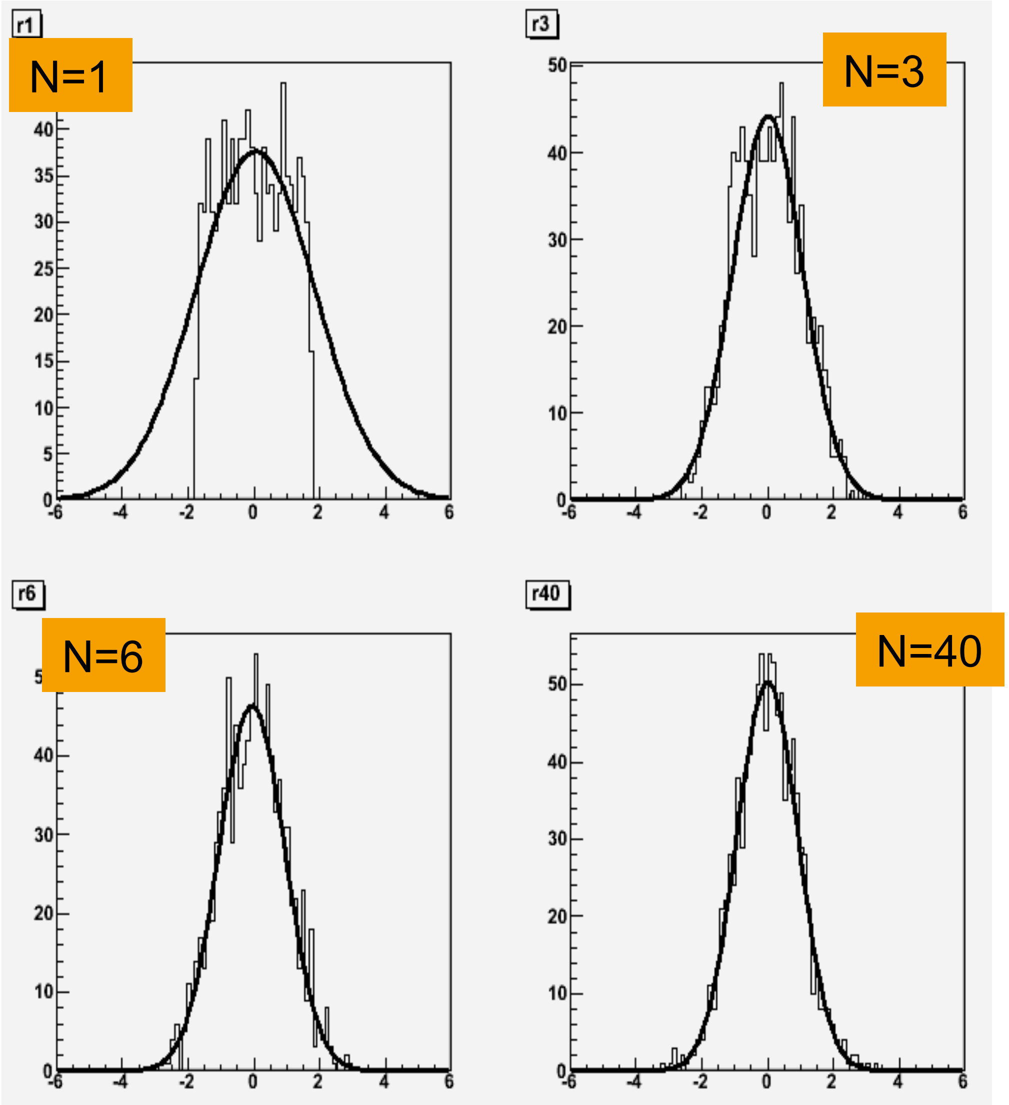

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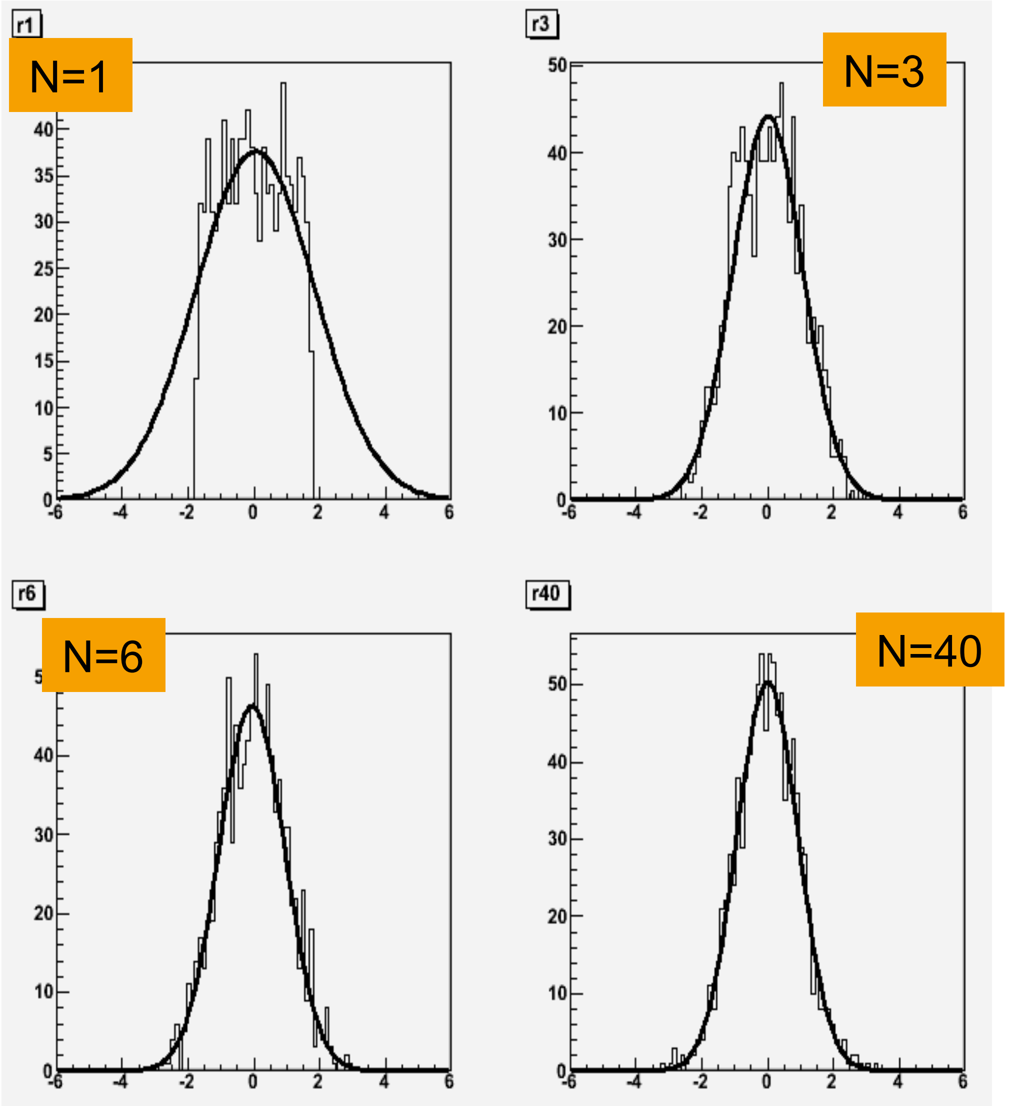


> To generate normal distribution centered at 0, variance 1, use:

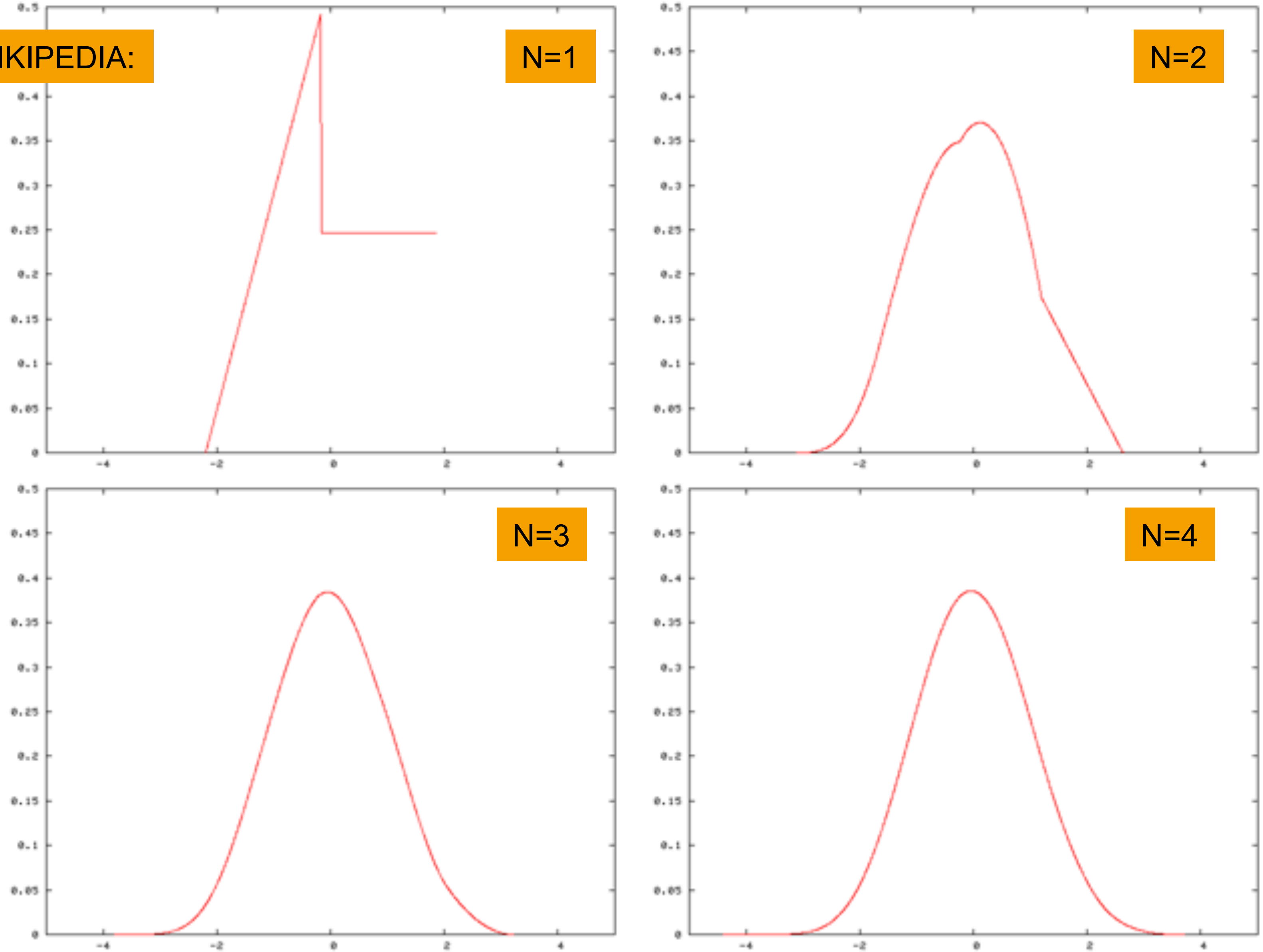
$$\frac{R_n - n/2}{\sqrt{n/12}} = \frac{\sum_{i=1}^{n} R_i - \sum_{i=1}^{n} \mu_i}{\sqrt{\sum_{i=1}^{n} \sigma_i^2}}$$

more generally:

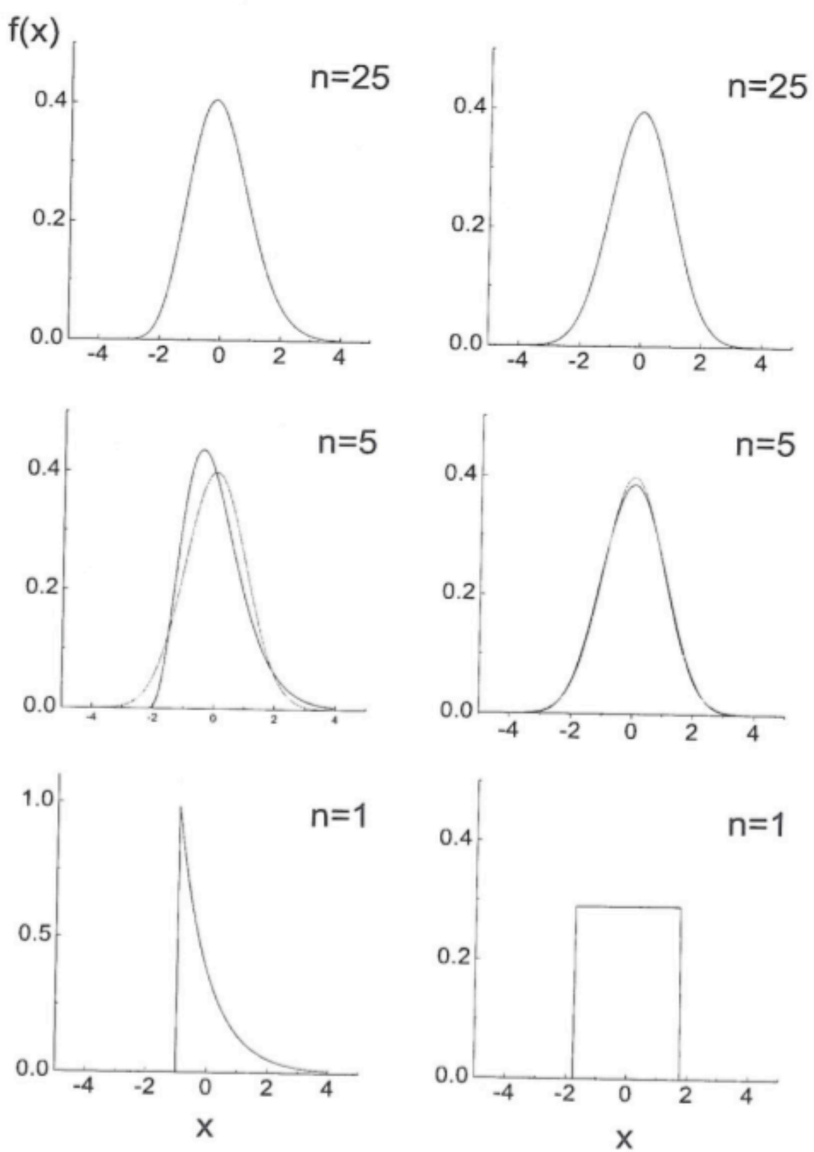
$$Z_n \equiv \frac{\sum_i x_i - n \cdot \mu}{\sqrt{n}\sigma} \longrightarrow N(0,1)$$

(MATHEMATICAL) BASICS

From WIKIPEDIA:

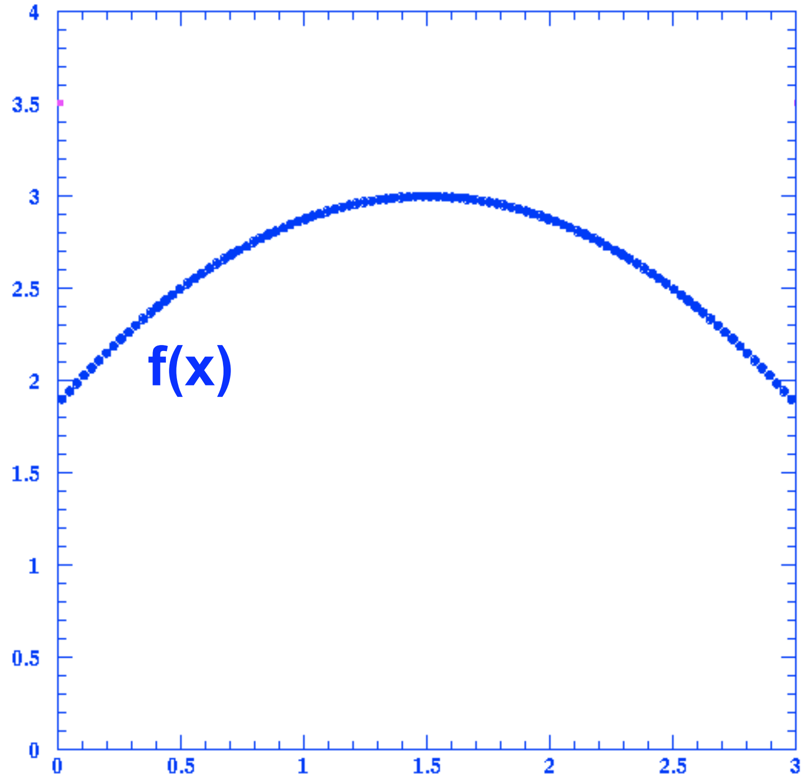


- Bohm&Zech: Einführung in die Statistik und Messwertanalyse:
  - Works for ANY starting distribution!!!!



GENERATING DISTRIBUTIONS (1)

- Assume you want to create events according to some distribution f(x)!
- Brute force or Hit&Miss method:
  - Works always – but not very elegant and not always efficient!



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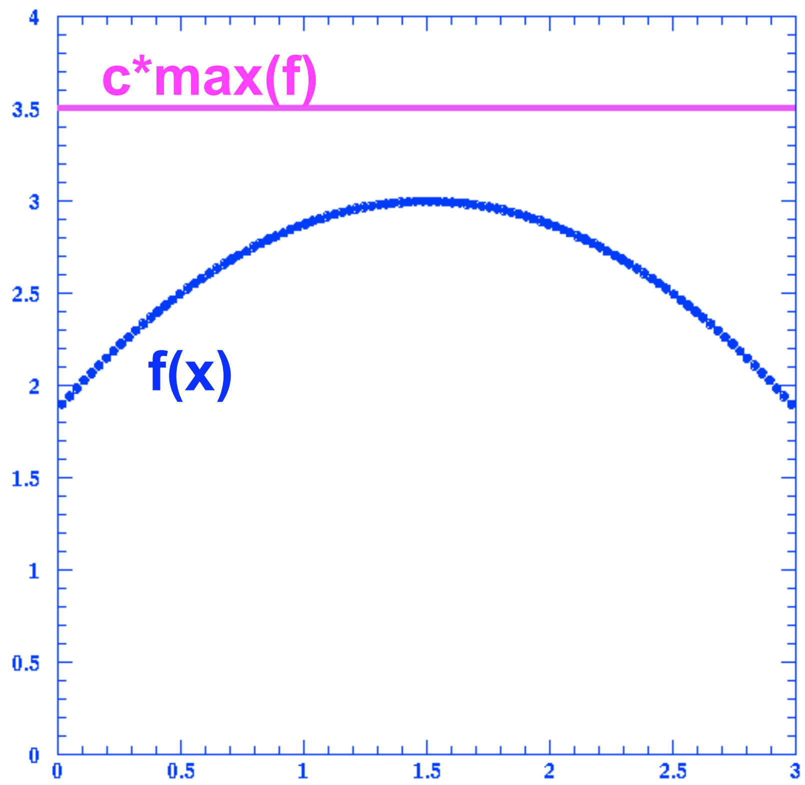

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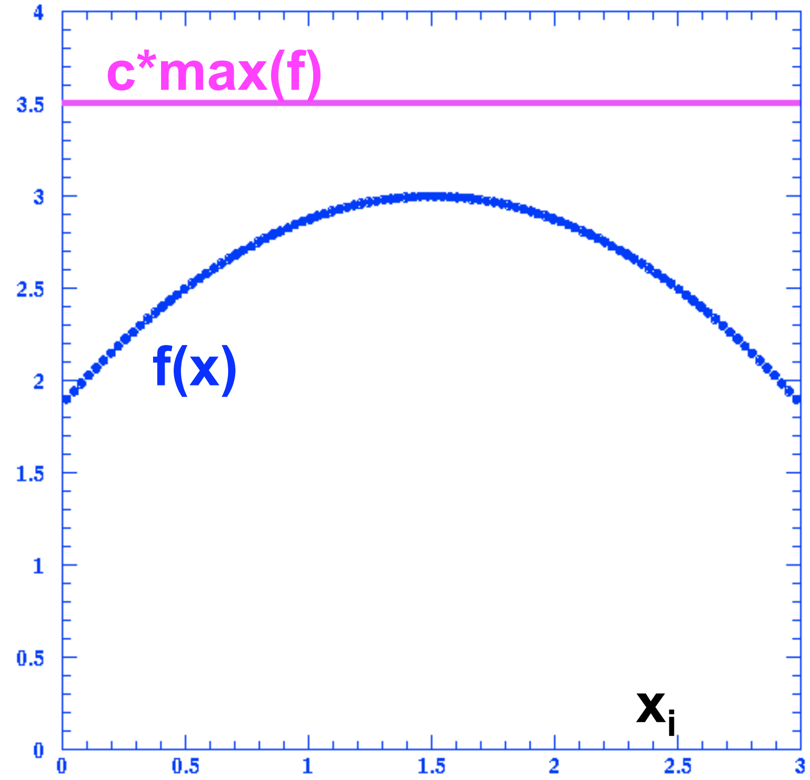
- Choose random number x_i.



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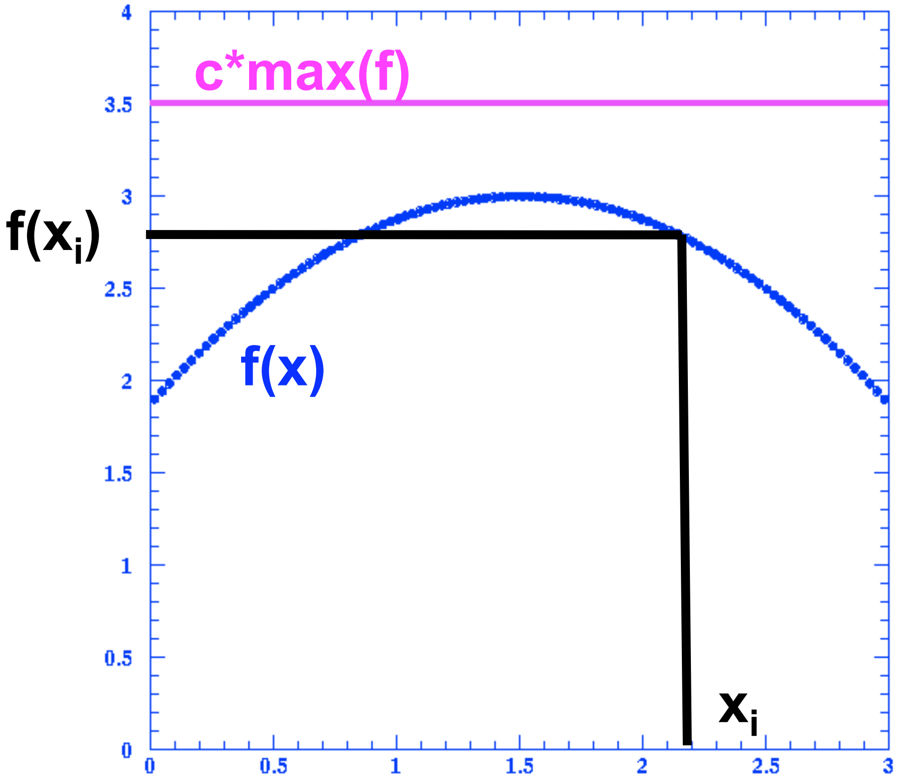
- Calculate $f(x_i)$.



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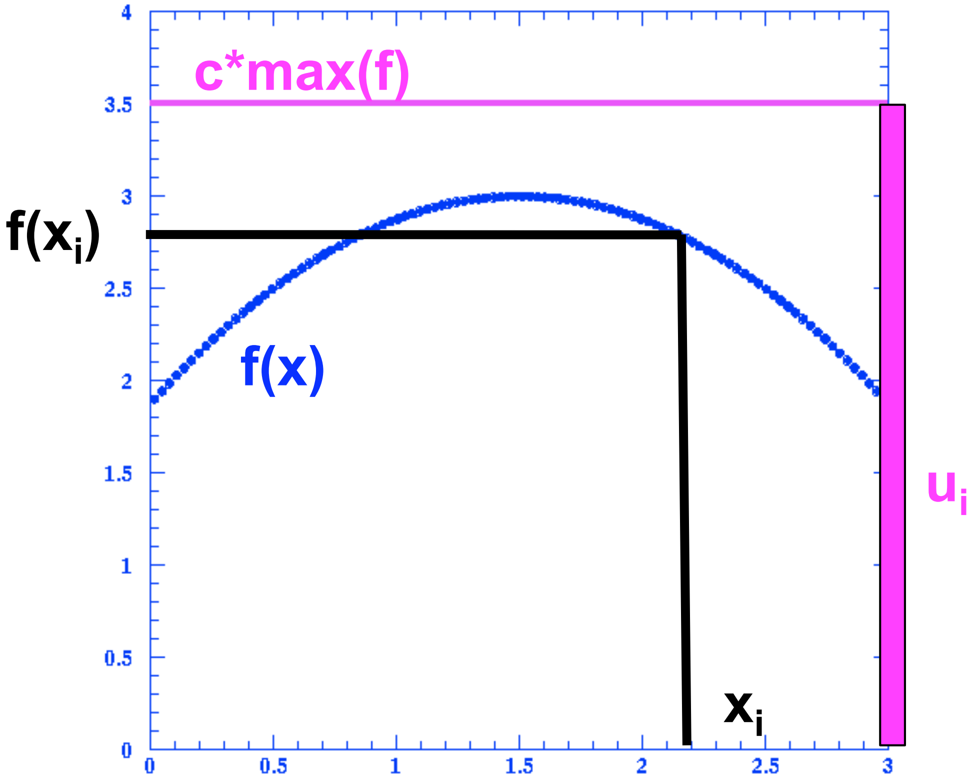

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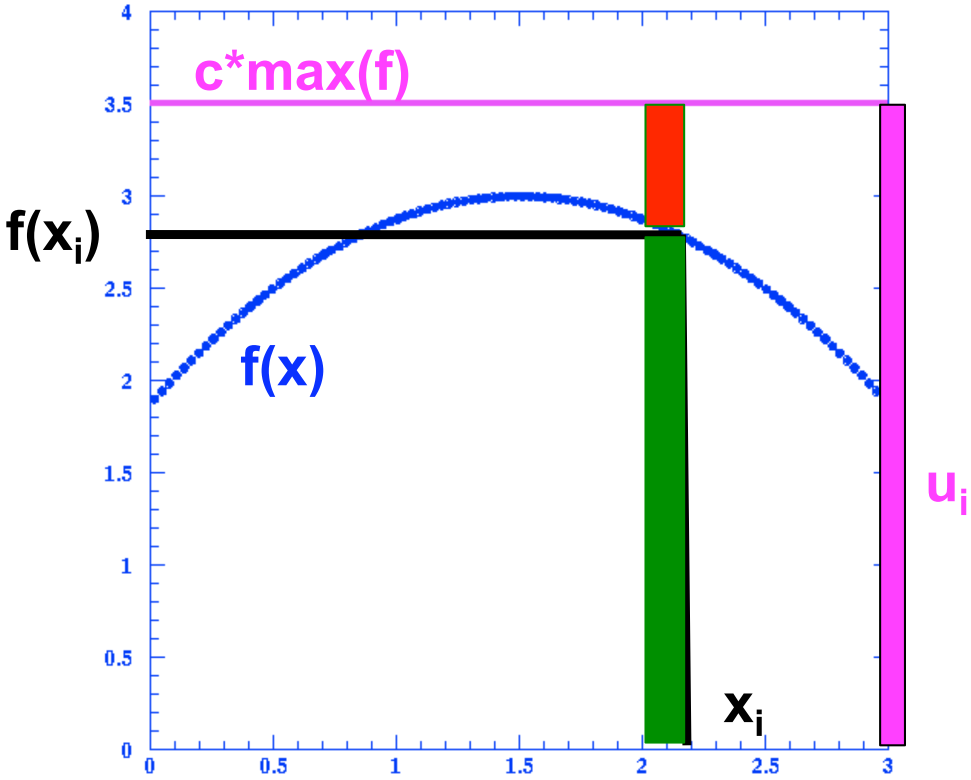
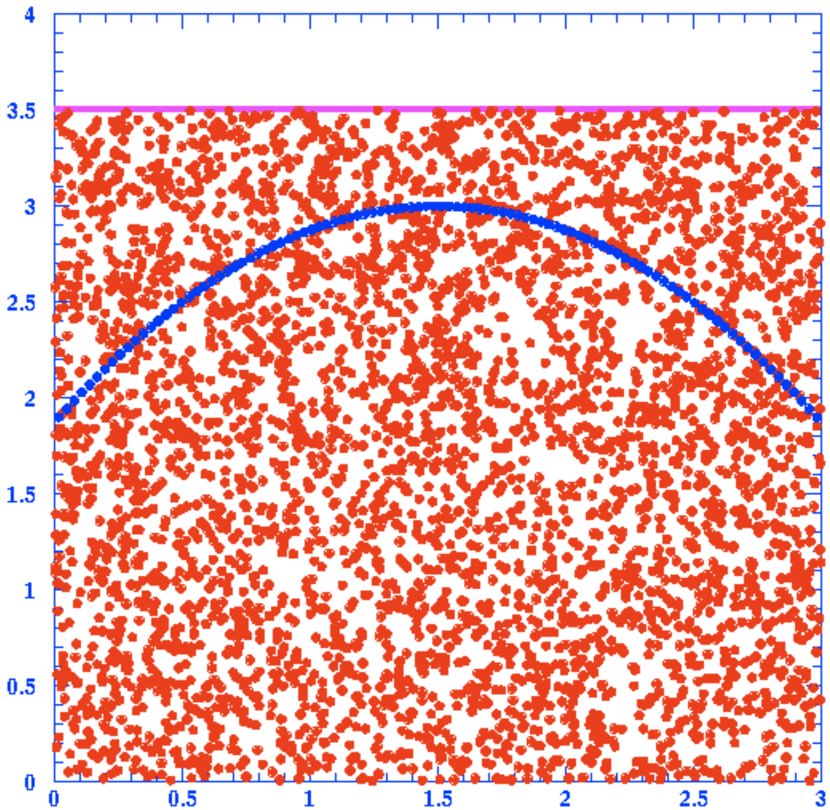
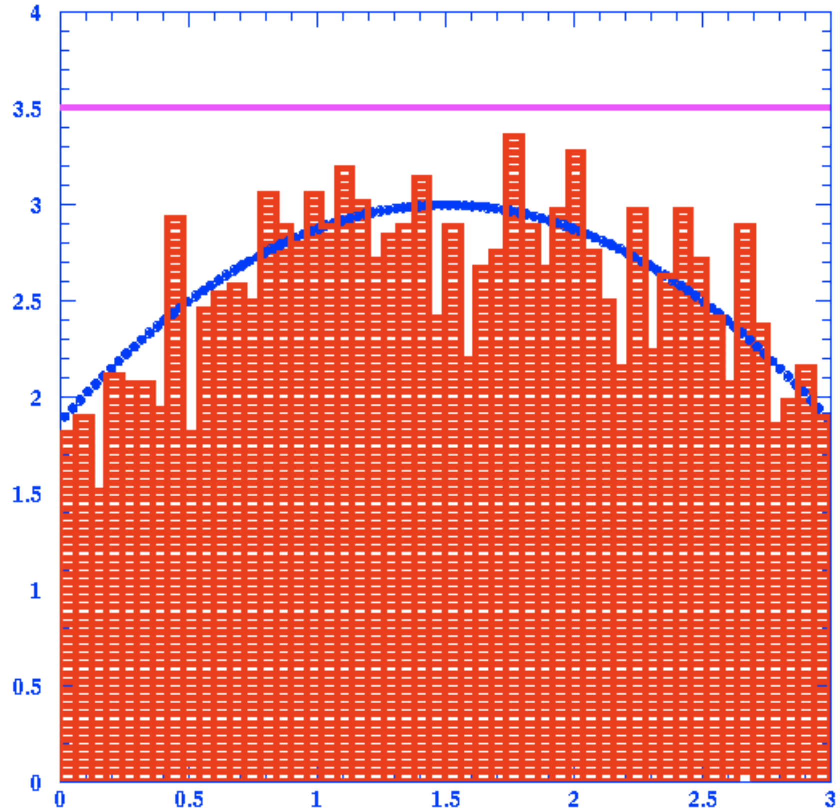
- If $u_i > f(x_i)$ **reject event**.
- Else **accept** (and make entry in histogram)!



GENERATING DISTRIBUTIONS (1)

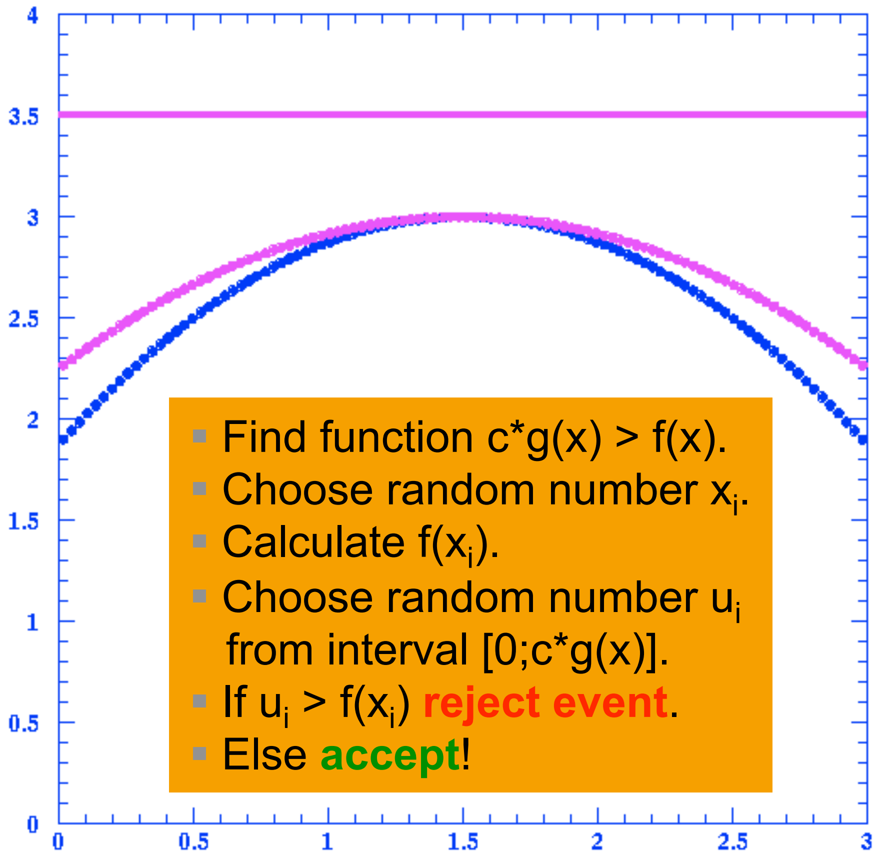
- Brute force or Hit&Miss method:
  - Preferred if no simple analytical solution exists!





GENERATING DISTRIBUTIONS (2)

- Modified brute force or Hit&Miss method:
  - Improve efficiency by variable transformation or better adjusted estimate of maximum!



- Find function c*g(x) > f(x).
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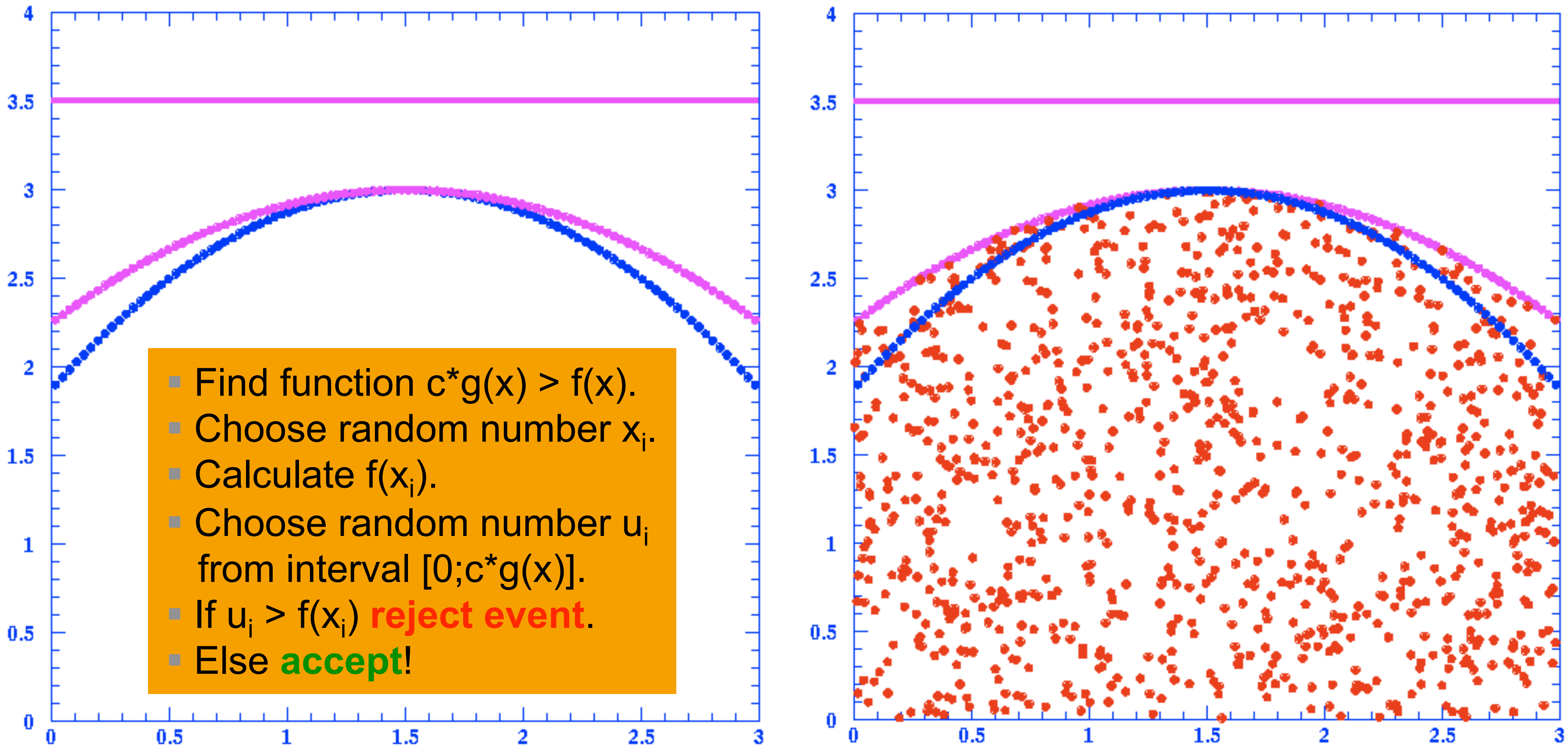

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GENERATING DISTRIBUTIONS (3)

> More elegantly – if analytically possible:

- Generation via "inversion of cumulative distribution function"

- Let f(t) be the function to simulate: $f(t)$
- First build the cumulative distribution ("Stammfunktion") $F(x) = \int_0^x f(t)dt$
- Build the inverse of F(x), $F^{-1}(Z)$.
- Proposition: With Z from [0.;1.] $F^{-1}(Z)$ is distributed as f(t). $x_i = F^{-1}(Z_i)$
- Proof in many books and lectures ;-).

> Works nicely and elegantly -

- … see examples on next pages.

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$$f(t)$$

$$F(x) = \int_0^x f(t)dt$$

$$x_i = F^{-1}(Z_i)$$

$$f(t) = 1/t$$

$$F(x) \propto \int 1/t \, dt \propto \ln t$$

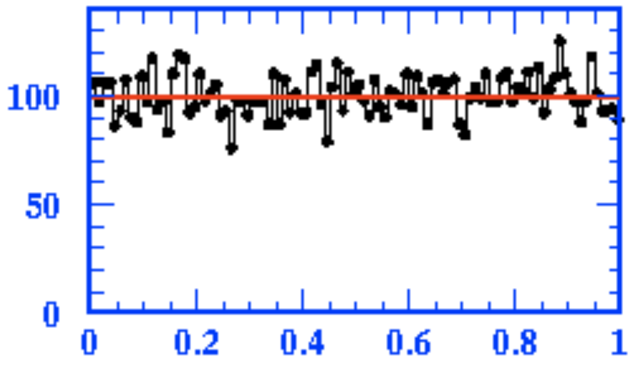
$$x_i = F^{-1}(Z_i) = \exp(Z_i)$$

Take uniform numbers Z_i and use as "random" number x_i.

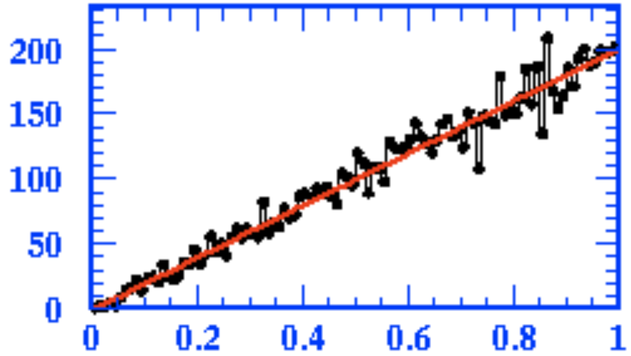
> Works nicely and elegantly -

- … see examples on next pages.

GENERATING DISTRIBUTIONS (3)

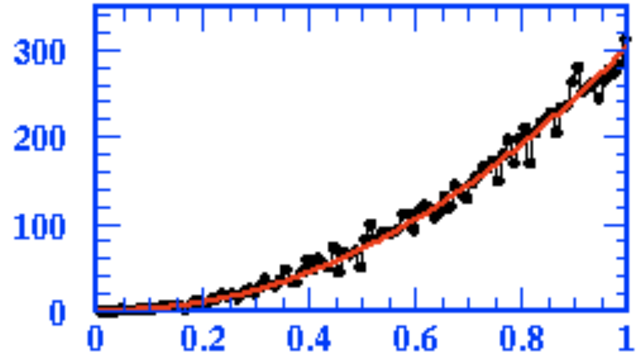


$$x_i = F^{-1}(Z_i) \quad Z \in [0.;1.]$$
$$F^{-1}(Z_i) = Z_i$$



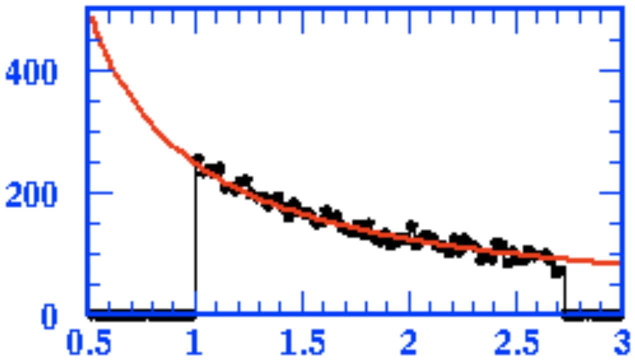
linear function

$$F^{-1}(Z_i) = \sqrt{Z_i}$$



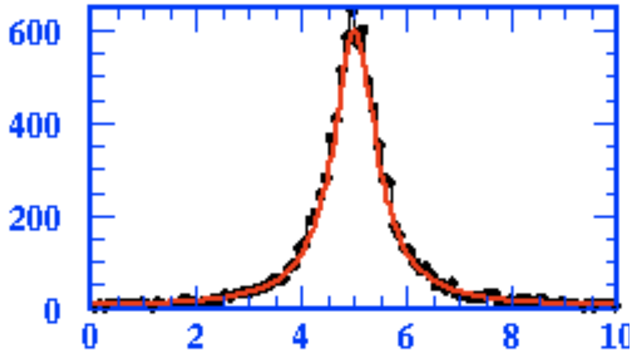
quadratic function

$$F^{-1}(Z_i) = \sqrt[3]{Z_i}$$



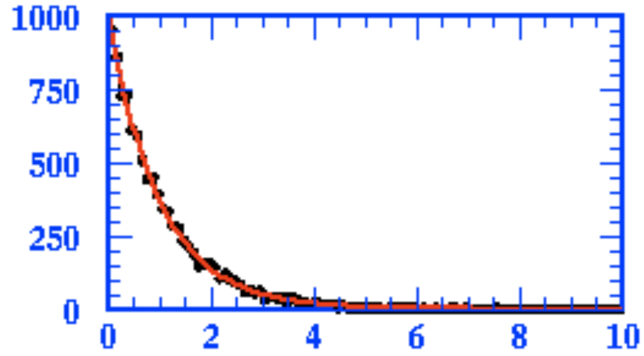
1/x function

$$F^{-1}(Z_i) = \exp(Z_i)$$



Lorentz curve

$$F^{-1}(Z_i) = a + b \cdot \tan(\pi \cdot Z_i - 1/2)$$

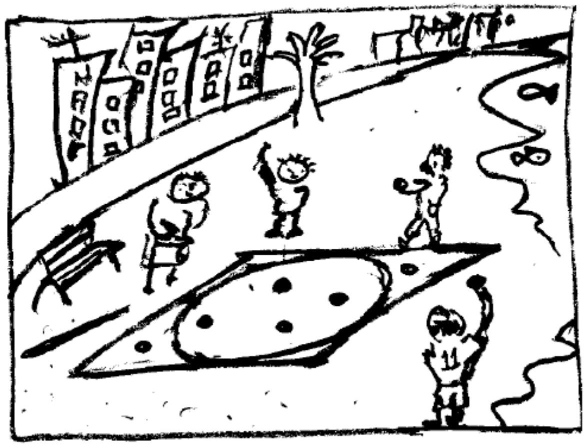


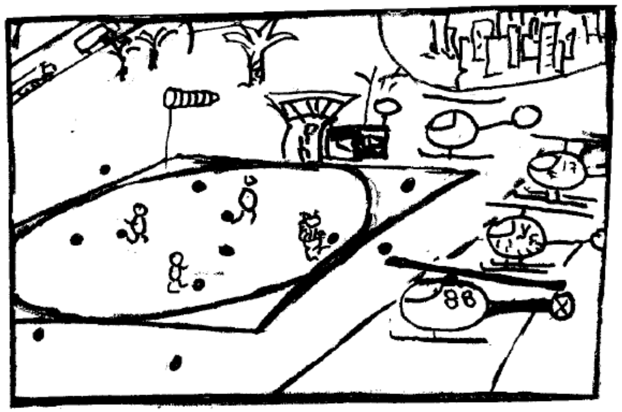
exponential

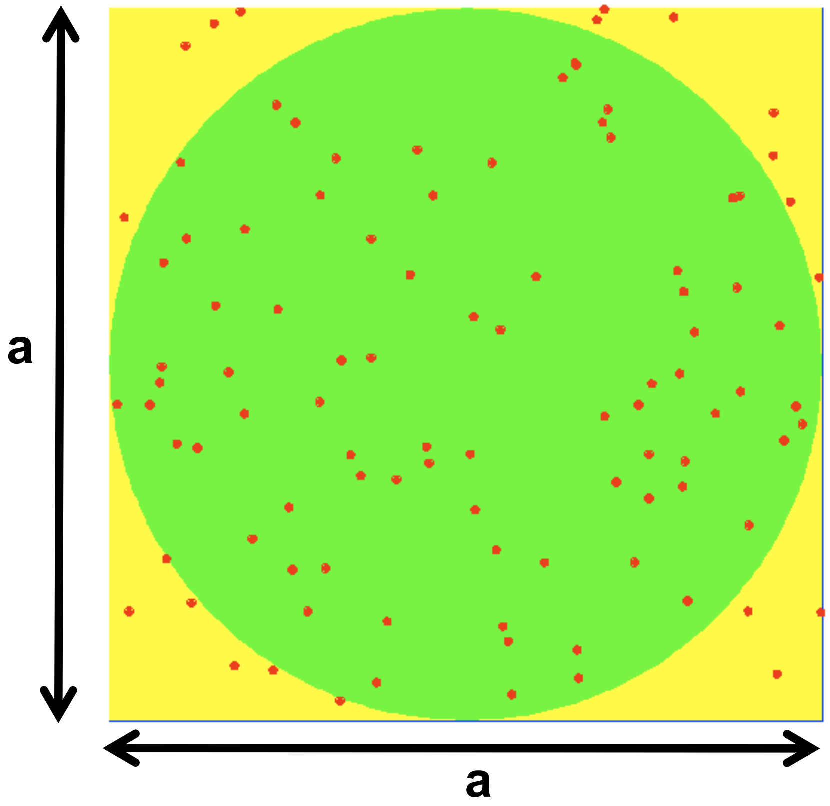
$$F^{-1}(Z_i) = -\ln Z_i$$

MC INTEGRATION (1)

- Another application of hit&miss: Calculating π using pebbles on the beach or helicopters in MC:







Area $\square$ = a^2

Area $\bigcirc$ = $\pi*(a/2)^2$

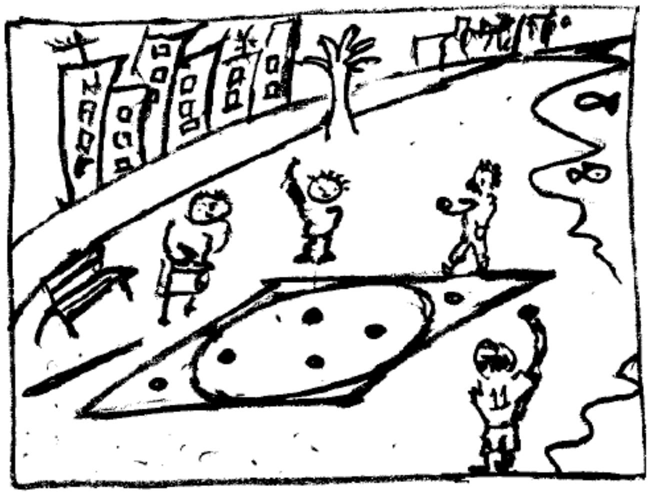
$\square / \bigcirc = 4/\pi \rightarrow N_{\square} / N_{\bigcirc}$

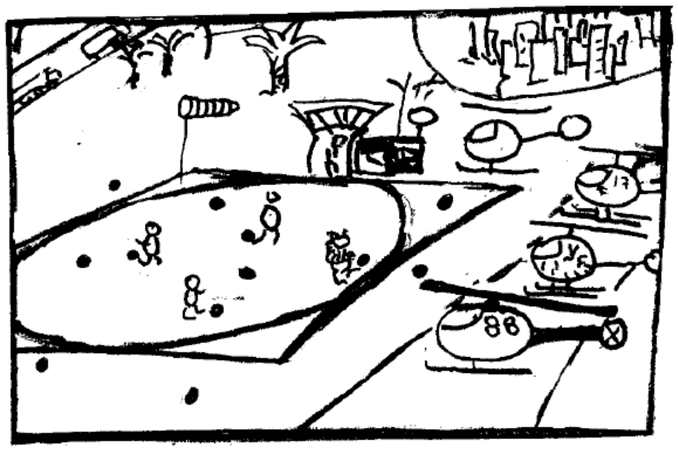
$\pi = 4*N_{\bigcirc} / N_{\square}$

… invoking again the law of large numbers …

MC INTEGRATION (1)

- Calculating π using pebbles on the beach or helicopters in Monte Carlo:





10^3:	3.056000
10^4:	3.132800
10^5:	3.145680
10^6:	3.141996
10^7:	3.141707
10^8:	…

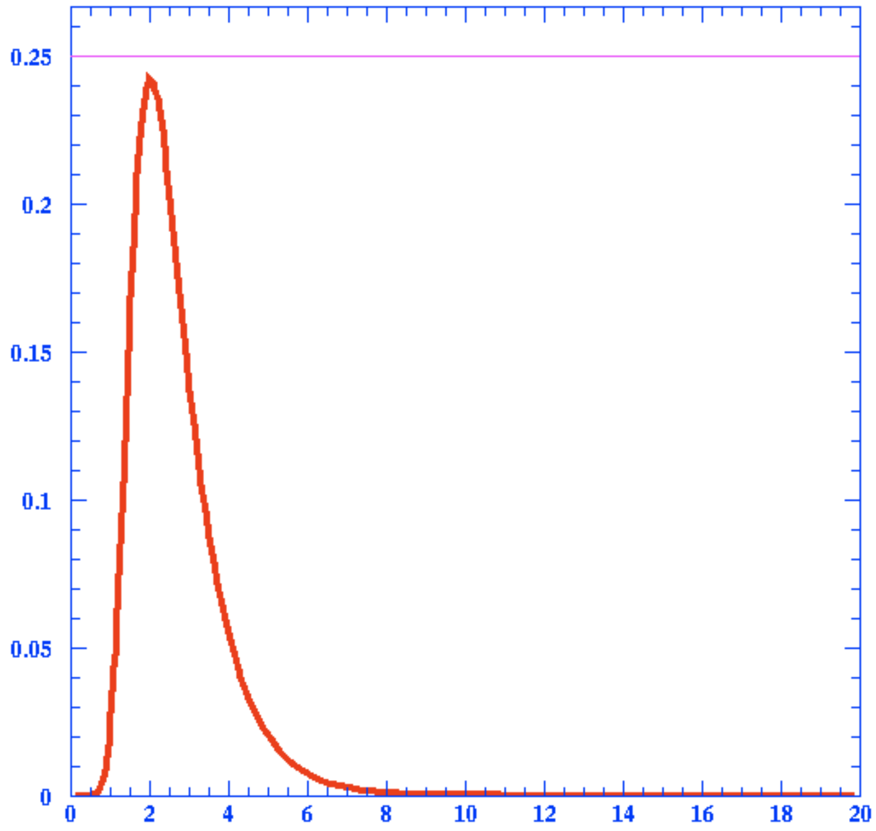
$\pi = 3.141592653\ldots$

MC INTEGRATION (2)

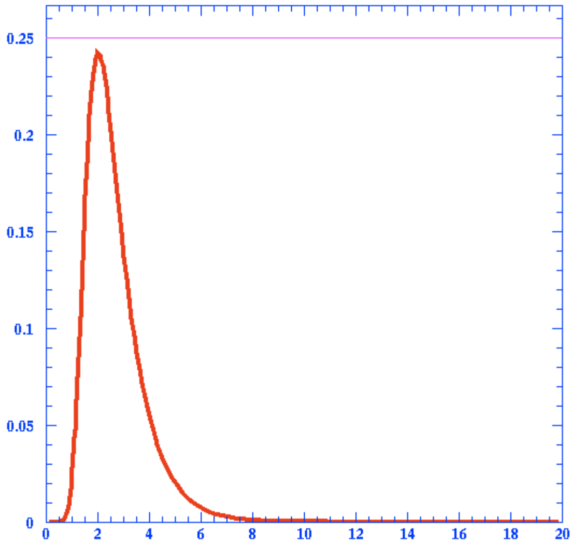
- Integration with Hit&Miss method:
  - Get random number R_1 for x axis in interval [0.;20.] (here).
  - Get random number R_2 for y axis between 0. and c*max(f).
  - Reject if $R_2 > f(R_1)$ (point "above" function).
  - Else accept.

➔ In principle comparison with area of known size!

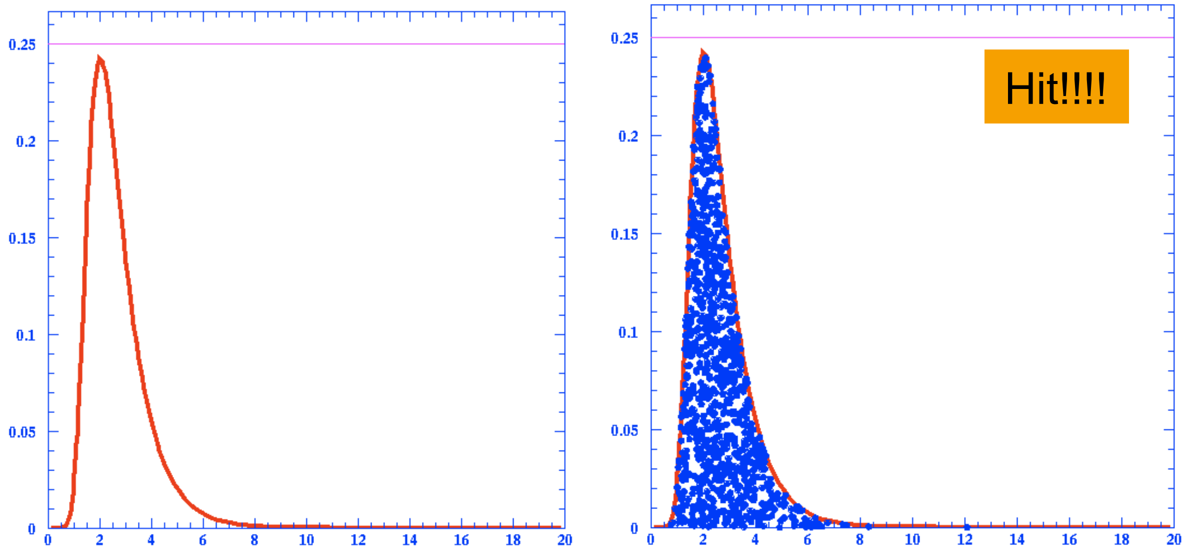
- Example: Landau distribution (energy loss of particles passing a thin layer of matter)
  - Strongly peaked signal
  - … now do hit and miss …



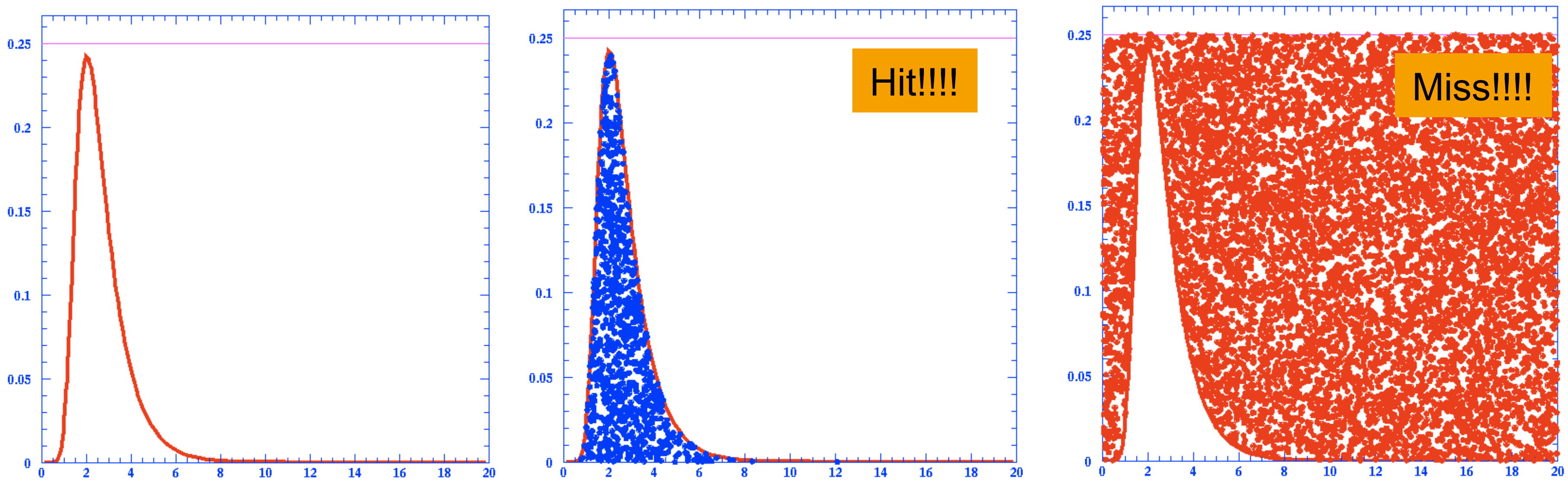
MC INTEGRATION (2)



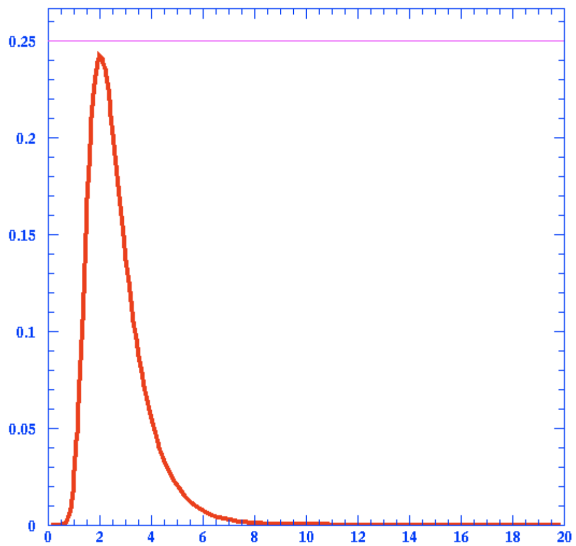
MC INTEGRATION (2)

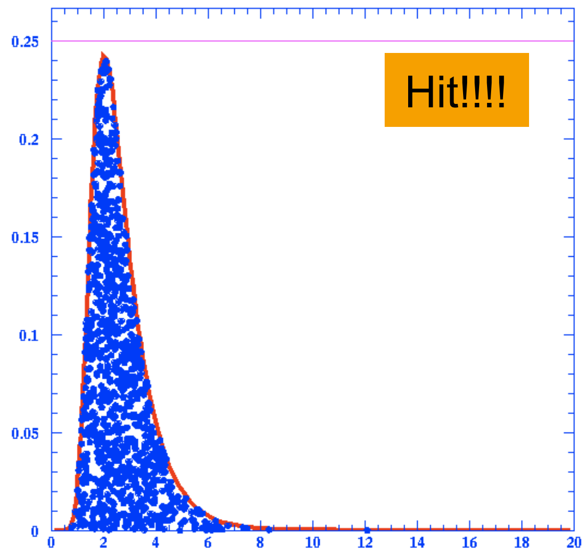


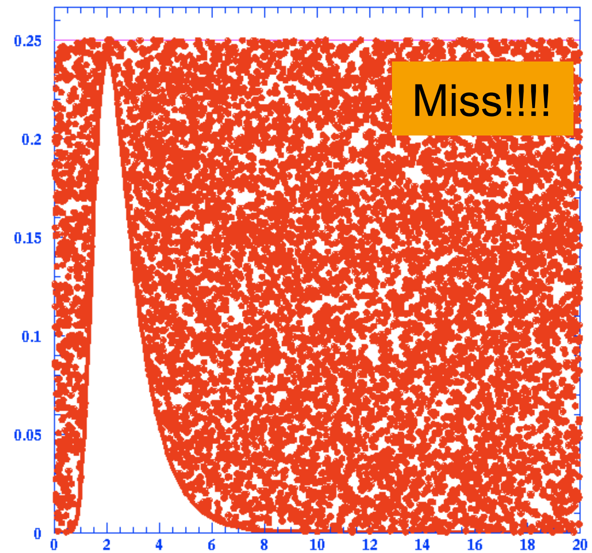
MC INTEGRATION (2)

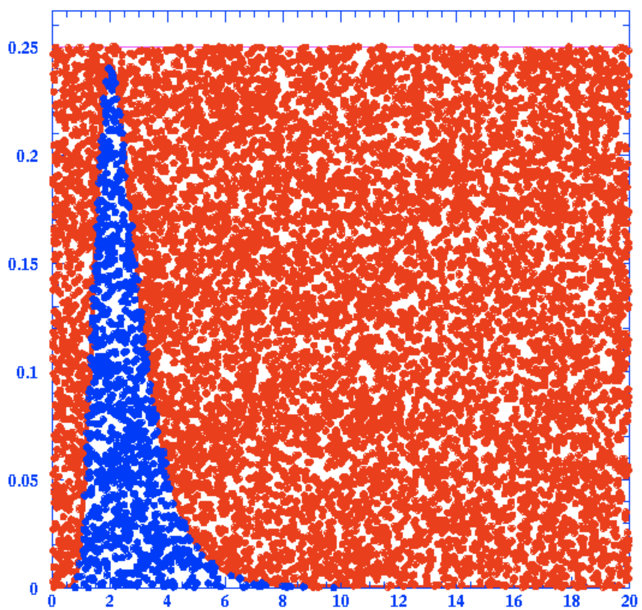


MC INTEGRATION (2)

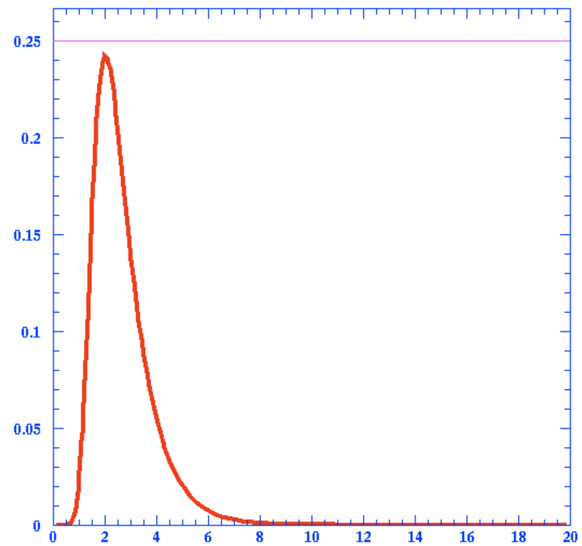
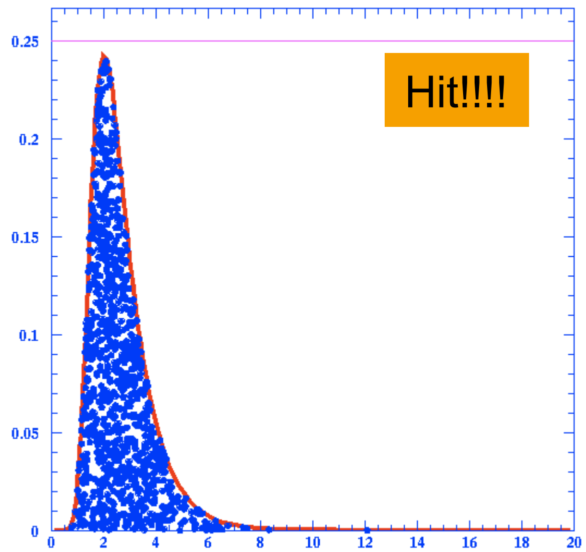


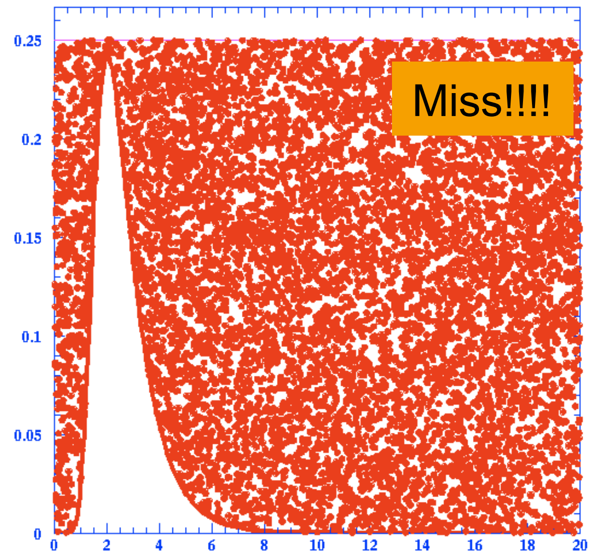


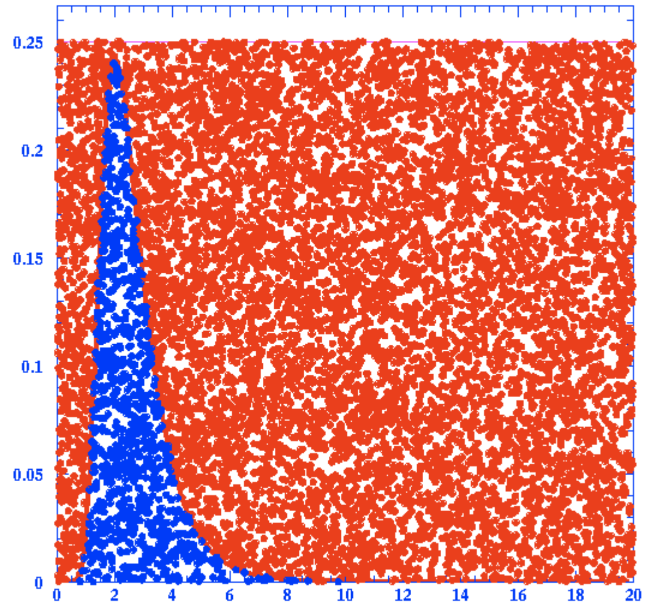




MC INTEGRATION (2)



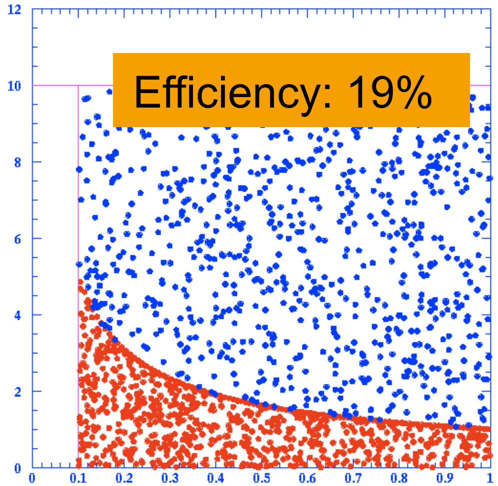


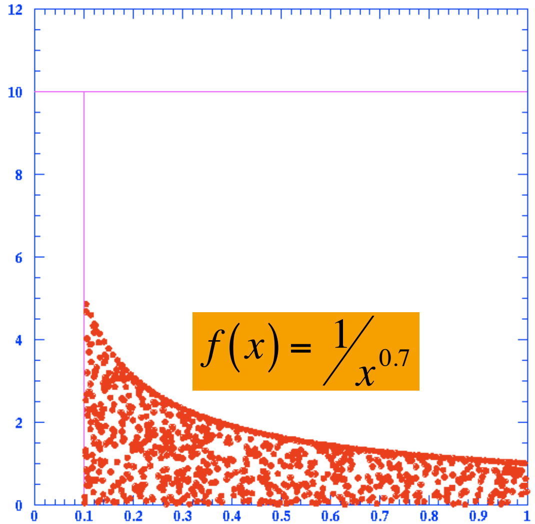
- Efficiency (ratio of hit/miss): 9% for hits example!
- 91% of “events” generated for the garbage
- Highly inefficient CPU usage!

➔ Can we do better?

MC INTEGRATION (3)

> Remember function generation by hit&miss: Increase efficiency by choosing better function maximum!





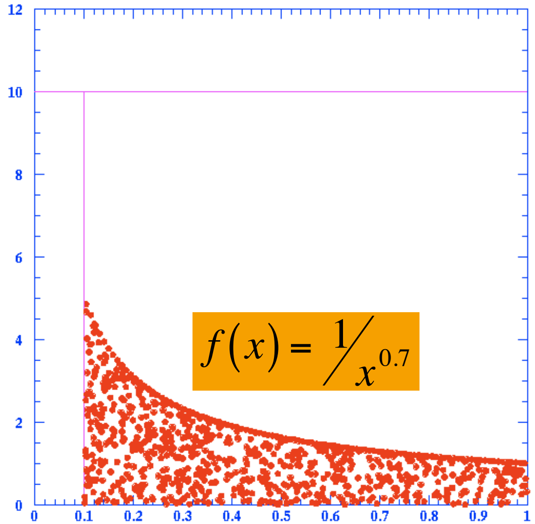
… now try something similar to distribution generation …
Choose g(x)~1/x …

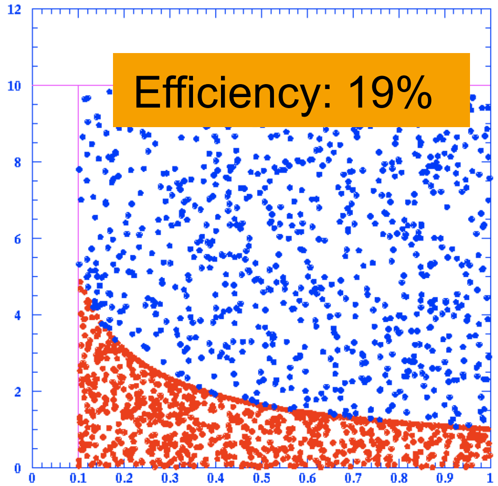
MC INTEGRATION (3)

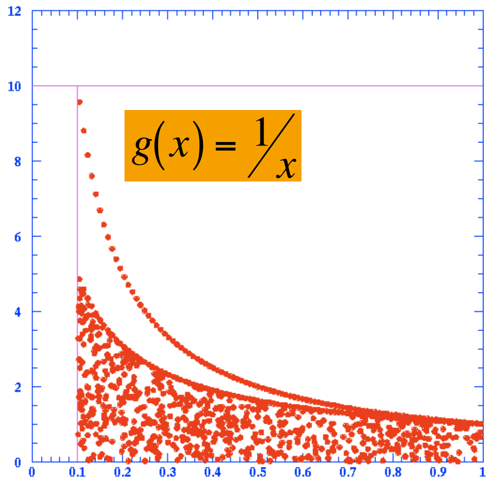
- Remember function generation by hit&miss: Increase efficiency by choosing better function maximum!

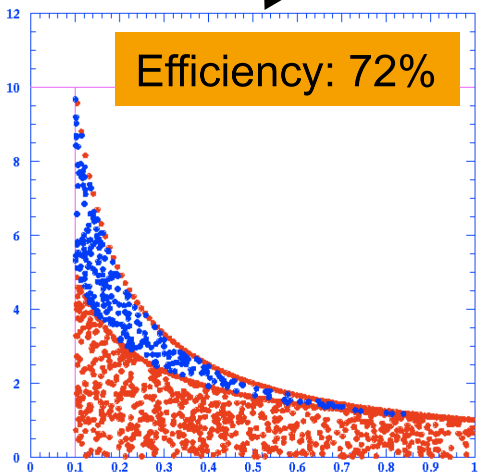
Side effect: potential reduction of variance:

$$\sigma = \frac{\sqrt{V(f)/V(g)}}{\sqrt{N}}$$







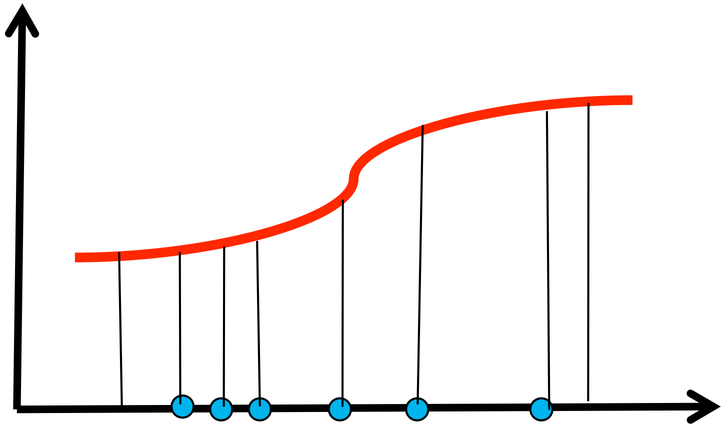


MC INTEGRATION (4)

- Mathematically: Solve

$$I = \int_a^b f(x)dx = (b-a)E(f(x))$$

(Mean value theorem)



- Remember Law of Large Numbers:

$$\tilde{E}(f(x)) = \frac{1}{N}\sum_{i=1}^{N} f(u_i) \to \frac{1}{b-a}\int_a^b f(u)du$$

MC estimate converges to true integral:

$$I \approx I_{MC} = \frac{b-a}{N}\sum_{i=1}^{N} f(x_i)$$

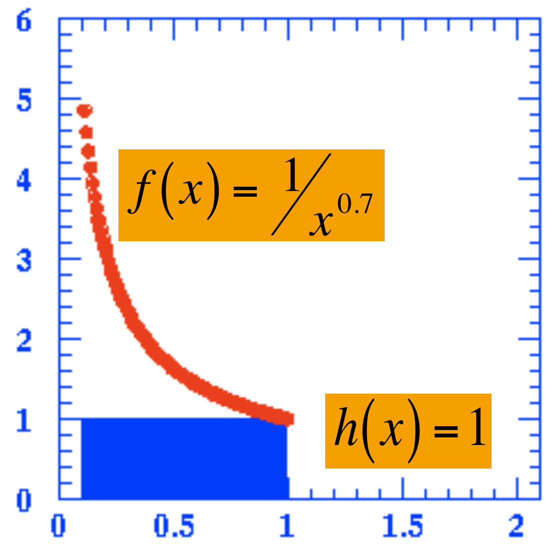
- Remember Central Limit Theorem:
  - MC estimate is asymptotically normally distributed, approaching Gaussian density with

$$\sigma = \frac{\sqrt{V(f)}}{\sqrt{N}} \propto \frac{1}{\sqrt{N}}$$

➔ to decrease estimate uncertainty, increase N!
(or try to reduce the variance of the relevant function)

MC INTEGRATION (4)

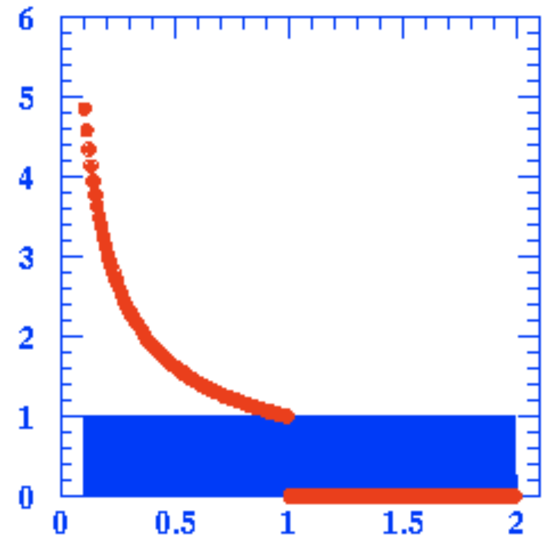
> **Importance sampling:** increase efficiency; start with `**barely relevant**' sampling



→ no sense to sample where function f(x) is 0 (or small).

- ➔ extending the integration (and the underlying probability density) to regions which don't contribute is … a waste of resources.

- ➔ concentrate on the relevant regions, and invest more CPU time in them!



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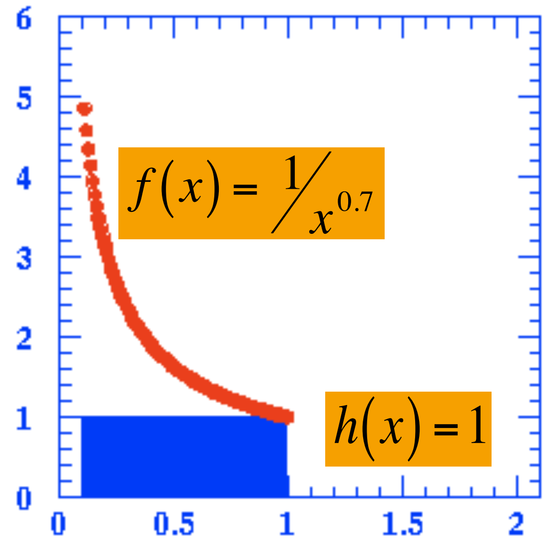
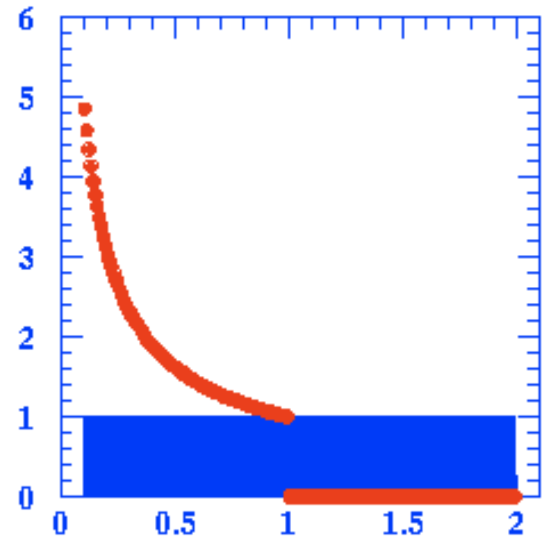




➔ Some mathematics:

[mean value theorem]

$$I[f(x)] = (b-a)E[f(x)]$$

$$E[f(x)] = E_h[f(x)] = \int f(x)dx = \int f(x)h(x)dx$$

Mostly assuming constant PDF (h(x)=1 here)

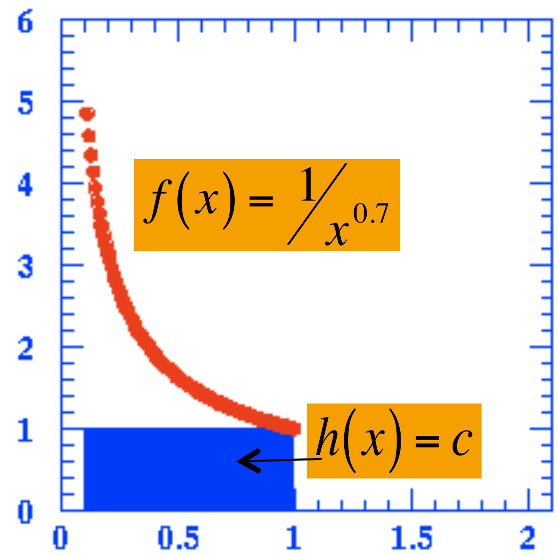
MC INTEGRATION (4)

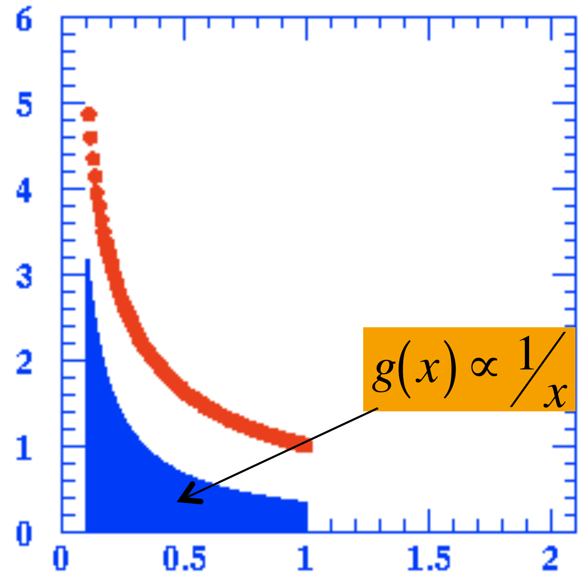
- Importance sampling more rigorously: $I[f(x)] = (b-a)E[f(x)]$
  ➔ Introduce a better suited PDF g(x):

$$E_h[f(x)] = \int f(x)h(x)dx = \int f(x)h(x)\frac{g(x)}{g(x)}dx$$
$$= \int f(x)\frac{h(x)}{g(x)}g(x)dx \equiv \int f(x)w(x)g(x)dx$$
$$= E_g[f(x)w(x)]$$

- Thus we can calculate the integral I by
  - Generating a sample x_i according to g(x)
  - Using $\frac{1}{n}\sum_{i=1}^{n} f(x_i) \xrightarrow{n\to\infty} E_h[f(x)]$ get I as:

$$I[f(x)] = (b-a)E_h[f(x)] = E_g[f(x)w(x)]$$
$$= (b-a)\frac{1}{n}\sum_{i=1}^{n} f(x_i)w(x_i)$$





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$$= E_g[f(x)w(x)]$$

Requirements on g(x):
- Integrable
- simple
- close in shape to f(x)
- Efficient to generate
- …

➔ Not always easy to find!

- Thus we can calculate the integral I by
  - Generating a sample x_i according to g(x)
  - Using $\frac{1}{n}\sum_{i=1}^{n} f(x_i) \xrightarrow{n\to\infty} E_h[f(x)]$ get I as:

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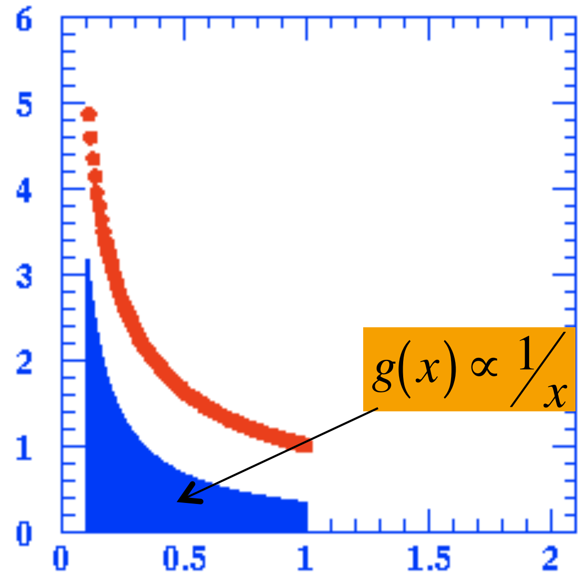
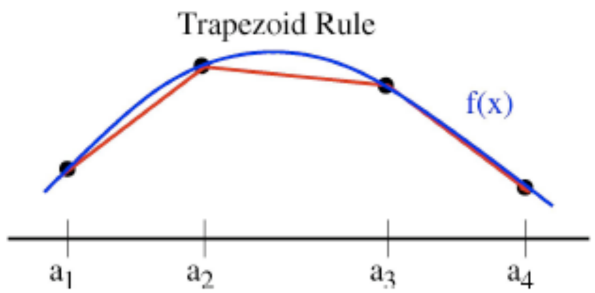
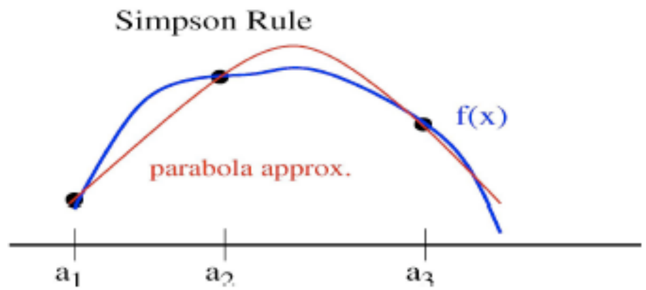


MC INTEGRATION (5)

- Comparison of MC integration with other numerical methods (from Hannes Jung):
  - Monte Carlo: Hit & Miss
  - Trapezoidal Rule: approximate integral in subinterval by area of trapezoid below (above) curve
  - Simpson quadrature: approximate by parabola
  - Gauss quadrature: approximate by higher order polynomial



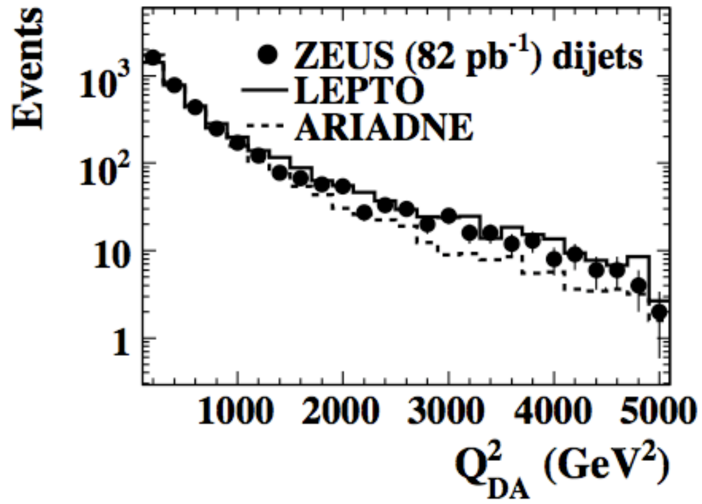


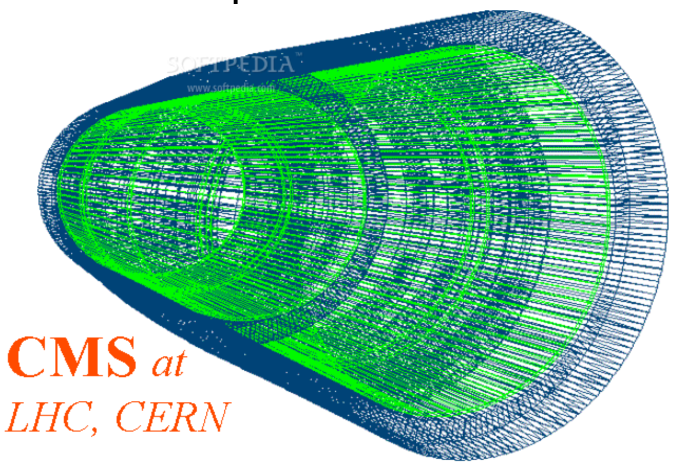
method	err (1d)	error
MC	$n^{-1/2}$	$n^{-1/2}$
Trapez	n^{-2}	$n^{-2/d}$
Simpson	n^{-4}	$n^{-4/d}$
Gauss	n^{-2m+1}	$n^{-(2m-1)/d}$

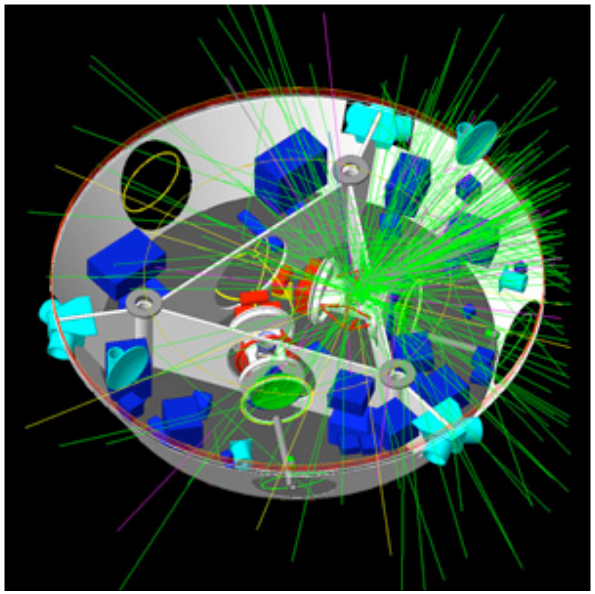
➔ Especially for higher dimensions, MC integration wins very often!

MC IN HEP

- “MC generators”: Computer programs to simulate “arbitrarily” complex physics following some distribution.
  - Higher-order calculations, parton shower …
  - HERWIG, PYTHIA, etc.
- Statistics: Markov chains etc.
- Detector simulation programs
  - Simulate interactions of particles with the matter.
  - … for example for detector corrections.







SUMMARY

- “MC methods”: no unique definition, but …
  - … invoking law of large numbers to approximate expectations …
  - … making use of “random” numbers for sampling purposes.
- (Pseudo)Random numbers:
  - Necessary ingredient, but not too easy to obtain. Different methods with more or less good properties.
- Generating distributions …
  - … by means of hit&miss or, for example, inversion of the cumulative function, …
- Integration as one of the main applications.
  - … hit and miss, …
  - … importance sampling …
- Numerous applications
  - … in HEP
  - … and elsewhere.