Computational methods for Medical Physics

Lecture 1
Monte Carlo Basics

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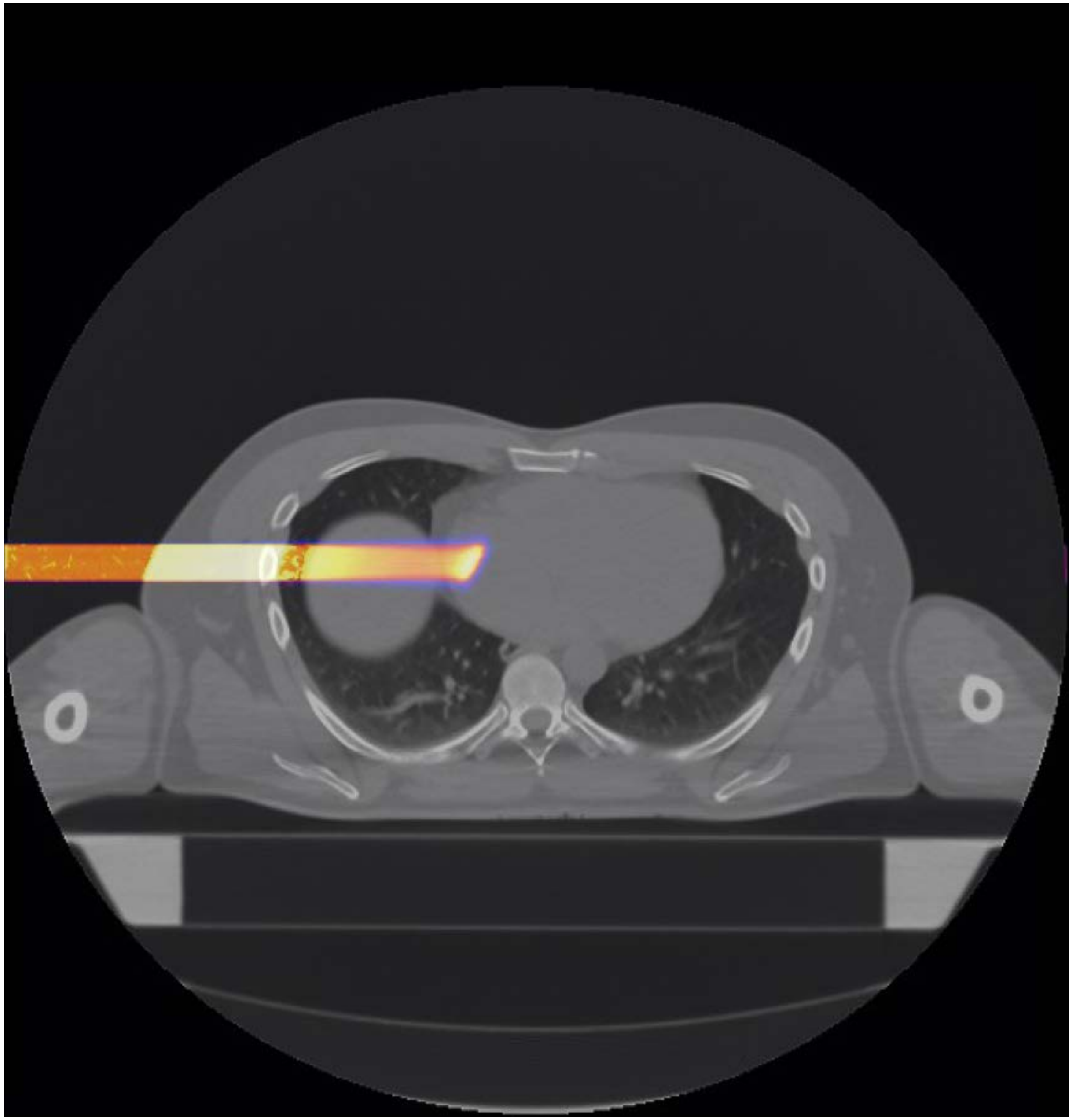
WS 2016-2017

LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

Past and next lectures’ content

- Next few lectures:
  - Monte Carlo technique basics
  - Simulation of particle transport using Monte Carlo

Motivation



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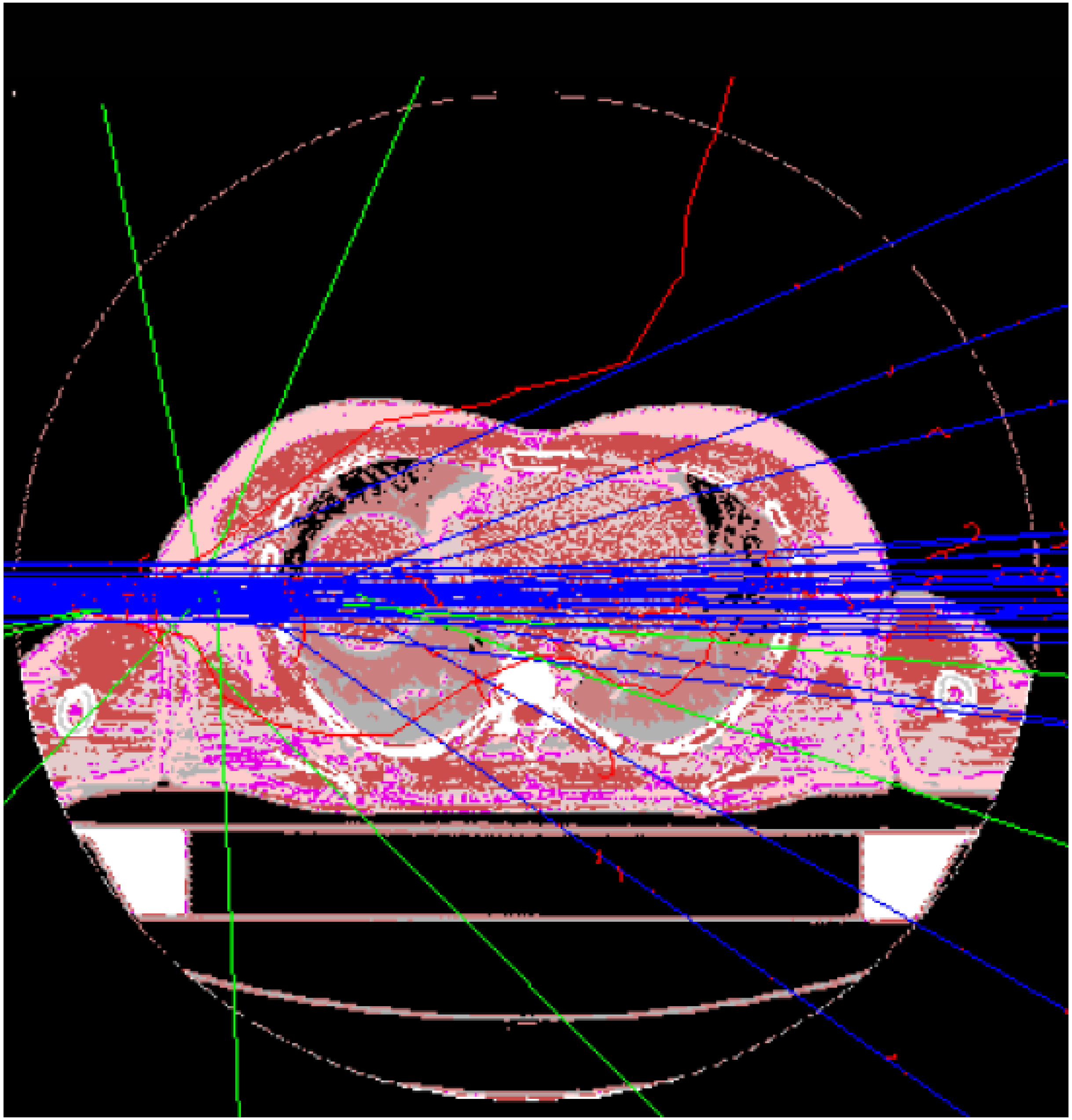

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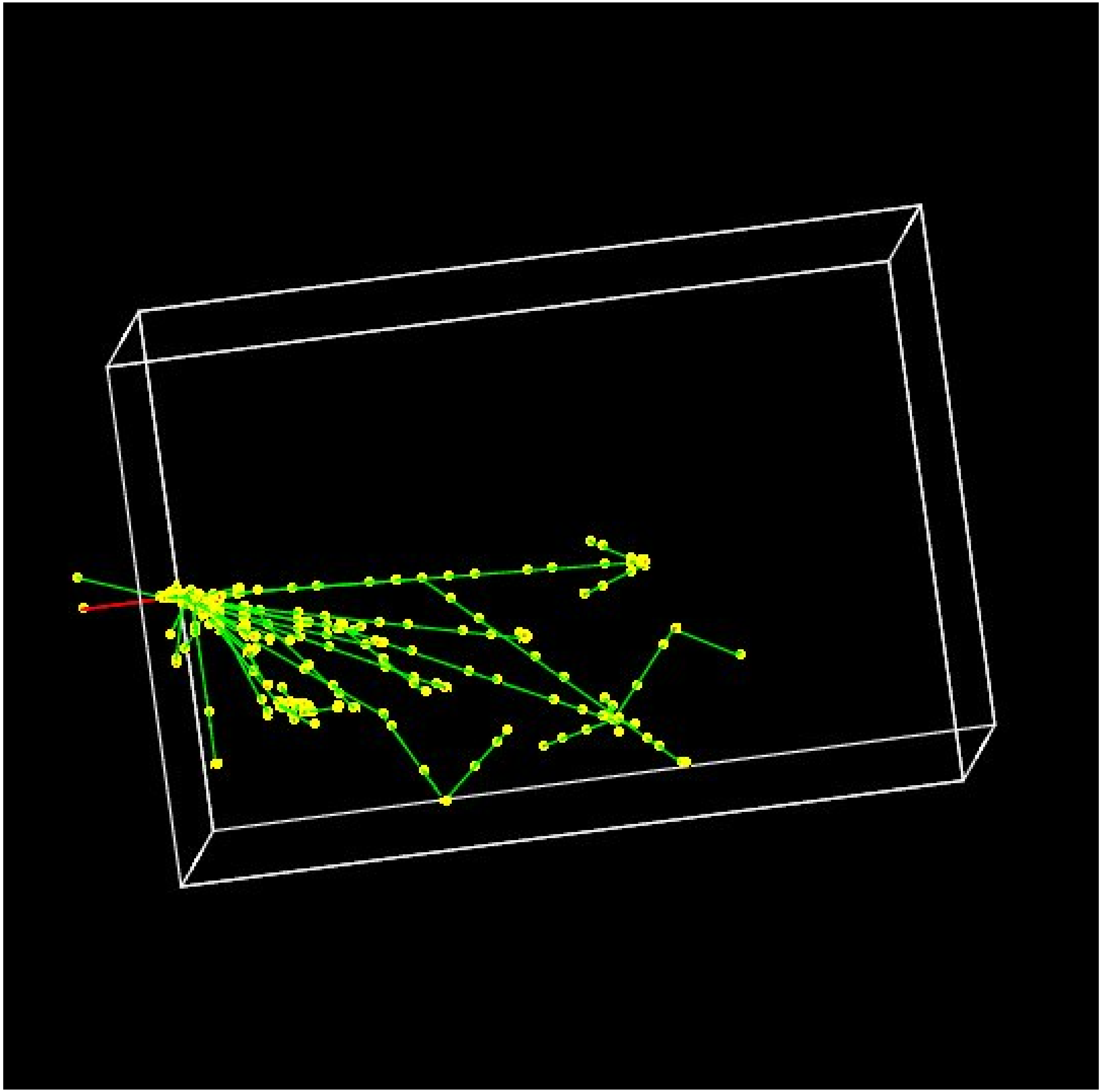
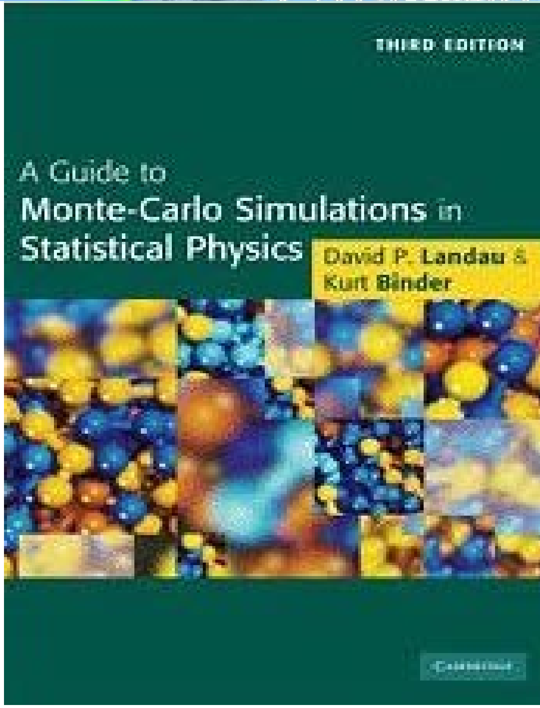


External material

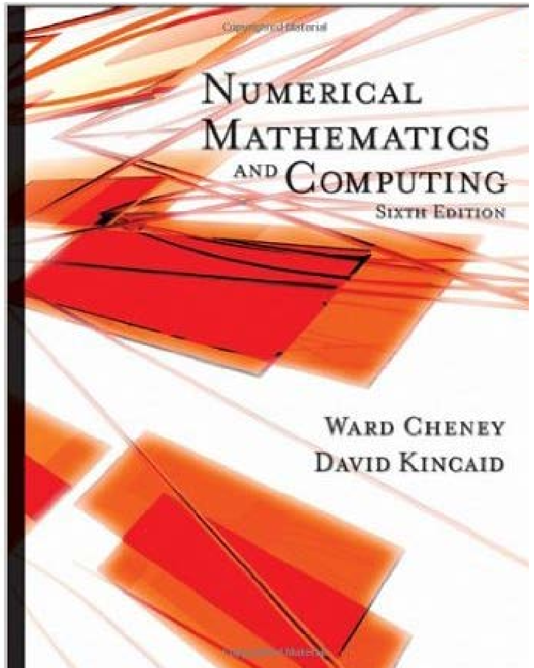
- Material form this lecture was taken from the following lectures:
  - Aalto University School of Science
    Department of Biomedical Engineering and Computational Science
    Lecture on Computational Science
    Dr. Ricu Linna
    Dr. Laura Juvonen
  - University of Helsinki
    Department of Physics
    Basics of Monte Carlo Simulations Lecture
    Priv. Doz. Dr. Flyura Djurabekova

External material

- Books:
  - A Guide to Monte Carlo Simulations in Statistical Physics
    David P. Landau, Kurt Binder



  - Numerical Mathematics and Computing
    Ward Cheney, David Kincaid



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- The question for this lecture is: MC is an interesting technique for what?
- To answer that, we will start from:
  - Some historical information about MC technique
  - Integration (numerical/MC)

- Probability theory started being used in order to understand games of chance
  - Pierre de Fermat and Blaise Pascal were asked by a professional gambler to solve some of his questions on dice games
  - In 1654 they solved the problem by using probabilities calculation
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Monte Carlo
Historical review

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- In 1812 Laplace published his "*Théorie analytique des probabilités*"

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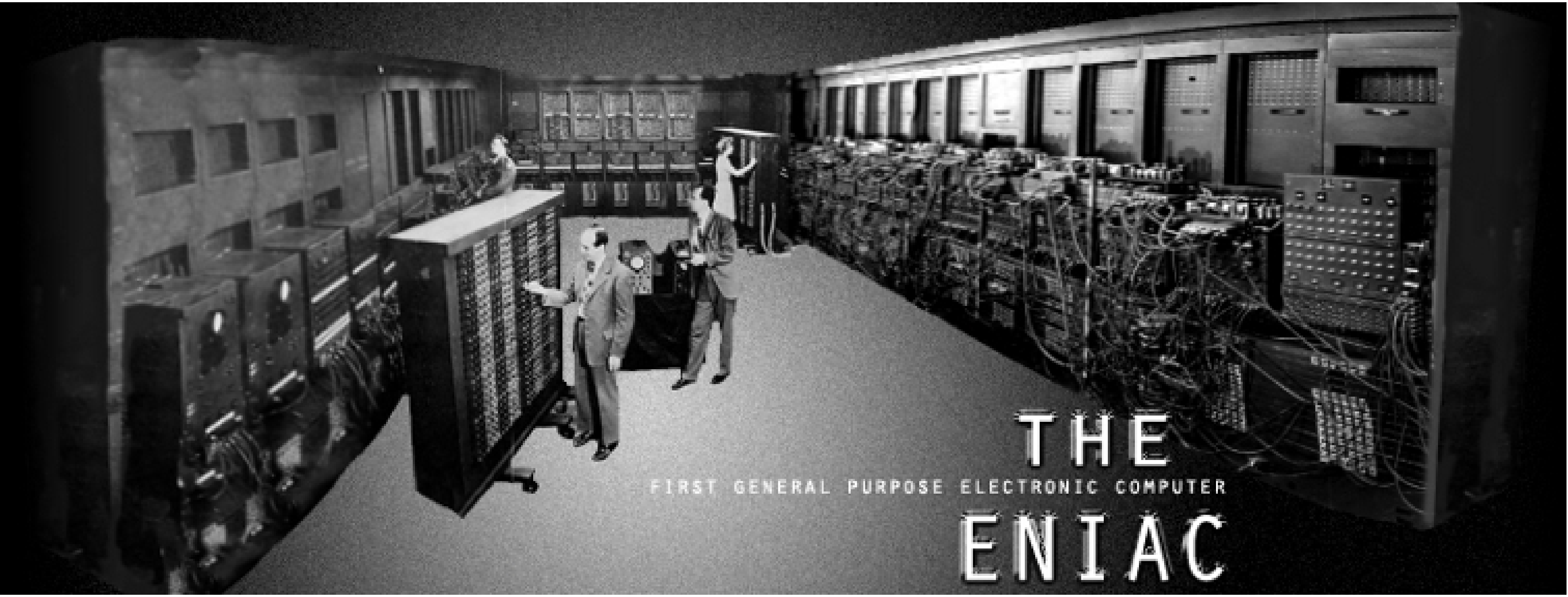
- 18.000 vacuum tubes and 500.000 shoulder joints!



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- In 1946 there was the idea to solve thermonuclear problems (neutron diffusion in fissile material) by using statistical sampling techniques
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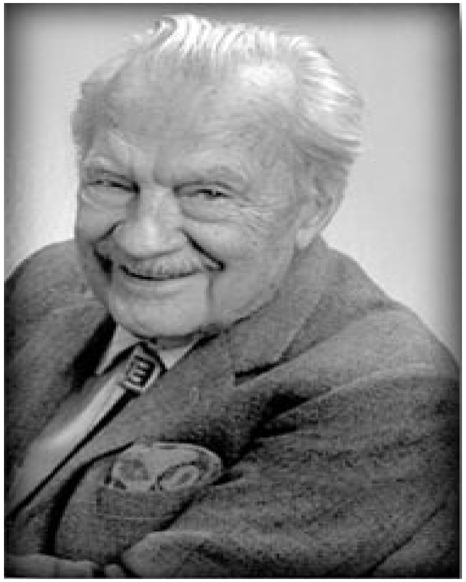
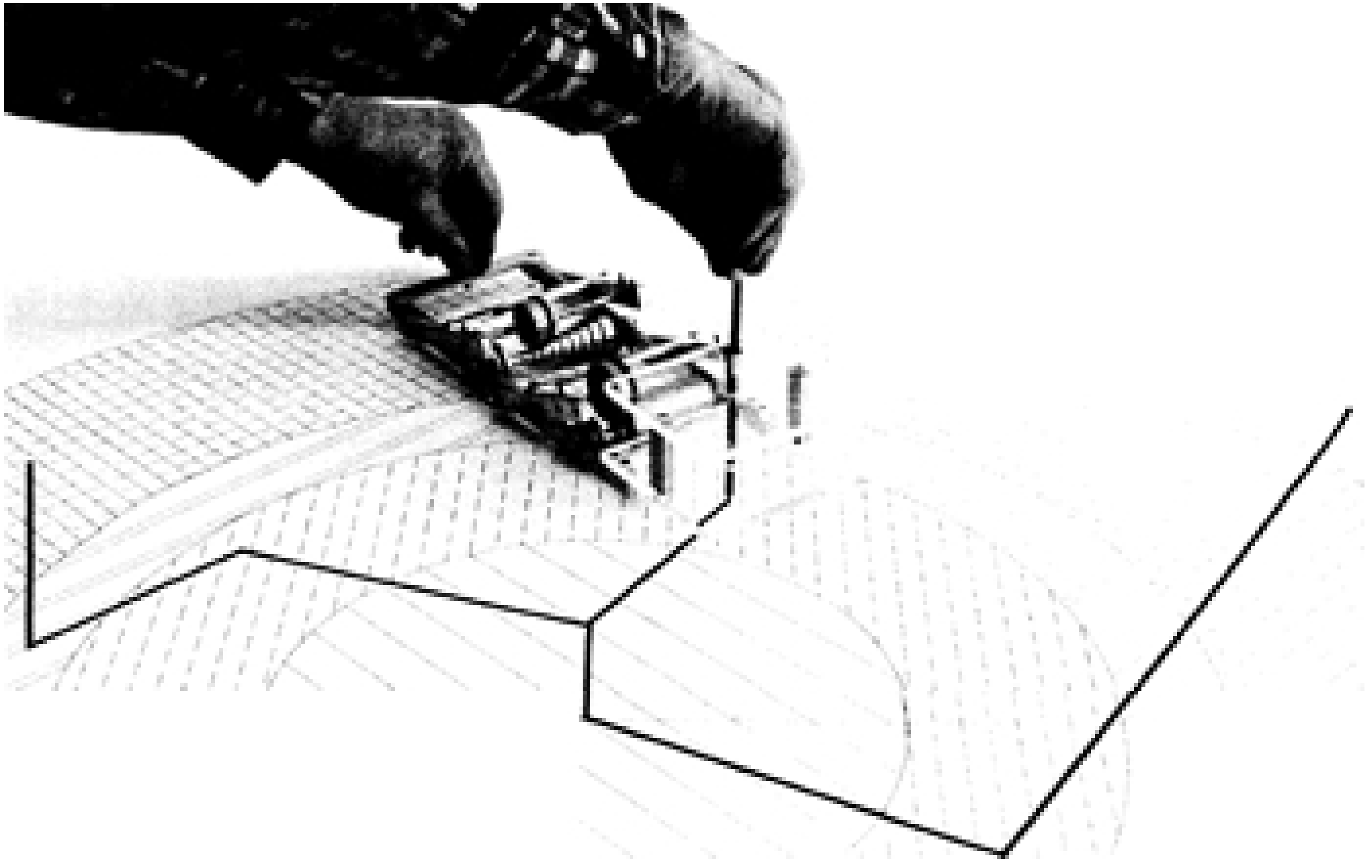
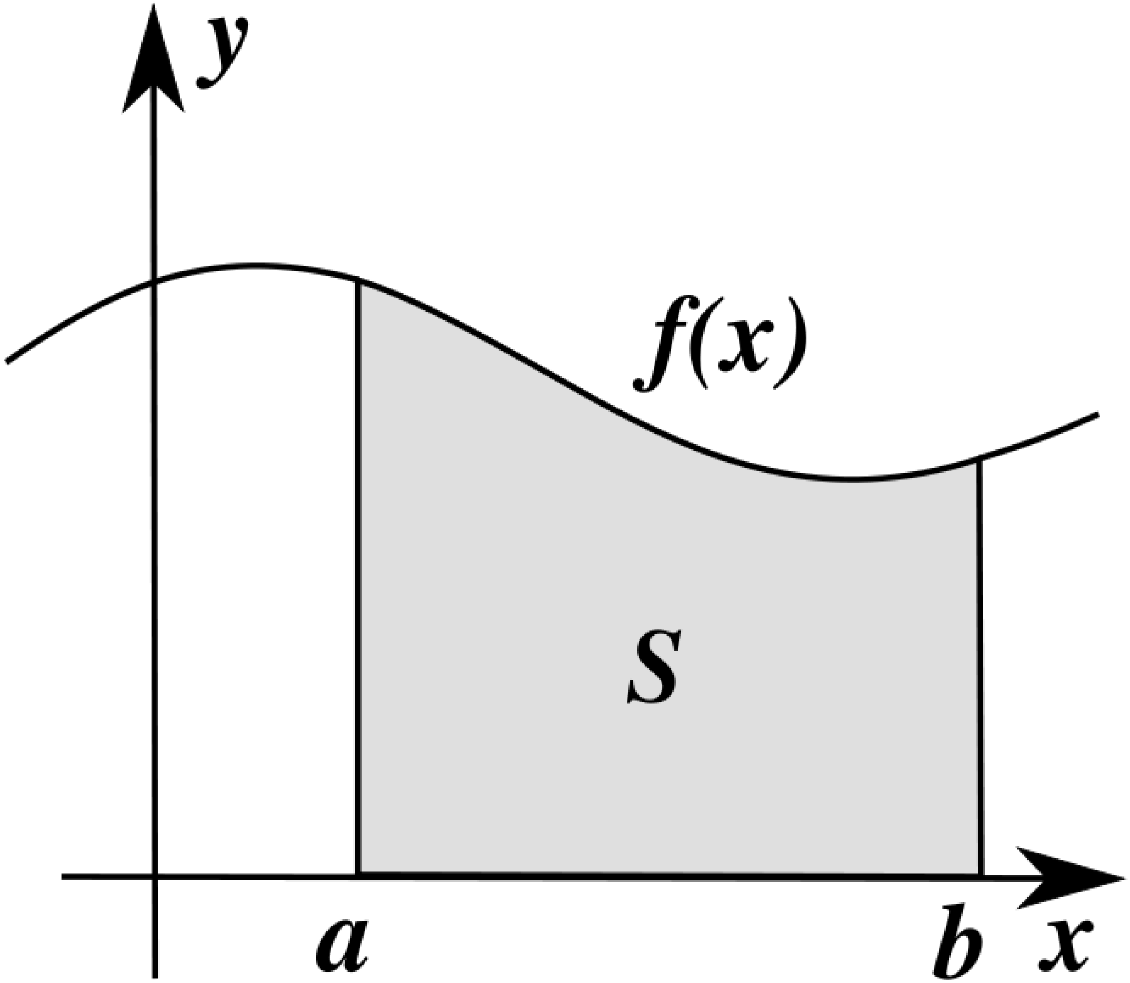
   

- An analog computer based on MC modeling of neutron transport in different materials

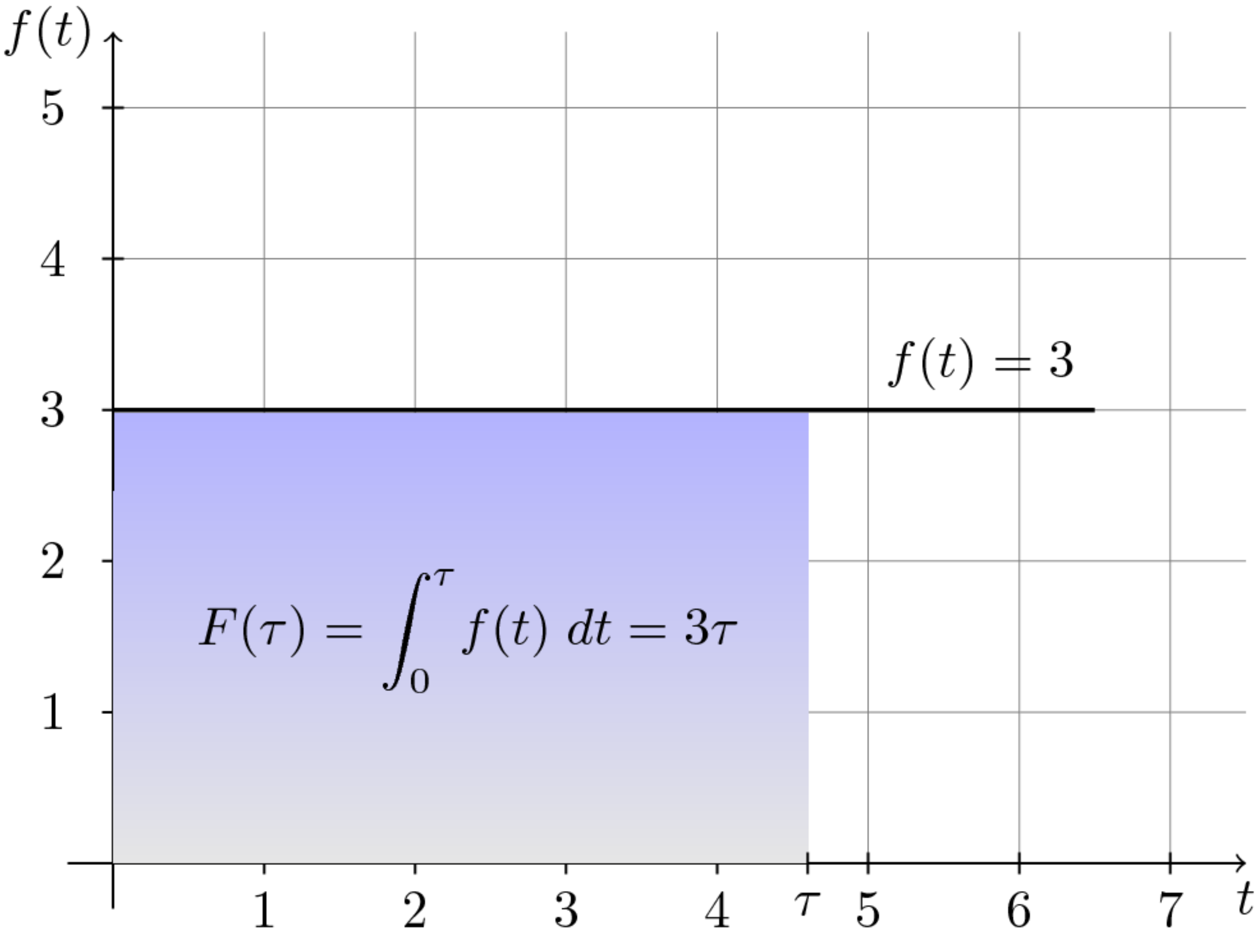


Integrals

- A single integral represents the signed area between the function and the axis where the integration variable is represented

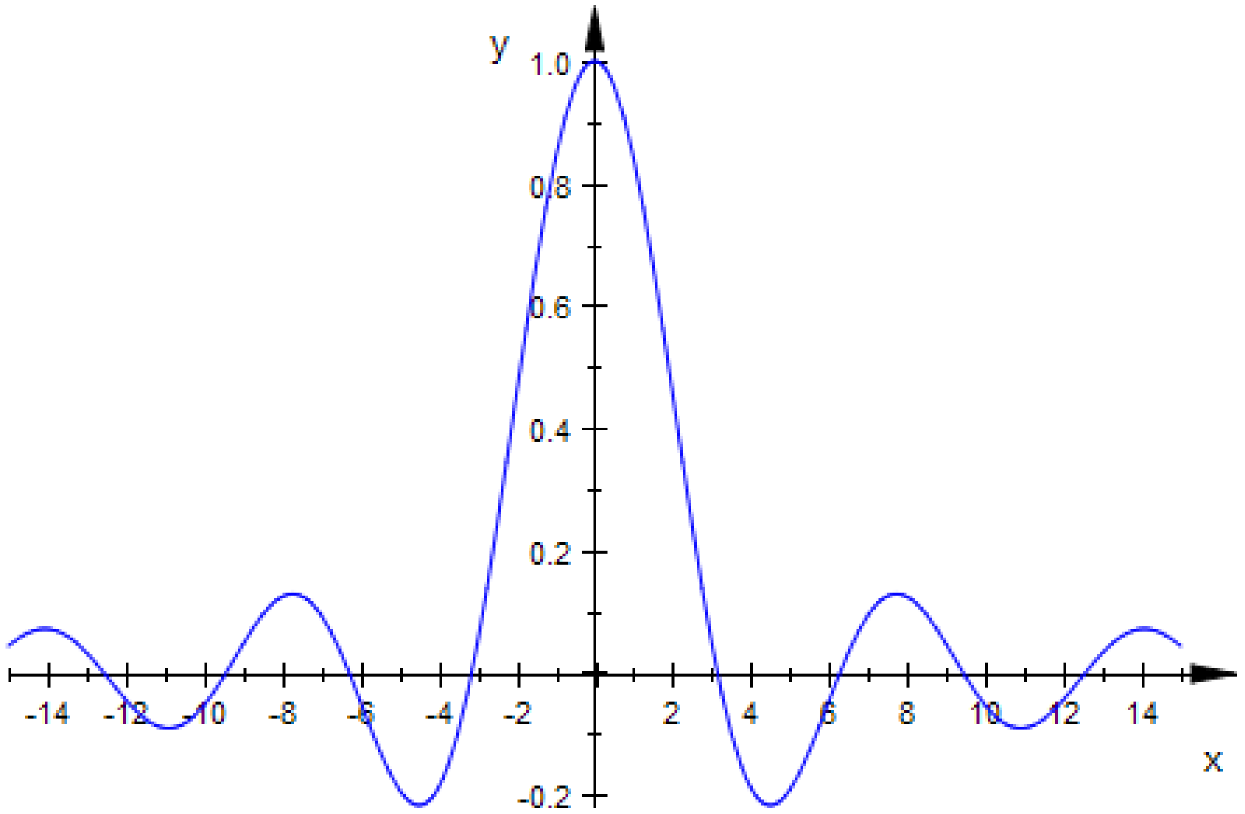


- There is a number of relatively simple functions that can be integrated analytically



Integrals

- Unfortunately, quite often the most interesting integrals cannot be solved analytically



- Such an example from a common physics problem is the magnetic field induced by a current flowing in a circular loop:

$$\boxed{H(x) = \frac{4Ir}{r^2 - x^2}\int_0^{\pi/2}\left[1 - \left(\frac{x}{r}\right)^2 sin^2\,\theta\right]^{1/2} d\theta}$$

- There is no analytical solution to the above integral
- We have to rely on numerical integration

- A non-analytically derivable definite integral can be estimated by means of lower and upper sums

- Assuming a function f and the area between f and the x-axis for xϵ[a,b]

  - We can partition [a,b] to n subintervals

$$\boxed{P = \{a = x_0 < x_1 < \cdots < x_{n-1} < x_n = b\}}$$

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  - With m_i being the greatest lower bound and M_i the least upper bound

$$m_i = inf\{f(x)\colon x_i < x < x_{i+1}\}$$

$$M_i = sup\{f(x)\colon x_i < x < x_{i+1}\}$$

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  - The lower sums (*L*) and upper sums (*U*)

$$\boxed{L(f;P) = \sum_{i=0}^{n-1} m_i\,(x_{i+1} - x_i)}$$

$$\boxed{U(f;P) = \sum_{i=0}^{n-1} M_i\,(x_{i+1} - x_i)}$$

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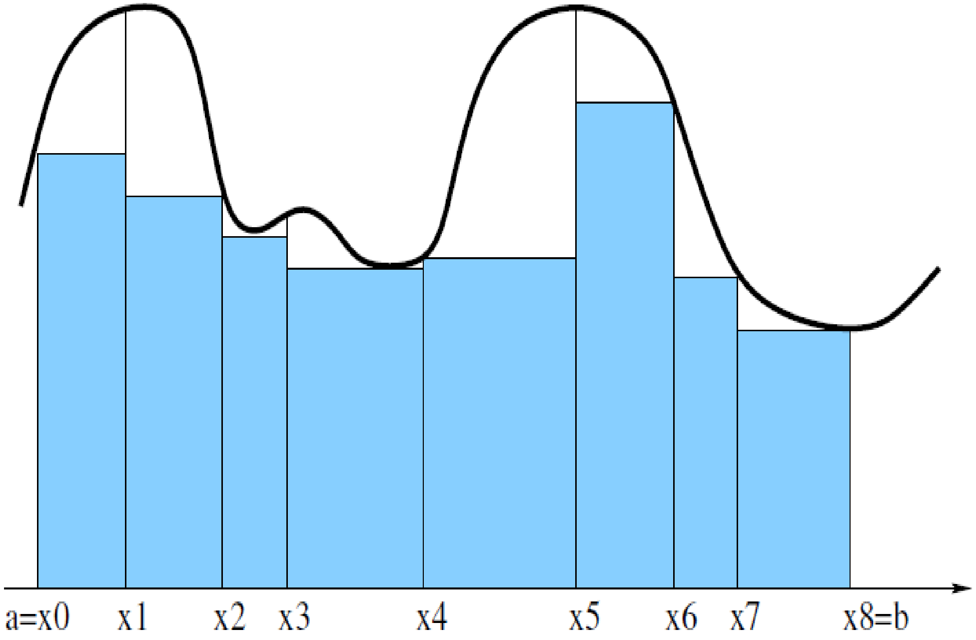

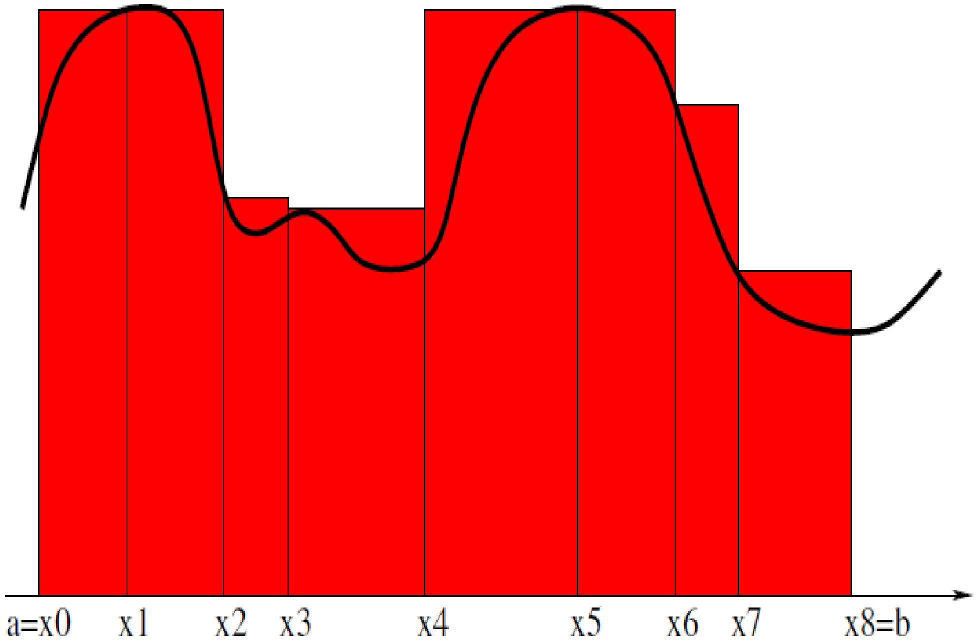

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Numerical integration
Trapezoid rule

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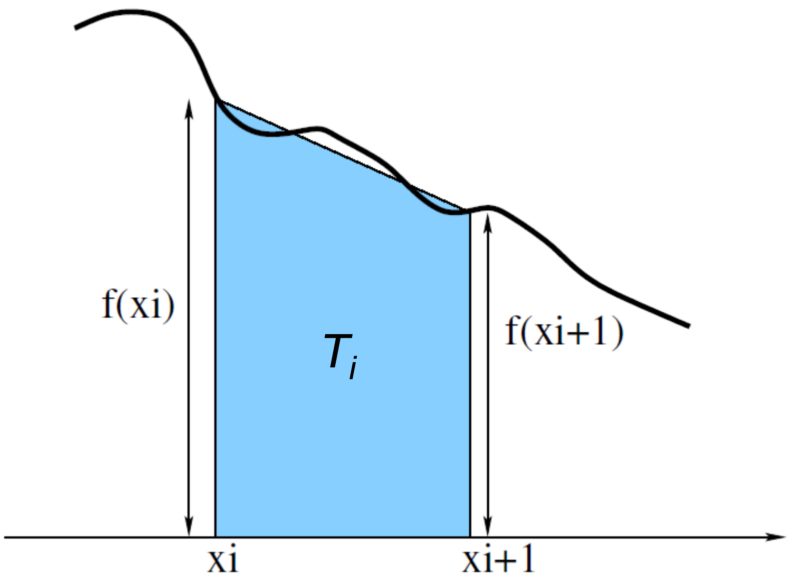

$$\int_{x_i}^{x_{i+1}} f(x)\,dx \approx T_i = \frac{1}{2}[f(x_i) + f(x_{i+1})](x_{i+1} - x_i)$$

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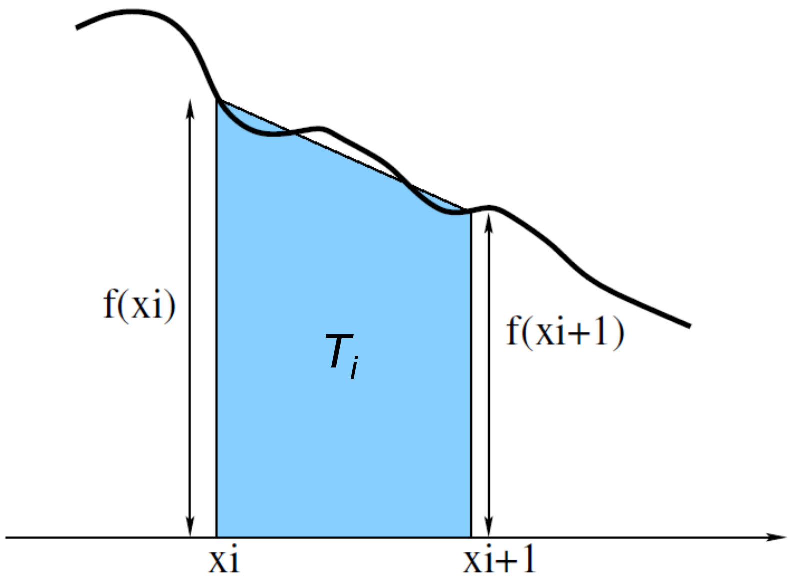

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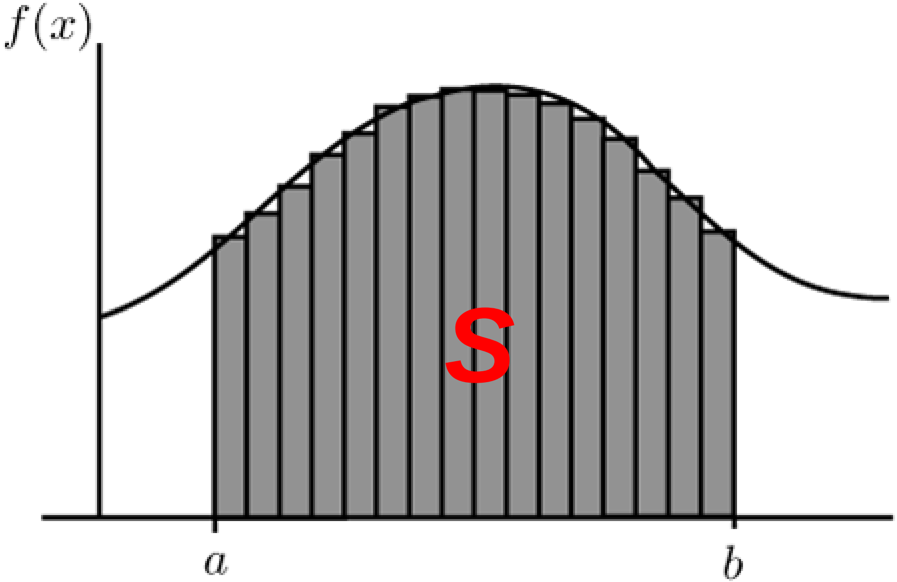
- Then the total area below the function A is:

$$\int_a^b f(x)\,dx \approx A(f;P) = \sum_{i=0}^{n-1} T_i = \frac{1}{2}\sum_{i=0}^{n-1}[f(x_i) + f(x_{i+1})](x_{i+1} - x_i)$$

- Let's start again from a simplified 1D numerical integration $\int_a^b f(x)\,dx$



Monte Carlo Integration
Sampling mean method

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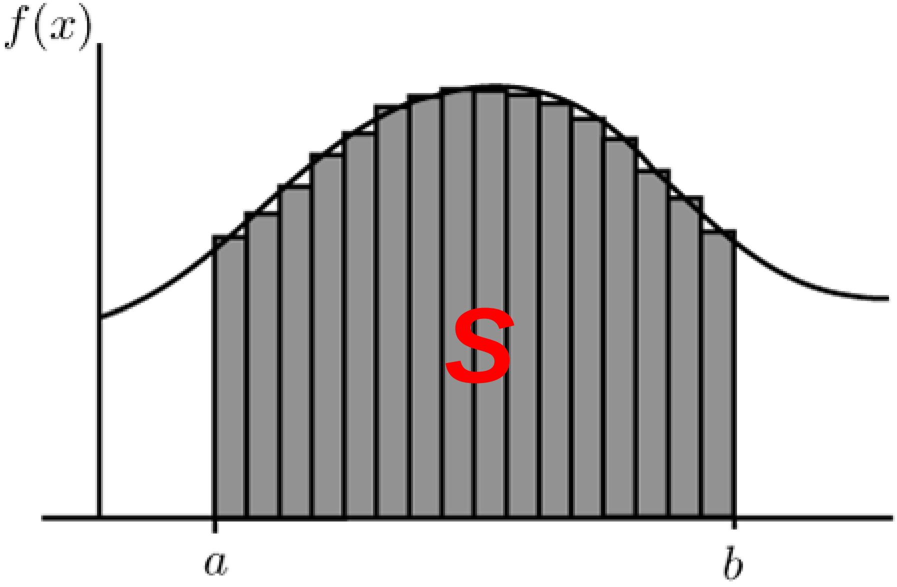

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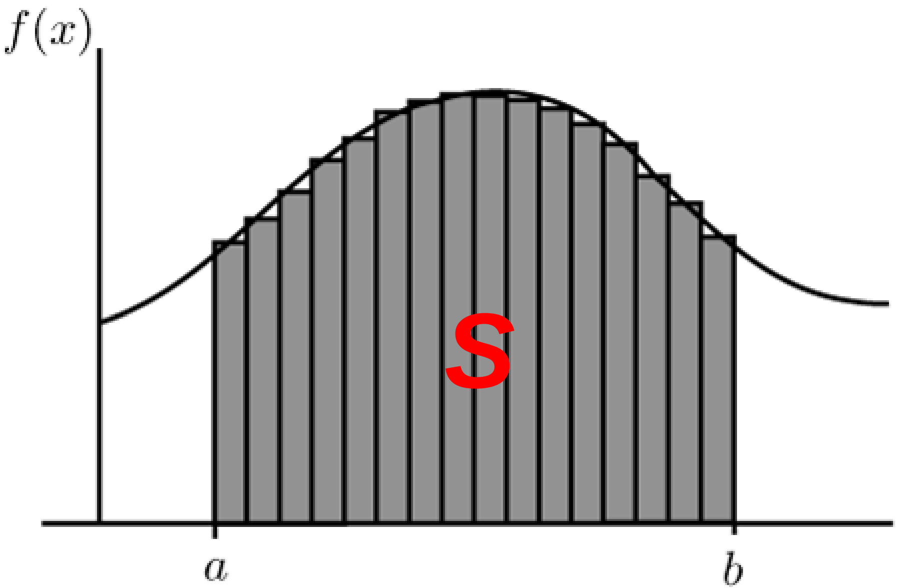

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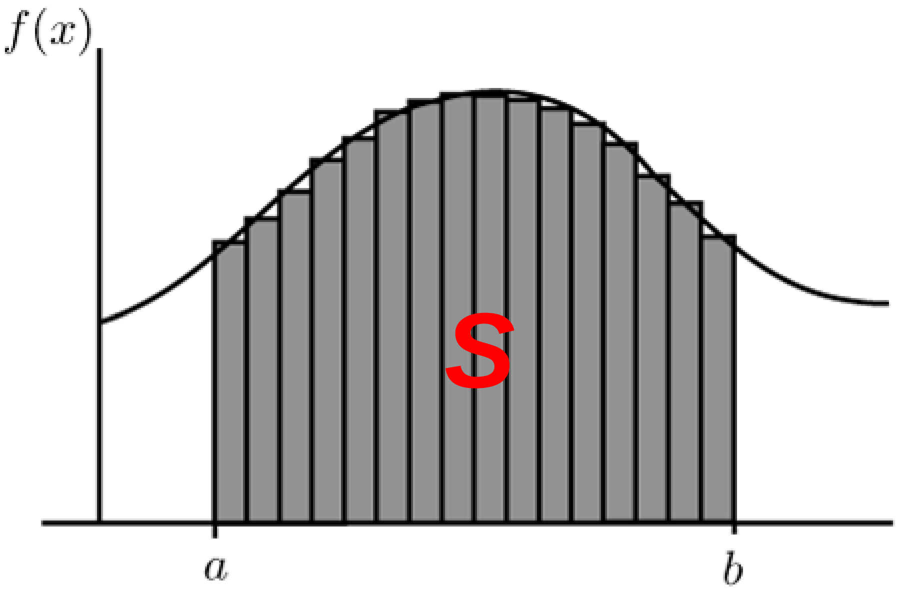

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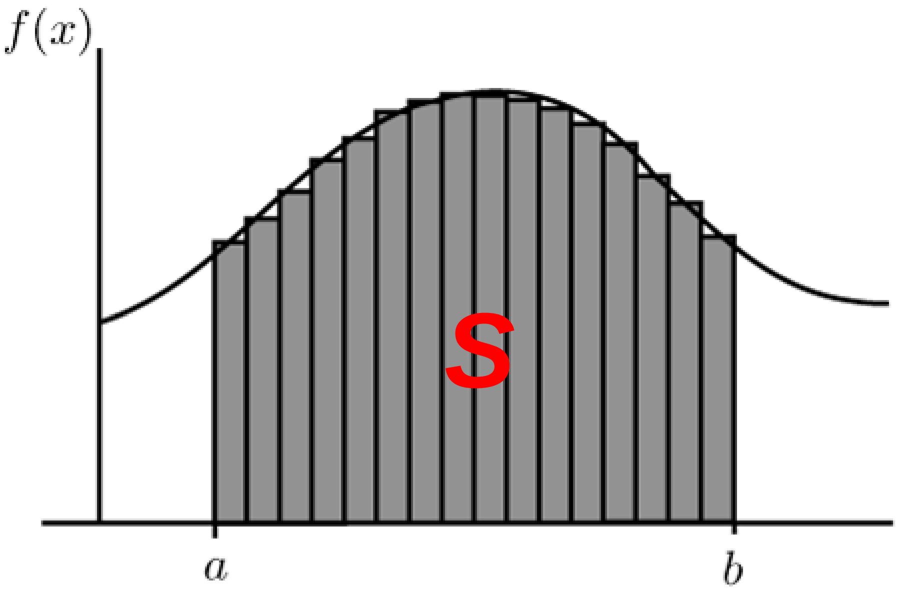

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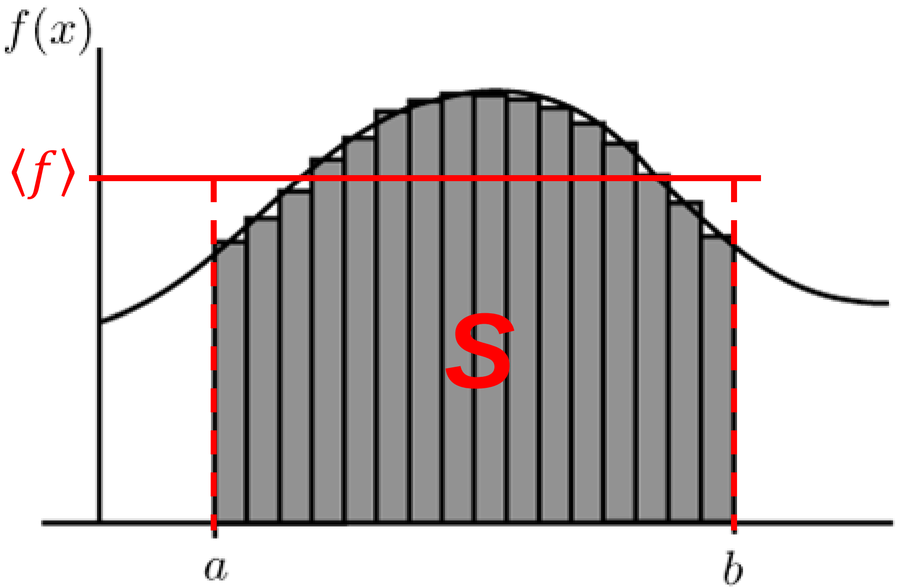

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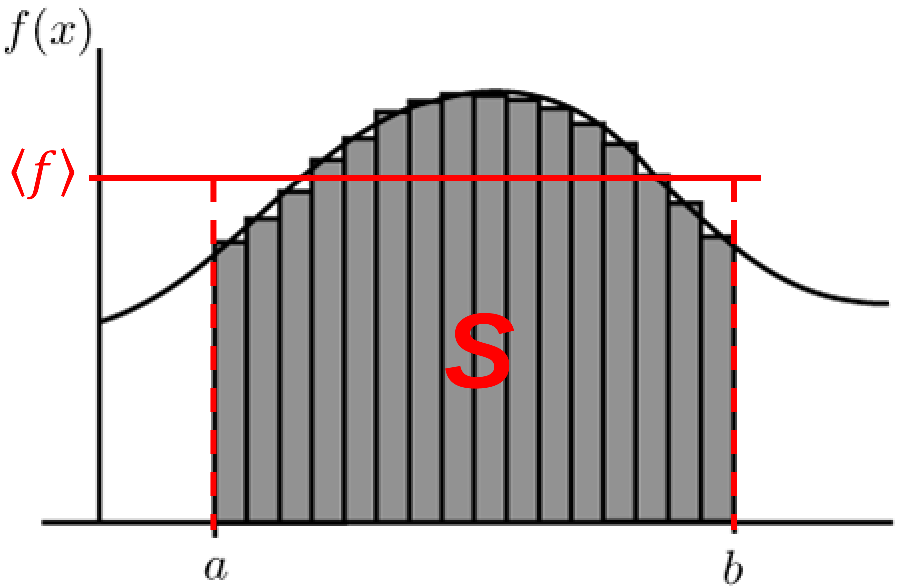

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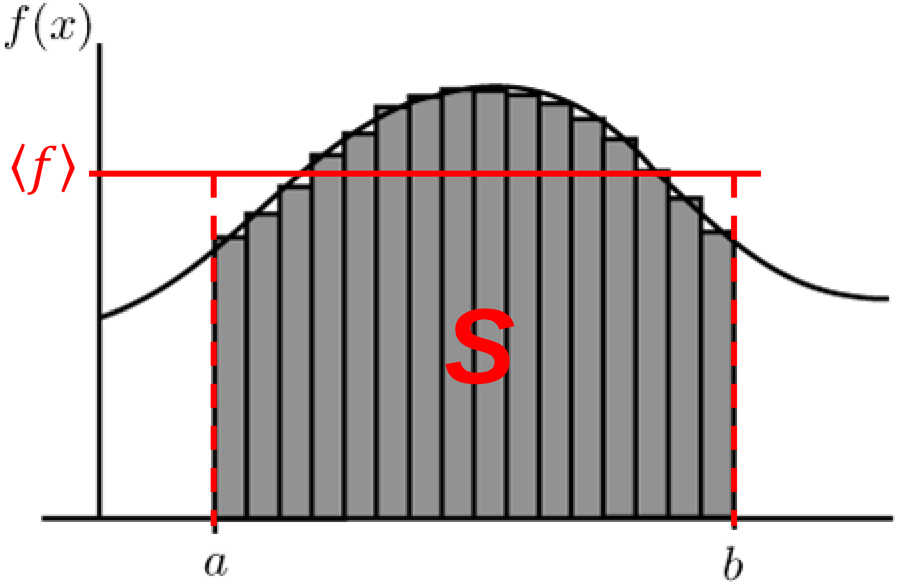

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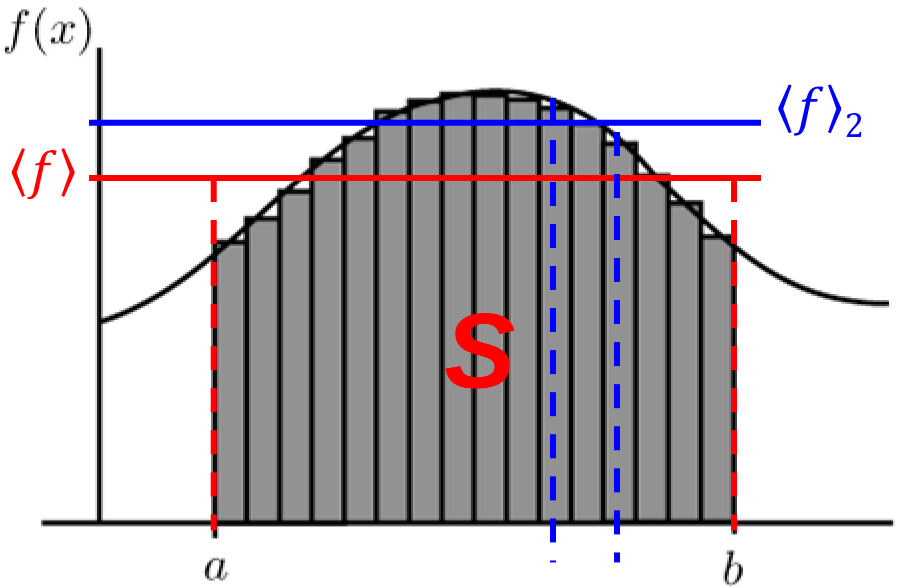

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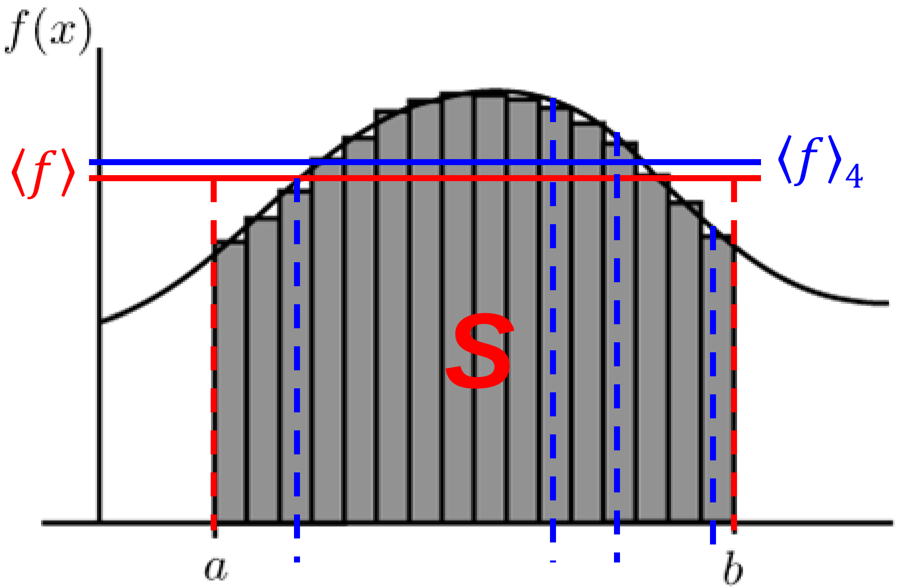

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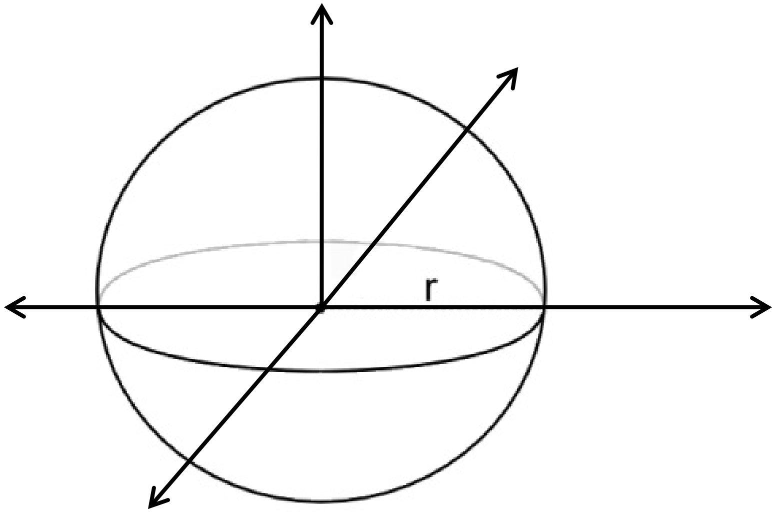
- Example estimation of a volume of a sphere (3D space):

$$r^2 = x^2 + y^2 + z^2 \Rightarrow z = \sqrt{r^2 - (x^2 + y^2)}$$

- So $f(x,y) = \sqrt{r^2 - (x^2 + y^2)}$ and we would like to estimate $\int_{-1}^{1} \int_{-1}^{1} f(x,y)\, dx\, dy$



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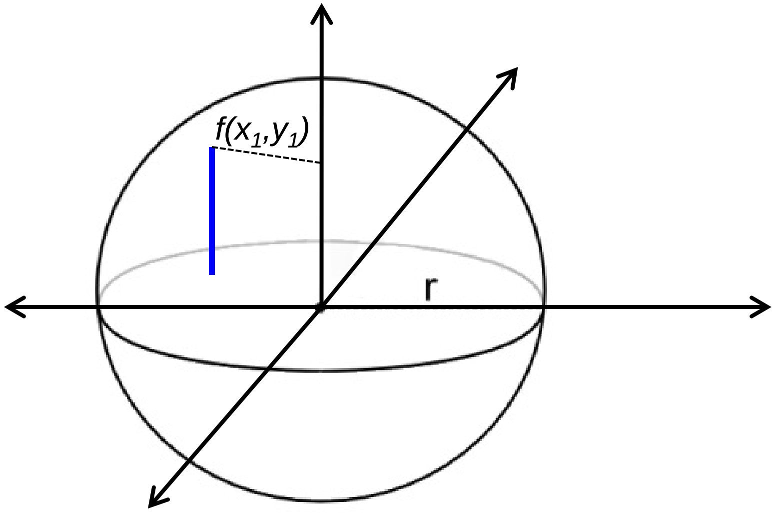

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Monte Carlo Integration
Sampling mean method

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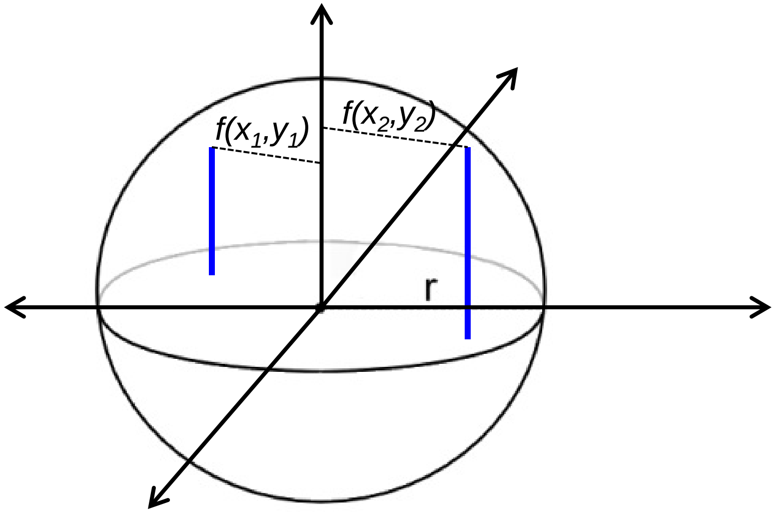

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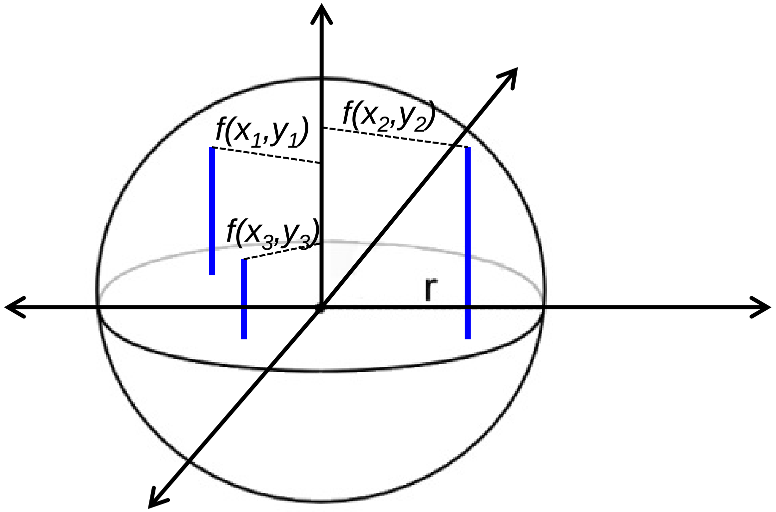

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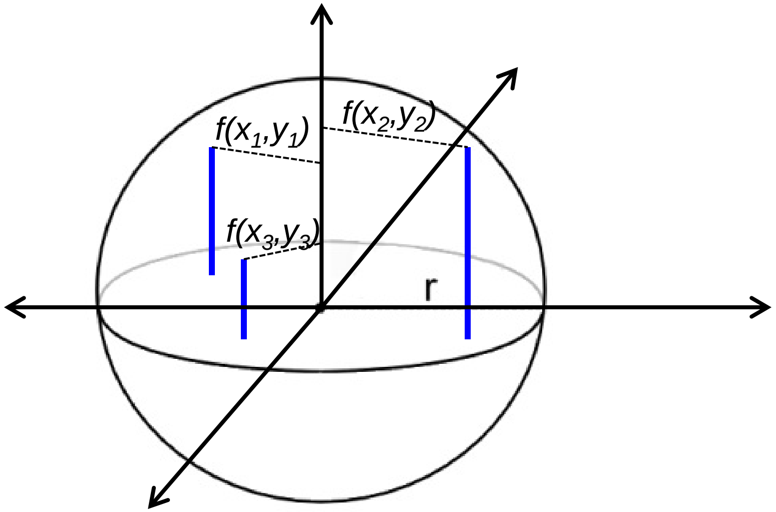

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- We estimate $\langle f \rangle$ from the sampling
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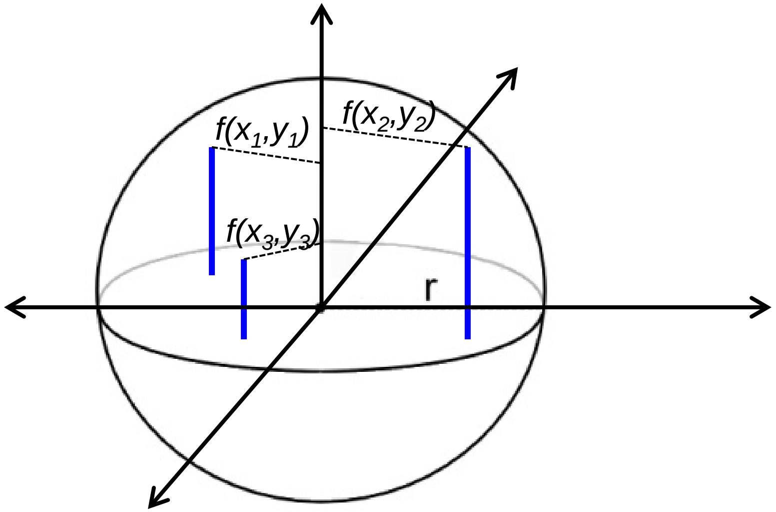


- We sample randomly in two dimensions (x,y)
- We estimate $\langle f \rangle$ from the sampling
- The three-dimensional space (volume of the sphere) will be $S^{M+1} = 2\pi r^2 \langle f \rangle$

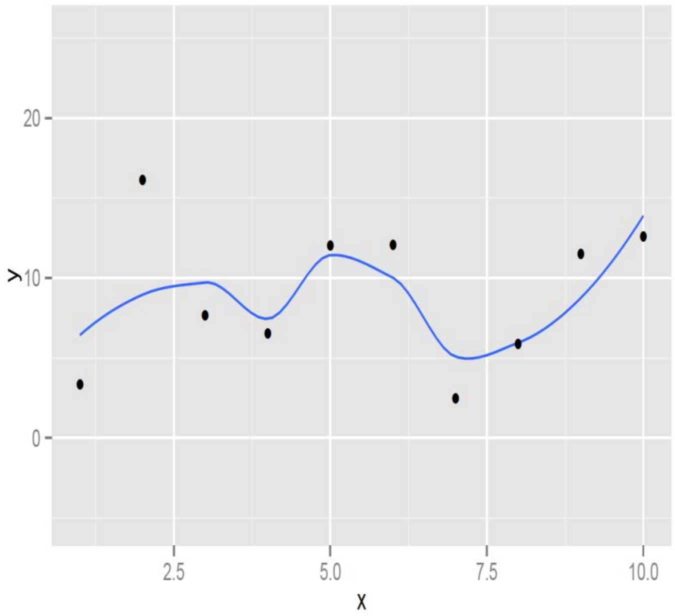
- Summarizing:
  - We want to calculate the integral over an M dimensional space of a function

$$\underbrace{f(x, y, z, \dots, m)}_{\text{M dimensions}}$$

  - The integral will be of M+1 dimension $S^{M+1} = S^{M}\langle f\rangle$
  - The problem is reduced to finding an accurate $\langle f\rangle$ by random sampling in M space
  - Finally we have to multiply the M dimensional sampling space with $\langle f\rangle$

Monte Carlo Integration
Hit or miss method

- Another approach of MC integration is the Hit-or-miss method
- Simpler logic than the sampling method
- We have a (complex/not well defined) function we need to integrate



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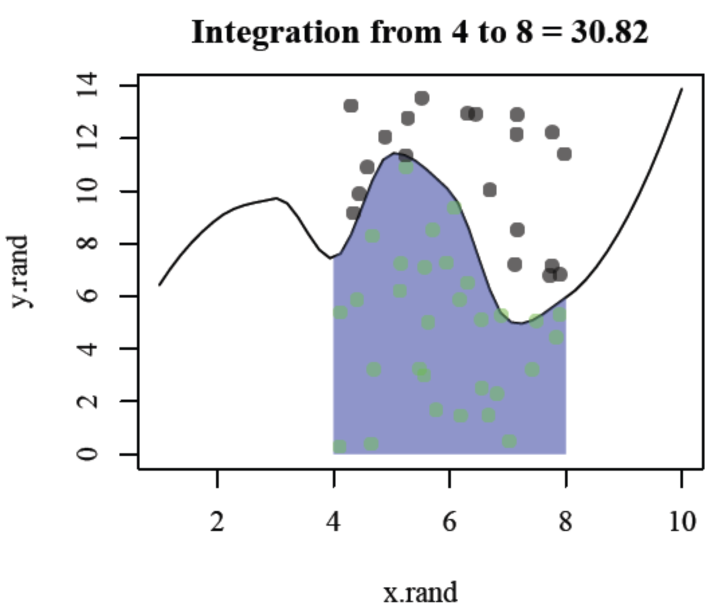
- In the webpage that I’ve found this nice example, it is called as the “Poor man’s” integration for those who have forgotten the “Dark Arts”
(tricks to help you derive analytically a complex integral)

- Another approach of MC integration is the Hit-or-miss method
- Simpler logic than the sampling method
- We have a (complex/not well defined) function we need to integrate



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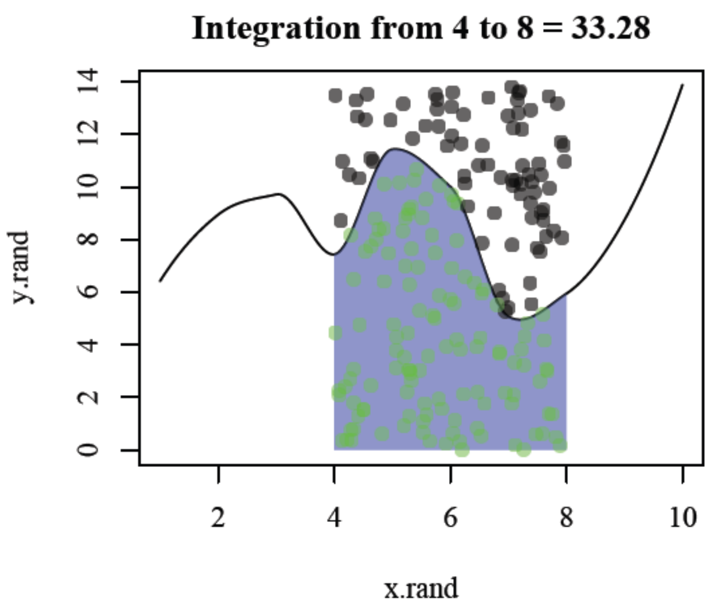

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Monte Carlo Integration
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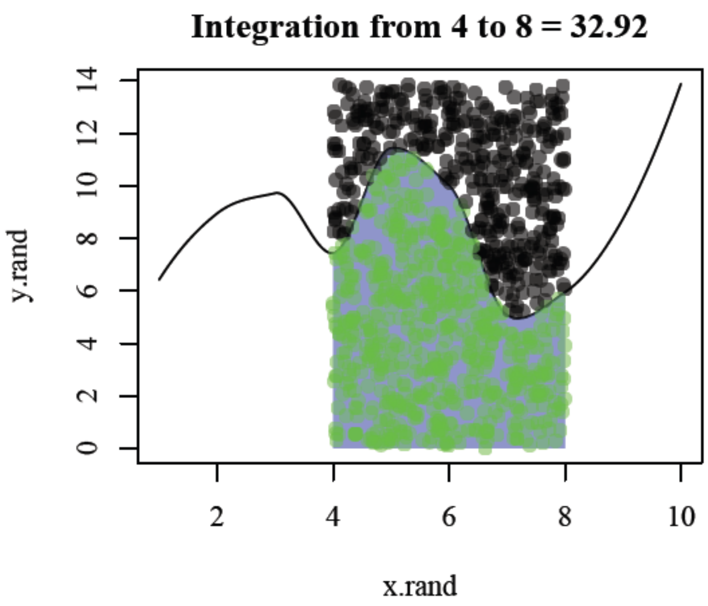

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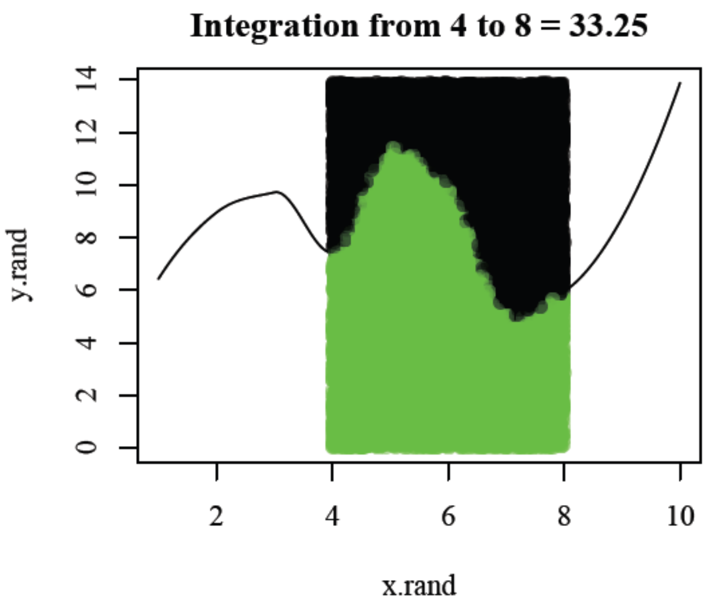

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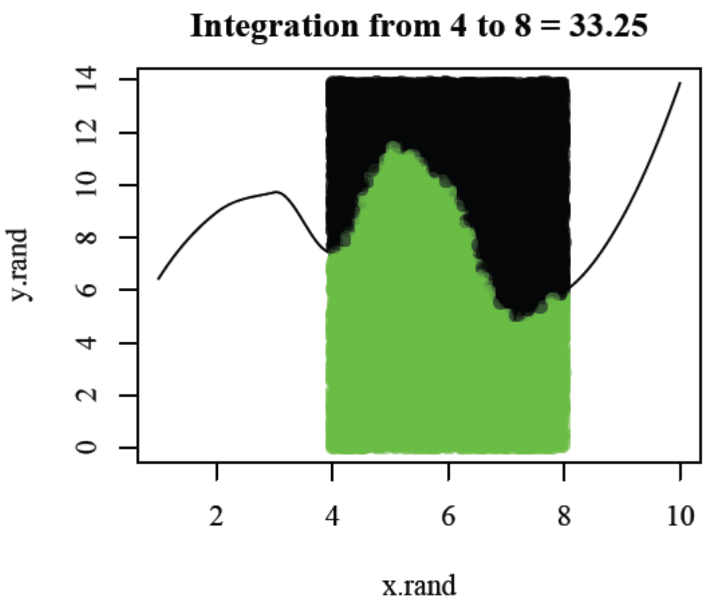

- We define a well known/easy to calculate volume/surface I_{known} that contains the complex volume/surface I_{est} we want to estimate
- We create random sampling of our known volume (as many as possible)
- Then $$\frac{N_{est}}{N_{known}} = \frac{I_{est}}{I_{known}}$$

- The famous π calculation
- Is simply the counting of the number of points in a circle and in a square containing this circle

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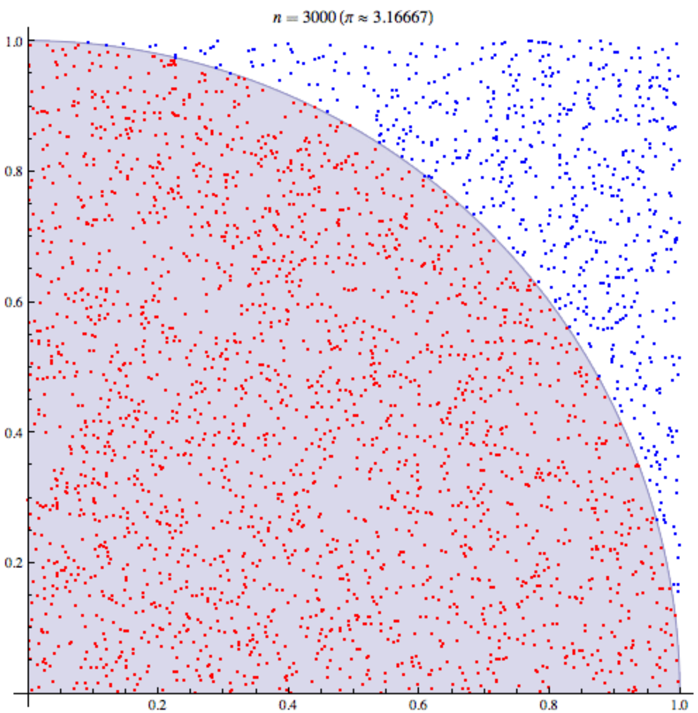


$$\frac{N_{circle}}{N_{sq}} = \frac{I_{circle}}{I_{sq}}$$

$$\frac{N_{circle}}{N_{sq}} = \frac{\pi r^2}{4r^2}$$

$$\pi = 4\frac{N_{circle}}{N_{sq}}$$

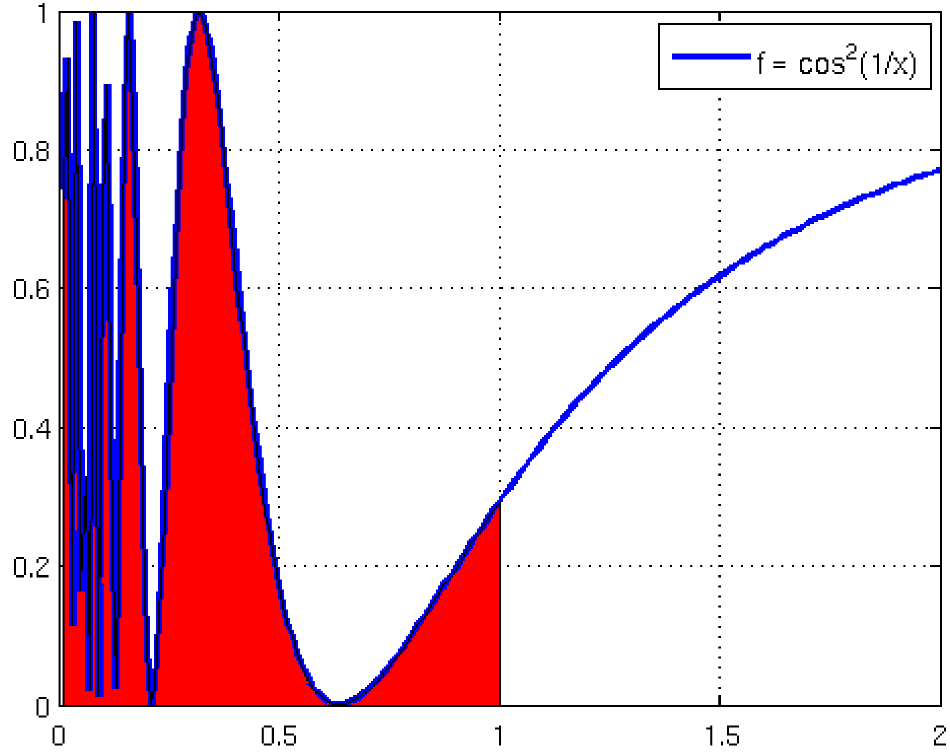
Monte Carlo Integration vs Numerical Integration

- It can be shown that the error of the traditional numerical methods scales as $N^{-1/M}$, where N is the number of intervals/points and M is the number of dimensions
- In the case of Monte Carlo Methods, the error for any number of dimensions M scales with $N^{-1/2}$

Dimensions M	Numerical Methods	Monte Carlo Technique
1	$1/N$	$1/\sqrt{N}$
2	$1/\sqrt{N}$	$1/\sqrt{N}$
>2	$1/\sqrt[M]{N}$	$1/\sqrt{N}$

- Monte Carlo methods become more efficient at higher dimensions

- Programming exercise 1:
  - Write two programs (in any programming language, preferable in C++, C, FORTRAN) that integrate $f(x) = \cos^2 \frac{1}{x}$ on [0,1] using the two MC integration techniques we learned:



- Programming exercise 1:
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    - Sampling (mean) MC method
    - Hit-or-miss method
  - For the two methods test and plot the convergence to the correct answer of 0.326543 (with 6 decimal digits)
  - For the two methods test and plot the variance (the spread of values obtained from a given set of samples)

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- One can use refined/intelligent methods in order to enhance MC performance
- We will discuss two advanced MC integration methods:
  - Importance sampling
  - Control variates

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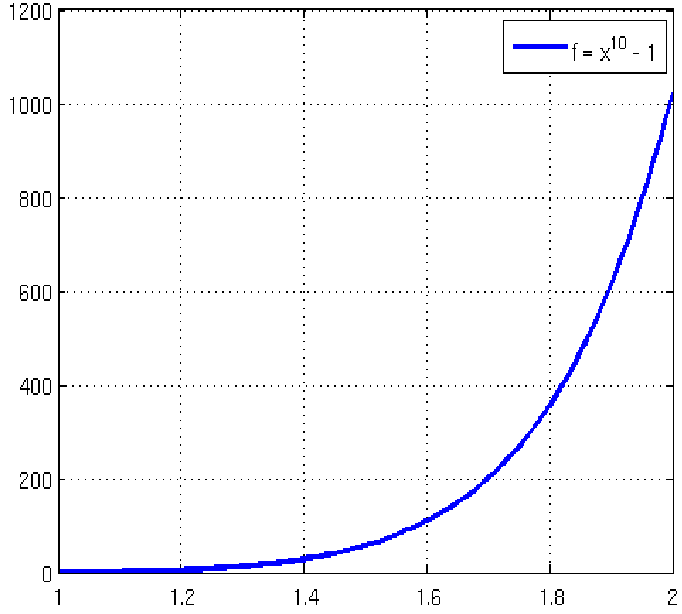

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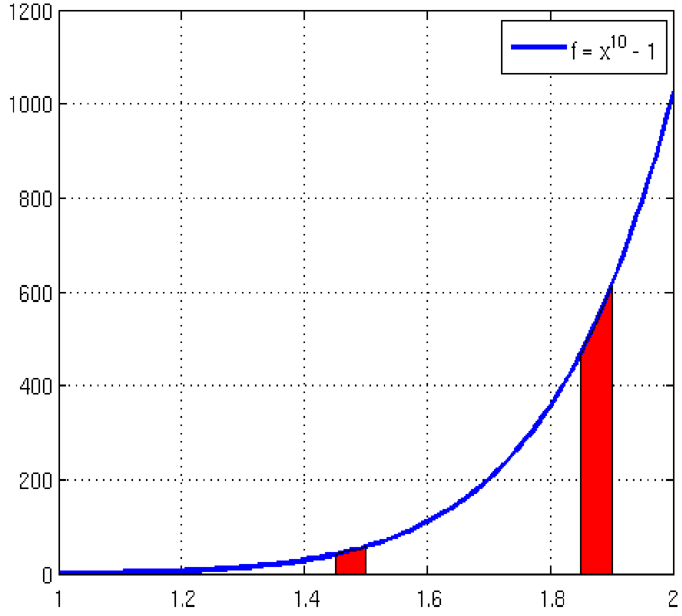

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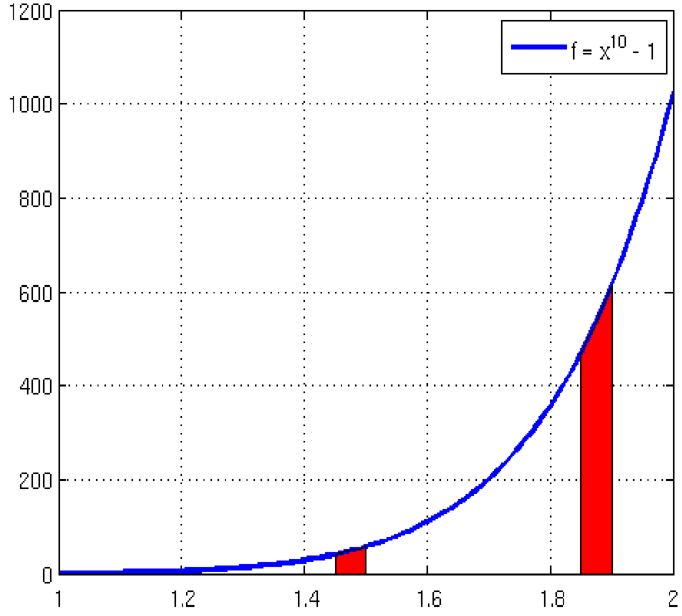

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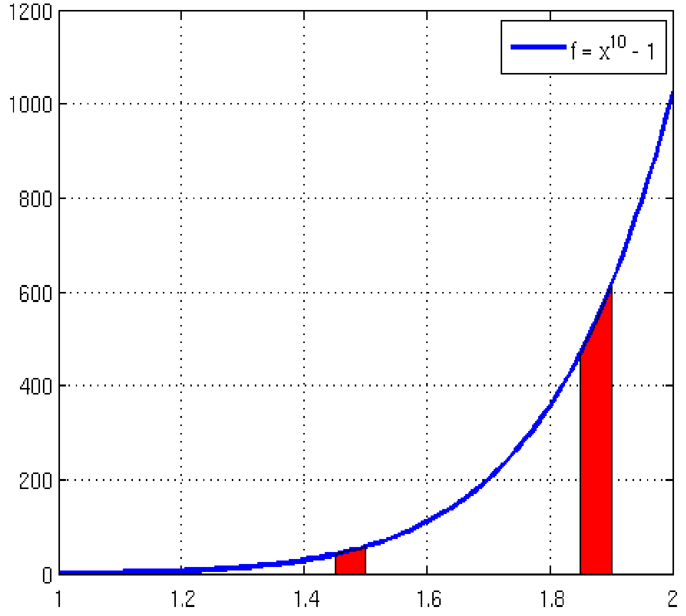

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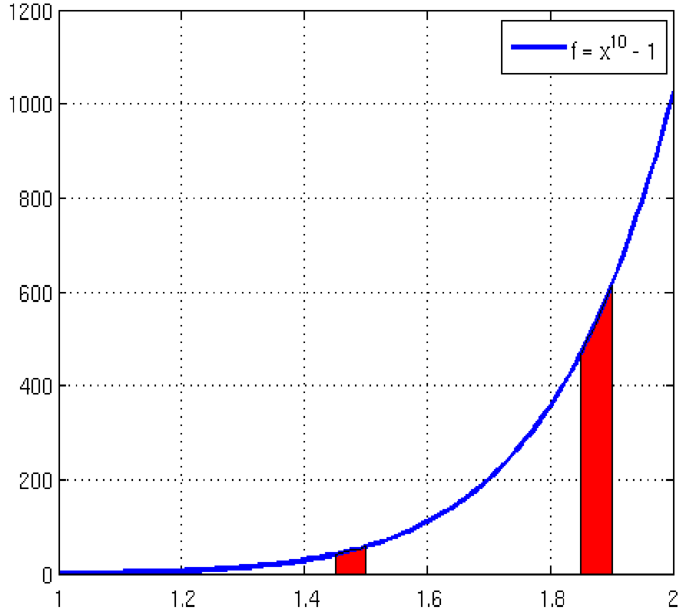

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$$I = \int_a^b f(x)\,dx = \int_a^b \frac{f(x)}{g(x)} g(x)\,dx = \int_{G(a)}^{G(b)} \frac{f(x)}{g(x)} dG(x)$$

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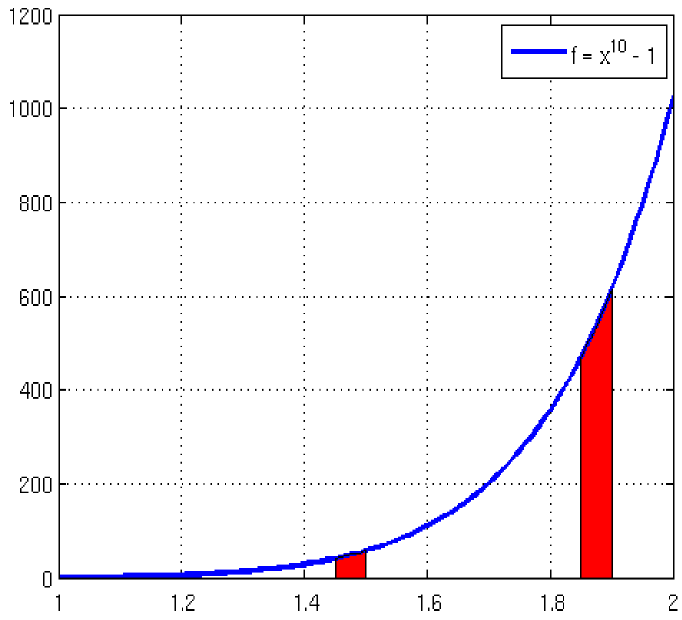

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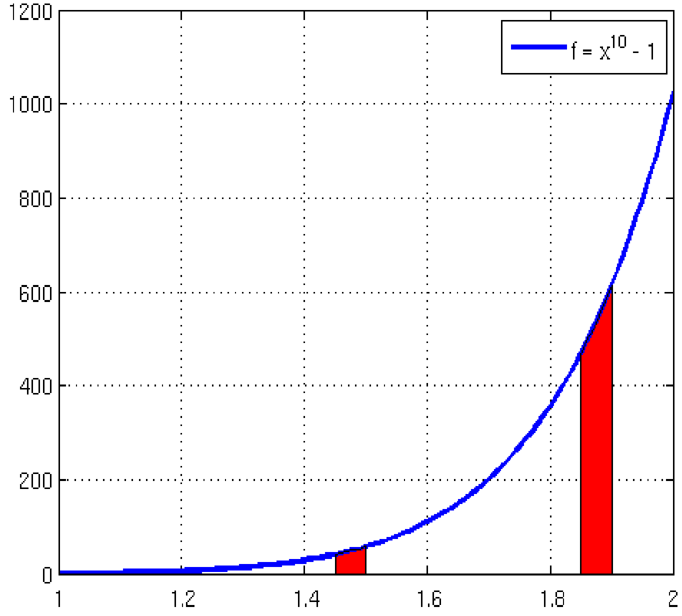

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- With $$G(x) = \int_a^x g(x)\,dx$$

- And the weighting function g(x) should be normalized in [a,b]: $$\int_a^b g(x)\,dx = 1$$

- Taking $$I = \int_a^b f(x)\,dx = \int_a^b \frac{f(x)}{g(x)} g(x)\,dx = \int_{G(a)}^{G(b)} \frac{f(x)}{g(x)} dG(x)$$

Monte Carlo Integration
Importance sampling

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- And doing a variable change $y = G(x)$ so that $x = G^{-1}(y)$

$$I = \int_a^b f(x)\,dx = \int_{G(a)}^{G(b)} \frac{f(G^{-1}(y)\,)}{g(G^{-1}(y)\,)} dy$$

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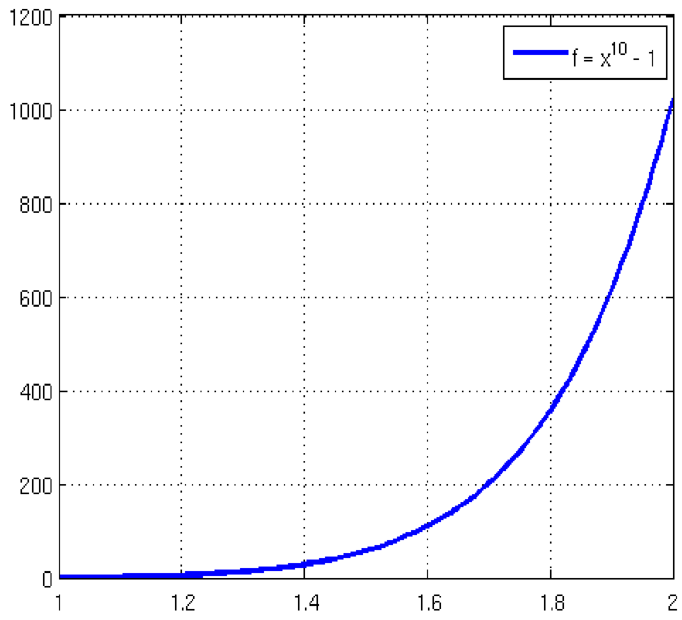
- The integral can be estimated as in the case of the simple sampling method

$$I = \frac{G(b) - G(a)}{N} \sum_{i=1}^{N} \frac{f(G^{-1}(y_i)\,)}{g(G^{-1}(y_i)\,)}$$

- Going back to the example of $f(x)=x^{10}-1$ in [1,2]



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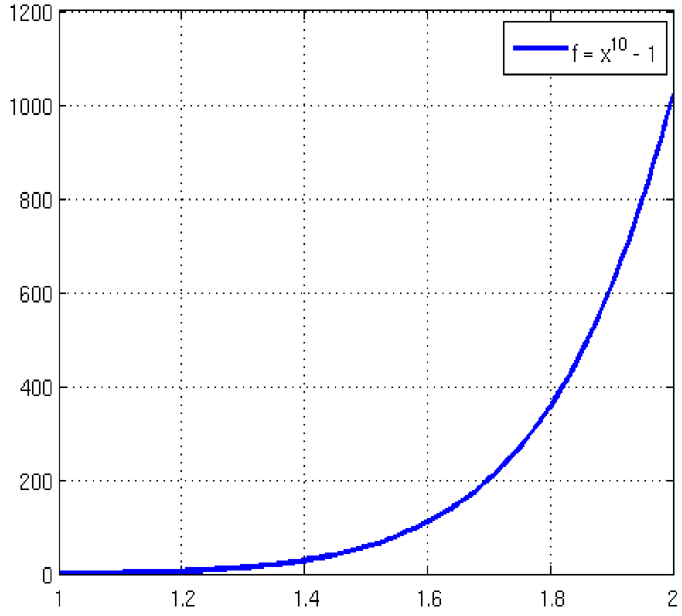

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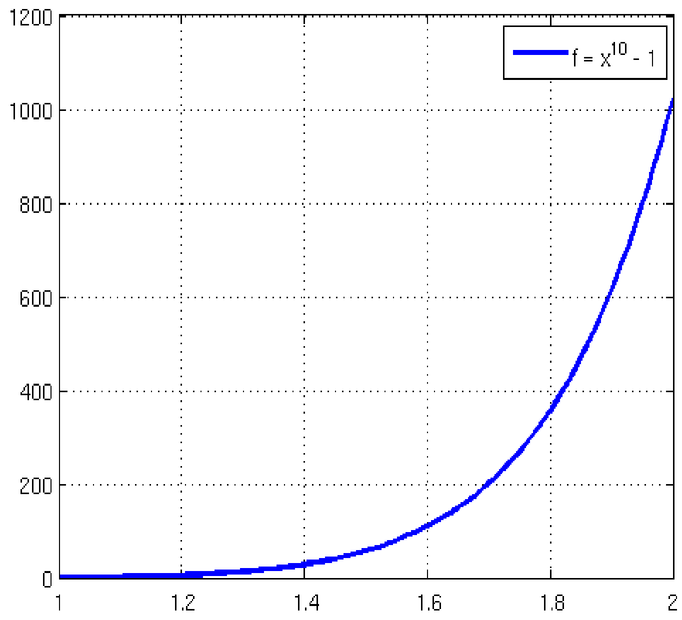

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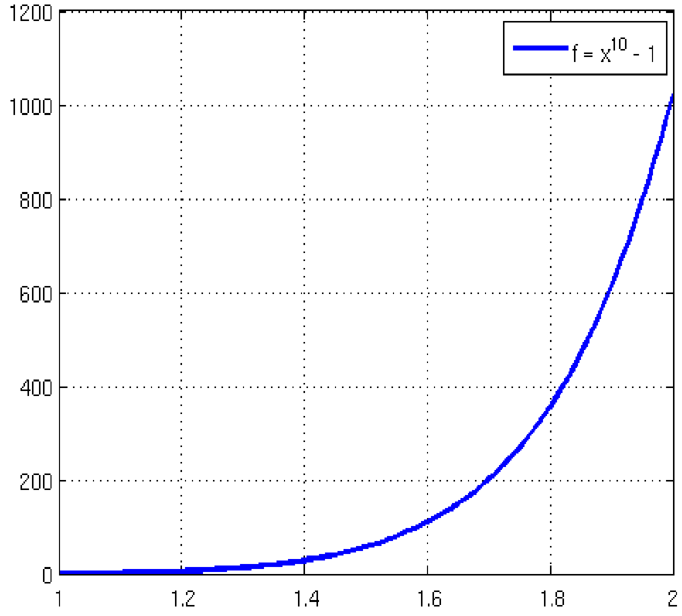

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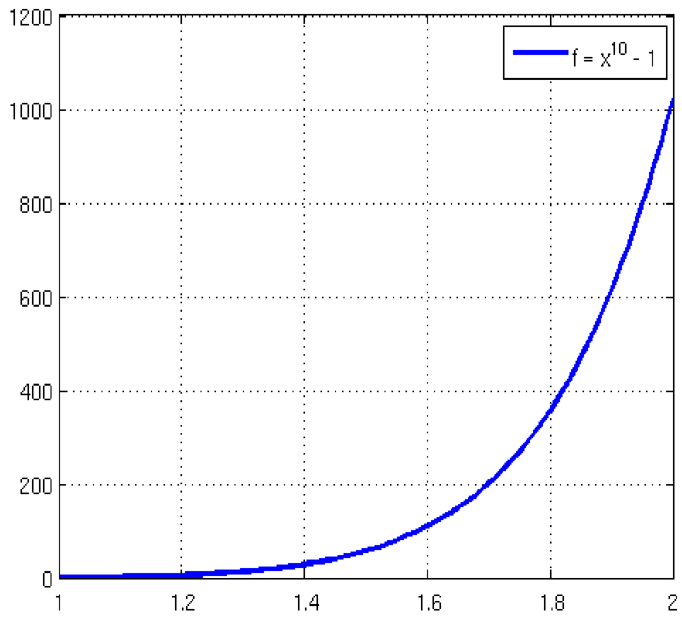

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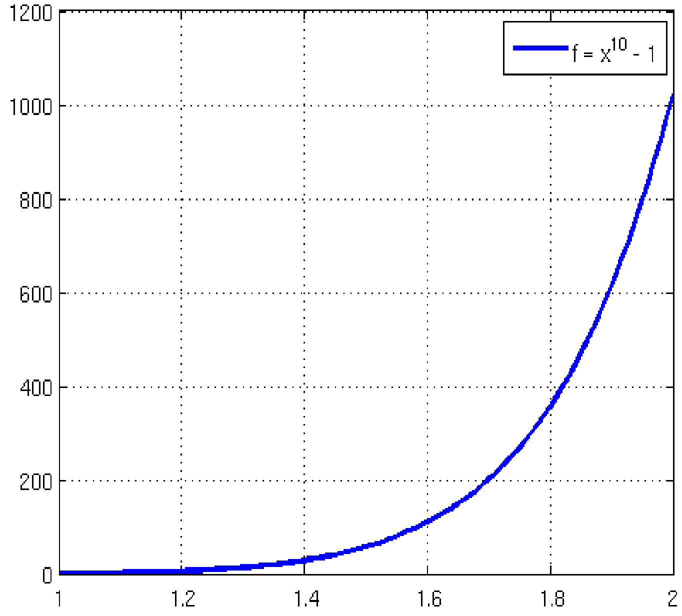
- So $G(x) = y = \frac{x^{11}-1}{2^{11}-1}$ and $x = G^{-1}(y) = [(2^{11}-1)y+1]^{1/11}$

- So the estimation of $I = \int_1^2 f(x)\, dx = \int_1^2 \frac{f(x)}{g(x)} g(x)\, dx = \int_{G(1)}^{G(2)} \frac{f(x)}{g(x)} dG(x)$



- Becomes: $\int_{G(1)}^{G(2)} \frac{f(G^{-1}(y)\ )}{g(G^{-1}(y)\ )} dy$

- With $G(1) = 0$ and $G(2) = 1$

- So that

$$I = \frac{1}{N} \sum_{i=1}^{N} \frac{f(G^{-1}(y_i)\ )}{g(G^{-1}(y_i)\ )}$$

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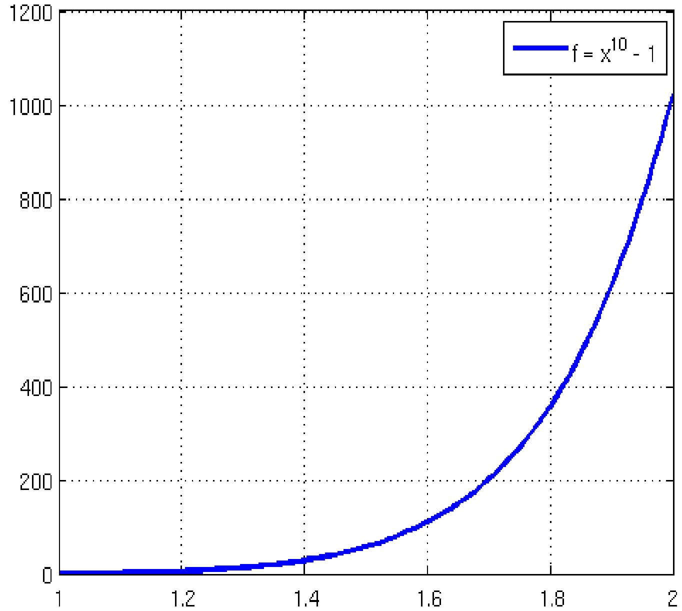

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- How is this of any help for my calculation?!?!?

- Forget for the moment the whole discussion about “flattening”

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- A re-interpretation of what happened is that we started from sampling the function f over the domain of uniformly distributed x

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- We reached at the point of sampling f/g again in the domain x but now starting from a uniformly distributed y

$$I = \frac{G(b)-G(a)}{N}\sum_{i=1}^{N} \frac{f(G^{-1}(y_i)\ )}{g(G^{-1}(y_i)\ )}$$

- With $x = G^{-1}(y)$

- So what we really did is to change from uniform sampling x to non-uniform sampling x because $x = G^{-1}(y)$

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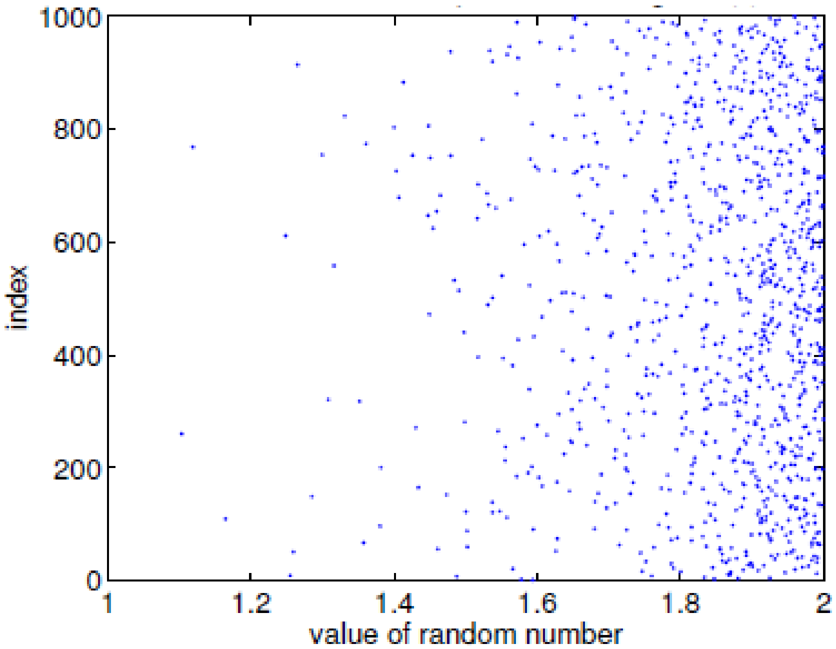

- In our example:

$$x = G^{-1}(y) = [(2^{11}-1)y + 1]^{1/11}$$

- With y uniform in [0,1]

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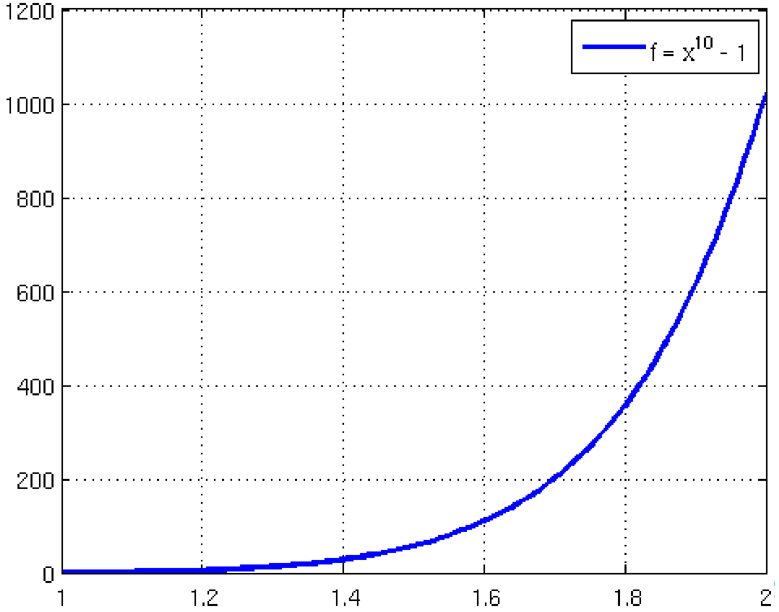

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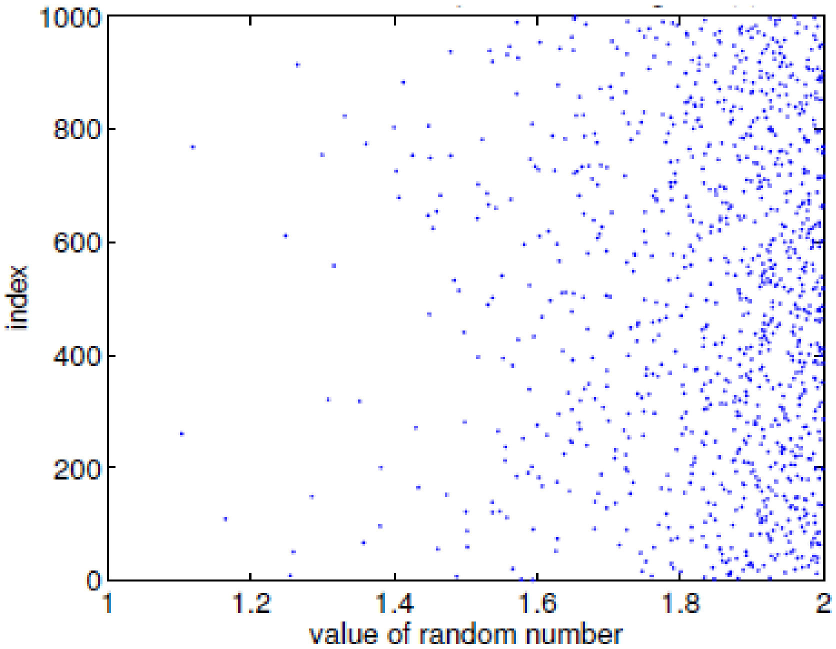

- In our example:

  $$x = G^{-1}(y) = [(2^{11}-1)y + 1]^{1/11}$$

- With y uniform in [0,1]

- Instead of using directly the flat random number generator, we transformed it to an engine that gives numbers according to a non-uniform probability density function (pdf) g(x) and a cumulative distribution function G(x)

- Programming exercise 2:
  - Write a program (in any programming language, preferable in C++, C, FORTRAN) that integrates a Gaussian function

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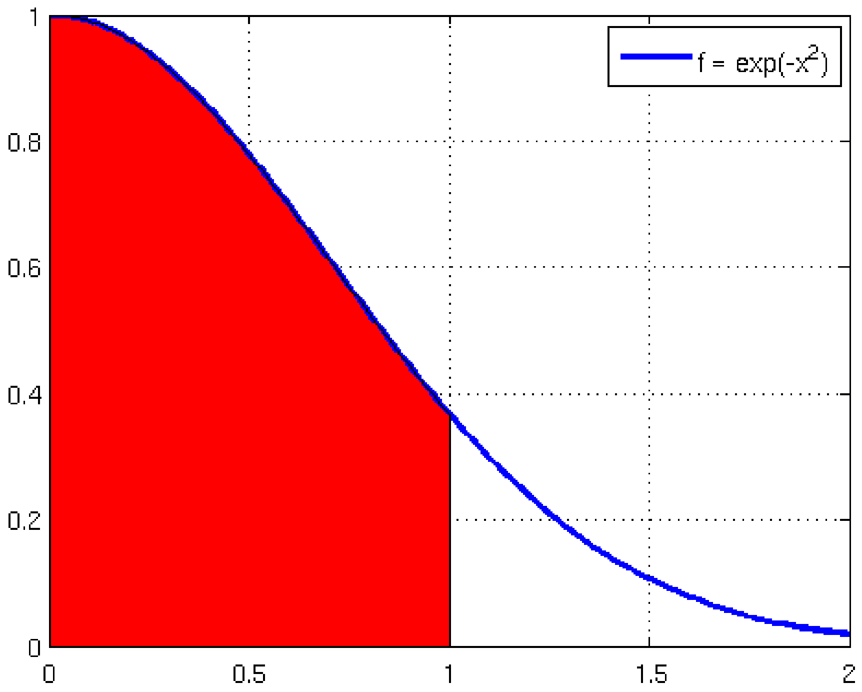

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    in [0,1] using two MC integration techniques:
    - MC Sampling
    - Importance sampling (hint use e^{-x} as your g(x))
  - Compare the two methods in terms of convergence and variance

- We mentioned a second advanced MC integration method, called Control Variates
- Will be discussed in the next lecture alongside with Random Number Generators
- …getting closer to MC particle simulation

- Website of the lecture material (slides):

http://www.physik.uni-muenchen.de/lehre/vorlesungen/wise_15_16/Vorlesung_-Computational-methods-in-medical-physics/index.html

- Exercises to be sent via email (G.Dedes@physik.uni-muenchen.de) as a zip file:

  - Containing all source code and make files
  - Short report on the findings

- The name of the zip file should be:
  - Exercise12_NameLastname.zip