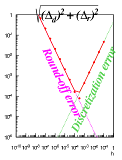
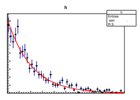
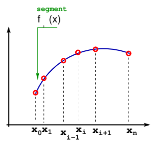
Computational Physics

numerical methods with C++ (and UNIX)







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Computational Physics

Monte-Carlo methods

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Monte Carlo integration

- ✔ we want to evaluate the following integral:

$$F = \int_a^b f(x)\,dx$$

- ✔ remember that the expectation value of the function $f(x)$ for x distributed according to a PDF $p(x)$

$$\langle f \rangle = \int_a^b f(x)\,p(x)\,dx \qquad \text{with: } \int_a^b p(x)\,dx = 1$$

- ✔ choosing x to be uniformly distributed in the interval $[a, b]$, one has:

$$\begin{aligned} p(x) &= \tfrac{1}{b-a} \\ \langle f \rangle &= \int_a^b f(x)\,p(x)\,dx = \tfrac{1}{b-a}\int_a^b f(x)\,dx \end{aligned}$$

MC integration

$$\begin{aligned} F &= \int_a^b f(x)\,dx \\ &= (b-a)\,\langle f \rangle \\ &= \tfrac{(b-a)}{N}\sum_{i=1}^N f(x_i) \end{aligned}$$

x_i is a random variable uniformly distributed in the interval $[a, b]$

error estimation

$$\begin{aligned} \sigma_F &= (b-a)\sigma_{\langle f \rangle} \\ \sigma_f^2 &= \left\langle f^2 \right\rangle - \langle f \rangle^2 \\ \sigma_{\langle f \rangle}^2 &= \frac{\sigma_f^2}{N} \end{aligned}$$

$$\boxed{\sigma_F = \frac{\sigma_f}{\sqrt{N}} = \frac{1}{\sqrt{N}}\sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(f(x_i)\right)^2 - \left(\frac{1}{N}\sum_{i=1}^{N} f(x_i)\right)^2}}$$

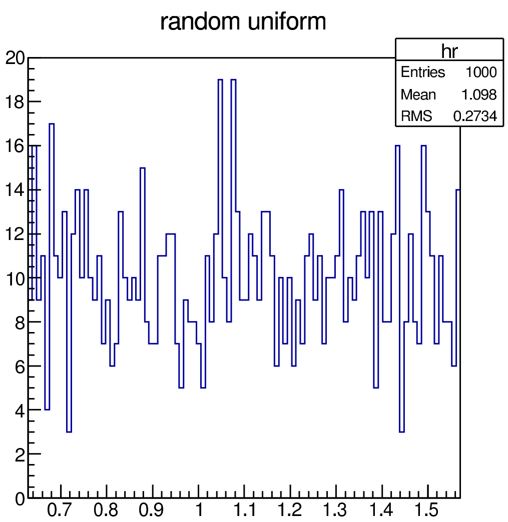
MC integration (cont.)

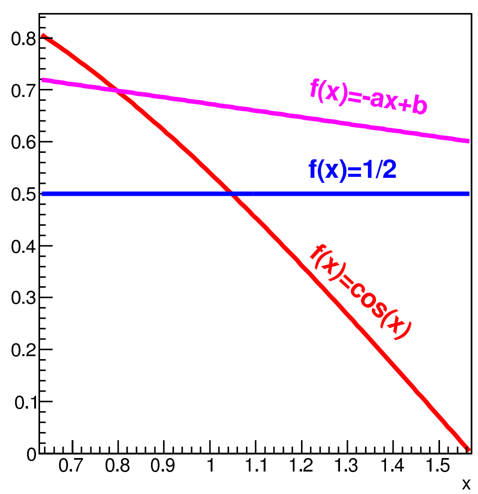
Let's compute the integrals of the functions:

$$\begin{aligned} &\int_{0.2\pi}^{0.5\pi} \frac{dx}{2} = 0.471239 \\ &\int_{0.2\pi}^{0.5\pi} cos(x)\,dx = 0.412215 \\ &\int_{0.2\pi}^{0.5\pi} (ax+b)\,dx = 0.622035 \end{aligned}$$

Throwing 100 random variable uniformly distributed we obtain the following results:

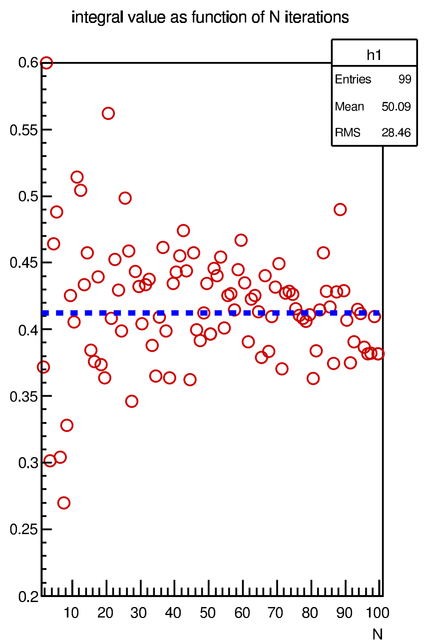
$$\begin{aligned} &\int_{0.2\pi}^{0.5\pi} \frac{dx}{2} = 0.471239 \pm 0.000000 \\ &\int_{0.2\pi}^{0.5\pi} cos(x)\,dx = 0.413671 \pm 0.007098 \\ &\int_{0.2\pi}^{0.5\pi} (ax+b)\,dx = 0.622280 \pm 0.001037 \end{aligned}$$

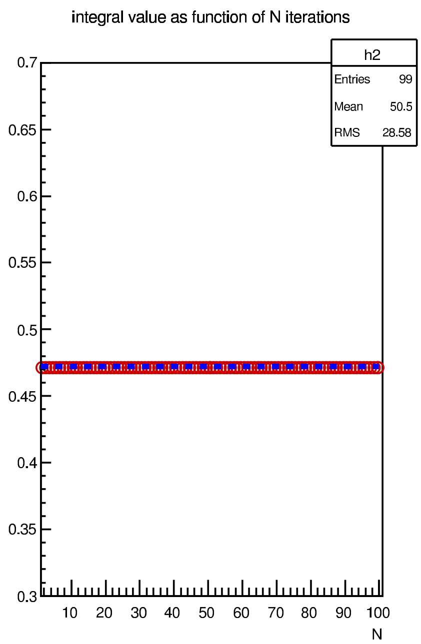


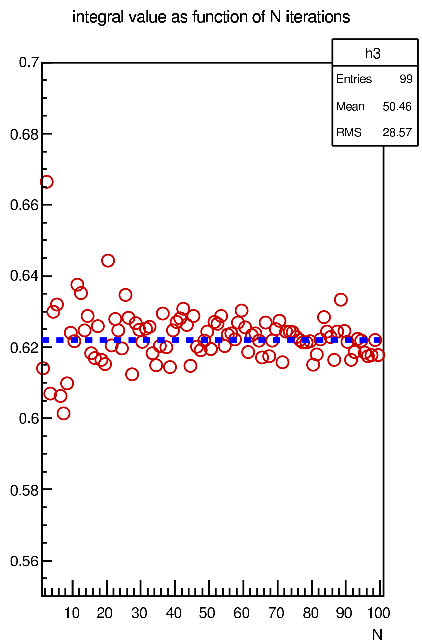


MC integration (cont.)

Let's check the integral value as function of the number of random variables generated N







$$F = \int_{0.2\pi}^{0.5\pi} cos(x)\, dx$$

$$F = \int_{0.2\pi}^{0.5\pi} \frac{dx}{2}$$

$$F = \int_{0.2\pi}^{0.5\pi} (ax + b)\, dx$$

Reduction variance techniques

✔ The $cos(x)$ function varies much more in the interval of integration that the others

✔ Its integral value evaluation presents the largest variance. Why?

☞ Because we are sampling uniformly and the regions close to zero where the function is more important are sampled with the same importance as others where the function is smaller!

☞ In the framework of the **importance sampling technique** an additional pdf $p(x)$ can be used to rend the integrand smooth!

Importance sampling

- Rend smooth our integrand by applying a pdf $p(x)$

$$F = \int_a^b f(x)\, dx = \int_a^b \frac{f(x)}{p(x)}\, p(x)\, dx$$

- If the pdf is normalized in the integral interval $[a, b]$

$$\int_a^b p(x)\, dx = 1$$

and x is a variable distributed according to $p(x)$, then

$$\left\langle \frac{f}{p} \right\rangle = \int_a^b \frac{f(x)}{p(x)}\, p(x)\, dx$$

- Let's make a variable change

$$\int_a^b \frac{f(x)}{p(x)} \underbrace{p(x)\, dx}_{p(y)dy}$$

$p(x)dx = p(y)dy$

if y is distributed uniformly in $[0, 1]$ then

$\int_0^1 p(y)dy = 1 \Rightarrow p(y) = 1$

The transformation between x and Y can be obtained by:

$\int_a^x p(x')dx' = \int_0^y dy' \quad \Rightarrow \quad \boxed{y = \int_a^x p(x')dx'}$

Importance sampling (cont.)

- From the transformation of variables we have a relation between x and y

$$\boxed{y = \int_a^x p(x')dx' \quad \Rightarrow \quad x(y)}$$

Generating a random variable y uniformly between $[0, 1]$ and applying the transformation relation $x(y)$ we get random variables x distributed according to $p(x)$

$$\boxed{F = \int_a^b f(x)\, dx = \int_a^b \frac{f(x)}{p(x)}\, p(x)\, dx = \int_0^1 \frac{f(x(y))}{p(x(y))}\, dy = \left\langle \frac{f}{p} \right\rangle_y = \frac{1}{N} \sum_{i=1}^{N} \frac{f(x(y_i))}{p(x(y_i))}}$$

- Exercise: make the following integral

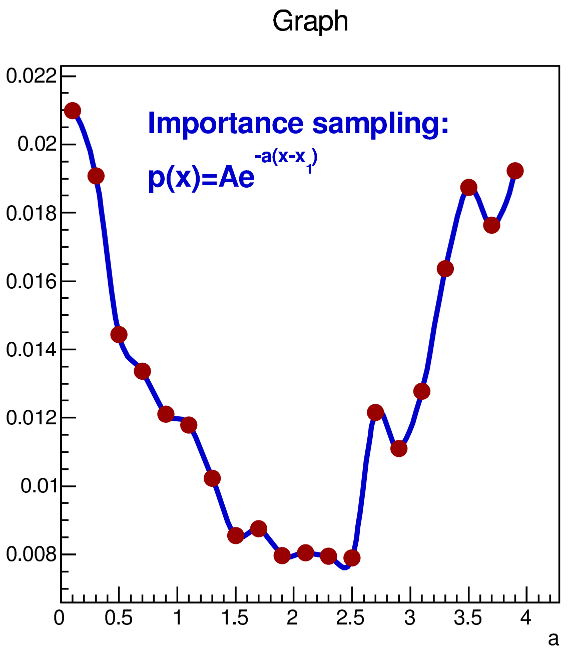
$$\int_{0.2\pi}^{0.5\pi} cos(x)dx$$

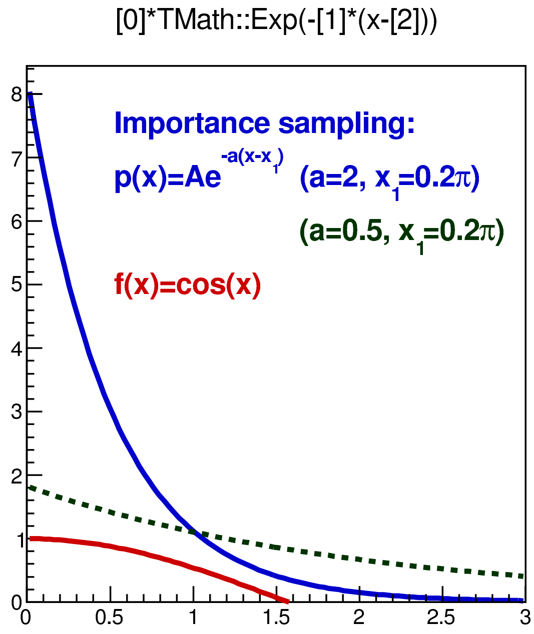
expected = 0.412215
MC = 0.432225 +/- 0.025083 (100 deviates generated)
What about using importance sampling with a pdf: $p(x) \propto e^{-ax}$?

Importance sampling (cont.)

The function PDF shape matters?

Let's study the variation of the integral error with the a parameter of the exponential





Importance sampling (cont.)