Theoretical Practical Course in Computational Physics

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Contents

1 Monte Carlo (MC) integration method

The Monte Carlo integration method is quite similar to the Riemann integration method with the subtle difference that one chooses the x_is randomly. This leads to the following approximative formula for the integral:

$$I = \frac{b-a}{N} \sum_{i=0}^{N-1} f(x_i) \xrightarrow{N\to\infty} \int_a^b f(x)\,\mathrm{dx} \tag{1}$$

We can estimate the integral of the function f by:

$$\int_a^b f(x), \mathrm{dx} \approx I \pm Error = V\langle f\rangle \pm V\sqrt{\frac{\langle f^2\rangle - \langle f\rangle^2}{N}} \tag{2}$$

Of course we do not know the standard deviation of f but we can approximate it "on the flight" when performing the Monte Carlo integration. In our program, we assume that the desired accuracy is reached, when:

$$accuracy \geq \frac{\sqrt{\frac{\langle f^2\rangle - \langle f\rangle^2}{N}}}{\langle f\rangle}$$

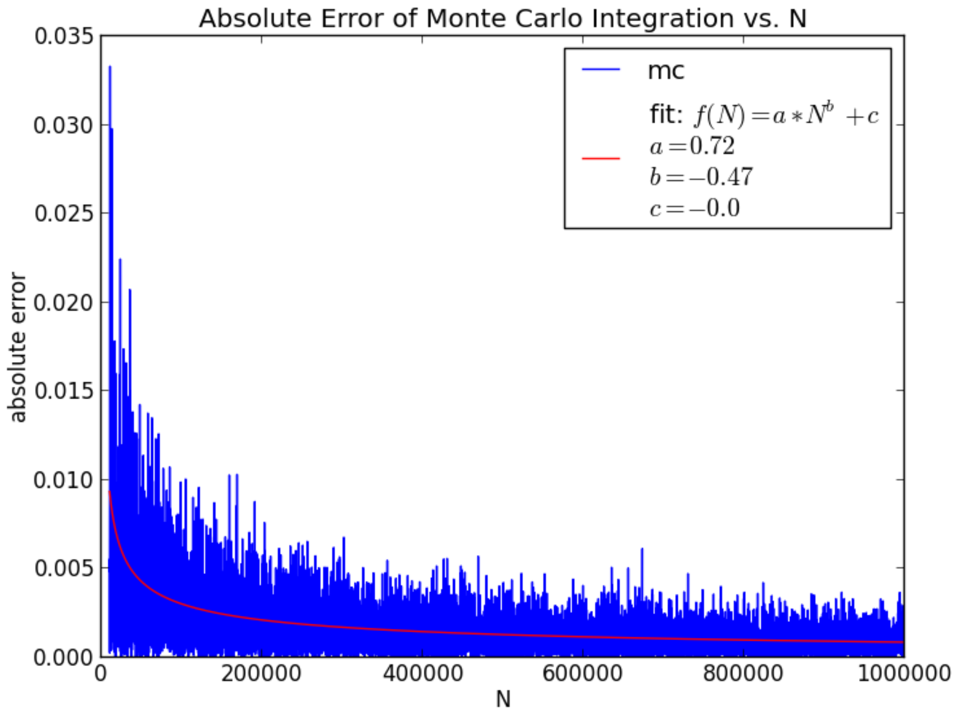
As one can see, the error decreases with $\sim \frac{1}{\sqrt{N}}$. To get an more detailed idea of what determines the error, we should notice that the individual function values at random points x_i one the x-axis are themselvs random numbers.The Integrand, being sum of random numbers is a random number too. The distribution of the integrated values approaches a Gaussian. By using the central limit theorem it can be shown that the following expression holds:

$$\sigma^2(I_N) = \frac{V^2}{N}\int_V (f(x) - \langle f\rangle)^2 \mathrm{dx} = \frac{V^2}{N}\sigma^2(f) \tag{3}$$

This leads to the important conclusion that the variance of I_N does not depend only on the quantity of random points N, but also on the volume V and the variance of the function $\sigma^2(f)$. To show this characteristic we define the ratio ρ.

$$\rho = \frac{N}{V^2}\frac{\sigma^2(I_N)}{\sigma^2(f)}$$

Figure 1: $f(x) = x$, volume: $[-1, 1]$, ratio: 1.051



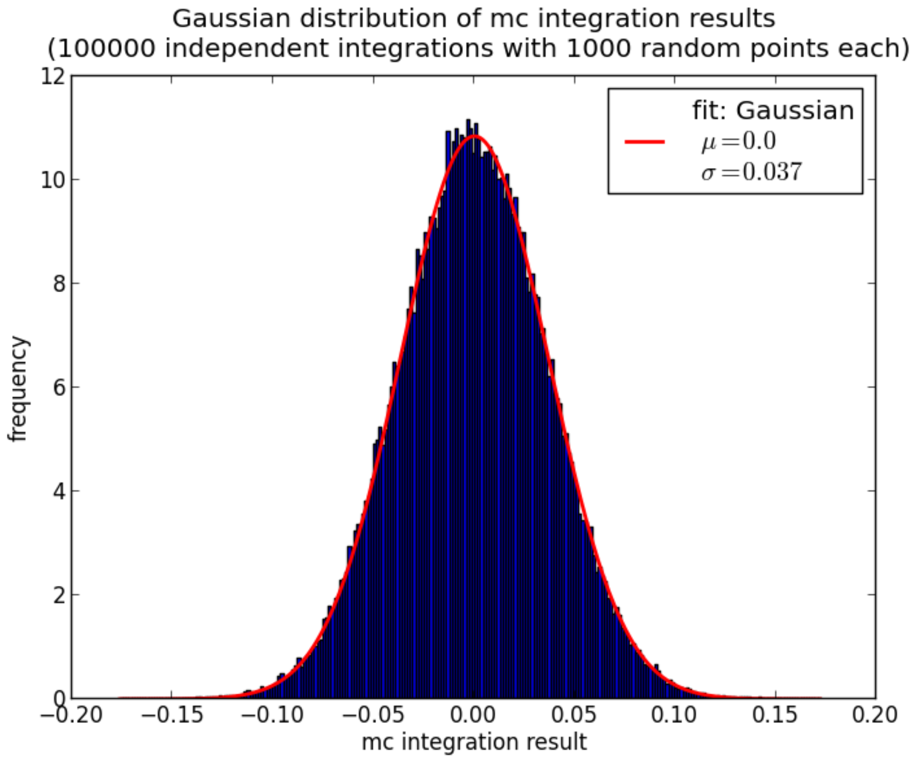
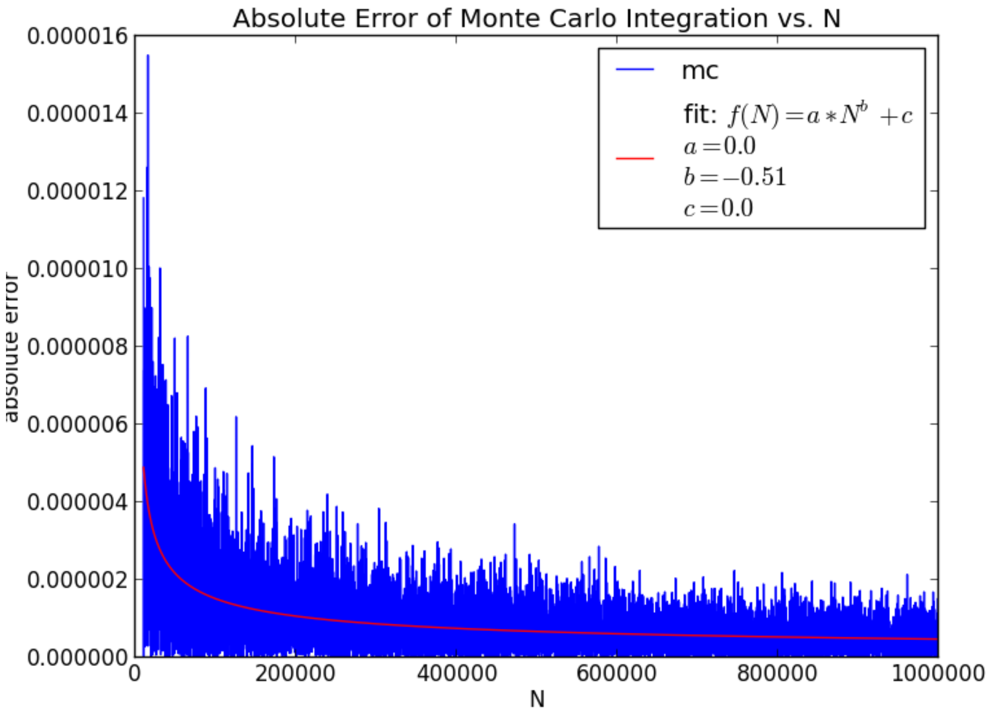


Figure 2: $f(x) = x^2$, volume: $[-1, 1]$, ratio: 1.043



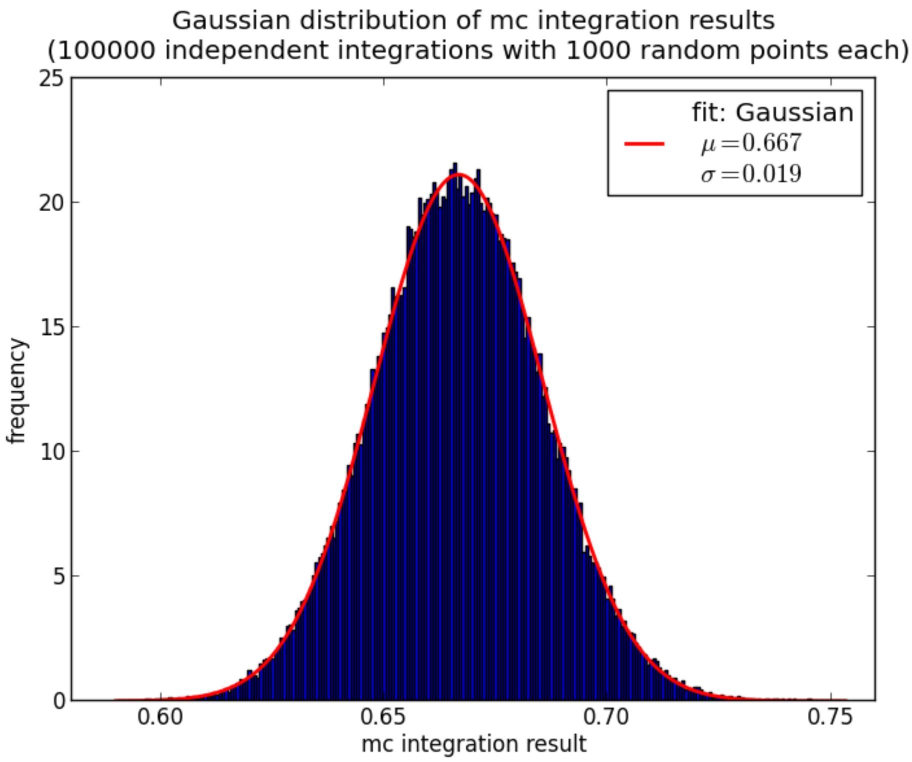
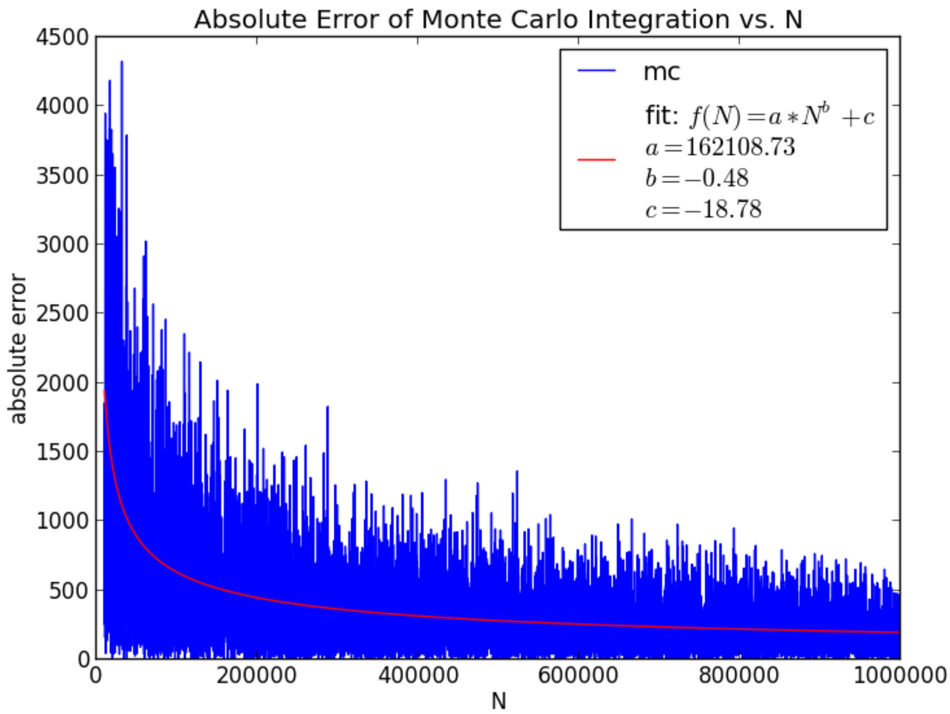


Figure 3: $f(x) = x^5$, volume: $[-1, 1]$, ratio: 0.951, (the fit function failed to find the correct fit paramters for the Gaussian)



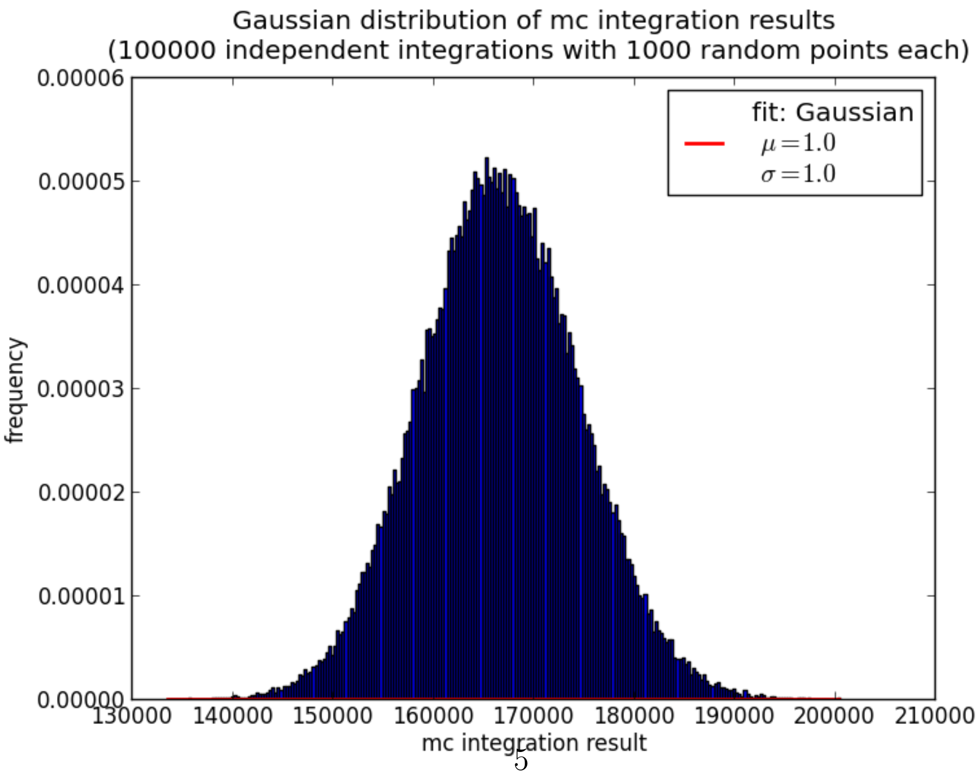
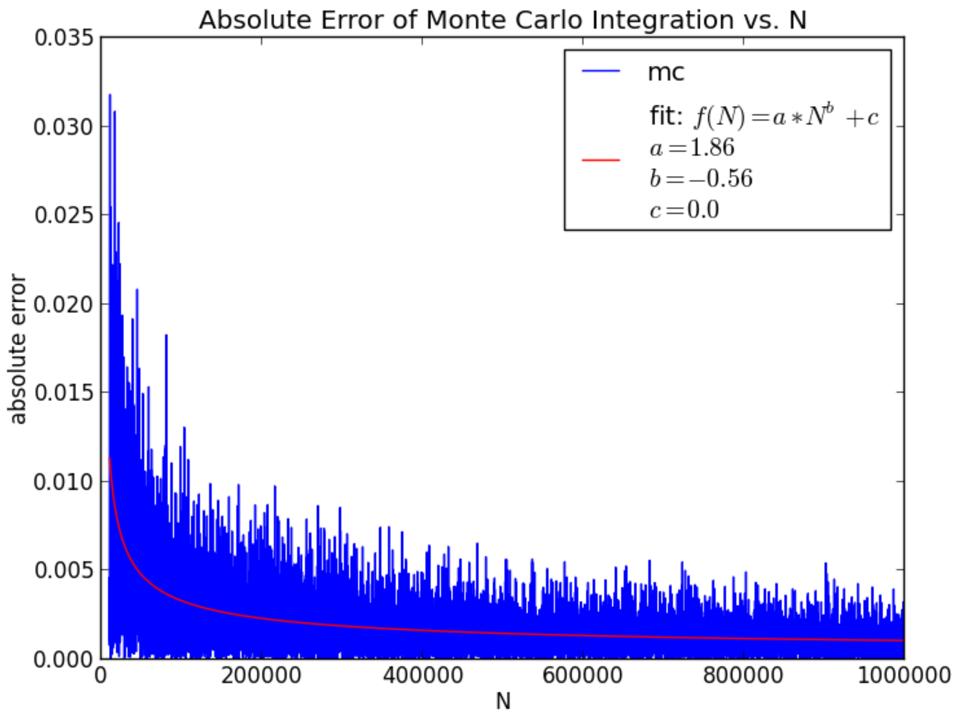


Figure 4: $f(x) = exp(x)$, volume: $[-1, 1]$, ratio: 0.932



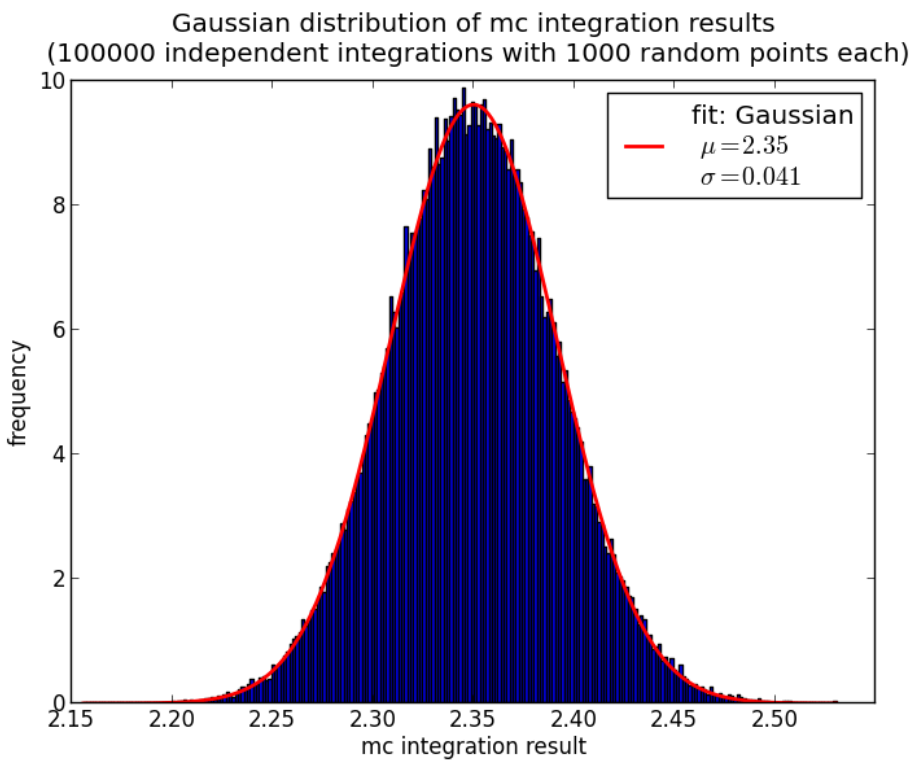


Figure 5: $f(x) = sin(x)$, volume: $[0, 2\pi]$, ratio: 1.085