# Introduction to Computational Physics – Exercise 10

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## Probability Distribution Functions

Consider a probability distribution function $p(x)$ given in the domain $[0,\, a\rangle$ by

$$p(x) = bx \tag{1}$$

Assume that $\{r_i\}$ is a random set of numbers, distributed uniformly between 0 and 1.

**Task:** Give the proper value of $b$ as a function of $a$ such that the probability distribution function is properly normalized.

**Task:** Use the rejection method to make a set $\{x_i\}$ that obeys Eq. (1) for $a = 0.5$.

**Task:** Make a histogram of the resulting numbers and check that the histogram indeed follows Eq. (1), i.e. overplot Eq. (1). Experiment with the size of the set (the number of random numbers drawn), to find out how large you have to make it to get (by eye) a reasonable fit.

## Determination of $\pi$ with Random Numbers

**Task:** Compute the number $\pi$ using a rejection method with the function $f(x) = \sqrt{1-x^2}$, for $0 \le x \le 1$. *Hint:* It is enough to use only one quadrant $x,\, f(x) > 0$. Vary the number of random numbers (RNs) widely (orders of magnitude) and plot the accuracy of the result as a function of the number of RNs. Use logarithmic variables for the plot.

To determine $\pi$ numerically, we first use a so-called *rejection method*: To do this, consider a quadrant $f(x) = \sqrt{1-x^2}$ $(0 \le x \le 1)$ with radius $r = 1$ that lies within a square with the side lengths $r = 1$. The following applies to the ratio of the areas of the quadrant and the square:

$$\frac{A_\mathrm{c}}{A_\mathrm{s}} = \frac{\pi r^2}{4r^2} = \frac{\pi}{4} \tag{2}$$

The goal is now to estimate the ratio of the areas in order to calculate $\pi$. We can devise an algorithm that generates two random numbers $x_i,\, y_i \in [0,\, 1]$ (random coordinates from the square) and checks whether the coordinate fell into the quarter circle or not (rejection method):

$$\left[\text{if} \quad y_i \le \sqrt{1-x_i^2} \quad \Rightarrow \quad \text{“take”}\right] \qquad \dot{\vee} \qquad \left[\text{if} \quad y_i > \sqrt{1-x_i^2} \quad \Rightarrow \quad \text{“reject”}\right] \tag{3}$$

The value of $\pi$ is then approximately given by the ratio of the number $N_\text{take}$ of points within the quadrant to the total number $N_\text{total}$ of points:

$$\pi \approx 4\, \frac{N_\text{take}}{N_\text{total}} \tag{4}$$

Another possibility for the numerical determination of $\pi$ is the so-called *Monte Carlo integration*: Monte Carlo integration is a technique for numerical integration using random numbers. We want to integrate the function $f(x)$ on the interval $[a,\, b]$. The idea with Monte Carlo integration is to evaluate the function $f(x)$ on $N$ randomly selected points $x_i$ $(i = 1,\, \ldots,\, N)$ (random sampling) in the interval $[a,\, b]$. In the case of equally distributed random numbers $x_i$, the value of the integral is simply the average of the function values $f(x_i)$:

$$\int_a^b f(x)\,\mathrm{d}x \approx \frac{b-a}{N} \sum_{i=1}^{N} f(x_i) \tag{5}$$

The fact that this method works is due to the law of large numbers, i.e. $N \to \infty$. We know that the integral of $f(x) = \sqrt{1 - x^2}$ on the interval $0 \leq x \leq 1$ gives a quarter of the area of the unit circle. The area of the unit circle (radius $r = 1$) is $A_\mathrm{c} = \pi r^2 = \pi$. With $N$ randomly selected values $x_i \in [0,\, 1]$, we obtain the following approximation formula for $\pi$ using Monte Carlo integration:

$$\frac{\pi}{4} = \int_0^1 \sqrt{1 - x^2}\,\mathrm{d}x \approx \frac{1}{N} \sum_{i=1}^{N} \sqrt{1 - x_i^2} \qquad \Longrightarrow \qquad \pi \approx \frac{4}{N} \sum_{i=1}^{N} \sqrt{1 - x_i^2} \tag{6}$$