# **Physics through Computational Thinking**

The Monte Carlo method

### **Auditya Sharma and Ambar Jain**

Dept. of Physics, IISER Bhopal

### **Outline**

In this module we look at

- 1. how to estimate ln(2) using the Monte Carlo method and a suitable definite integral.
- 2. how to estimate  $\pi$  using a Monte Carlo method to compute a suitable definite integral.

# An elementary integral

Consider the integral

$$I = \int_0^1 \frac{1}{1+x} \, dx. \tag{1}$$

It is straightforward for us to find this integral. It is simply given by:

$$I = \ln(2). \tag{2}$$

In fact, we can get Mathematica to evaluate it for us:

Integrate 
$$\left[\frac{1}{1+x}, \{x, 0, 1\}\right]$$

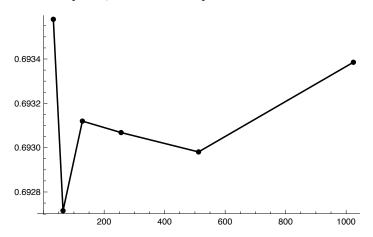
Log[2]

Let us use the Monte Carlo method to estimate this integral, and therefore obtain an estimate for ln(2). The idea is to do a random sampling of points between zero and unity, and simply find an average of the value of integrand evaluated at these points.

$$\begin{aligned} \text{data = Table} \Big[ n &= 2^k; \\ & \Big\{ n, \, \text{Mean} \Big[ \text{Table} \Big[ \frac{1}{(\text{RandomReal}[]+1)}, \, \{n\} \Big] \Big], \, \{1000\} \Big] \Big] \Big\}, \, \{k, \, 5, \, 10\} \Big]; \end{aligned}$$

#### TableForm[data]

32	0.693579
64	0.692715
128	0.69312
256	0.693068
512	0.692981
1024	0.693385



errdata = Table 
$$n = 2^k$$
;

$$\left\{n, \, Mean\Big[Table\Big[Abs\Big[Mean\Big[Table\Big[\frac{1}{(RandomReal[]+1)}, \, \{n\}\Big] - Log[2]\Big]\Big], \, \{1000\}\Big]\right]\right\}, \, \{k, \, 5, \, 10\}\Big];$$

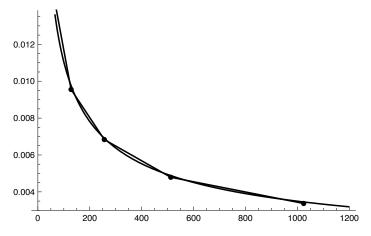
### TableForm[errdata]

$$fn[x_] = ax^b;$$

$$\label{eq:fit_errdata} \mbox{fit} = \mbox{FindFit} \Big[ \mbox{errdata,} \; \Big\{ \mbox{a} \; \mbox{x}^b \Big\}, \; \{ \mbox{a,} \; b \} \; , \; \{ \mbox{x} \} \, \Big]$$

$$\{a \to 0.110299, b \to -0.499775\}$$

 $Show[Plot[fn[x] /. fit, \{x, 0, 1200\}], ListPlot[errdata, Joined \rightarrow True]]$ 



So, the error goes roughly as  $\frac{1}{\sqrt{n}}$ .

# Estimating $\pi$

Now, let us consider the integral

$$I = \int_0^1 \frac{4}{1+x^2} \, dx. \tag{3}$$

It is straightforward for us to find this integral. It is simply given by:

$$I = \pi. (4)$$

We can get *Mathematica* to check it for us:

Integrate 
$$\left[\frac{4}{1+x^2}, \{x, 0, 1\}\right]$$

π

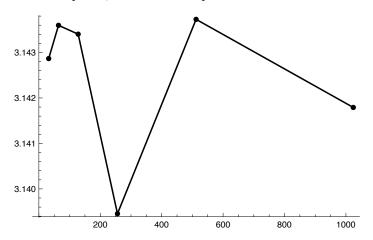
Let us use the Monte Carlo method to estimate this integral, and therefore obtain an estimate for  $\pi$ . The idea is to do a random sampling of points between zero and unity, and simply find an average of the value of integrand evaluated at these points, as before.

$$\text{data = Table} \Big[ n = 2^k; \\ \Big\{ n, \, \text{Mean} \Big[ \text{Table} \Big[ \frac{4}{\Big( \left( \text{RandomReal} \left[ \right] \right)^2 + 1 \Big)}, \, \{n\} \Big] \Big], \, \{k, \, 5, \, 10\} \Big];$$

#### TableForm[data]

32	3.14287
64	3.1436
128	3.1434
256	3.13946
512	3.14373
1024	3.14179

#### ListPlot[data, Joined → True]



$$\left\{n,\,\mathsf{Mean}\Big[\mathsf{Table}\Big[\mathsf{Abs}\Big[\mathsf{Mean}\Big[\mathsf{Table}\Big[\frac{4}{\big(\left(\mathsf{RandomReal}[\,]\right)^2+1\big)},\,\{n\}\,\Big]-\pi\Big]\Big],\,\{100\}\,\Big]\right\},\,\{k,\,5,\,10\}\Big];$$

### TableForm[errdata]

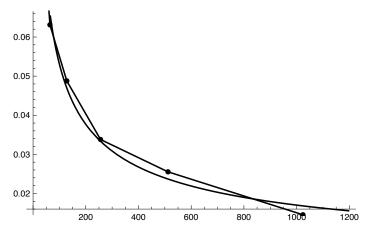
32 0.0941386 64 0.0631196 128 0.0487795 256 0.0337932 512 0.025524 1024 0.0145453

$$fn[x_] = ax^b;$$

fit = FindFit[errdata,  $\{ax^b\}$ ,  $\{a, b\}$ ,  $\{x\}$ ]  $\{a \rightarrow 0.515859, b \rightarrow -0.493919\}$ 

fn[x] /. fit;

### $Show[Plot[fn[x] /. fit, \{x, 0, 1200\}], ListPlot[errdata, Joined \rightarrow True]]$



So, once again, we see that the error goes roughly as  $\frac{1}{\sqrt{n}}$ .