

Monte Carlo method

Introduction to MC method

- It have been invented in the context of the development of the atomic bomb in the 1940's.
- Monte carlo methods are a class of computational algorithms, it can be applied to vast ranges of problems.
- It is not a statistical tool, it rely on **repeated random sampling**.
- **It** provide generally approximate solutions, and are used in cases where analytical or numerical solutions don't exist or are too difficult to implement

MC methods have applications in various fields such as Material Science, Statistical Physics, Chemical and Bio Physics, nuclear physics, flow of traffic and many others.

Monte-Carlo methods generally follow the following steps:

1. Determine the **statistical properties** of possible inputs
2. Generate many **sets of possible inputs** which follows the above properties
3. Perform a **deterministic calculation** with these sets
4. Analyze **statistically** the results

The error on the results typically decreases as $1 / \sqrt{N}$

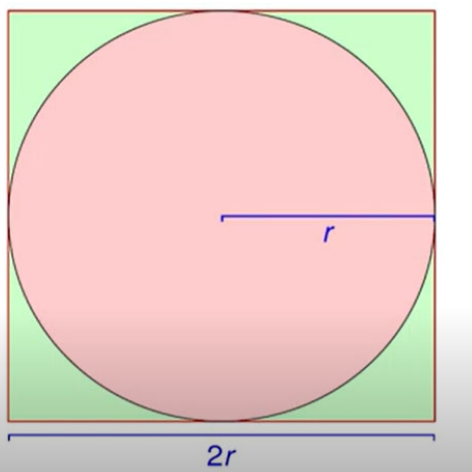
A simple example of MC

Can we determine the value of π using a Monte Carlo method ?

- Consider a square with sides of length $2r$.
- Draw a circle inside the square with radius r .

$$S_{\text{square}} = (2r)^2 = 4r^2.$$

$$S_{\text{circle}} = \pi r^2.$$



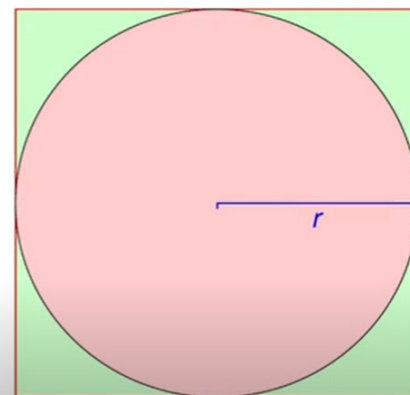
- Then the ratio is

$$\frac{S_{\text{circle}}}{S_{\text{square}}} = \frac{\pi r^2}{4r^2} = \frac{\pi}{4}.$$

- Multiplying 4 on both sides of the equation yields

$$4 \times \frac{S_{\text{circle}}}{S_{\text{square}}} = 4 \times \frac{\pi}{4}$$

$$4 \times \frac{S_{\text{circle}}}{S_{\text{square}}} = \pi$$



$$\pi = 4 \times \frac{S_{\text{circle}}}{S_{\text{square}}}$$

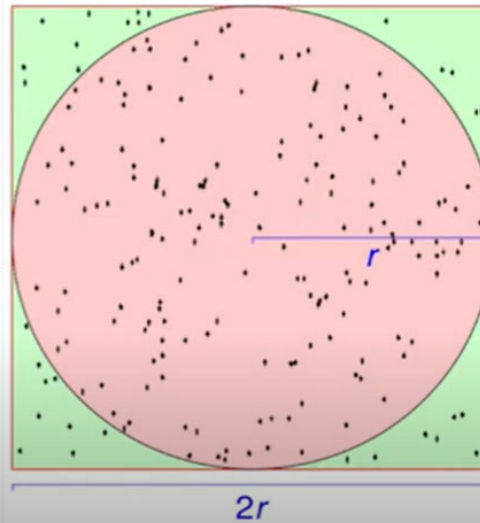
- Since $\pi = 4 \times \frac{S_{\text{circle}}}{S_{\text{square}}}$

- We have

$$\pi = 4 \times \frac{S_{\text{circle}}}{S_{\text{square}}}$$

\approx

$$4 \times \frac{\text{Points within the circle}}{\text{Points within the Square}}$$



Draw a square on the ground, then inscribe a circle within it. Uniformly scatter some objects of uniform size (grains of rice or sand) over the square.

Count the number of objects inside the circle and the total number of objects.

The ratio of the two counts is an estimate of the ratio of the two areas, which is $\pi/4$. Multiply the result by 4 to estimate π .

Solving Boltzmann Transport equation using Monte-Carlo method

Direct simulation Monte Carlo (DSMC – by Dr. Bird at 1963) method is one of a popular choice for solving Boltzmann transport equation (BTE) in the field of rarefied gas dynamics due to a number of factors:

First, the high dimensionality associated with $f(t, x, p)$ makes numerical methods based on discretization computationally expensive, both in terms of CPU time and storage

second, the particle formulation employed by DSMC is ideal for accurately and *stably* capturing the propagation of traveling discontinuities in the distribution function resulting from the advection operator in the Boltzmann equation.

finally, the DSMC algorithm combines simplicity with an intuitive formulation that naturally employs importance sampling for improved computational efficiency

DSMC solves the Boltzmann equation using discretization in time; each time step of length Δt is split into a collisionless advection and a collision substep. Numerically, this corresponds to a splitting scheme in which the collisionless advection substep integrates

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \mathbf{F} \cdot \nabla_{\mathbf{v}} f = 0$$

while the collision substep integrates

$$\frac{\partial f}{\partial t} = \left[\frac{\partial f}{\partial t} \right]_{\text{coll}}$$

During the advection substep, particles move ballistically (according to their velocities and accelerations).

During the collision substep, the distribution function is updated by processing binary collisions between collision pairs chosen from within the same computational cell of linear size Δx , using an acceptance-rejection procedure.

This introduces the second important mode of discretization in this algorithm, as it corresponds to treating the distribution function as spatially homogeneous within each cell.

