Exercise 3. Crude "hit or miss" Monte Carlo method

Objective: Use "hit or miss" Monte Carlo method for calculating the volume inside a sphere in different dimensions.

The volume delimited by a sphere of radius R in D dimensions is

$$V_{sphere} = \int ... \int \theta(R^2 - x_1^2 - ... - x_N^2)\, dx_1...dx_N \tag{1}$$

where the theta function is defined as

$$\theta(x) = \begin{cases} 0, & \text{if } x < 0 \\ 1, & \text{if } x > 0. \end{cases}$$

Integral (1) can be calculated sampling uniform distributions,

$$\begin{aligned} V_{sphere} &= \int_{-R}^{R} ... \int_{-R}^{R} \left[(2R)^D \theta(R^2 - x_1^2 - ... - x_N^2)\right] p_{uniform}(x_1, ..., x_N)\, dx_1...dx_N & (2) \\ &\approx \langle (2R)^D \theta(R^2 - x_1^2 - ... - x_N^2) \rangle_{uniform} & (3) \end{aligned}$$

The statistical error in the estimation of the average of a quantity a can be estimated as $\sigma/\sqrt{N_{iter}}$ where the variance is

$$\sigma^2 = \langle a^2 \rangle - \langle a \rangle^2 \tag{4}$$

In the case of Eq. (3), the quantity to be averaged is $a = (2R)^D \theta(R^2 - x_1^2 - ... - x_N^2)$.

1 Area of a circle in 2D

Consider a circle of unit radius, $R = 1$, in two dimensions. Generate N_{iter} random numbers $-1 < x < 1$ and $-1 < y < 1$ using uniform random distribution. Calculate the probability that point (x, y) lies inside of the circle, i.e. if $x^2 + y^2 < 1$. Use the obtained probability to approximate the area of the circle S. Compare it to the exact result, $S_{exact} = \pi R^2$, report the statistical error $\sigma/\sqrt{N_{iter}}$ and compare it with the actual error.

Make a log-log plot showing (i) statistical error, $\sigma/\sqrt{N_{iter}}$ (ii) actual error, $|S - S_{exact}|$ as a function of the number of iterations.

2 Volume of a sphere in 3D

Consider a circle of unit radius, $R = 1$, in three dimensions. Generate N_{iter} random numbers $-1 < x < 1$, $-1 < y < 1$ and $-1 < z < 1$ using uniform random distribution. Calculate the probability that point (x, y, z) lies inside of the sphere, i.e. if $x^2 + y^2 + z^2 < 1$. Use the obtained probability to approximate the volume of the sphere. Compare it to the exact result, $V = \frac{4}{3}\pi R^3$, and report the statistical error.

3 Volume of a sphere in D dimensions

Consider a circle of unit radius, $R = 1$, in D dimensions. Generate N_{iter} random numbers $-1 < x_i < 1$, $i = 1, ..., D$ using uniform random distribution. Calculate the probability that point $(x_1, ..., x_D)$ lies inside of the sphere, i.e. if $\sum_{i=1}^{D} x_i^2 < 1$. Use the obtained probability to approximate the volume of the sphere. Compare it to the exact result, $V = \pi^{D/2} R^D / \Gamma(D/2+1)$, and report the relative error.

What is the largest space dimensionality, in which this method can be reliably used? What is the ratio between the volume of the sphere of diameter $2R$ and a cube with side $2R$ in D dimensions?

4 * Volume inside a sphere in $D = 100$ dimensions

The crude Monte Carlo method does not work well if the sphere volume is significantly smaller than the volume of the cube. Algorithmically, this means that even if even one of the random values x_i is close to R, the resulting distance from the center of the sphere most probably will be larger than R and will provide zero contribution to the integral.

A possible way out is to sample more frequently the region close to the origin by using an importance sampling technique.

$$V_{sphere} = \int_{-\infty}^{\infty} ... \int_{-\infty}^{\infty} \left[(2\pi)^{D/2} \sigma^D e^{\frac{x_1^2 + ... + x_N^2}{2\sigma^2}} \theta(R^2 - x_1^2 - ... - x_N^2) \right] p_{normal}(x_1, ..., x_N) \, dx_1 ... dx_N \quad (5)$$

$$\approx \langle (2\pi)^{D/2} \sigma^D e^{\frac{x_1^2 + ... + x_N^2}{2\sigma^2}} \theta(R^2 - x_1^2 - ... - x_N^2) \rangle_{uniform} \quad (6)$$