Exercise sheet 5

Random directions

PUE Advanced Computational Physics

University of Vienna - Faculty of Physics

14 Uniform random points on a sphere

Choosing a random point on the unit sphere is an often encountered problem, for example when one chooses a random rotation axis for a molecule. Consider the following approaches to this problem:

i. Choose 3 random numbers between -1 and 1 and interpret them as a vector, $\vec{v}$. The random point is then given by $\vec{v}/|\vec{v}|$.

ii. Choose 3 random numbers between -1 and 1 and interpret them as a vector, $\vec{v}$. Discard all vectors with $|\vec{v}| > 1$ and normalize the rest, as above.

iii. Choose 2 random numbers $\phi \in [0, 2\pi)$ and $\vartheta \in [0, \pi]$ and interpret (ϑ, ϕ) as the spherical coordinates of the vector.

iv. Choose 2 random numbers $\phi \in [0, 2\pi)$ and $\cos(\vartheta) \in [-1, 1]$ and interpret (ϑ, ϕ) as the spherical coordinates of the vector.

v. Pick four numbers x_0, x_1, x_2, and x_3 from a uniform distribution on $[-1, 1]$, accept only choices with $x_0^2 + x_1^2 + x_2^2 + x_3^2 \leq 1$ and apply the following transformation:

$$x = \frac{2(x_1x_3 + x_0x_2)}{x_0^2 + x_1^2 + x_2^2 + x_3^2}$$
$$y = \frac{2(x_2x_3 - x_0x_1)}{x_0^2 + x_1^2 + x_2^2 + x_3^2}$$
$$z = \frac{x_0^2 - x_1^2 - x_2^2 + x_3^2}{x_0^2 + x_1^2 + x_2^2 + x_3^2}$$

The goal is to generate a sample of uniformly distributed points on the unit sphere (i.e. the probability density of the points is rotationally invariant).

a. Generate samples using the above methods and visualize them in a suitable way.

b. Which methods work? Which methods do not—and why?

c. Between methods iii and iv, argue which of these methods is correct.

d. Which method would you choose to be as computationally efficient as possible?