PHILIPPS-UNIVERSITAET MARBURG, THE DEPARTMENT OF PHYSICS

Computational Physics II : Assignment 3

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1 RANDOM WALK WITH MEMORY

We first picked up 100000 points for $x_0 = 0$, then we evaluate them for 1000 steps with memorized random walks

$$x_0 = 0, \quad x_1 = x_0 + l_0, \quad \cdots, \quad x_{n+1} = x_n + l_n \tag{1.1}$$

where

$$l_0 = \begin{cases} 1 & \text{with probability of } 0.5 \\ -1 & \text{with probability of } 0.5 \end{cases}, \quad l_n = \begin{cases} l_{n-1} & \text{with probability of } 0.5 + \varepsilon \\ -l_{n-1} & \text{with probability of } 0.5 - \varepsilon \end{cases} \tag{1.2}$$

for $\varepsilon \in \{0.1, 0.2, 0.3, 0.4\}$. The results are presented in Figure 1.1.

By using the fitting parameters σ, the diffusion constant can be determined. But hardly we can find

ε	0.1	0.2	0.3	0.4
diffusion constant D	1.4977	2.3225	3.9958	9.0068

Table 1.1: the diffusion constant for memorized random walk with $\varepsilon \in \{0.1, 0.2, 0.3, 0.4\}$.

the trend of the diffusion constants.

2 RANDOM WALKS IN 3D

We first constructed the random vectors generators by following the interpretation. Our strategies go as:

(i) Spherical coordinates

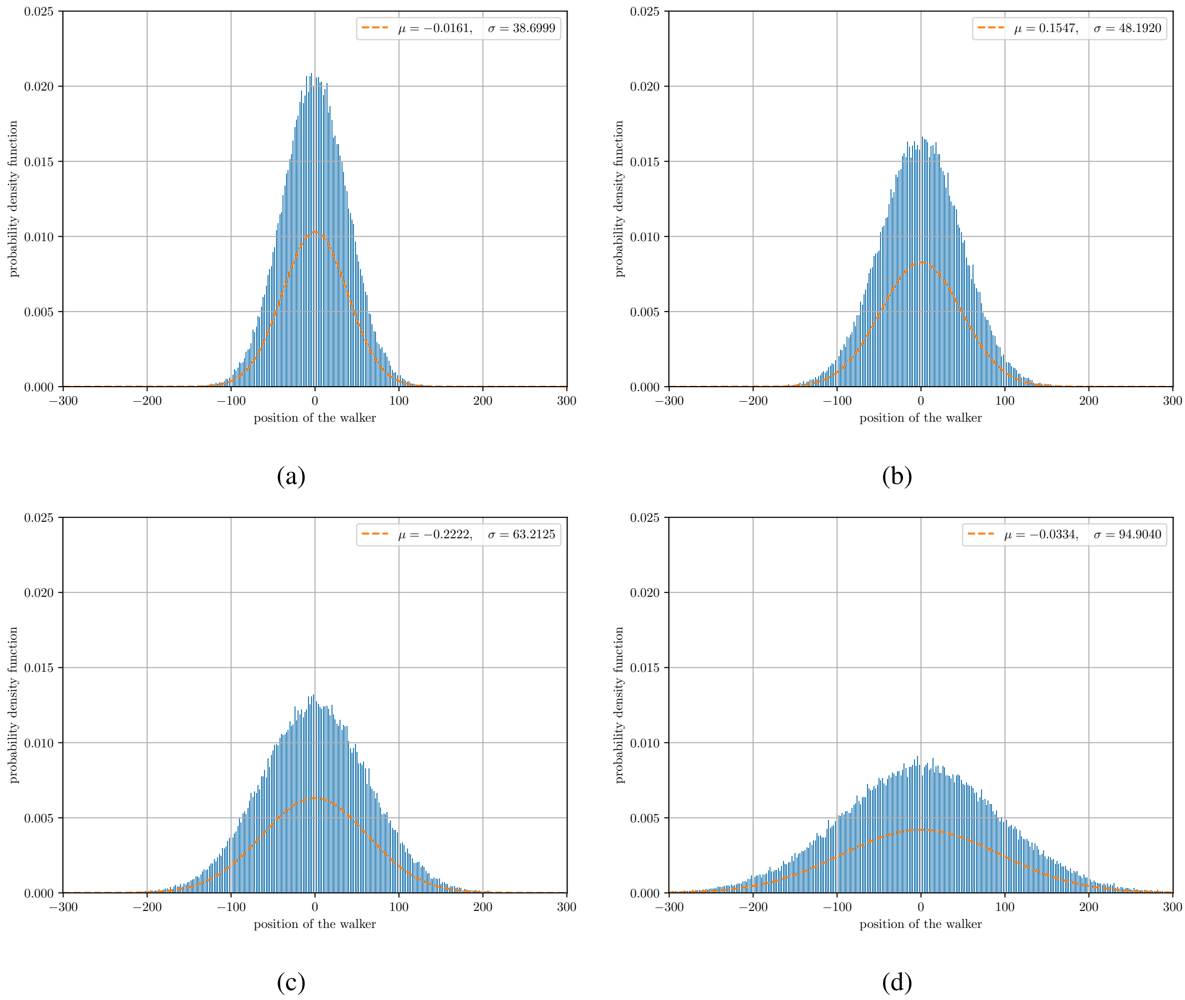


Figure 1.1: the statistics for the memorized random walk with $\varepsilon = 0.1, 0.2, 0.3, 0.4$ corresponding to (a), (b), (c), (d), and their fitting curve for Gaussian distribution.

The direction is given by $n = (\sin\theta\cos\phi, \sin\theta\cos\phi, \cos\theta)$, whose probability density is determined as $d\Omega = \sin\theta d\theta\phi$. If the θ and ϕ are determined from uniform random number in the range of (0,π) and range (0,2π), then the directional distribution is is not uniform shown in Figure 2.1 (a).

To build uniform distribution of direction $d\Omega = d\zeta d\eta$ where ζ and η are uniform random variable in (-1,1).

$$d\Omega = d(-\cos\theta)d\phi = d\zeta d\eta, \quad \theta = \arccos(-\zeta) \quad \& \quad \phi = \eta \tag{2.1}$$

The results are proved to have high homogeneity which are shown in Figure 2.1 (b).

(ii) Sperical Volume

Sphere is iostropic in all direction and directional density is also idential. So the randomly picking a point in sphere volume gives uniform direction distribution. To simulate sphere with radius 1, three random numbers $x_i \in (-1, 1)$ with $||x|| < 1$ are picked. The points directions are represented in Figure 2.1 (c).

(iii) Gaussian random distribution

With normally distributed random number ; ζ, η, ξ for cartesian coordinates, the probability density only depends on r. This mean for each direction the probability is identical. The results shown in Fig 2.1 (d).

$$d\zeta d\eta d\xi = (\frac{1}{\sigma\sqrt{2\pi}})^3 e^{-\frac{x^2+y^2+z^2}{2\sigma^2}} dxdydz = (\frac{1}{\sigma\sqrt{2\pi}})^3 e^{-\frac{r^2}{2\sigma^2}} dxdydz \tag{2.2}$$

After that, in order to calculate the diffusion constant out, we plot the radius distribution of the final position. And do curve fitting with

$$f(r)\, dr = \int_0^{\pi} \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi \left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^3 \exp\left(-\frac{r^2}{2\sigma^2}\right) r^2 \sin\theta \mathrm{d}r = \frac{\sqrt{2}}{\sqrt{\pi}\sigma^3} \exp\left(-\frac{r^2}{2\sigma^2}\right) r^2 \mathrm{d}r. \tag{2.3}$$

The results are shown in Figure 2.2. By using the σ here, the diffusion constant are found out at $D = 0.3352$.

3 Brownian motors and ratchets

We are unable to solve this task.

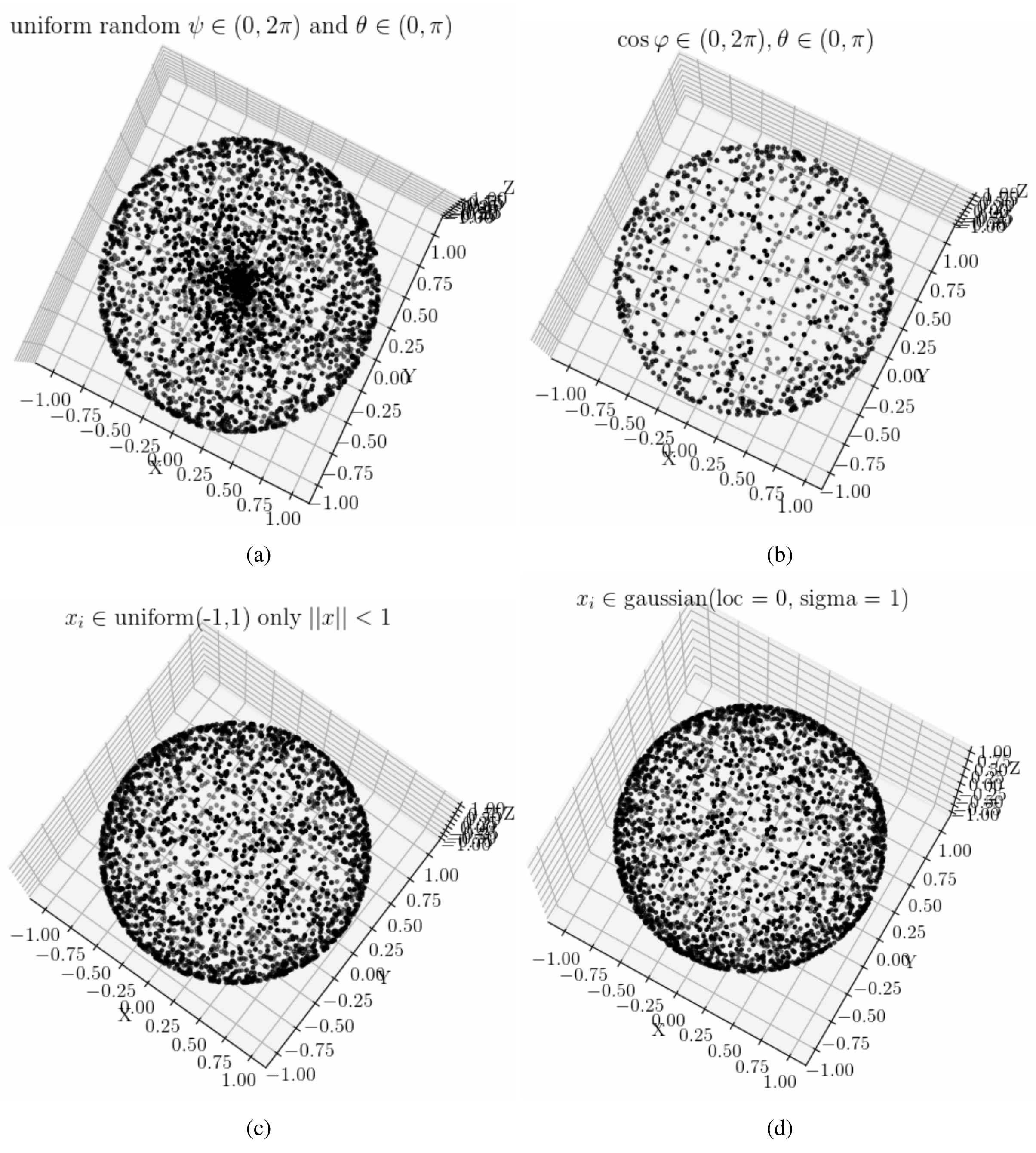
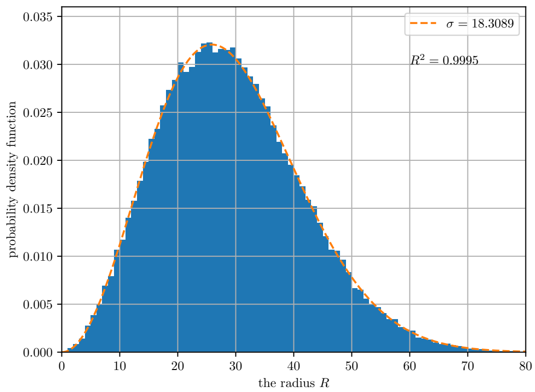
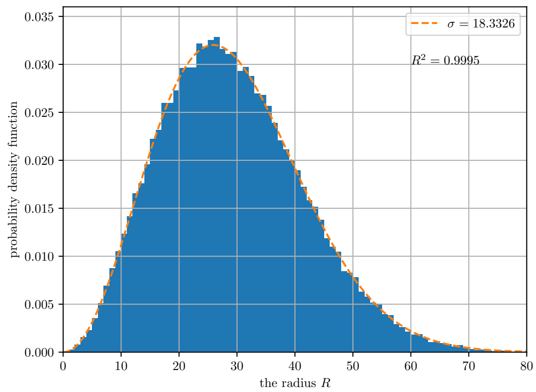


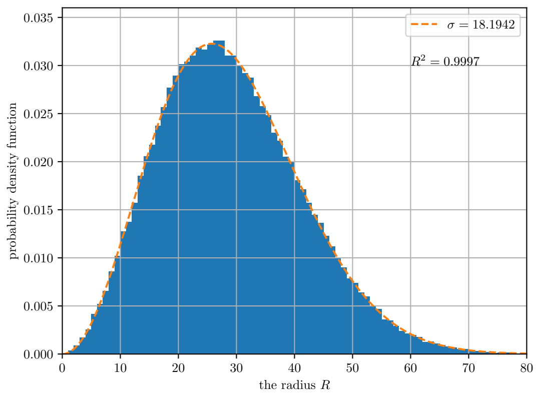
Figure 2.1: Direction distribution with 4 different way of random variable



(a)



(b)



(c)

Figure 2.2: the radius distributions for three types of 3D random walk: (a) spherical; (b) spherical volume; (c) Gaussian.