2D Brownian motion simulation

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Introduction

Brownian motion of a single particle is simulated using random numbers drawn from a normal distribution.

Model equations

At each timestep the particle moves a distance $d\mathbf{s} = \mathbf{v}\delta t$ so the location $\mathbf{s}$ of the particle is given by:

$$\mathbf{s} = \mathbf{s} + \mathbf{v}\delta t \tag{1}$$

Where $\mathbf{v}$ is the velocity of the particle and δt the size of the timestep. The velocity $\mathbf{v}$ is calculated by:

$$\mathbf{v} = k\mathbf{R} \tag{2}$$

$\mathbf{R}$ is a vector (R_x, R_y) with normalized and normally distributed random components and k a constant of proportionality, defined as $k = \sqrt{2D\delta t}$ with D the diffusion coefficient. At each timestep the velocity vector is updated with a new pair of random numbers.

Results

The mean squared displacement $d = x_c^2 + y_c^2$, with x_c the x coordinate and y_c the y coordinate, of the particle of interest is proportional with time. A plot of the results is given in figure 1, where the mean squared displacement is plotted against time.

The number of particles in some given region between r and $r + \delta r$ observed in simulations at time t_f is compared with the number of particles in the same region predicted theoretically using the solution to the diffusion equation. The comparison is shown in figure 2.

Discussion

Simulations show that the mean squared displacement d is approximately proportional with time. This implies that the probability density of the particle of interest can be given by:

$$\rho(r,t) = \frac{1}{4\pi Dt} e^{-r^2/4Dt} \tag{3}$$

Since the mean squared displacement is equal to the variance of equation (3):

$$d = \int_0^\infty \frac{1}{4\pi Dt} e^{-r^2/4Dt} \cdot 2\pi r \cdot r^2 dr = 4Dt \tag{4}$$

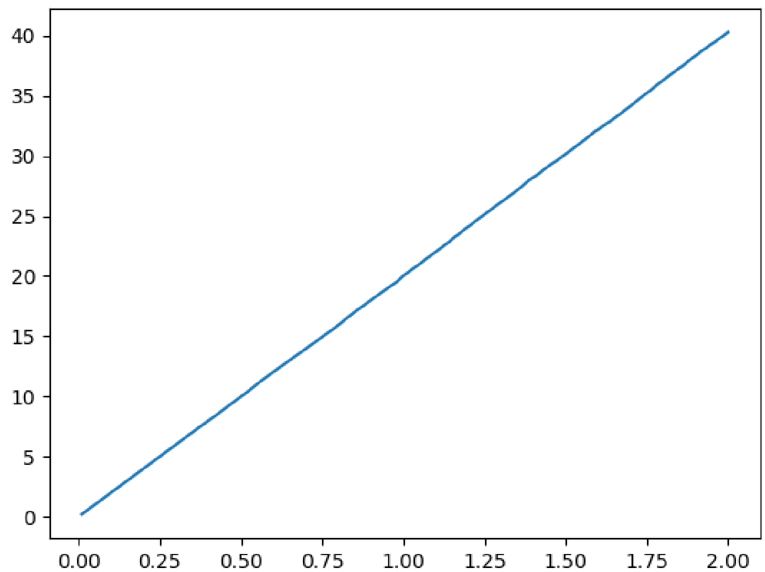

Figure 1: The mean squared displacement as a function of time.

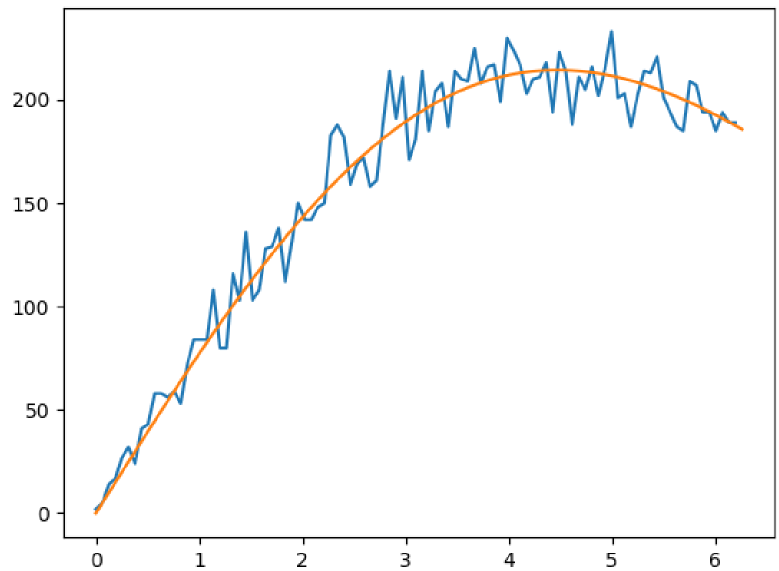

Figure 2: The blue line shows the computed number of particles within a given region between r and $r + \delta r$ vs the radial coordinate and the orange line shows the theoretical prediction of the number of particles within the same region.

Where D is the diffusion coefficient and r the radial coordinate. The probability density function given by equation (3) is the solution to the transient diffusion equation:

$$\frac{\partial \rho}{\partial t} = \frac{D}{r}\frac{\partial}{\partial r}(r\frac{\partial \rho}{\partial r}) \tag{5}$$

With boundary conditions at time $t = 0$:

$$2\pi \int_0^\infty \rho(0,0) r dr = 1 \tag{6}$$

$$\rho(r,0) = 0 \tag{7}$$

And for times $t > 0$ the following conditions apply:

$$\frac{\partial \rho(\infty, t)}{\partial r} = 0 \tag{8}$$

$$\frac{\partial \rho(0, t)}{\partial r} = 0 \tag{9}$$

The number of particles between r and $r + \delta r$ can be estimated theoretically by:

$$\frac{1}{4\pi D t} e^{-r^2/4Dt} \cdot 2\pi r \delta r \tag{10}$$

Which can then be compared with the number of particles between r and $r+\delta r$ observed in simulations. A comparison between theoretical prediction and simulation is given in figure 2. The figure shows that, although there are oscillations, the number of particles within a given region predicted theoretically does not deviate much from the number of particles within a given region observed in simulations. This, together with the fact that the mean squared displacement is proportional with time, implies that the motion of the particle of interest can be described reasonably well using the standard law of diffusion.