Exercise 1

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Diffusion equation

The diffusion equation for the one-dimensional Brownian motion is written as

$$\frac{\partial f(x,t)}{\partial t} = D\frac{\partial^2 f(x,t)}{\partial x^2}\,, \tag{1}$$

where $f(x,t)$ is a density function that describes the time-evolution of a Brownian particle (e.g. a pollen grain suspended in a liquid) and D is the diffusion constant.

Pen-and-paper exercise Solve the diffusion equation for the initial condition

$$f(x,0) = \delta(x-x_0)\,, \tag{2}$$

where δ is the Dirac delta function, and

- Infinity boundary conditions:

$$\lim_{x\to\pm\infty} f(x,t) = 0 \tag{3}$$

- Reflecting boundary conditions

$$\begin{aligned} f\left(-\frac{L}{2},t\right) &= f\left(+\frac{L}{2},t\right) \\ -D\frac{\partial f}{\partial x}\bigg|_{x=\pm\frac{L}{2}} &= 0 \end{aligned} \tag{4}$$

  where L is the size of a one-dimensional box.

Computational exercise Using your favorite programming language:

- Write a program that simulates the one-dimensional Brownian motion.
  Hint: Trajectories that simulate the Brownian motion can be generated using the Euler-Maruyama scheme:

$$x_{k+1} = x_k + \sqrt{2D\,\Delta t}\,\eta\,, \tag{5}$$

  where x_k denotes the position of the particle at time $t = k\cdot\Delta t$, x_{k+1} denotes the position of the particle at time $t+\Delta t$, Δt is a small timestep and η is a random number drawn from a standard normal distribution $\mathcal{N}(0,1)$.

- Generate a large number of trajectories, and estimate the distribution $f(x,t)$ at different timesteps.
  Hint: to estimate the distribution, build the histogram of the trajectories.

- Compare the results from your numerical experiment with the analytical solution of eq. 1.

- Repeat the numerical experiment for both the given boundary conditions.

- Stress your program by changing the input parameters, and test the conditions under which the analytical solution accurately reproduces the numerical results.