Physics through Computational Thinking

Random walks

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Outline

In this module we

1. see how the diffusion equation may be obtained from the random walk problem.

The diffusion equation

When we take the continuum limit (in both space and time) the random walk problem yields the diffusion equation. Let us work this out explicitly in one dimension and extend it to the general three dimensional problem thereafter.

Let $P(x, t)$ be the probability density of finding the particle at position x at time t. In the time step Δt the particle undergoes a change

$$x(t + \Delta t) = x(t) + l(t), \tag{1}$$

where $l(t)$ is a random variable drawn from a distribution $W(z)$. We will assume that $l(t)$ has mean zero and variance a^2. To find the probability distribution $P(x, t + \Delta t)$, we will need to integrate over all space in the previous step weighted with an appropriate probability for the jump as follows:

$$P(x, t + \Delta t) = \int_{-\infty}^{\infty} P(x - z, t)\, W(z)\, dz. \tag{2}$$

Doing a Taylor expansion in z and keeping terms up to second order, we have

$$\begin{aligned} P(x, t + \Delta t) &\approx \int_{-\infty}^{\infty} \left(P(x, t) - z \frac{\partial P}{\partial x} + \frac{z^2}{2} \frac{\partial^2 P}{\partial x^2} \right) W(z)\, dz \\ &= P(x, t) + \frac{1}{2} a^2 \frac{\partial^2 P}{\partial x^2}, \end{aligned} \tag{3}$$

where we have used the fact that $W(z)$ is normalized, has mean zero and variance a^2. Taking Δt to be small we have

$$P(x, t + \Delta t) - P(x, t) \approx \frac{\partial P}{\partial t} \Delta t \tag{4}$$

using which we get the diffusion equation

$$\frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial x^2}, \tag{5}$$

where $D = \frac{a^2}{2 \Delta t}$ is the diffusion constant. In three dimensions the diffusion equation generalizes to

$$\frac{\partial P}{\partial t} = D \nabla^2 P. \tag{6}$$

The general solution of this problem too turns out to have a Gaussian form wherein once again the variance of the displacement goes linearly with time, just like in the case of the discrete random walk.

$$P(x, t) = \frac{1}{\sqrt{4 \pi D t}} e^{-x^2/4 D t} \tag{7}$$

Such a time dependence goes by the name of diffusive motion, and is seen in a variety of contexts whenever stochastic forces are in play.

Homework

- Verify that the above Gaussian function does solve the original diffusion equation, by directly plugging into the partial differential equation. The exact solution may be derived by a technique called the Green function method, about which you may learn in a course on Mathematical Methods.
- For $P(x, t)$ to be a legitimate probability density, it must be normalized. Check if this is true, and if indeed it remains true at all times.
- Plot the function $P(x, t)$. What happens as you decrease t? What about in the limit $t \to 0$? Interpret this physically.

Remarkable Generality

The linear dependence of the variance of the displacement with time turns out to be very general, and holds regardless of whether time, space or both are discrete or continuous. It also works for a range of distributions of the walker at each step. Again, it is independent of dimensionality effects. The reason for this remarkable universality is rooted in a very deep theorem called the central limit theorem. Roughly it says that the sum of a large number of independent random variables has a Gaussian distribution, independent of the precise details of the distributions of all the constituent random variables in question.