Physics through Computational Thinking

Random walks

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Outline

In this module

1. revisit how the diffusion equation may be obtained from the random walk problem. Check the analytical results.

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.

Exercise

- 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.
- Find the mean $<x>$ and plot it as a function of time. What about the variance $\sigma^2 = <x^2> - <x>^2$. How does this quantity vary with time? Plot it.

Solution

```
Integrate[1/Sqrt[4 π Ds t] Exp[-x^2/(4 Ds t)], {x, -∞, ∞}];

Ds = 1;

Manipulate[Plot[{1/Sqrt[4 π Ds t] Exp[-x^2/(4 Ds t)]}, {x, -5, 5}, PlotRange → {0, 1}], {t, 0.001, 1}];

Integrate[x/Sqrt[4 π Ds t] Exp[-x^2/(4 Ds t)], {x, -∞, ∞}];

Integrate[x^2/Sqrt[4 π Ds t] Exp[-x^2/(4 Ds t)], {x, -∞, ∞}];
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