question 2 views

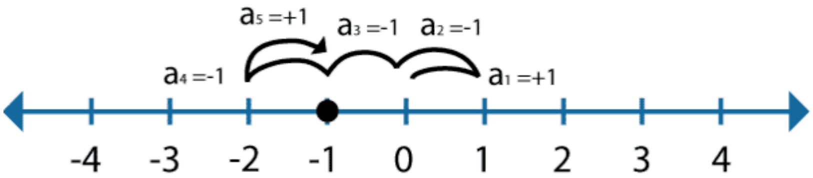
Daily Challenge 24.2

(**Due: parts (a) - (d) due Tuesday 3/12 at 12:00 noon Eastern; parts (e) - (i) due Wednesday 3/13 at 12:00 noon Eastern**)

Today I've designed a mini-project on random walks and diffusion to get us started with probability theory. This is longer than a usual DC so I've given you two days.

(1) Problem: Random walks and the diffusion equation.

Consider a particle on a one-dimensional line which begins at the origin at time $t=0$. At each time step δt, the particle takes one step of length δx, moving either to the left or to the right with equal probabilities. In the simple case $\delta x = 1$, the picture might look like the following,



where $a_0 = 0$ is the particle's position at time $t=0$, $a_1 = 1$ is its position at time 1, and so on. In this problem, we will leave the time step δt and the spatial step δx arbitrary, rather than setting $\delta t = 1 = \delta x$.

Assume that, at time $t = 0$, we release a large number of random walkers at the origin $x = 0$. Let $P(x,t)$ be the **density** of random walkers near a position x at time $t > 0$. We ignore $t = 0$ since the density at the origin is infinite.

Equivalently, you can think of $P(x,t)$ as the *probability density* for a single random walker. But the interpretation as physical density for a large number of walkers is more relevant if we think of this process as diffusion -- perhaps the real line is a column of water, and we release a large number of ink molecules are the origin at time $t = 0$, which then diffuse outward.

(**Part a**) Because each random-walker moves to the left or to the right with equal probabilities, I claim that the density function satisfies

$$P(x, t+\delta t) = \frac{1}{2}P(x-\delta x, t) + \frac{1}{2}P(x+\delta x, t).$$

Briefly explain why this is true in a sentence or two. [Hint: particles can't stand still under our assumptions, so the only way a particle can reach position x is by stepping to the right from $x - \delta x$ or stepping to the left from $x + \delta x$.]

(**Part b**) Define a number

$$D = \frac{(\delta x)^2}{2\delta t},$$

called the *diffusion constant*.

Begin with the equation of part (a) and do some algebra (begin by subtracting $P(x,t)$ from both sides, multiply both sides by appropriate constants, etc.) to show that

$$\frac{P(x,t+\delta t) - P(x,t)}{\delta t} = D\frac{P(x-\delta x,t) + P(x+\delta x,t) - 2P(x,t)}{(\delta x)^2}.$$

(**Part c**) We will now take the double limit $\delta t \to 0, \delta x \to 0$. The left side of your equation is clearly

$$\lim_{\delta t \to 0} \frac{P(x,t+\delta t) - P(x,t)}{\delta t} = \frac{dP(x,t)}{dt}.$$

Note that, on this side of the equation, we are taking a derivative with respect to t and holding x constant.

Next let's handle the right side. Prove that

$$\lim_{\delta x \to 0} \frac{P(x-\delta x,t) + P(x+\delta x,t) - 2P(x,t)}{(\delta x)^2} = \frac{d^2P(x,t)}{dx^2},$$

where this time we take derivatives with respect to x but hold t constant. [Hint: follow the steps in the top-voted answer by Brian Scott here.]

(**Part d**) You have proven that the density equation satisfies the condition

$$\frac{dP(x,t)}{dt} = D\frac{d^2P(x,t)}{dx^2},$$

which is called the *diffusion equation* or *Fick's second law of diffusion*. You will hear more about this in Week 10 of 3.091.

Show that the solution is

$$P(x,t) = \frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right)$$

by explicitly taking the appropriate derivatives of this equation and showing that they obey the condition. This is the Gaussian distribution we met last time!

Be careful about what is a variable and what is a constant! In a $\frac{d}{dt}$ derivative, x is constant and t is a variable; in a $\frac{d}{dx}$ derivative, t is constant and x is a variable.

(**Part e**) Clearly the average position of the particles at any time will be zero, since particles are equally likely to move right as to move left. To measure how much they have spread out, therefore, we will compute the average *squared distance* from the origin.

Using ~~the definition of expectation value~~ (technically LOTUS, but we will discuss later), compute the average squared displacement at time t:

$$\begin{aligned} E[x^2] &= \int_{-\infty}^{\infty} x^2 P(x,t)\,dx \\ &= \int_{-\infty}^{\infty} x^2 \frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right)dx. \end{aligned}$$

You should find $E[x^2] = 2Dt$. Therefore, the square root of the average squared distance is

$$\sqrt{E[x^2]} = \sqrt{2Dt},$$

which is the famous square-root-of-time behavior you noticed.

Hint: by symmetry, we can just double the integral from zero to infinity:

$$E[x^2] = \frac{1}{\sqrt{4\pi Dt}}\cdot 2\cdot\int_0^{\infty} x\exp\left(-\frac{x^2}{4Dt}\right)\,(x\,dx)\,,$$

where notice that I have split the x^2 into one factor of x in front and a second factor $x\,dx$ with the dx, which will help us with the u-sub in a moment.

Make the change of variables $\frac{x^2}{4Dt} = u$ so that $\frac{x\,dx}{2Dt} = du$. Likewise, $x = \sqrt{4Dtu}$. Then the integral becomes

$$E[x^2] = \frac{2}{\sqrt{4\pi Dt}}\cdot\int_0^{\infty}\sqrt{4Dtu}\,\exp(-u)\,\,(2Dt\,du)\,,$$

where the first factor comes from $x = \sqrt{4Dtu}$ and the last factor comes from $x\,dx = 2Dt\,du$. The result is

$$E[x^2] = \frac{2}{\sqrt{4\pi Dt}}\cdot\sqrt{4Dt}\cdot(2Dt)\cdot\int_0^{\infty}\sqrt{u}\,\exp(-u)\,du,$$

But now the integral is exactly the definition of the gamma function we saw before,

$$\Gamma(z) = \int_0^{\infty} u^{z-1}e^{-u}\,du,$$

with the value $z = \frac{3}{2}$. Simplifying constants, we have

$$E[x^2] = \frac{1}{\sqrt{\pi}}\cdot(4Dt)\cdot\Gamma\left(\frac{3}{2}\right)$$

Now we must resort to looking up a table of values of the gamma function, which tells us $\Gamma\left(\frac{3}{2}\right) = \frac{1}{2}\sqrt{\pi}$. So we conclude

$$E[x^2] = 2Dt,$$

which is what we wanted to show.

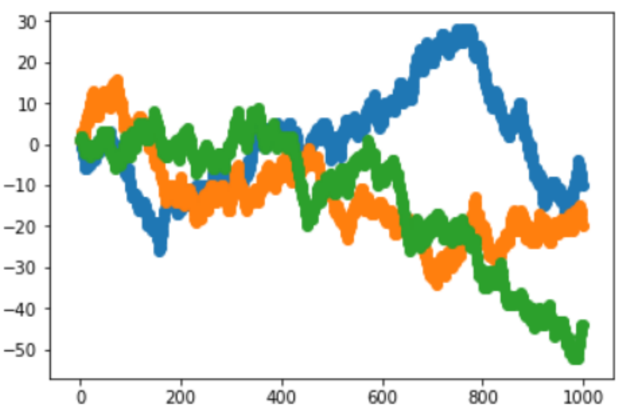
(**Part f**) Now open Python. For the simulations, we can set $\delta x = 1$ and $\delta t = 1$.

Write a function that does one run of a random walk, but make sure the function returns a **list** of the positions at each time, not just the final time.

```
def random_walk(n_steps=1000):
    step_list = 0

    ## Go through a loop `n_steps` times, and on each time step, pick either +1 or -1 with equal
    ## probabilities. Add this to your most recent step, then append the result to the running list.

    return step_list
```

(**Part g**) To practice plotting with matplotlib, run 3-5 random walks and plot the results. You can use the syntax screenshotted below:

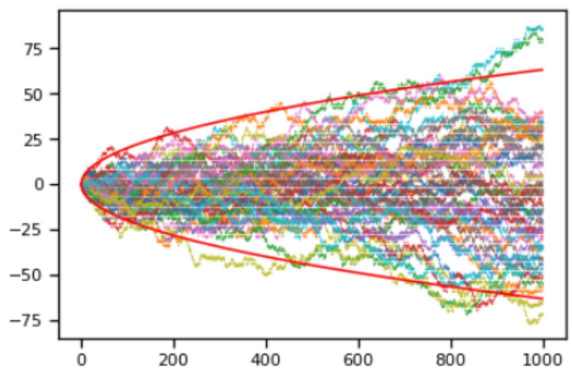
```
In [7]: import matplotlib.pyplot as plt
        %matplotlib inline

        times = range(1000)

        walk1 = random_walk()
        walk2 = random_walk()
        walk3 = random_walk()

        plt.scatter(times, walk1)
        plt.scatter(times, walk2)
        plt.scatter(times, walk3)

Out[7]: <matplotlib.collections.PathCollection at 0x2c63e331cf8>
```



(**Part h**) Now make a plot that shows both a collection of random walks, along with the "envelopes" of $\sqrt{E[x^2]} = \pm 2\sqrt{t}$ using the root-mean-squared displacement. You might look at my code below for some tips on formatting the plots.

In [47]:
```
import matplotlib.pyplot as plt, seaborn as sns
sns.set_context("notebook")
%matplotlib inline

n_steps = 1000
n_walks = 50
walk_list = []

for walk in range(n_walks):
    this_walk = random_walk(n_steps)
    walk_list.append(random_walk(n_steps))
    plt.scatter(times, this_walk , s=0.1)

upper = 2*np.sqrt(range(n_steps))
lower = -2*np.sqrt(range(n_steps))

plt.plot(times, upper, 'r-')
plt.plot(times, lower, 'r-')
```

Out[47]:
```
[<matplotlib.lines.Line2D at 0x2c642ae9668>]
```



(**Part i**) Explain in words (but no need to implement in code) how you might modify your script in the following ways.

- How could you change the diffusion constant D?
- How could you add a small "drift" term, so that the random walk is not unbiased but prefers one direction?
- How would you generalize to an n-dimensional random walk, i.e. where the walker's position is a set of integers $(k_1, k_2, \cdots, k_n)$ and on each turn he randomly chooses one direction to increment by ± 1?

daily_challenge

Updated 1 month ago by Christian Ferko

the students' answer, *where students collectively construct a single answer*

:GWvertiPeepoSadMan:

Updated 1 month ago by Logan Pachulski

the instructors' answer, *where instructors collectively construct a single answer*

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