1. **Simulating the 1D Random Walk** In lecture and in the first problem set, we have extensively considered a random walker that moves in one dimension with probability p for taking a step to the right and probability $q = 1 - p$ for taking a step to the left. We called the total displacement X and computed the average displacement $\langle X \rangle_T = (p - q)T$ and variance $\langle \delta X^2 \rangle_T = 4pqT$ after time T. In this problem we will simulate the behavior of the random walker.

   You may complete these exercises by writing code from scratch or you may follow along with the Mathematica notebook called ps2Mathematica.nb, which provides examples that should be helpful.

   (i) Setting $p = q = 1/2$, simulate 10,000 random walkers to make a histogram estimating the probability distribution $P_T(X)$ for $T = 100$. More explicitly, you will plot how many of the random walkers ended up at $X = -100, X = -99, \ldots, X = 100$ (out of 10,000 walkers it's highly unlikely that any of them will land much outside the range from -45 to 45). Why is the final position X an even number for every single random walkers? On top of your histogram, plot the exact values for $P_T(X)$. Evidently sampling 10,000 random walkers gives a pretty good sense of the shape of the distribution. Since you've already written the code, you might choose to repeat with only 100 random walkers to see that 100 is really not enough walkers to get a good approximation for $P_T(X)$.

   (ii) Still using $p = q = 1/2$, sample random walkers to estimate the average drift $\langle X \rangle_T$ and the mean squared displacement $\langle \delta X^2 \rangle_T$ for T ranging between 0 and 100. Plot your estimates as functions of T. Include error bars that indicate the uncertainty that arises from the fact that your estimates came from averaging over a finite number of random walkers. (The Mathematica notebook has an example of computing and including the error bars. This is a great thing to get used to doing in all of your work!). If you could use an infinite number of random walkers, you should get our exact results: $\langle X \rangle_T = (p - q)T$ and $\langle \delta X^2 \rangle_T = 4pqT$. Include these exact results on your plot as a comparison.

   (iii) Redo parts (i) and (ii) with $p = 0.65$ and $q = 0.35$.

   (iv) With $p = 0.65$ and $q = 0.35$, sample random walkers to plot histograms of $P_T(X)$ for $T = 10, 25, 50,$ and 100. As before, you should be able to use 10,000 walkers per choice of T. Plot all of these histograms on the same graph.

   (v) Let $x = X/T$ be the rate per unit time of the transport. For each random walker, you can compute x. The average value of these x's should converge to $\langle x \rangle$. In terms of p and q, what should be the value of $\langle x \rangle$? Does it depend on T?

   (vi) Again with $p = 0.65$ and $q = 0.35$, plot histograms of $P_T(x)$ (lower case x now!) for $T = 10, 25, 50,$ and 100. Plot all these histograms on the same graph. Discuss why $P_T(X)$ gets broader as T increases but $P_T(x)$ gets narrower.

2. **Asymmetric random walker with a twist!** In lecture I introduced a variation on the asymmetric random walker. In this variation, the random walker can either go right with probability p, left with probability q, or stay in the same position with probability r. Because the walker must choose one of these three choices, $p + q + r = 1$.

   (i) Setting $p = 0.3, q = 0.2$ and $r = 0.5$, simulate this new random walk for $T = 100$ steps. Is it still the case that each random walker yields an even value of X?

   (ii) Plot $\langle X \rangle_T$ and $\langle \delta X^2 \rangle_T$ as a function of T as in (ii) of Problem 1. Does $\langle X \rangle_T$ still increase in proportion to T? Does it still equal $(p - q)T$ as in Problem 1? Does the mean squared deviation still increase in proportion to T? Does it still equal $\langle \Delta X^2 \rangle = 4pqT$?

(iii) Rather than simulate this model, we could have computed the mean and mean squared deviation analytically. To do so, first compute the moment generating function $Z_T(\beta) = \left\langle e^{-\beta X} \right\rangle_T$.

(iv) By differentiating the cumulant generating function $\ln Z_T(\beta)$ with respect to β and evaluating at $\beta = 0$, determine $\langle X \rangle_T$ and $\left\langle \delta X^2 \right\rangle$. Check your answers against your simulation results.

(v) The point of considering this random walker with a twist is to see that some phenomena depend on the details of the microscopic model we construct while other details are not sensitive to the microscopic model. Imagine I now introduce a random walker with one more twist. In addition to p, q, and r, this final model has a probability of jumping two steps to the right or two steps to the left. Make predictions about how those big jumps will impact the random walker's mean squared displacement. Will $\left\langle \delta X^2 \right\rangle = \text{Constant} \times T$? If so, how will the constant compare to the constants from the previous two models?

3. **Do you smell that?** I'm worried people are going to fall asleep in lecture, so I decide to open up a bottle of perfume at the front of the room the moment I see someone start to nod off. Let's try to figure out how long it will take before they smell it.

   (i) Let us first assume that the random walk models we've worked so laboriously to understand can help us explain the situation! In other words, we assume that each perfume molecules can be modeled as moving in some direction until it collides with an air molecule, at which point the perfume randomly gets kicked in a new directly. We have seen that the spread of the random walkers (in this case perfume molecules) goes like $\left\langle \delta \boldsymbol{R}^2 \right\rangle_T = 2dDT$, where d is the dimensionality and D is the perfume's diffusion constant. Since we live in a three dimensional world, $\boldsymbol{R}^2 = X^2 + Y^2 + Z^2$ and $d = 3$. If perfume has a diffusion constant in air of 10^{-6} m^{2}s^{-1}, estimate the time for the perfume to reach the dozing student 5 meters away.

   (ii) Is your answer to (i) reasonable? What else could be going on?

   (iii) While we're crunching numbers, let's think about the *self-diffusion* of water, that is to say one molecule diffuses in a background of other water molecules (as opposed to the perfume in a background of air). The self-diffusion constant for a water molecule in liquid water is about 10^{-5}cm^2/sec. Assuming the liquid is at equilibrium and not stirred, what are the typical times for a water molecule to move one molecular diameter (about 0.3 nm)? What about across the surface of a protein (about 1 nm)? Finally, a macroscopic distance (about 1 cm)?