Stochastic Simulations of Brownian Motion

Introduction

The observation that, when suspended in water, small pollen grains are found to be in a very animated and irregular state of motion, was first systematically investigated by Robert Brown in 1827, and the observed phenomenon took the name Brownian Motion because of his fundamental pioneering work. He showed that the motion is present in any suspension of fine particles, but the riddle of Brownian motion was not solved until 1905, when Einstein published [1] an explanation of the effect on the basis of intrinsic thermal fluctuations resulting from random collisions of the particle with the molecules of the liquid.

Observation of Brownian Motion

You will first observe Brownian motion through a microscope. The sample is a suspension of 0.5 μm diameter latex spheres in a glycerol/water mixture, enclosed between a microscope slide and cover slips, sealed with clear epoxy glue. The particles are too small to resolve, but their diffraction circles are visible. Focus on one *moving* particle (some are stuck to the glass surfaces), and follow it for a little while. Sketch a schematic drawing of your observation in your notebook.

Simulation of Brownian Motion

Brownian motion can be simulated stochastically due to its random character. As an illustration of these methods, you will perform a simple one- and two-dimensional stochastic model simulation, called the *random walk*, which is closely related to Brownian motion. These simulations can easily be expanded to describe Brownian motion completely (see below). The formulation of the random walk problem may seem rather abstract and to bear little relation to physical problems, but this is not so. A number of phenomena of interest, such as molecular diffusion, or the average dimension of a long polymer molecule, can be treated as random walk problems in three dimensions.

One-Dimensional Random Walk

An example for a one-dimensional random walk is someone (you could imagine an intoxicated person if you like) walking along a sidewalk, unable to decide at each step whether to go forward or backwards. The direction of each step is random. If the chance of going forward or backwards is equal, you can simulate the "decision process" with a coin flip.

Try one such simulation as an illustration:
1. Assign forward and backward steps of the person to heads and tails
1. Flip a coin
1. Have the person step forward or backwards. Keep track of the movements of the person on graph paper until you run out of room on your sheet.
1. Go back to 2.

This generates a single one-dimensional trajectory of the position of the person on the sidewalk A second simulation run would of course generate a different trajectory, so the value of a trajectory seems very limited. However, a large collection of those trajectories will allow you to predict average quantities for an ensemble of hundreds of drunks on a sidewalk, for example how far they will have moved away on average after a certain time.

You probably do not want to generate hundreds of one-dimensional random walk trajectories by flipping a coin for every step and every drunk on the sidewalk. It's much easier to have a computer do the busy work. A common program capable of this is Excel. Fig. 1 shows a possible spreadsheet that flips a coin and keeps track of the drunk's position. Excel flips coins with the function "RAND()" which delivers a random number between 0 and 1. "ROUNDUP(RAND()*2 - 1,0)" transforms this random number into a "coin flip" with 1 and –1 as possible outcomes. Adding the new step to the old position (for example "C3 = C2 + B3") keeps track of the persons progress on the sidewalk. Type in the first row of equations and use "fill down" to generate a

sample of N steps. Plot the position as a function of time. Calculate a new trajectory by pressing the Apple key and =.

	A	B	C
1	Index	coin	position
2			0
3	=ROW()-3	=ROUNDUP(RAND()*2 - 1,0)	=C2+B3
4	=ROW()-3	=ROUNDUP(RAND()*2 - 1,0)	=C3+B4
5	=ROW()-3	=ROUNDUP(RAND()*2 - 1,0)	=C4+B5

Figure 1: Example of an Excel spreadsheet for the simulation of a one-dimensional random walk

Ensemble Averages

To calculate averages for an ensemble of drunks (molecules, particles…) sum up the variable of choice for every time step. First, you need to keep track of your number of runs: add a new line between line 1 and line 2, and enter a "1" into the field in line 2 of your column of interest (here: C2). Summing the position to generate the average will now also count the number of runs calculated. You can generate the sums by copying the values between C2 and C1000 (here: position from t=0 to t=998) and adding them to the corresponding values in column D (which will be the sum of the position at a particular time step for all runs). To do this, select C2 to C1000, choose Edit>copy, select D2 to D1000, choose Edit>paste special>(select "values" and "add"). Repeat this operation with the keyboard shortcut "Apple (Command) Y" a number of times.

This will add up the ones, giving you the number of runs N as well as the positions of all runs. Generate the average by creating a new column with the average values $\langle x \rangle_t$ (here: column E. Enter "=D3/D$2" into field E3, select from E3 to the end of your trajectory and "fill down". The $ sign in D2 keeps Excel from changing the index while you copy down)

After a number of runs you can plot the average vs. time. Create plots for the following averages:

    a. $\langle x \rangle_t$
    b. $\langle x^2 \rangle_t$

For the latter average you'll have to create a new column with the square of each x_t and modify your procedure to select this column instead (or as well) and add it to a new column with the sum of the squares.

From your plots, can you predict the relationship between $\langle x \rangle_t$ (or $\langle x^2 \rangle_t$) and the time step t? Diffusion obeys Fick's laws which yield the result:

$$\langle x^2 \rangle_t = 2Dt \tag{1}$$

Compare this result to your calculation. Approximately how far does a typical molecule in a liquid (with a diffusion coefficient of about 10^{-5} cm^2/s) diffuse in one second?

Two-Dimensional Random Walk

The one-dimensional random walk is easily extended into two dimensions. Instead of a drunk on a sidewalk, imagine a blindfolded, disoriented person wandering aimlessly across a field. To simulate, roll dice to pick a direction and use the isometric construction paper provided (triangular pattern) to keep track of the progress of the lost person (start at the center dot).

Figure 2 shows an example of an Excel spreadsheet calculating a single trajectory for such a disoriented person. He or she will always take steps of equal length, but the direction of the steps is random. In general, the person could go east, south, west, or north, or anywhere in between. This

random choice is best simulated with a random angle between 0 and 360 degrees: θ = RAND()*360. In a Cartesian coordinate system the new position (x_t, y_t) is then given by:

$$x_t = x_{t-1} + \cos\theta \qquad\qquad (2)$$

$$y_t = y_{t-1} + \sin\theta \qquad\qquad (3)$$

In Excel-speak this translates to C3 = C2 + COS(B3) and D3 = D2 + SIN(B3). Again, type in the first line, select, and "fill down". Pick the origin for the starting position (see C2 and D2).

	A	B	C	D
	A	**B**	**C**	**D**
1	step	angle	x position	y position
2			0	0
3	=ROW()-3	=RAND()*360	=C2+COS(B3)	=D2+SIN(B3)
4	=ROW()-3	=RAND()*360	=C3+COS(B4)	=D3+SIN(B4)
5	=ROW()-3	=RAND()*360	=C4+COS(B5)	=D4+SIN(B5)

Figure 2: Example of an Excel spreadsheet for the simulation of a two-dimensional random walk

Plot a random trajectory of a length of your choice. (Plot y versus x for the entire set. Select a line graph. Make the field of view square and preset both axis limits to the same range with the origin in the center). How far away from the origin did the person get?

Hit "Apple=" to see a few new trajectories. Does the distance of the endpoint to the origin change? Calculate the mean square displacement $<r^2>$ from the origin as before for several runs. Plot $<r^2>_t$ versus t. Interpret this result in terms of molecular diffusion (in two dimensions). What is the diffusion coefficient?

Do the plots of the trajectories remind you of anything? Anything chemical? That's right, you can also use the same model as a simulation of a two-dimensional "random coil", a prediction of the structure of macromolecules, such as synthetic polymers or amino acid chains. Interpret $<r^2>$ in terms of the size of the macromolecule. How does the root mean square start-end distance $\sqrt{<r^2>}$ change with the number of monomers?

Further Exploration: Langevin Dynamics

These simulations can be extended into three dimensions in a straightforward manner. How does the three-dimensional root mean square displacement scale with t?

A more advanced extension of these simulations uses the Langevin equation, which models a particle that is exposed to random *pushes* instead of a particle that steps into random directions. Each random push is a random force $f(t)$ that accelerates the particle, while friction in the medium γ slows the particle down.

$$m\ddot{x} - \gamma\,\dot{x} = f(t) \qquad\qquad (4)$$

After a short induction period the simulation reaches a steady state, which resembles Brownian motion. Try it! Your simulation will have to do a two-step now: first calculate a new velocity from the old one with your new random force ($v_t = \gamma v_{t-1} + f(t)$), then calculate the new position with your velocity ($x_t = x_{t-1} + v_t$). An example is shown below:

	A	B	C	D
1		friction:	0.2	
2	index	coin	velocity	position
3			0	0
4	=ROW() - 3	=ROUNDUP(RAND()*2 - 1,0)	=C$1*C3+B4	=D3+C4
5	=ROW() - 3	=ROUNDUP(RAND()*2 - 1,0)	=C$1*C4+B5	=D4+C5
6	=ROW() - 3	=ROUNDUP(RAND()*2 - 1,0)	=C$1*C5+B6	=D5+C6

Figure 3: Example of an Excel spreadsheet for the simulation of Langevin dynamics

Report for this Experiment

Print out the plots for your one-dimensional random walk, the two-dimensional random coil, and the respective mean square displacements as a function of time (or length). Print out your results of the Langevin diffusion and note how the induction period depends on your choice of γ.

Reference

1. A. Einstein, *Ann. Phys.* (Leipzig) **21**, 549 (1905).

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