Physical Principles in Biology
Biology 3550
Spring 2024

Lecture 11:

Random Walks Continued

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Parameters for a One-dimensional Random Walk

- x_0: The starting position on the x-axis.
- n: The total number of steps.
- l: The step length (if all steps have the same length).
- p_+ and p_-: The probability of a step in the positive or negative direction.
- δ_i: The displacement along the x-axis in step i.
- x_i: The position after step i.
- x_n: The position at the end of the walk.

Some Different Kinds of Average

For N random walks of n steps each:

- The mean:

$$\langle x_n \rangle = \frac{1}{N} \sum_{j=1}^{N} x_{n,j}, \text{ for large } N$$

  Angle brackets, $\langle\ \rangle$, indicate average over a large sample.
  $x_{n,j}$ is the final position of the j^{th} walk.

- The mean-square average:

$$\langle x_n^2 \rangle = \frac{1}{N} \sum_{j=1}^{N} x_{n,j}^2$$

- The root-mean-square (RMS) average:

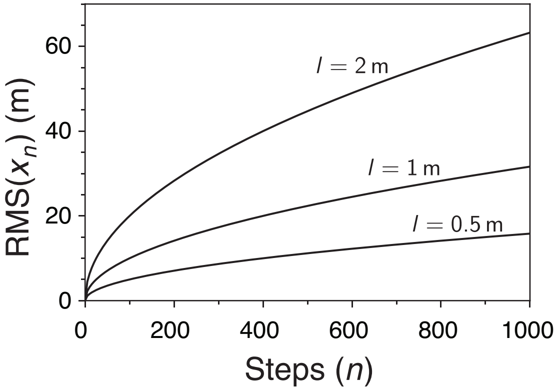
$$\mathrm{RMS}(x_n) = \sqrt{\langle x_n^2 \rangle} = \sqrt{\frac{1}{N} \sum_{j=1}^{N} x_{n,j}^2}$$

For the One-dimensional Random Walk

- The mean final position: $\langle x_n \rangle = nl(2p_+ - 1)$
- The mean-square final displacement: $\langle x_n^2 \rangle = nl^2$, if $p_+ = p_- = 0.5$
- The root-mean-square displacement: $\mathrm{RMS}(x_n) = \sqrt{\langle x_n^2 \rangle} = l\sqrt{n}$, if $p_+ = p_- = 0.5$
- How would $\langle x_n^2 \rangle$ and $\mathrm{RMS}(x_n)$ change if $p_+ > p_-$?

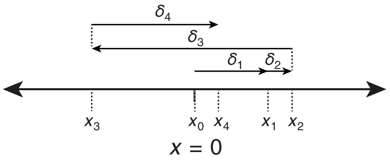
The Root-mean-square Displacement for a One-dimensional Random Walk

$$\mathrm{RMS}(x_n) = \sqrt{\langle x_n^2 \rangle} = \sqrt{n}\, l$$



- THE most important thing to remember about random walks!

A One-dimensional Random Walk with Variable Step Length



- Mean displacement:

$$\langle \delta_i \rangle = \frac{1}{n} \sum_{i=1}^{n} \delta_i$$

- Mean-squared displacement:

$$\langle \delta_i^2 \rangle = \frac{1}{n} \sum_{i=1}^{n} \delta_i^2$$

- If $\langle \delta_i \rangle = 0$:

$$\langle x_n^2 \rangle = n \langle \delta_i^2 \rangle$$

$$\mathrm{RMS}(x_n) = \sqrt{n}\sqrt{\langle \delta_i^2 \rangle}$$

$$= \sqrt{n}\,\mathrm{RMS}(\delta_i)$$

- For generality, redefine: $l = \mathrm{RMS}(\delta_i)$, so that $\mathrm{RMS}(x_n) = \sqrt{n}l$ applies to both fixed and variable step lengths.

Some Group Problems

from 2022 Quiz 2

A Random Walk

- A six-sided die, with numbers -3, -2, -1, 1, 2 and 3 on the sides.
- With each roll of the die, take the indicated number of strides in the positive or negative direction.
- The length of each stride is 0.5 m.
- The random walk is made up of 100 rolls of the die, representing 100 “steps” of variable length. ($n = 100$)

Problem #1

- What is the average number of strides per roll of the die?

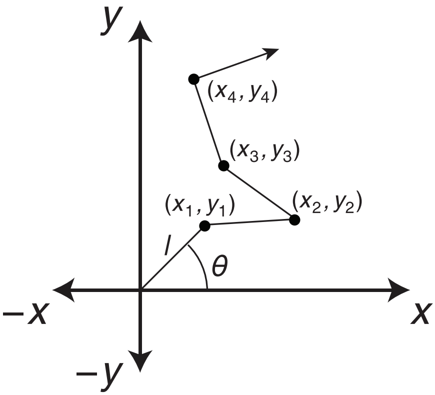
Problem #2

- δ_i is the displacement for each roll of the die.
- Calculate the average value of δ_i, $\langle \delta_i \rangle$.
- Calculate $\langle \delta_i^2 \rangle$
- Calculate $\mathrm{RMS}(\delta_i) = \sqrt{\langle \delta_i^2 \rangle}$

Problem #3

- If the random walk is repeated a large number of times, predict the RMS displacement between the beginning and end of the walks.

A Random Walk in Two Dimensions



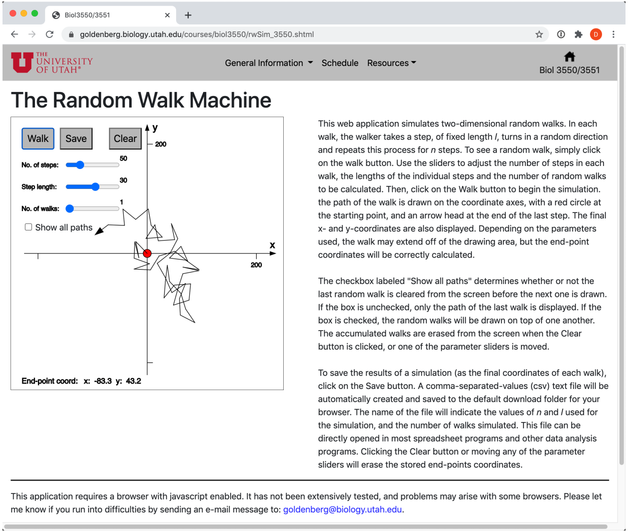
1. Start at (x, y) coordinates (0,0).
2. Choose a random direction, defined by the angle θ from the x-axis.
3. Move distance l in the chosen direction.
4. Repeat another $(n - 1)$ times.

- What can we say about the distribution of positions at the end of the random walk?

Two Approaches to Probability Problems

- Clever mathematical analysis.
  - Provides rigorous results, when applicable.
  - May be intractable for more complex problems.
- Computational simulation.
  - Different from just getting a bigger calculator to calculate bigger numbers!
  - Requires simulating the process a large number of times, using simulated random variables, collecting the results and analyzing them.
  - Can be applied to very complex processes that may not be amenable to analytical approach.
  - Can provide a more concrete or visual understanding of the process.
- Both approaches are important.

An Online Random Walk Simulator



Biol3550/3551

goldenberg.biology.utah.edu/courses/biol3550/rwSim_3550.shtml

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General Information Schedule Resources

Biol 3550/3551

The Random Walk Machine

Walk Save Clear

No. of steps: 50

Step length: 30

No. of walks: 1

Show all paths

y 200 x 200

End-point coord: x: -83.3 y: 43.2

This web application simulates two-dimensional random walks. In each walk, the walker takes a step, of fixed length *l*, turns in a random direction and repeats this process for *n* steps. To see a random walk, simply click on the walk button. Use the sliders to adjust the number of steps in each walk, the lengths of the individual steps and the number of random walks to be calculated. Then, click on the Walk button to begin the simulation. the path of the walk is drawn on the coordinate axes, with a red circle at the starting point, and an arrow head at the end of the last step. The final x- and y-coordinates are also displayed. Depending on the parameters used, the walk may extend off of the drawing area, but the end-point coordinates will be correctly calculated.

The checkbox labeled "Show all paths" determines whether or not the last random walk is cleared from the screen before the next one is drawn. If the box is unchecked, only the path of the last walk is displayed. If the box is checked, the random walks will be drawn on top of one another. The accumulated walks are erased from the screen when the Clear button is clicked, or one of the parameter sliders is moved.

To save the results of a simulation (as the final coordinates of each walk), click on the Save button. A comma-separated-values (csv) text file will be automatically created and saved to the default download folder for your browser. The name of the file will indicate the values of *n* and *l* used for the simulation, and the number of walks simulated. This file can be directly opened in most spreadsheet programs and other data analysis programs. Clicking the Clear button or moving any of the parameter sliders will erase the stored end-points coordinates.

This application requires a browser with javascript enabled. It has not been extensively tested, and problems may arise with some browsers. Please let me know if you run into difficulties by sending an e-mail message to: goldenberg@biology.utah.edu.

https://goldenberg.biology.utah.edu/courses/biol3550/rwSim_3550.shtml

Clicker-point Assignment

1. Carry out four sets of simulations, of $N = 100$ random walks each, using different values of n (no. of steps) and l (step length).
2. Each person will use four parameter pairs specified in the Canvas assignment.
3. From the simulator web page, download the four csv files containing the endpoint coordinates for the individual random walks and open them in a spreadsheet program, such as Excel.
4. For each random walk, calculate the distance, r, from the endpoint to the origin ($x = 0$, $y = 0$).

$$r = \sqrt{x^2 + y^2}$$

For Each Set of 100 Random Walks:

1. Calculate the averages of the x- and y-endpoint coordinates:

$$\langle x \rangle = \frac{\sum x}{N}, \quad \langle y \rangle = \frac{\sum y}{N}$$

2. Calculate the average of the end-to-end distances:

$$\langle r \rangle = \frac{\sum r}{N} = \frac{\sum \sqrt{x^2 + y^2}}{N}$$

3. Calculate the mean-square average of the x- and y-endpoint coordinates:

$$\langle x^2 \rangle = \frac{\sum x^2}{N}, \quad \langle y^2 \rangle = \frac{\sum y^2}{N}$$

For Each Set of Random Walks

4. Calculate the mean-square average of the end-to-end distance:

$$\langle r^2 \rangle = \frac{\sum r^2}{N} = \frac{\sum (x^2 + y^2)}{N}$$

5. Calculate the root-mean-square average of the x- and y-endpoint coordinates:

$$\mathrm{RMS}(x) = \sqrt{\langle x^2 \rangle}, \quad \mathrm{RMS}(y) = \sqrt{\langle y^2 \rangle}$$

6. Calculate the root-mean-square average of the end-to-end distance:

$$\mathrm{RMS}(r) = \sqrt{\langle r^2 \rangle}$$

Clicker-point Assignment

- For each value of n and l, report all of the averages in the Canvas assignment, using the provided template.
- Due by 11:59 PM, Sunday, 4 February.
- For help calculating these averages in Excel, see: https://www.techwalla.com/articles/how-to-get-the-rms-in-excel