PHSX815: Computational Methods in Physical Sciences
Project 1
Title: Simulation of Random Walk in 1D

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Introduction

In Science, we are often interested in a set of outcomes rather than a single event. Stochastic simulations allow us to generate and examine a series of simulations of a system in which the steps are governed by random choice. A simple algorithm for flipping of coin can be a useful tool to 'choose' if a step in a phenomenon will occur or not. Consider a drunkard trying to walk along the pavement in the middle of the night. In their drunk state of mind, they can only move sideways-either to the left or the right from their current position. Whether they take a step to the left or the right can be dictated by flipping a coin and checking if the outcome is 'Heads' or 'Tails'. The philosophy behind the seemingly simple thought experiment has a wide range of appli- cation in physics, chemistry as well as biology; to describe the diffusion of gas molecules, simulate bacterial motion and learn the pattern of genetic drift.

How the code works

Flipping of coin

The first section consists of importing the necessary modules for computation and plotting. We then begin by flipping the coins and understanding their output. To see why this is relevant in random walk, think of a gas molecule that has equal probabilities of moving either to the left of the right. To dictate whether the molecule moves to the left or the right by flipping a coin. This will obviously change every time that we run the code cell. To convert this to a 'heads' and 'tails' readout, we can assume that this is a totally fair coin. This means that the probability of getting "heads" to get P(H) is the same as flipping a "tails" P(T) such that P(H)+P(T)=1 . This means that for a fair coin, P(H)=P(T)=0.5 . To convert our coin flips above, we simply have to test if the flip is above or below 0.5 . If it is below, we'll say that the coin was flipped "heads", otherwise, it is "tails".

Testing if the coin-toss is fair

Now, in order to check if our coin-toss is fair, we toss it multiple times, say 1000 times. Let's flip a coin one thousand times and compute the probability of getting "heads".
The simulated probability is very close to our expected P(H)=0.5, but not exactly. This is the nature of stochastic simulations-it's based on repetitions. If we were to continue to flip a coin more number of times, our simulated P(H) would get closer and closer to 0.5 . This is why doing many repetitions of stochastic simulations is necessary to generate reliable statistics.

Plotting

In order to relate this to a gas molecule or a drunkard walking on a pavement, we start at position zero and flip a coin at each time step. If it is less than 0.5, we take a step left. Otherwise, we take a step to the right. At each time point, we keep track of our position and then plot our trajectory.
As our steps are based on the generation of random numbers, this trajectory will change every time the code is run. The power of stochastic simulation comes from doing them many times over. The next step would be to run the steps, say, one thousand times and plot all of the traces. Let's plot the mean at each time point as a blue line.

Interpretations and further scope

Let us take a look at the importance of repeated trials in stochastic simulations. The following plots are those of 10, 100, 1000 and 1000 trials respectively.

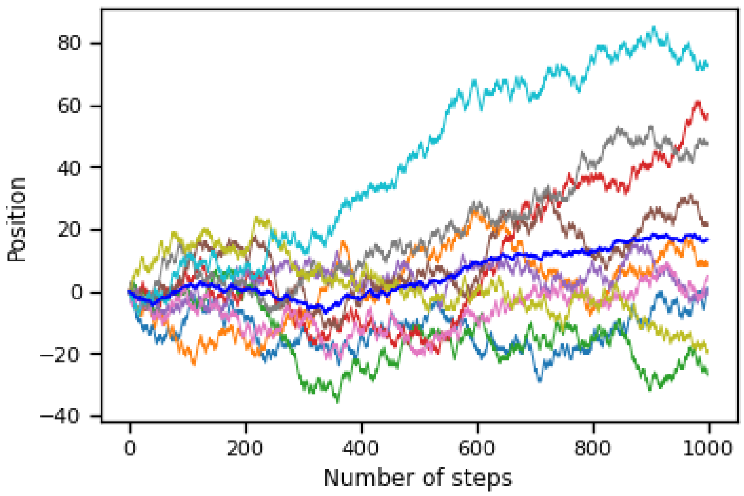

Figure 1: n=10

At n=10, we see that the mean computed at each step (the blue track) isn't exactly a straight line positioned at y=0, as we would expect for a typical random walk.

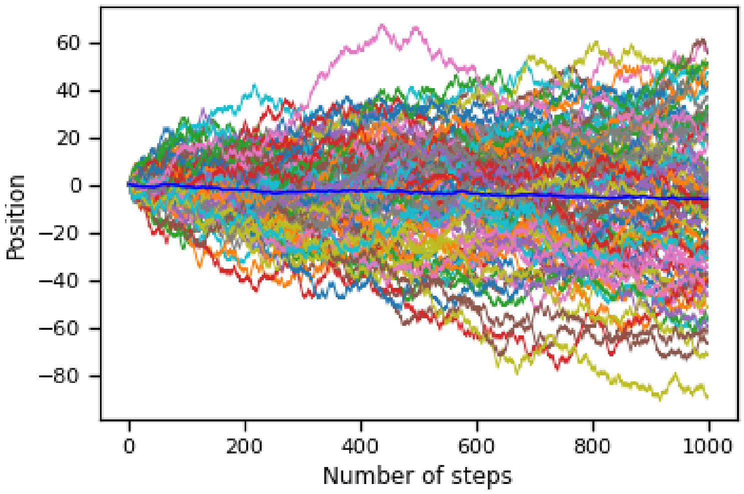

Figure 2: n=100

At n=100 we see that the data points or tracks get thicker as we move towards Position=0, from either top or bottom. The blue 'curve' which represents the mean computed at each point resembles a straight line better, at y=0.

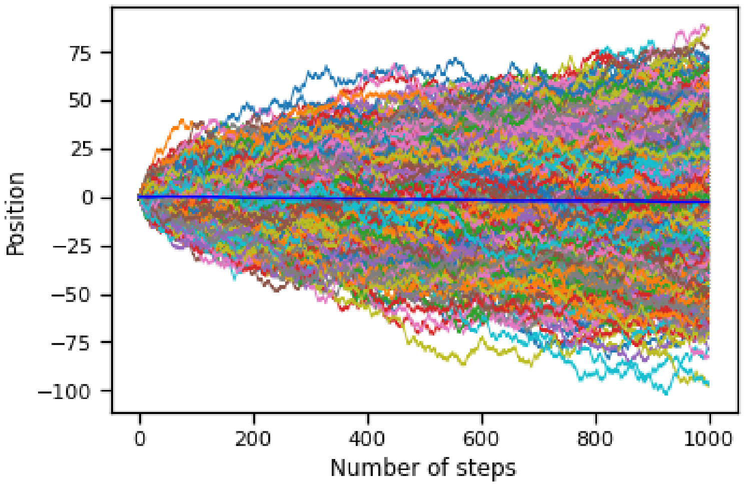

Figure 3: n=1000

The comparison of the position and the straightness of the blue curve representing the mean at each point makes it clear how important repetition of trials are.

Taking a look at the histogram of the probability distribution of the directions of the steps, at a given step provides an insight into the stochastic nature of the random walk. Here's a histogram for the distribution at Step=0.

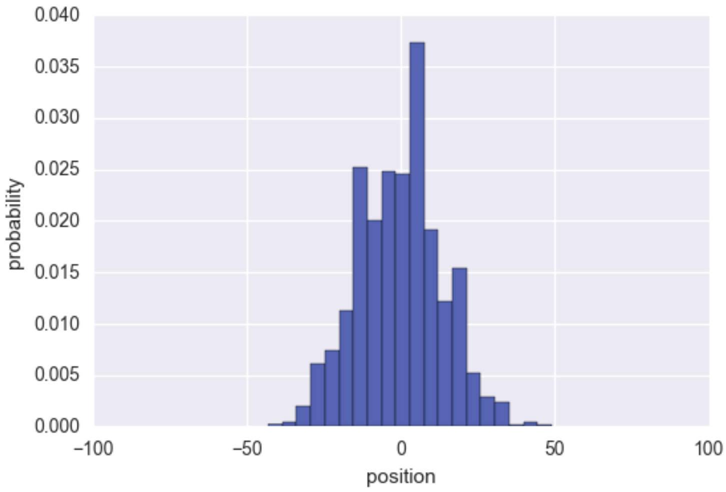

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Figure 4: Step=0

We see that the distribution is Guassian.