CS302: Modeling And Simulation
Lab 6 Report

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1 Radioactive decay

1.1 We have in the initial lectures modeled radioactive decay as a deterministic process. But radioactive decay is a non-deterministic process which can be simulated very naturally using the Monte-Carlo method. Suppose that the probability of any atom decaying over a time interval Δt is given by λ where $0 < \lambda < 1$. Then the history of a single atom can be simulated by choosing a sequence of random numbers x_k, k = 1,2,...m uniformly distributed on [0,1]. The atom survives until the the rst value of x_k for which $x_k < \lambda$. Use this approach to simulate an ensemble of atoms remaining after k intervals. Take $\lambda = 0.1$ and m = 50 and try values n = 10, 100, 1000 and 10000. How does the value of n (ensemble size) affect the smoothness of the resulting curve. Experiment with other values λ, n and m.

1.1.1 Varying the number of Initial atoms

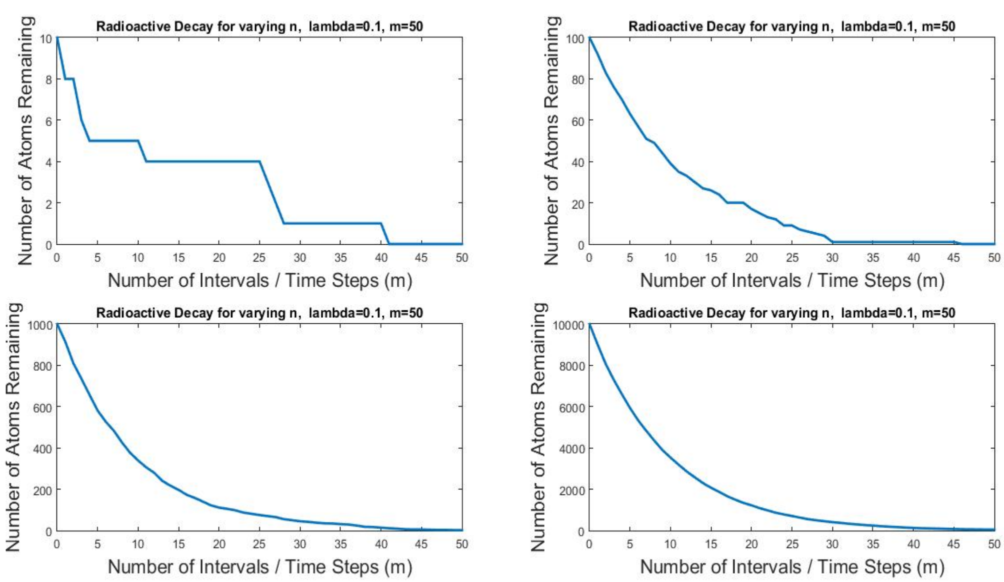

Figure 1: Radioactive Decay using probabilistic model for varying number of initial atoms

Observations:

- From the above figure, it is clear that as the number of atoms (n) increase, the smoothness of the curve increases.
- For small number of atoms, due to large time, the graph contains steps. This is because at some time steps, there are no atoms decayed while at some time steps there are significant atoms decayed.
- Due to randomness these steps cannot be removed unless the number of atoms increase.
- As number of atoms increase. The fraction of number of atoms decayed becomes approximately equal to decay factor. This makes the curve more smoother because approximately equal amount of atoms decayed in same time interval.
- On the whole, time remaining constant, the smoothness of the curve increases as the number of atoms increase.

1.1.2 Varying the decay rate λ

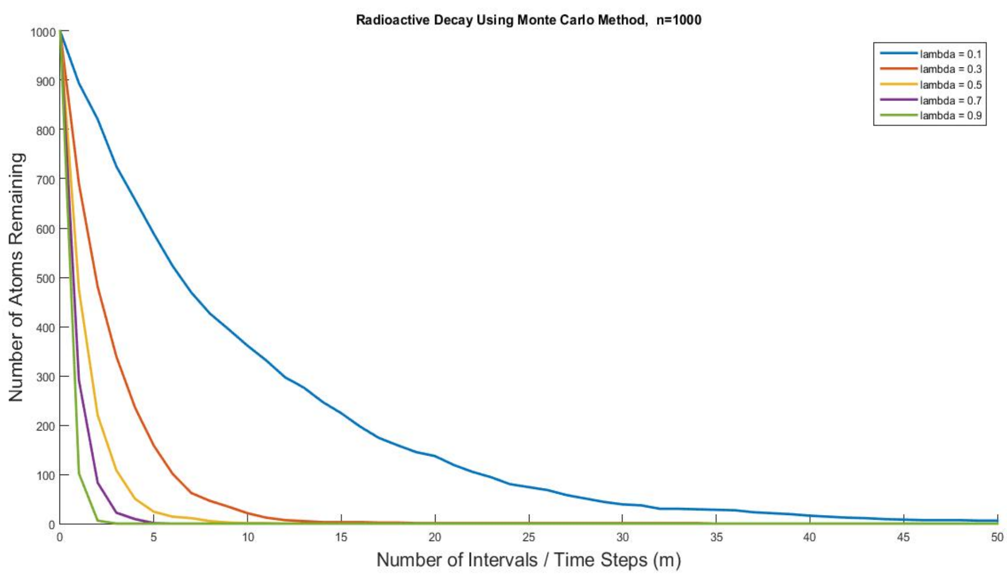

Figure 2: Radioactive Decay using probabilistic model for varying decay constant λ

Observations:

- Here the number of atoms initially present is same in all the cases and the time interval of simulation is also same.
- As the value of decay rate lambda increases, the steepness of the graph increases. The atoms decay quickly which is why the number of atoms not decayed reduces extremely fast.
- Intuitively also, as the decay rate increases, more atoms are decayed in the same time interval. Hence the observed behaviour is justified.
- Whatever may be the decay rate, eventually the system will reach the same state wherein all the atoms are decayed.

1.1.3 Varying the total time of simulation

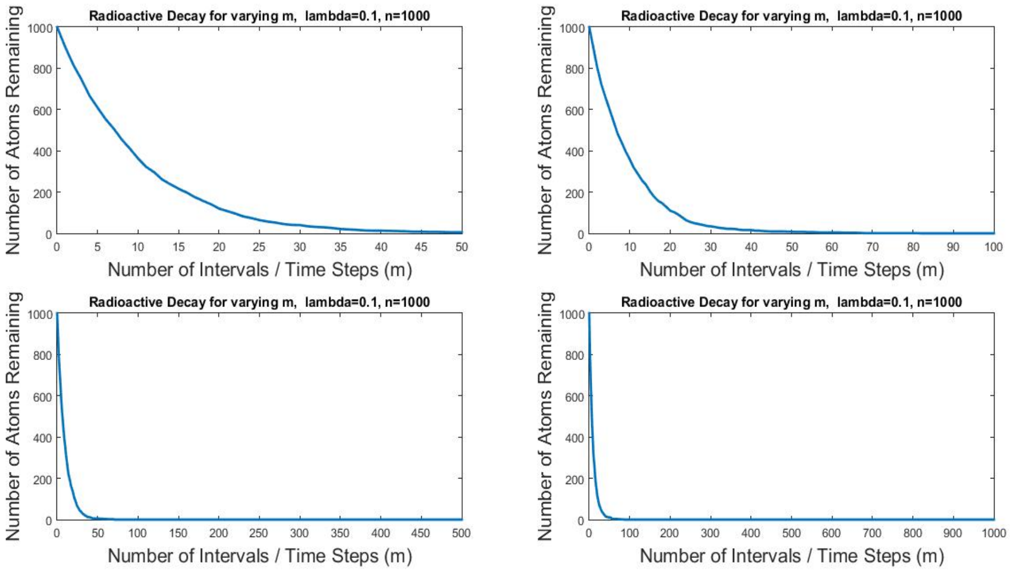

Figure 3: Radioactive Decay using probabilistic model for varying time

Observations:

- These graphs are pretty trivial. Here only the time of simulation changes which does not affect the actual decay behaviour since it depends on the decay rate and the initial number of atoms.

1.2 Compare your results with the continuous, deterministic model of radioactive decay.

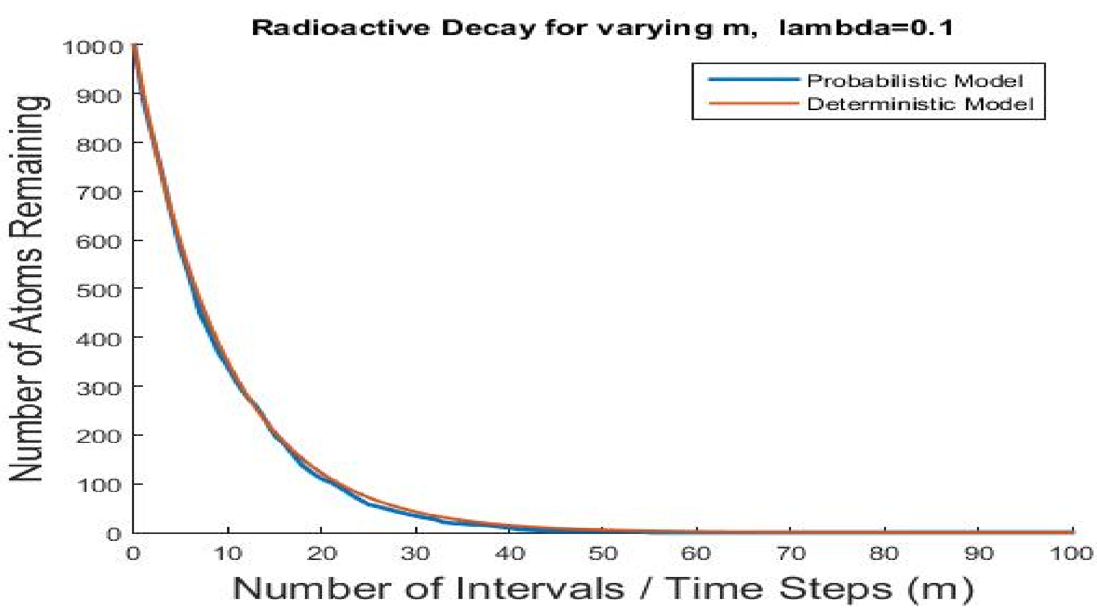

Figure 4: Graph of Radioactive Decay comparing the probabilistic model and deterministic model

Observations:

- When we compare the probabilistic model with the deterministic model. We see that the two graphs overlap to a large extent. This means both the models are able to capture the behaviour of the system.
- There are minor differences in the graphs. This is mainly because of the probabilistic model which exhibits inherent randomness.
- But still this randomness eventually is able to capture the deterministic behaviour.

1.2.1 Q. Which model do you think is closer to the way nature actually behaves and why?

- The probabilistic model is closer to the way the nature actually behaves. This is because the nature also has that inherent randomness. It is not deterministic.
- In this particular case, in nature, we cannot determine exactly which atoms will decay or how many atoms will decay. The rate of decay just gives the probability that a particular nucleus will decay by a particular amount in time interval Δt.
- Hence it cannot be determined precisely. There may be smaller aberrations but the general behaviour can be determined approximately. This is exactly what we have in the probabilistic model. Hence it is more closer to the nature.

2 1D Random walk

2.1 Symmetric random walk

In this first part we will simulate the symmetric random walk. Let the probability of a random walker going left or right be the same p = q = 1/2. The walk starts from the site 0 and proceeds by successive steps of unit length. For direction we adopt the convention that right is positive and left is negative. Write a program to implement the random walk of n steps, using a uniform random number generator to choose the direction of each step. Run your code to calculate the mean and mean square displacement(msd). What is the size of the ensemble beyond which you observe Einstein's relationship (Show in a single gure by taking ensemble of dierent sizes). What is the value of Diusion constant? Make a histogram of of the distribution 2 of p_n(m) obtained from your data, where p_n(m) is the probability of being at the m^{th} site after n steps.

The experiment is about simulating a discrete random walk with unit steps and experimentally determining the Expected Displacement and Expected Squared Displacement from the origin.

In this part, since random walk is symmetric, we expect the first quantity i.e. the mean displacement to tend to zero for a large number of observations because the probability of going to either side of the origin is equal.

To get an idea of **"how much has the random walker traversed"** i.e. the magnitude of the displacement of the random walker, we instead look at the mean squared displacement which is always non-negative. This is because even though negative motion is subtracted from the displacement of the random walker, it still contributes to the sum total of the movement of the random walker. Squaring is thus a simple way of getting rid of the negative terms.

It can be shown that theoretically, the Expected displacement is zero [makes sense if the random walk is symmetric] and that the Expected squared displacement is linear to the Number of steps taken in a random walk.

We verify these claims, by simulating a symmetric random walk using the ensemble average method. With enough number of ensembles, the ensemble average should approach the expected value due to the "law of large numbers".

At every step of random walk, we calculate the average displacement and average squared displacement using a certain number of ensembles(repetitions).

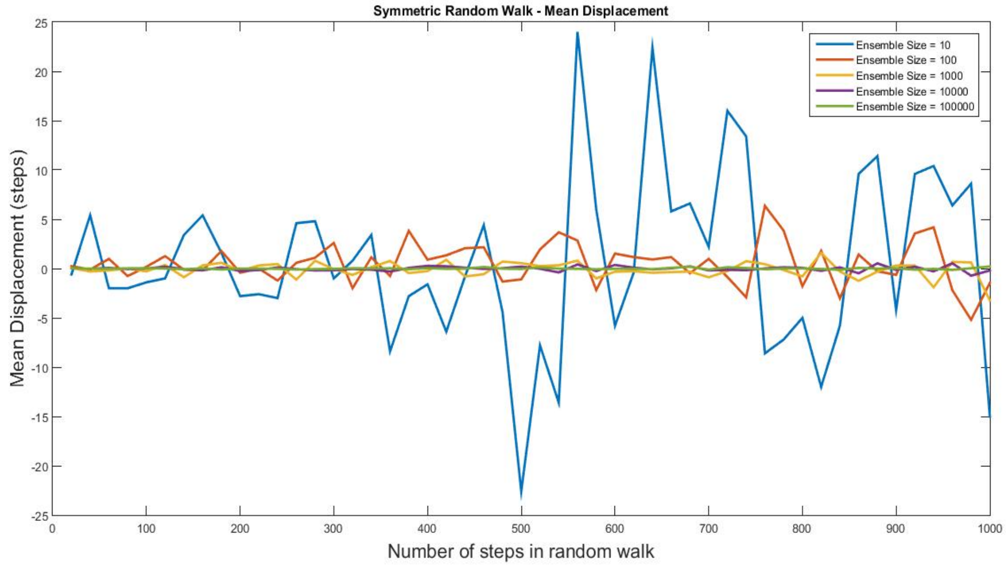

Figure 5: Graph of mean displacement in symmetric random walk

Observations:

- From the above figure, it is clear that as the ensemble size increases, due to the law of large numbers, the behaviour of the random walk emulates the long term behaviour of symmetric random walk.
- Deviation from the line with mean displacement reduces and the mean displacement almost remains 0 throughout for all the step size.

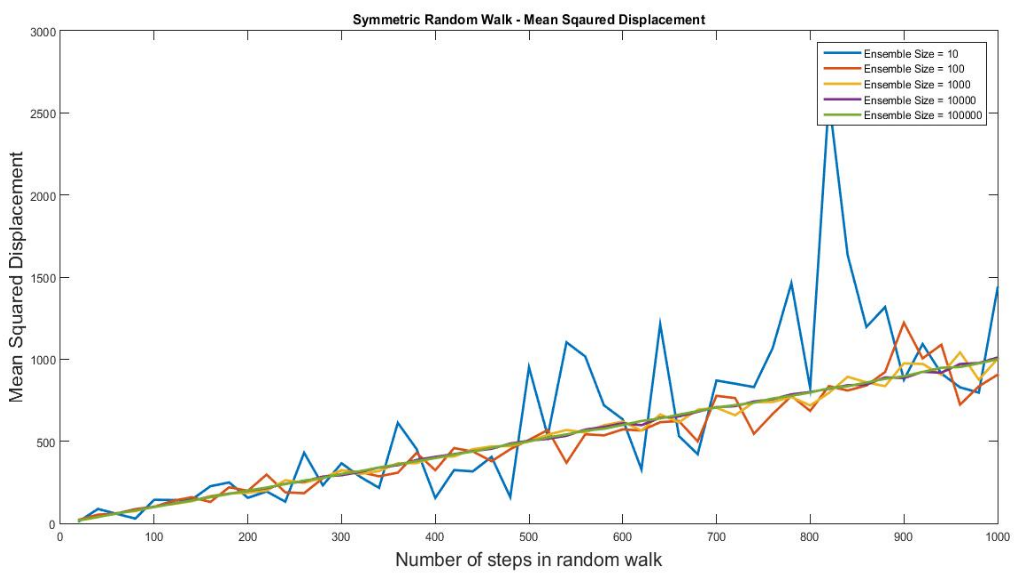

Figure 6: Graph of mean squared displacement in symmetric random walk

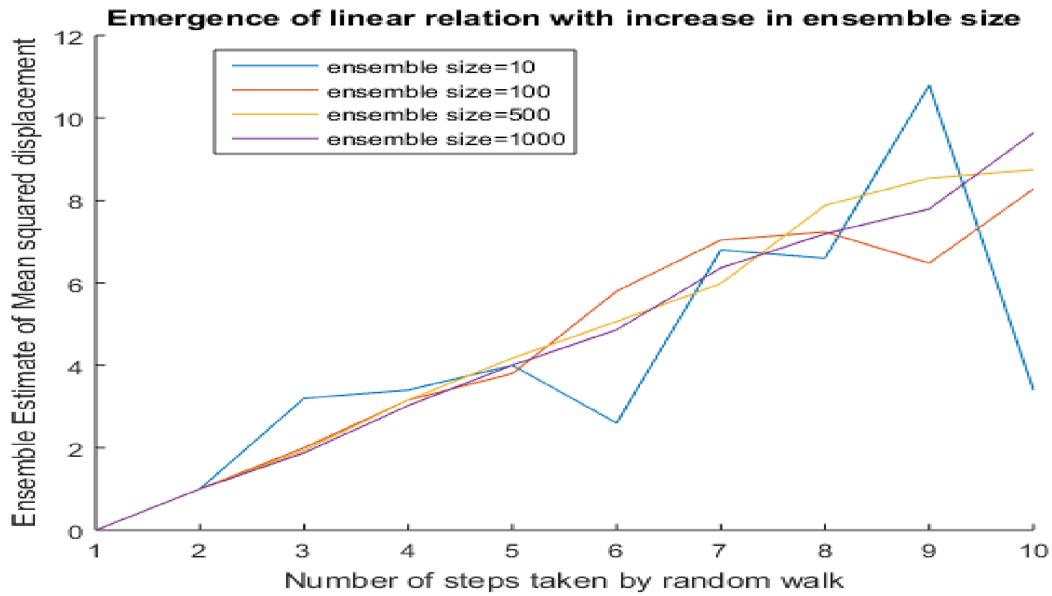

Figure 7: Graph of mean squared displacement in symmetric random walk

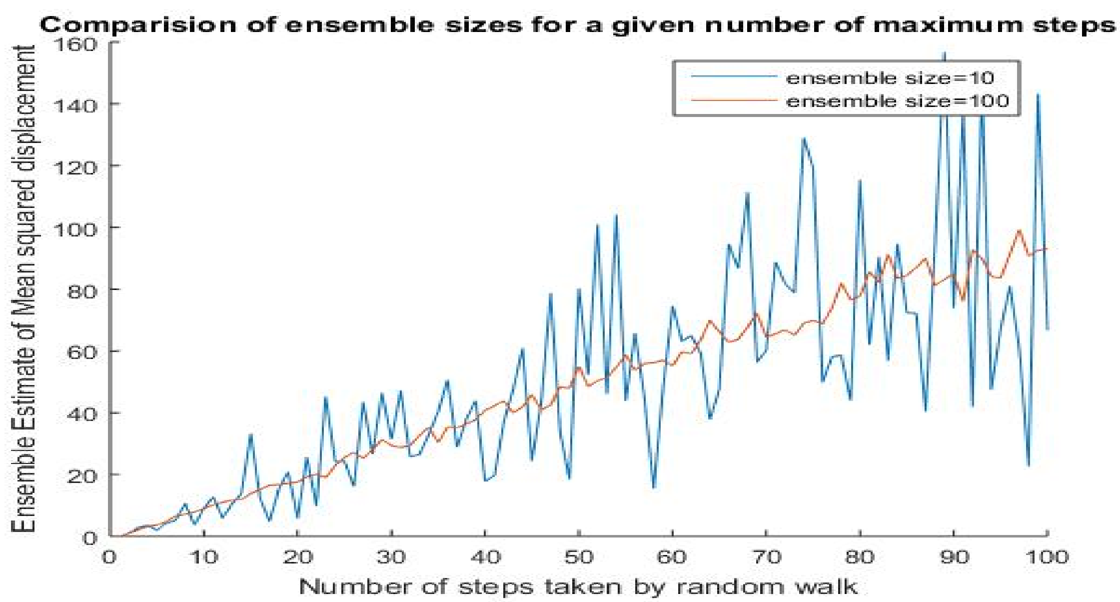

Figure 8: Graph of mean squared displacement in symmetric random walk

Observations:

- From Figure 6, 7 and 8: we clearly notice that for larger number of ensembles, we get a graph which is closer to the linear theoretical prediction. This is intuitive because for a fixed number of random walk steps, for larger number of ensembles we get a "clearer picture" of the stochastic process so to say. In other words, the more number of ensembles present the estimate gets better and better.
- For small number of ensembles, the estimate is not good enough and varies a lot from the theoretical long term behaviour.

- Even for 10 steps, with 500 ensembles (see Figure 7), It gives a reasonably linear graph of Expected Squared Displacement with step size. Note that for a larger step size, the possible values for the Expected quantity increase, hence we need more number of estimators in that case. So, for a step size of 100 for example, the following figure compares with ensembles of size 10 and 500 respectively. From Fig. 8 it is evident that for a given number of steps , a larger number of ensembles gives a better estimate.

2.1.1 What is the size of the ensemble beyond which you observe Einstein's relationship

Here for ensemble size of approximately 10000 and beyond, we observe the Einstein's relationship wherein the mean-squared displacement is directly proportional to the number of steps of the random walk.

2.1.2 What is the value of Diusion constant?

For maximum steps of 100, and for 1000 ensembles, we get a slope of around 0.97. The diffusion constant is therefore 0.97 / 2 = 0.485.

Theoretically, the diffusion constant is given by the following formula:

$$D = L/2\Delta t \tag{1}$$

where L = step size = 1, Δt = 1 unit of time

Therefore, D = 0.5

This shows that the theoretical and actual values of diffusion constant are very close. They may have something to do with the symmetry of the problem. We will reexamine this when we look at asymmetric random walks.

2.1.3 Make a histogram of of the distribution 2 of p_n(m) obtained from your data, where p_n(m) is the probability of being at the m^{th} site after n steps.

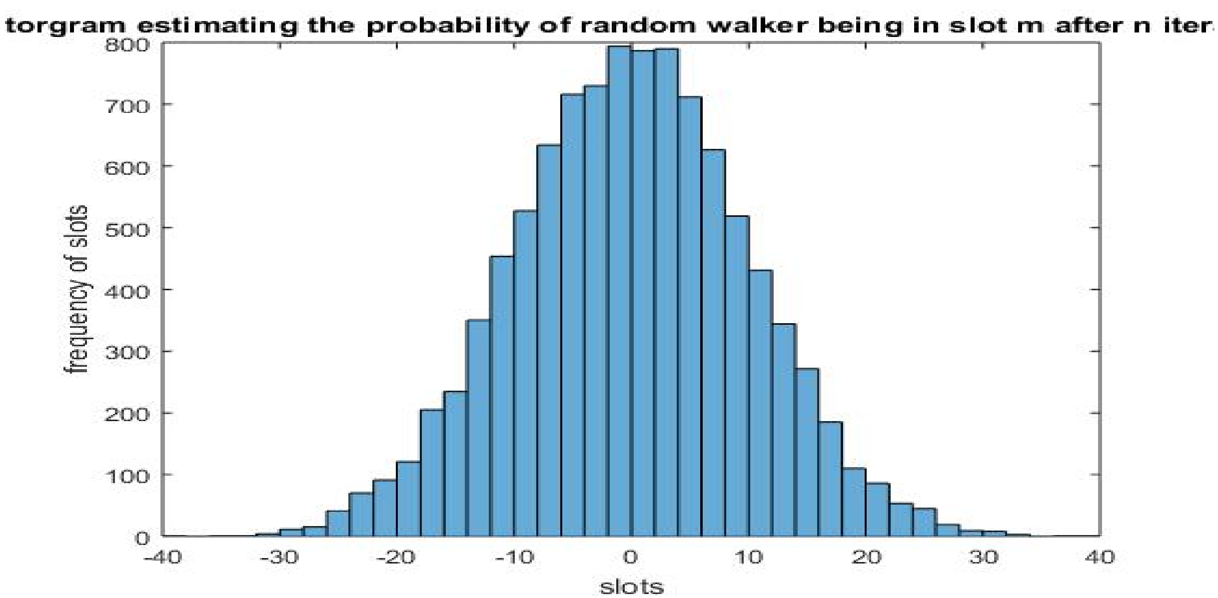

Figure 9:

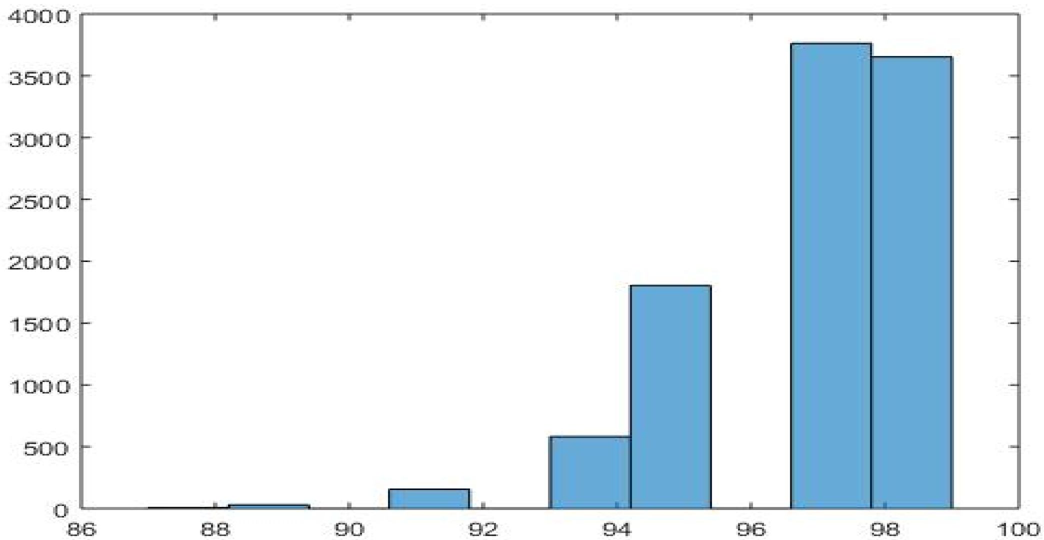

Figure 10: The probability distribution for a biased random walk with P(right)=0.99

Observations:

- The distribution is binomial
- Since we have taken a large number of trails, it is looking very similar to the normal distribution.
- So the probability of being close to zero is very high and the farther we get from the origin, the lesser is the probability. This is intuitive because it is much less likely to reach the endpoints if at all slots the probability of left or right is same. ie being at the endpoints is a very rare event. Recall, that in a binomial coefficient, maximum is when both number of heads and tails is equal. This happens near the origin.
- Fig 10 is the distribution for an extremely positively biased random walk. The distribution is clearly skewed towards the right. This is because the random walker is likely to go to the right than left. Hence it is much likely to be present far away from the origin towards the right.

2.2 Asymmetric random walk

Let us now consider the case of unequal probabilities of going left or right. Such a situation arises quite often when we force the random walker to prefer one of the directions. Think of the motion of an electron inside the metal in the presence of electric eld. Let p be the probability of going right and q = 1 - p be the probability of going left. Assuming that the random walker takes unit steps at each step what is the mean distance and mean squared displacement. Compare with the previous case.

Here the bias introduces drift, i.e. we are forcing the random walker to prefer one particular direction over other. This means that the mean displacement of the random walker will not be equal in both the directions.

When such situation happens, the diffusion which is the natural spread of the random walk decreases. This is because as we give drift to the motion, the probability of the random walk deviating from the mean position decreases. This means that the variance from the mean position decreases. To observe this situation, we must look at the variance of the mean displacement which is given by subtraction of mean-squared displacement and the square of the mean value.

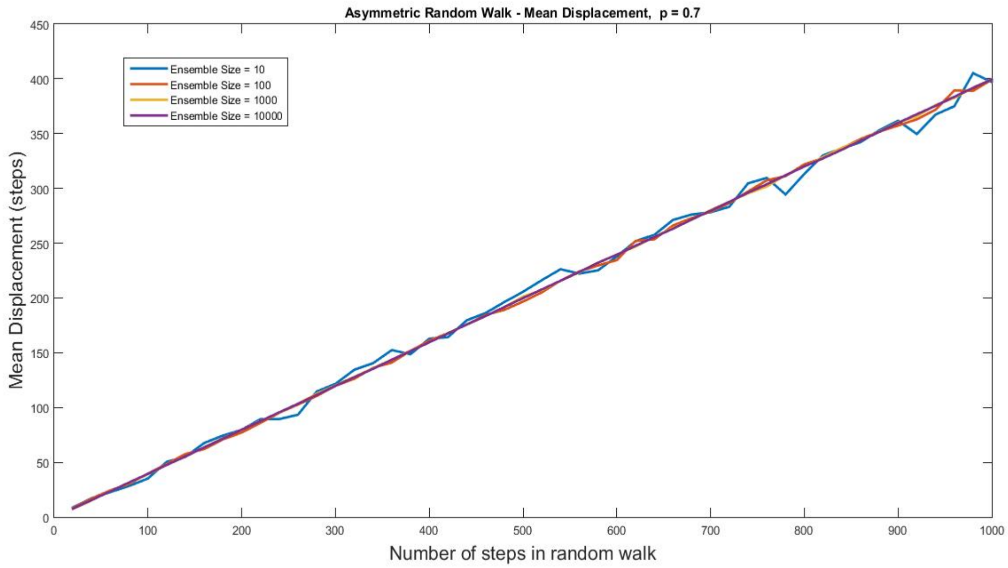

Figure 11: Graph of mean displacement in asymmetric random walk.

Observations:

- In the above figure, due to the positive bias, the motion will favour the positive direction. As p = 0.7, in the random walk of 1000 steps, for a large ensemble, the average steps in the positive direction would be 700 while the average steps in the negative direction would be 300. Since the step size is constant, the net movement should be 400 steps in the positive direction which is what is shown in the figure.
- Here also, as the ensemble size increases, the deviation in the graph decreases. The graph is linear indicating that the as the number of steps in the random walk increases, the effect of positive bias ensures that motion in the rightward direction remains proportional to it.
- Note here that the amont of deviation from the linear line is much smaller than the deviation seen in case of symmetric random walk. This must be attributed to the fact that as the drift increases. the diffusion decreases.

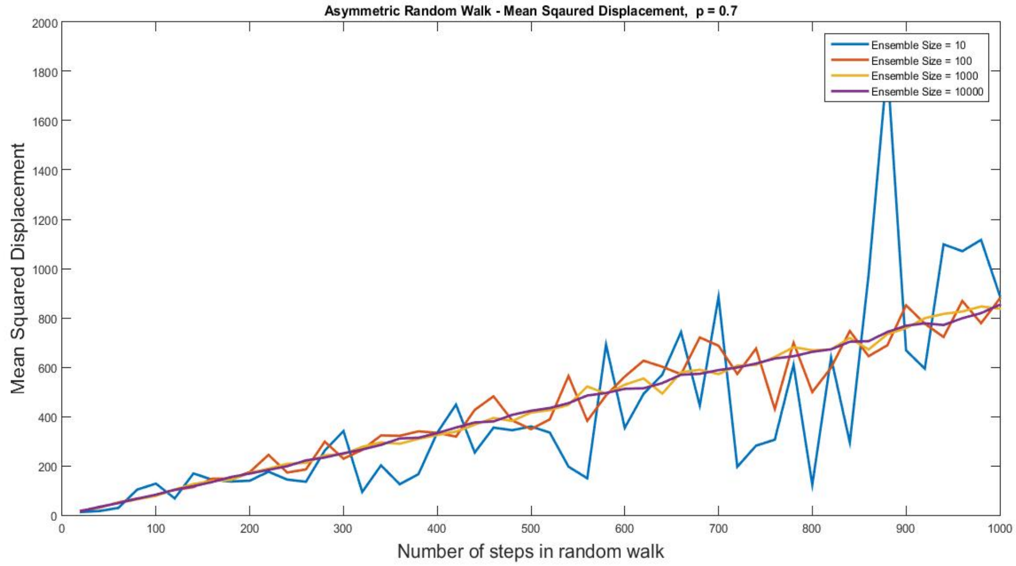

Figure 12: Graph of variance in asymmetric random walk

Observations:

- The above diagram shows the variance about mean position of the random walk.
- Here we see that the variation is more when the ensemble size is less. the variation in variance decreases as the ensemble size increases. This is because, the determination of variance is more accurate when the experiment is performed a large number of times.
- Also the slope of the graph has reduced and the variance converges to a value which is less than the linear value. This must be because, as the drift is introduce, certain deterministic behaviour comes into the system and hence the variance decreases.

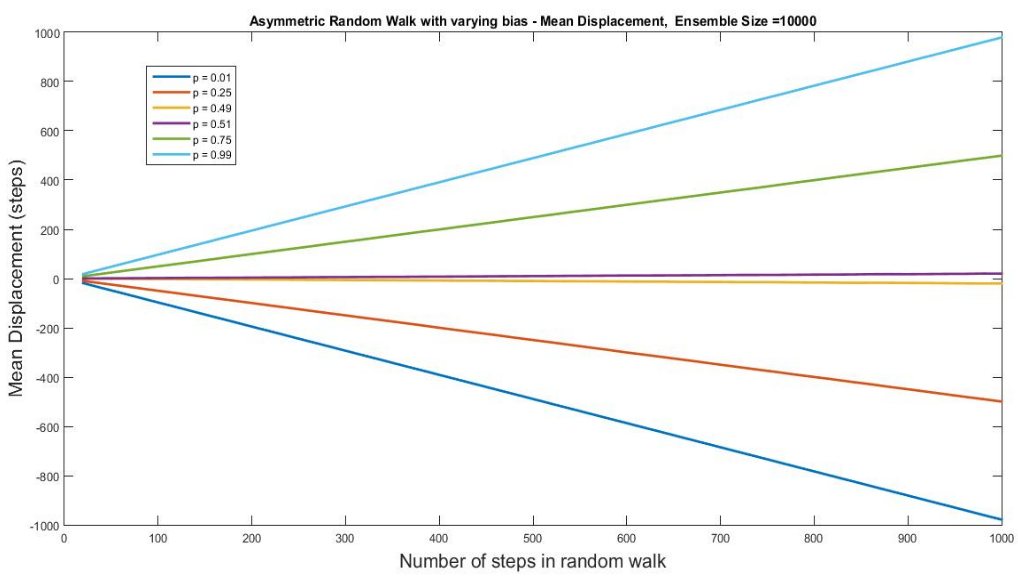

Figure 13: Graph of mean displacement in asymmetric random walk for varying bias

Observations:

- This graph fairly matches with the previous observation that as the bias increases, the motion is in that direction
- As the bias increases, the graph becomes more and more linear. This is because we force the random walk to prefer one particular direction.

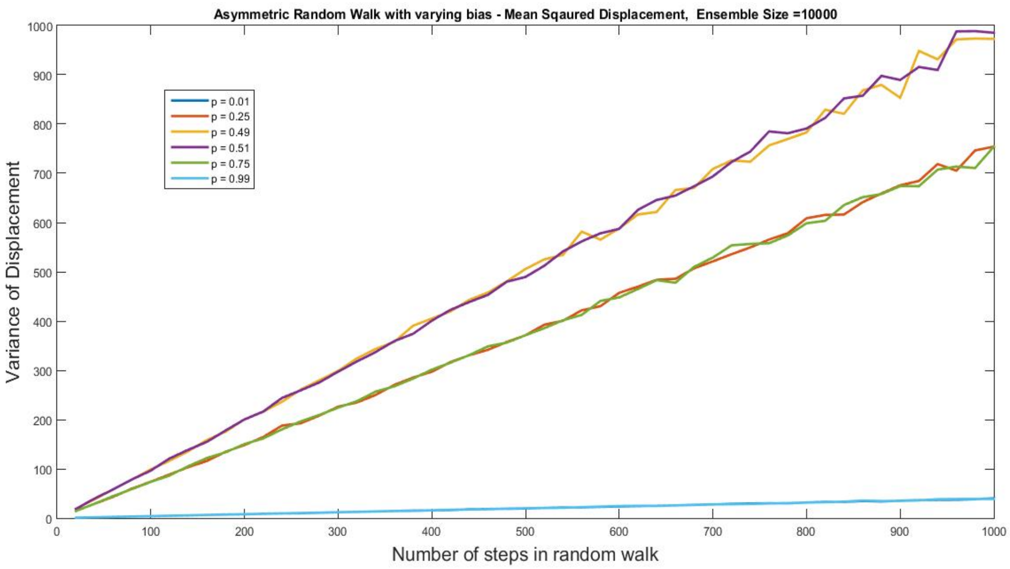

Figure 14: Graph of variance in asymmetric random walk for varying bias.

Observations:

- This graph is very important. Here as the bias increases in either direction, the variance of displacement decreases, that is the actual displacement is more closer to the mean displacement.
- This means that the problem becomes more deterministic as more drift is introduced and the effect of diffusion which is indicated by the slope of this line.

2.3 Walk of varying lengths

Let us now allow the random walker to take steps of varying lengths. While we can in principle take any distribution for the step length let us assume that the length of the steps are normally distributed with with mean 0 and variance 1. From your simulations comment on the general behavior of the random walker in terms of the mean and msd, and calculate the diffusion constant. If the distribution was not standard normal but rather $N(\mu, \sigma)$ do you observe any dierence in the behavior.

In this case, we take the length of step (L) to be varying according to a normal distribution and find its effect on motion of random walker.

2.3.1 L follows Standard Normal Distribution where $\mu = 0$ and $\sigma = 1$

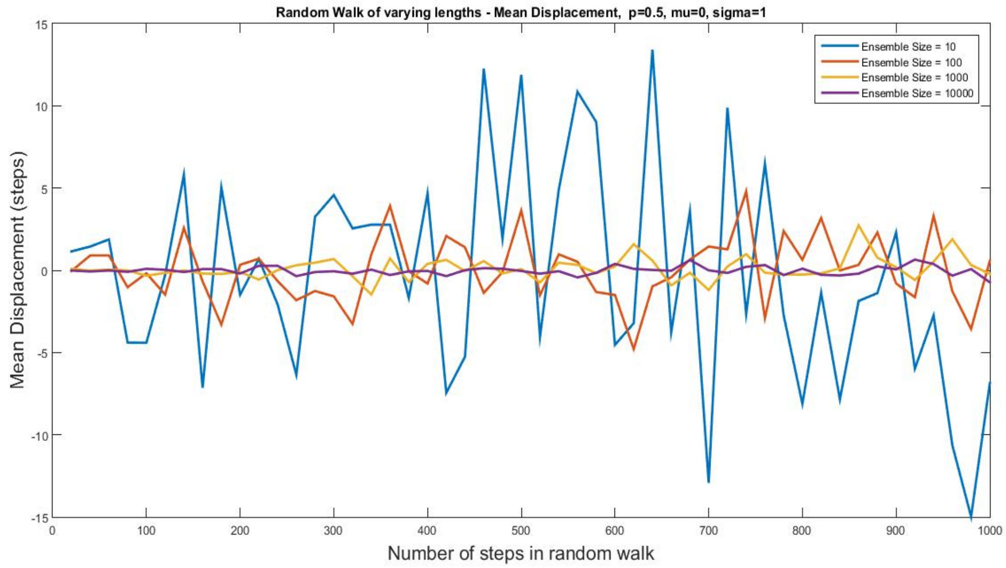

Figure 15: Graph of mean displacement in random walk for varying lengths.

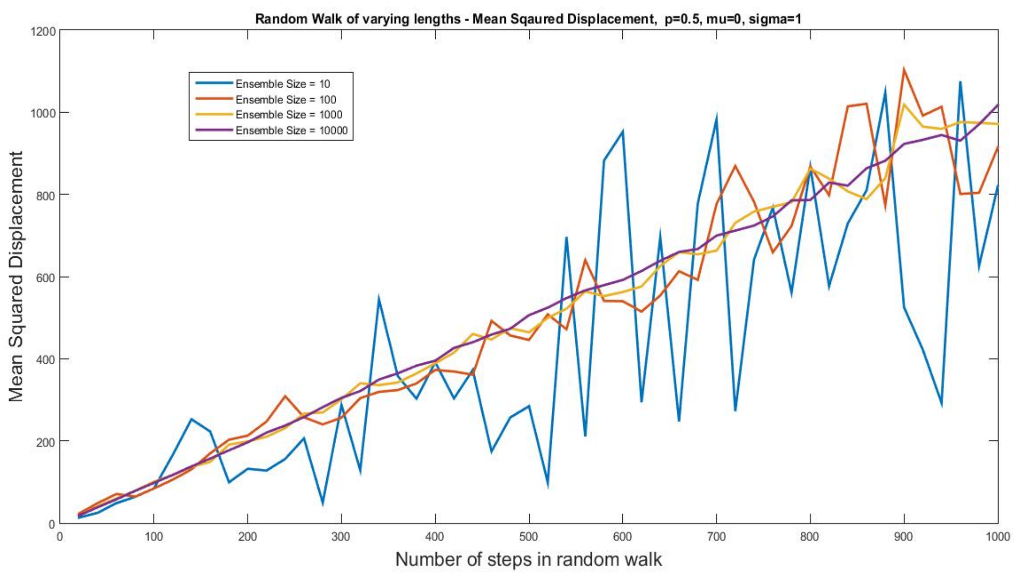

Figure 16: Graph of mean square displacement in random walk for varying lengths.

Observations:

- These graphs are similar to the symmetric random walk graphs. This must be because the step length is a standard normal distribution which when performed a large number of times would be symmetric around the mean = 0 and hence would move with equal amounts in both the directions. Hence net displacement would be zero which is what is seen in the graph.

- The similarity is a consequence of the law of large numbers. Since, we are taking the observations for a large number of times and the only difference being the step size varying, performing the experiment large number of times ensures that the random walker travels in both directions and every step of certain length in one direction is thus cancelled out by a similar step in the opposite direction

- Thus one could say that the behaviour of this random walker is essentially similar to the symmetric case

Calculation of expected squared displacement analytically for this case and the diffusion constant. We can go through a similar derivation as for the constant L. The only difference being the fact that now L is not a constant by a Normally distributed random variable with mean 0 and variance 1. We make use of the fact that that ϵ and L at a particular iteration are independent. We finally get that the mean square displacement is actually x_o + N. We have taken x_o as 0 so mean square displacement is simply the number of steps taken by the random walker. This is as if each step of the random walk contributes 1 to the mean square displacement. We can verify this from **Fig 16**. Mean square displacement is exactly equal to the number of steps. Thus, even if L is not constant, the expected value of L^2 is 1 (equal to its variance). So, taking Δ t =1 again, we get D = 0.5 theoretically. From the figure we can verify our theoretical calculation.

2.3.2 L follows Normal Distribution where $\mu = 10$ and $\sigma = 50$

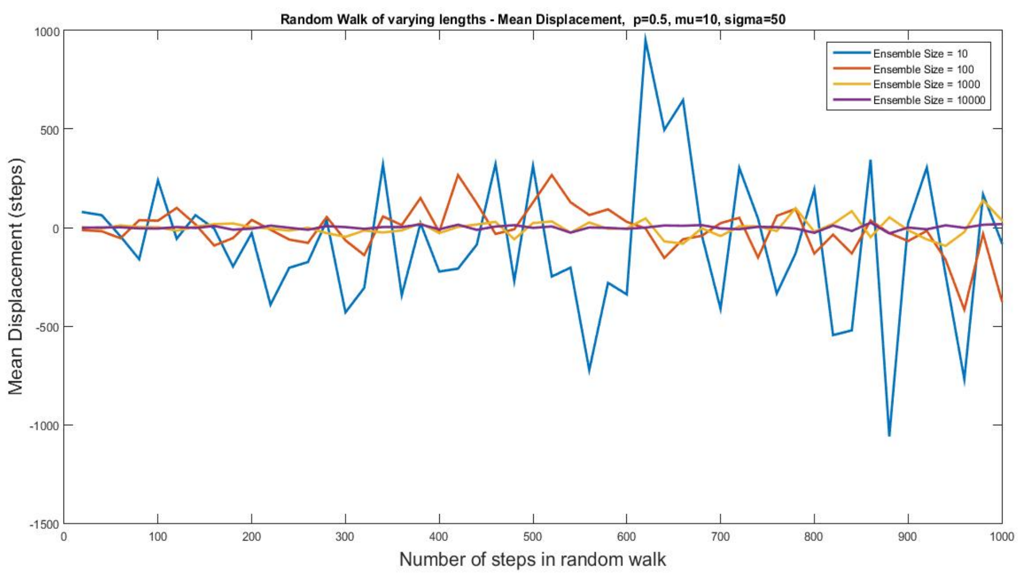

Figure 17: Graph of mean displacement in random walk for varying lengths.

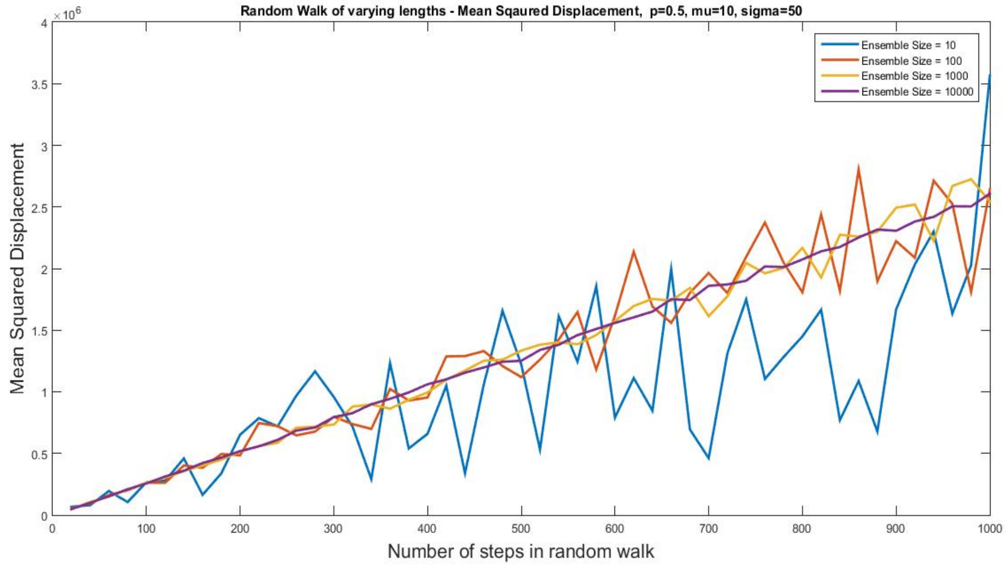

Figure 18: Graph of mean square displacement in random walk for varying lengths.

Observations:

- Again we notice that the mean displacement is zero. This can again be attributed to the symmetric nature of the normal distribution and the unbiased nature of the random walk.
- The mean squared displacement however is larger. This is simply because the mean step size is larger and hence the mean squared displacement is larger.

Calculation of expected squared displacement analytically for this case and the diffusion constant.

Here the L normally distributed variable with some μ and σ.

We again go through the same derivation and get the following result.

The mean squared displacement = $(\mu^2 + \sigma)$N. Here $x_0 = 0$. Thus for 1000 steps we get a large mean square displace of 2.5e6. This can be verified from Fig.18

Thus, the mean squared displacement is still linearly dependent on N which indicated Einstein's diffusion constant can still be defined. This gives us a large diffusion constant of 2.5e6. This is because a larger variance in step size leads to a larger mean squared displacement. Here as mean displacement is 0, variance[diffusion] is equal to mean square displacement. Thus, we conclude diffusion is large.

2.3.3 L follows Standard Normal Distribution for positive bias

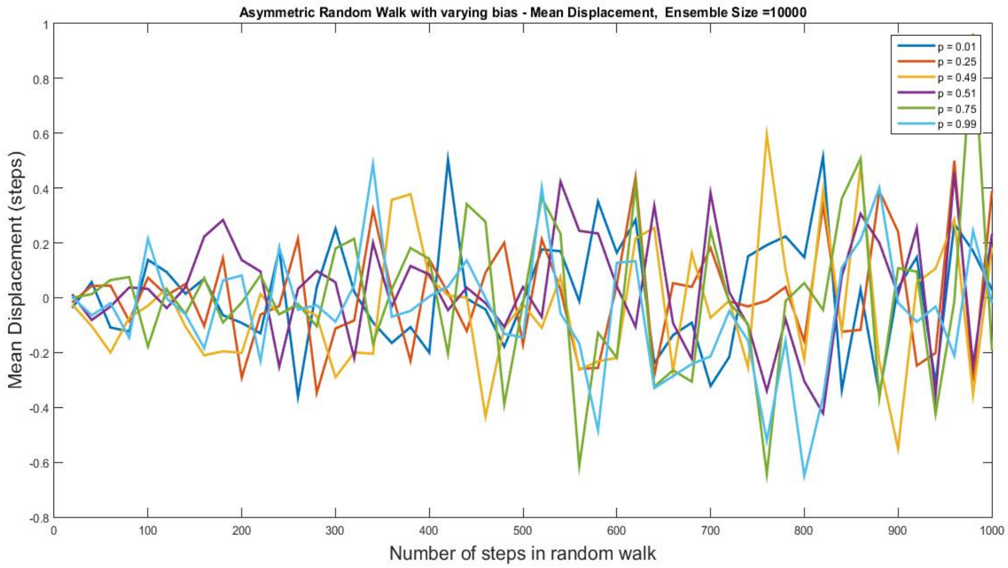

Figure 19: Graph of mean displacement in random walk for varying lengths.

Observations:

- This is an interesting observation. Here as we put bias in the system, the system starts to deviate from 0 but there is no fixed value to which the system goes. This is because the size of step is not fixed and hence the deterministic behaviour introduced by the bias is balanced.

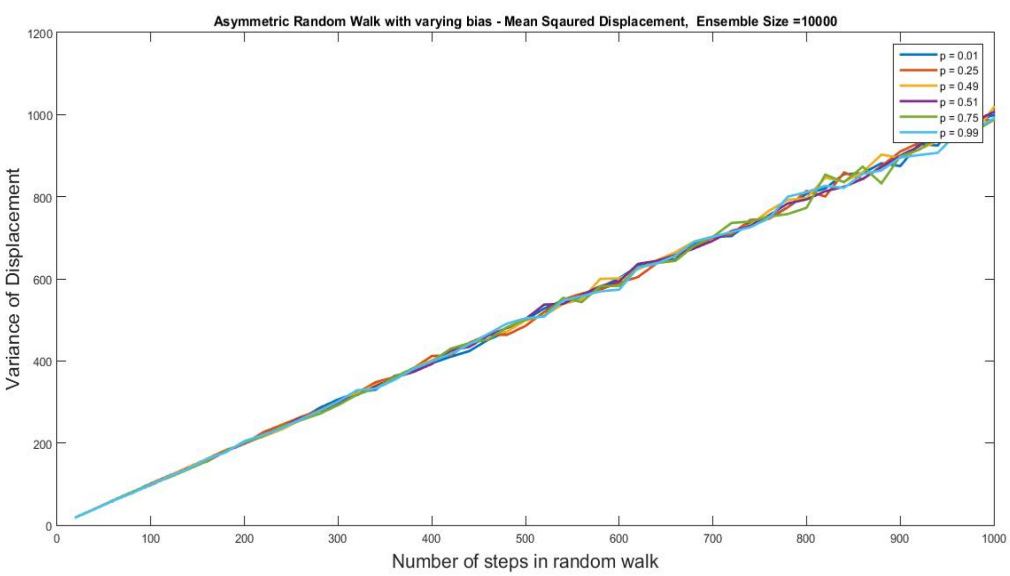

Figure 20: Graph of mean square displacement in random walk for varying lengths.

Observations:

- Contrary to the above graph. The variance of the system follows a fixed pattern wherein it shows the same Einstein behaviour even when bias is introduced.