Computational Physics & Astronomy (188B)

Project IV: Random Processes

Erik Lamb

March 1, 2016

1 Brownian Motion

1.1 Introduction

Brownian motion is the random motion of particles suspended in a fluid after colliding with molecules or atoms of the fluid. An easy was to think of Brownian motion is as the motion of beach ball being pushed around in the bleachers of a stadium, where the ball is a particle and spectators are molecules. This random movement particles in a fluid can in fact be described by the following diffusion equation

$$\frac{\partial w(x,t)}{\partial t} = D\frac{\partial^2 w(x,t)}{\partial x^2} \tag{1}$$

where D is a constant proportional to the mean square displacement (defined later) of a particle subjected to Brownian motion. The solution to Eqn. 1 is in a fact the probability density for particles in the Brownian fluid. The time discretized solution to the diffusion equation is a Gaussian distribution function of the form

$$w_n(x) = \frac{1}{\sqrt{2\pi\sigma_n^2}} \exp -\frac{x^2}{2\sigma_n^2} \tag{2}$$

for discrete time step n and where σ_n^2 is related to the mean square displacement by $\overline{X_n^2} = \sigma_n^2$. A probability density is a statistical quantity with that property that it is equal to unity when integrated over all space, e.g.

$$\int w(x)dx = 1 \tag{3}$$

More explicitly, the probability density is the derivative of a probability function $P(x)$, and is formally expressed as

$$w(x) = \lim_{\Delta x \to 0, Z \to \infty} \frac{Z(x,\Delta x)/Z}{\Delta x} = \frac{dP(x)}{dx} \tag{4}$$

where $Z(x,\Delta x)$ is the total number of measurements that fall inside the interval $[x-\Delta x/2, x+\Delta x/2]$. $Z(x,\Delta x)$, in fact, generates a histogram and quantity $Z\Delta x$ in (4) is the area of a particular "bin" of a histogram and is a normalizing quantity so that the probability density behaves (3). Therefore, we can construct a probability density discretely by creating a histogram for particle quantity. The only caveat is that we must have a very large system, large Z, so the limit in (4) is satisfied.

This relates to Brownian motion because we can discretely approximate the solution of (1) by creating a histogram for the appropriate quantity. That quantity is naturally the position of the particle relative to the origin of the container of the Brownian fluid. Because Brownian motion is a random, statistical process, we can use a *random walk* to both simulate a particle in a Brownian fluid and generate the necessary position data for creating the histogram. The random walk and other necessary statistical methods are discussed in the next section.

1.2 Methods

A random walk can be used to simulate Brownian motion by making the assumptions that particles move in a series of discrete steps and that they move at a constant velocity and in given direction until a collision with a molecule or a wall occurs at the next step, at which point the particle changes its motion to a new random direction. We only consider two-dimensional Brownian motion, and therefore random walks in the $x - y$ plane. The process of implementing the 2-D random walk model for Brownian motion is as follows. We first define a container size L for the Brownian fluid to which the particles contained and can only have positions with $x, y \in (-L/2, L/2)$, a step length l, the total number of steps N, and the total number of particles Z, which must be large. We then create two two-dimensional $(N + 1) \times Z$ arrays X and Y to store all of the position data for all of the particles which will be used to plot the random walk and to create the histogram that will make the probability density. The first rows for both arrays are set to zero so that all particles start at the origin. The nth rows of the 2-D arrays are time steps and columns are different particles. Next, we must create $(N + 1)*Z$ random numbers $U_{n,i}$ such that $U_{n,i} \in [0, 1]$, enough for each particle at each time step. We created random numbers using the Python random library function python.uniform(0,1). Now that we have taken care of all of the preliminaries, we implement the random walk model by first creating position increments for each particle over all time steps using the random numbers $U_{n,i}$ and the formulas

$$\begin{aligned} \phi_i &= 2\pi U_{n,i} \\ \Delta X_i &= l\cos(\phi_i) \\ \Delta Y_i &= l\sin(\phi_i) \end{aligned} \tag{5}$$

The size of the container comes into consideration as a boundary condition. If the new particle increments defined by (5) satisfy $|X_{n,i} - \Delta X_i| \geq L/2$ and/or $|Y_{n,i} - \Delta Y_i| \geq L/2$, then we must change the sign of ΔX_i and/or ΔY_i in order to keep the particles within the container. This condition leads to particles bouncing and getting "stuck" against the walls as we will see later. Using (5), we can finally create a random walk simulation by incrementing over time steps n and all particles i and filling the 2-D arrays X and Y with the equations

$$\begin{aligned} X_{n_1,i} &= X_{n,i} + \Delta X_i \\ Y_{n_1,i} &= Y_{n,i} + \Delta Y_i \end{aligned} \tag{6}$$

In this, very straightforward, way we generate all of the position data necessary for plotting the random walk trajectories that simulate Brownian motion. We also use the data in the 2-D arrays X and Y to generate probability densities, which can be checked by the actual solution (2). In order to use (2), however, we need to determine σ_n^2 for a particular time step. Using $\sigma_n^2 = \overline{X_n^2}$, we can determine σ_n^2 with following equations,

$$\begin{aligned} \overline{X_n} &= \frac{1}{Z}\sum_{i=0}^{Z-1} X_{n,i} \\ \overline{X_n^2} &= \frac{1}{Z}\sum_{i=0}^{Z-1} X_{n,i}^2 \end{aligned} \tag{7}$$

and similarly for $\overline{Y_n}$ and $\overline{Y_n^2}$. We now have all of the statistical tools needed to fully implement the random walk model for Brownian motion. Throughout the report we consider the primary simulation which determines Figure 1 as well as two other special cases.

1.3 Results

1.3.1 Random Walk Simulations

Our initial random walk simulation for Brownian motion had the following parameters: a box dimension size $L = 100$, meaning the domain and range run from -50 to 50; a maximum spatial step of size $l = 1$; $N = 400$ total time steps; a very large system of $Z = 10000$ particles; an initial starting point at the origin. The results of this simulation are shown in the figure below,

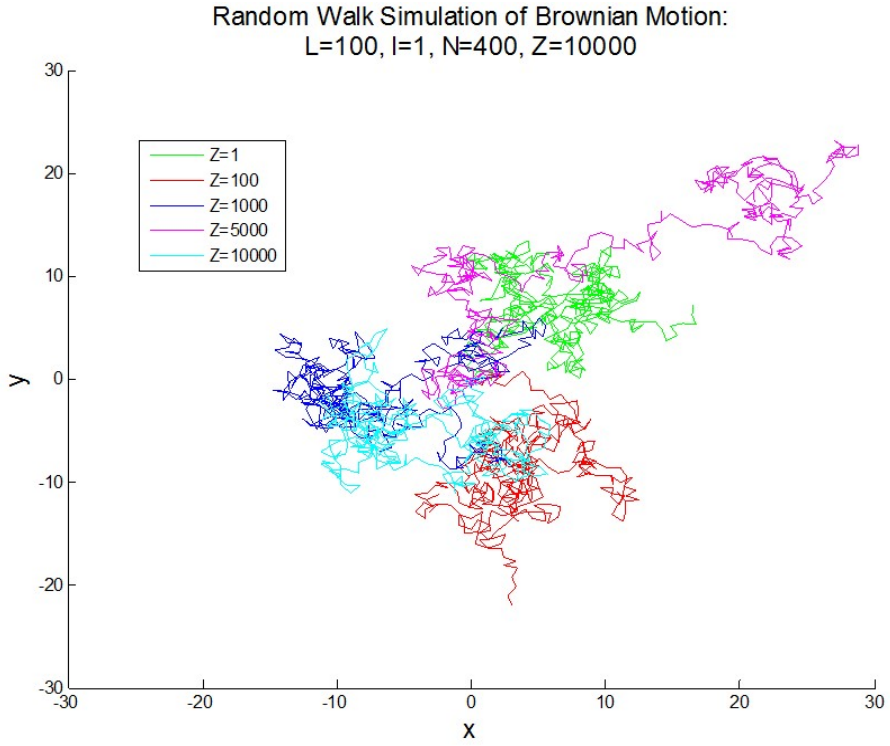

Figure 1: Random walk simulation representing Brownian motion for five different particles. Each trajectory corresponds with a different particle, the number of which is given by the index. Notice how most of the paths are grouped about the center of the square domain.

From the above random walk trajectories we can determine some qualitative features of Brownian motion. The most obvious of these features is the inconsistent random path taken by the particles, which was expected and was motivated us to use the random walk simulation in the first place. In the context of Brownian motion these random paths are due to the enormous amount molecules in a liquid constantly bumping into each other, which leads to particles experiencing imbalanced forces and random motion. Despite this, Fig. 1 also reveals that particles undergoing Brownian motion tend to stay in a predictable region, centered about the origin, for short times. Indeed, most of all five random walk trajectories depicted in Fig. 1 are located within the region of $x, y \in [-10, 10]$ by the end of the 400th time step. We can interpret this as also being a result of the many molecules in a liquid, whose presence acts as a sort of potential a particle at the origin must overcome in order to reach the boundaries of the container. Therefore, the many molecules present in a liquid are responsible for random motion, but they also appear to constrain particles to a particular region for a given period of time by reducing their energy through collision. This is not to say the particles do not want to move away from the origin as they clearly do, but rather it means that it is very difficult to do it, and long times are needed to escape the strong "potential." Indeed the $Z = 5000$ particle appears to have escaped the center of the container by the 400th time step by pure luck.

We then adjusted our simulation slightly by increasing the number of time steps to $N = 2000$.

The random walk trajectories for this simulation are shown below.

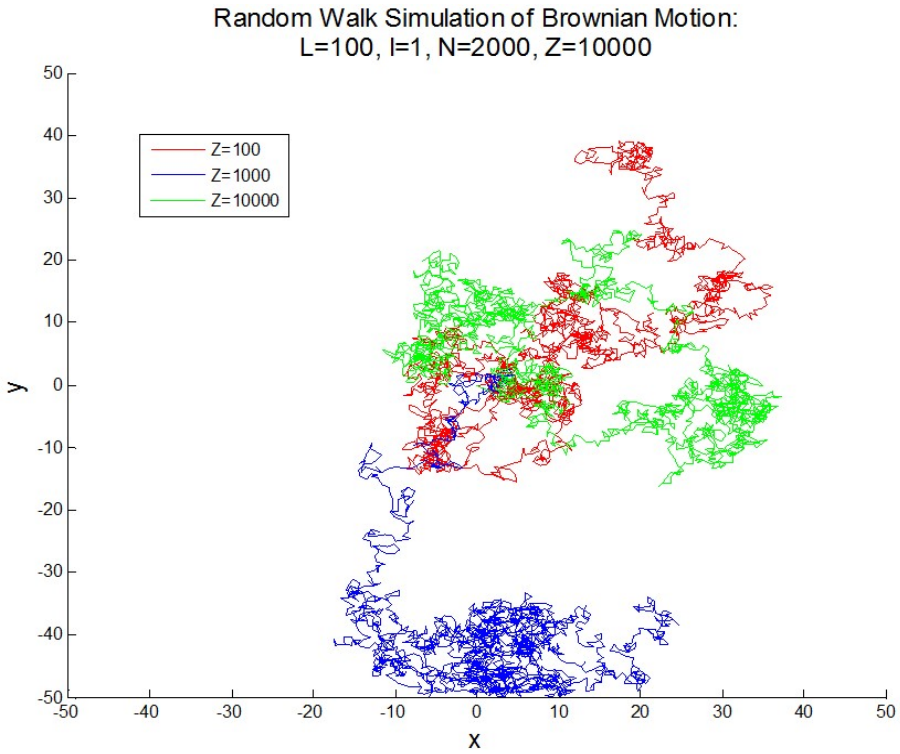

Figure 2: Random walk simulation representing Brownian motion for three different particles. Notice how all three paths have moved far away from the origin by the 2000th time step. The $Z = 1000$ particle in particular has reached the walls of the container.

We have increased the run time of the simulation shown in Fig. 1 by five times, which is shown in Fig. 2. Clearly the run time of this simulation is long enough to demonstrate the ability and tendency of particles to move away from the region about the origin when given enough time. Indeed all three trajectories have reached at least $x, y = |40|$, meaning that they have nearly reached the wall of the container. However, even though the particles have escaped the origin region, we see them once again being confined to other regions for the same reason; molecules are preventing them from moving around freely. A special case is that of the blue $Z = 1000$ trajectory which has actually made it to the container wall. Once a particle reaches a container wall it "bounces" off of it. This, however, leads to particles getting "stuck" against the wall of the container since they now have less random paths available. The blue trajectory, for example, appears to have reached the container wall early and remained in that region for most of the simulation. The blue particle cannot easily move through the sea of molecules above it and it cannot move through the wall below it, meaning that the blue particle can only move parallel to the container wall.

Finally, we ran third simulation where $N = 400$ and l is random number between 0 and 5. The random walks for this simulation are shown below, Recall that l is maximum spatial increment a particle can make in a given time step. By allowing l to be a larger random value, we attempted to create a simulation that was perhaps more realistic than the previous simulations, since the random l value would represent the inconsistent forces of varying magnitude and direction a particle experiencing Brownian motion would encounter, whereas before l was always $l = 1$. How realistic this model is is dubious, however we will discuss it further as it represents high energy Brownian motion. Because the particles experience higher energy collisions due to larger l, they have larger jumps in position and can "bypass" molecules that would have inhibited their motion in the case of Fig. 1. Particles then travel farther faster, and by the 400th time step all trajectory paths have

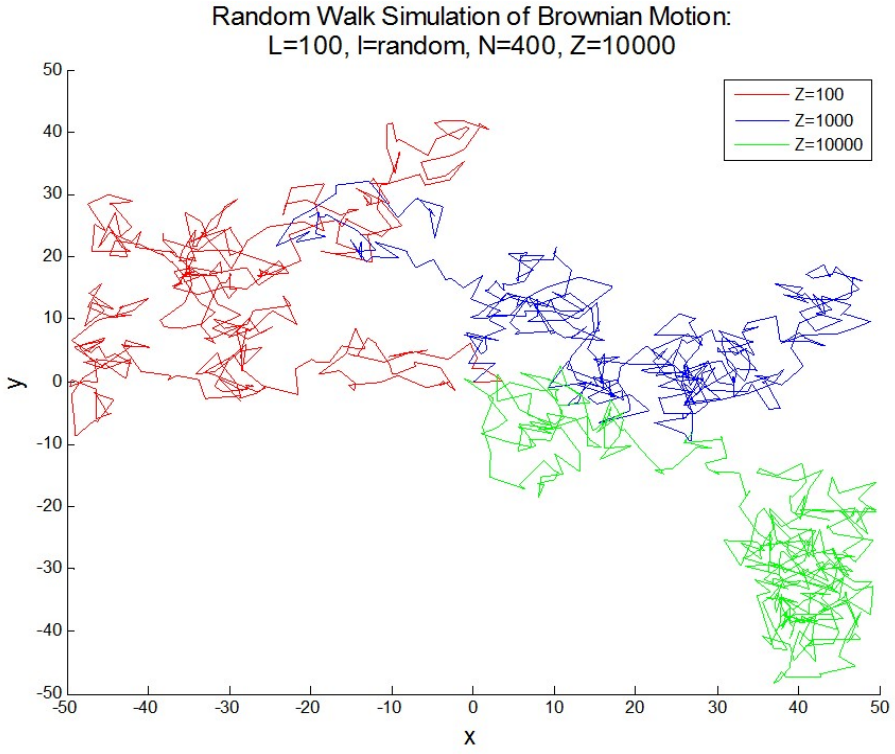

Figure 3: Random walk simulation representing Brownian motion for three different particles. Notice how all three paths have moved far away from the origin by the 400th time step due to the larger, random maximum step size l. The step size l is analogous to the energy imparted onto a particle, and therefore allows for larger jumps in the same time step as before.

reached the container walls in this simulation. We will come back to this simulation in the next section when we discuss probability density.

1.3.2 Probability Density

We next plotted the probability densities, with respect to x, of our original simulation for an early and late time. The probability densities were constructed by creating a regular histogram and normalizing the area under the curve, just as for a continuous probability density. The square of the spread used in creating the Gaussian envelope is equal to the average squared displacement of for the time step under consideration. We first plotted the probability density for the early time of $N = 20$ for the simulation in Fig. 1, shown below.

We know the above probability density is correct from how well it agrees with the Gaussian distribution. This has more to do with the choice of parameters than anything else, as we will see shortly. By examining this probability density we come to the same conclusions as we did from examining the random walk trajectories; particles are mostly concentrated within the region $x, y \in [-10, 10]$ at earlier time steps due to molecules colliding and preventing them from moving farther away from the origin. This point is evidenced by the sharp peak about $x = 0$ indicating this is the region where one is most likely to find a particle.

The probability distribution with respect to y has a nearly identical result to Fig 4., shown on the next page. The probability densities $w(x)$ and $w(y)$ are identical because of the random trajectories taken. Randomness does not distinguish between dimensions, therefore we should expect that for random walks and the Brownian motion modeled by them a sort of symmetry between motion in the x-direction and motion in y-direction.

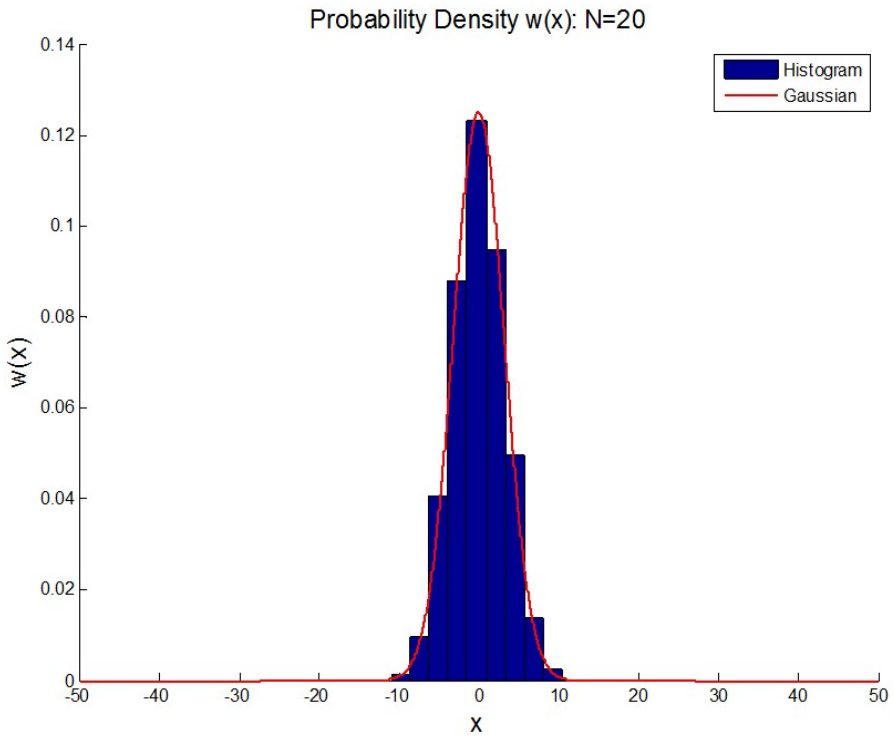

Figure 4: . Probability density with respect to x for the random walk simulation shown in Fig. 1 for $N = 20$. Notice the correct Gaussian envelope and the concentration about $x = 0$.

We then plotted the probability density, with respect to x, for a much later time step at $N = 400$ for the simulation in Fig. 1. This result is shown in Fig. 6. Compared to Fig. 4, we see that the peak in the probability density about $x = 0$ is not as sharp and is smaller in magnitude. Additionally, the spread in the probability density is greater in Fig. 6 for late times than in Fig. 1 for earlier times. Once again, these differences indicate qualities of Brownian motion we have mentioned before, most importantly that as time progresses particles manage to overcome being contained within a particular region about the origin and "jiggle" their way to farther away regions. This increases the probability of a particle being found in region farther away from the origin, and therefore increases the spread and decrease the amplitude of the probability density.

discuss the two probability densities for the two additional systems mentioned previously. The probability density for a very late time of $N = 2000$ is given in Fig. 7. This probability density corresponds with the simulation shown in Fig. 2. From Fig. 7 we see that the spread in the probability density is very large and the peak is much less sharp than any $N = 400$ density. This is due to the usual explanation that for a very late time $N = 2000$, particles have had the opportunity to permeate throughout fluid in the container and thus have a high probability of being found anywhere. Figure 7 also appears to be leveling out and approaching some limit where the probability of a particle being found is the same throughout the entire container. This result is also predicted by theoretical Brownian motion as the the Gaussian becomes constant when the spread is infinite.

Finally, we return to the simulation shown in Fig. 3 where l is a random value from 0 to 5. From Fig. 8 we see that rather than increasing the number of time steps the same effect of having particles permeate throughout the entire system can achieved by increasing the energy and randomness of molecular collisions by making the spatial increment parameter large and random. Indeed if a particle "accidentally" received a large amount of energy upon a collision it would have a less likely chance of colliding with molecule since this means the particle is moving faster and the entire system is higher energy, meaning the density low. If this occurs frequently, all particles will quickly

permeate throughout the container. By only the 400th time step, Fig. 8 shows that a particle has nearly the same probability of being found anywhere in the chamber, except for at the boundaries which is due to reflection at the walls, due to the large amount of energy in the system. Also of note is how poorly the probability density is approximated by the Gaussian distribution, which indicates that this "high energy" random walk diverges from theoretical Brownian motion.

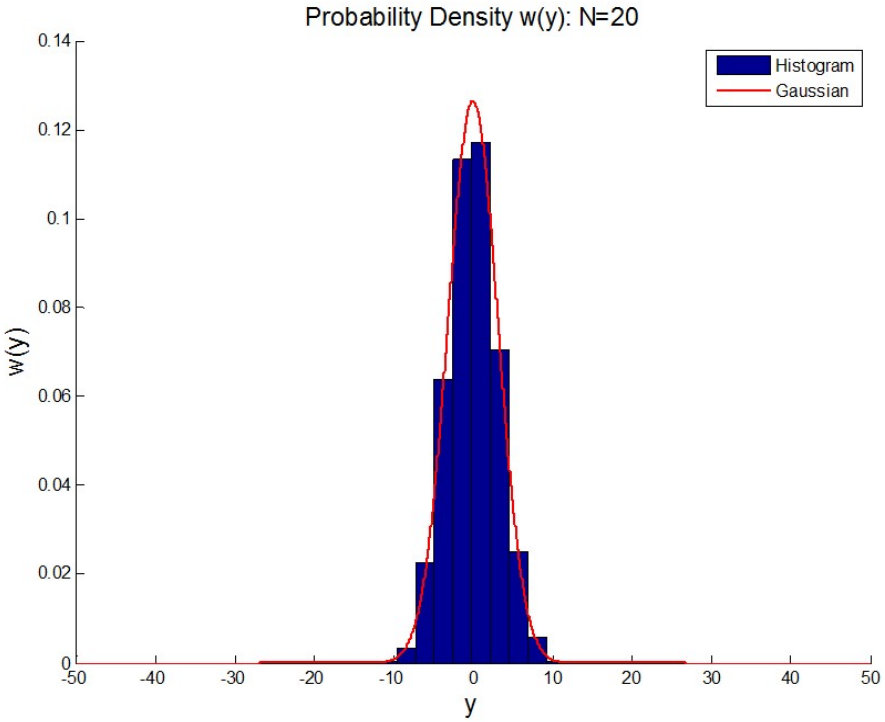

Figure 5: . Probability density with respect to y for the random walk simulation shown in Fig. 1 for $N = 20$. Notice the correct Gaussian envelope and the concentration about $x = 0$. Also notice how it is virtually identical to the probability density with respect to x in Fig. 4.

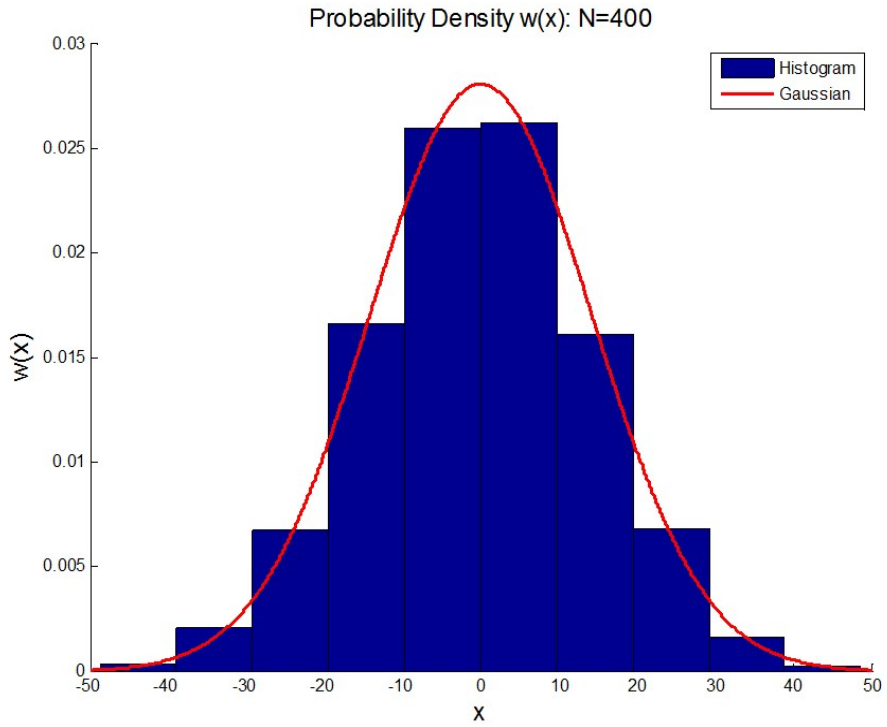

Figure 6: . Probability density with respect to x for the random walk simulation shown in Fig. 1 for $N = 400$. Notice how the peak about $x = 0$ is much less sharp, and that the spread in values is larger.

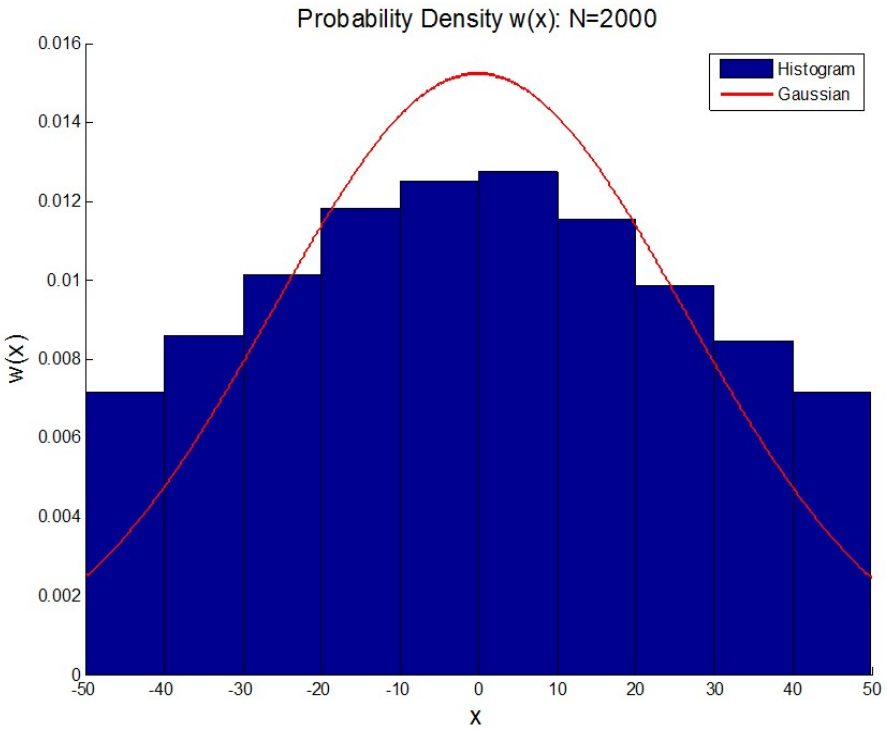

Figure 7: . Probability density with respect to x for the random walk simulation shown in Fig. 2 for $N = 2000$. Notice how the peak about $x = 0$ is much less sharp than any of the previous probability densities.

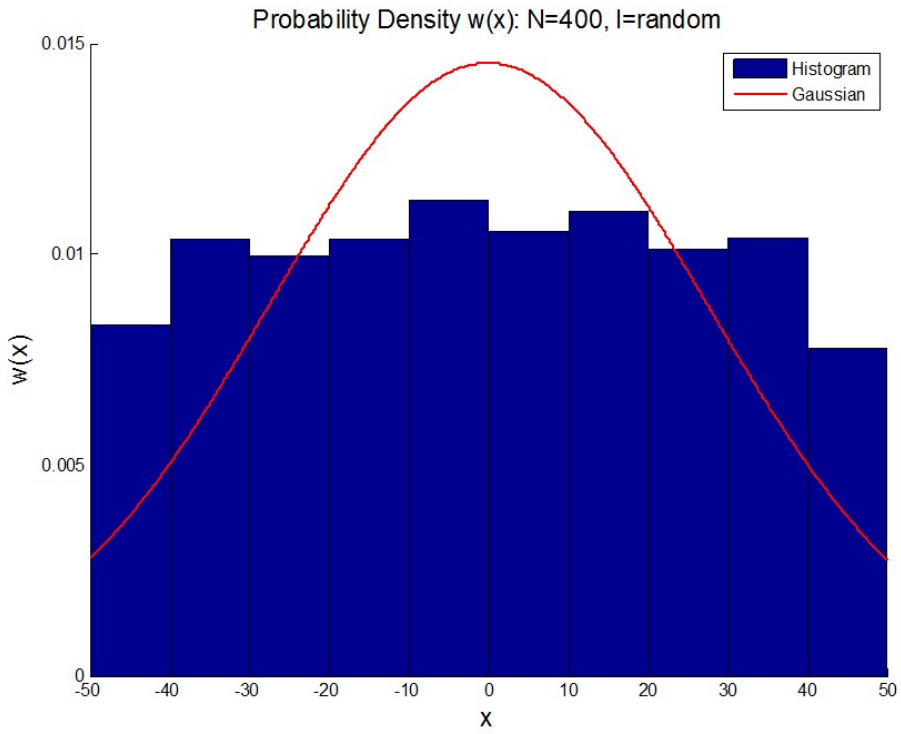

Figure 8: . Probability density with respect to x for the random walk simulation shown in Fig. 2 for $N = 400$ and l is a random value between 0 and 5. Notice how the probabilities are virtually same throughout all space, with the exception of the boundaries where reflection occurs making the probability less.

1.3.3 Expectation Values

For this section we were to plot the expectation values $\overline{X_n}$, the average displacement from the origin, and $\overline{X_n^2}$, the average squared displacement from the origin, for the simulation in Fig. 1. I also chose to plot their y-axis corollaries $\overline{Y_n}$ and $\overline{Y_n^2}$. We first plot the average displacement as a function of the time step n, shown in Fig. 9.

The goal of this task was to show that a plot of the average displacement versus the time step n would be about zero for all time for a system where the maximum number of time steps is $N \leq 400$; show that $\overline{X_n}, \overline{Y_n} \approx 0$. Figure 9, at first glace, does not appear to confirm this property, but rather, it exhibits jagged, almost oscillatory behavior about $\overline{X_n}, \overline{Y_n} = 0$. This, of course, is a result of the many random changes in the displacement of the 10000 particles of the system as well as a result of the cosine and sine dependence of the spatial increments. Upon further inspection of Fig. 9 we realize that the y-axis scale is small and if we increase the scale to the that of the container we produce Fig. 10. Figure 10 clearly shows that the average displacements are indeed zero for all n for an $N \leq 400$ system. We expected this result for reasons mentioned earlier. All Brownian motion in the liquid is essentially random. Random movement is characterized by there being a equal probability of moving in *any* direction. Because our system is incredibly large with many particles, it is a statistical certainty that movement will in fact occur in nearly every direction. Therefore when we average the displacement among all of the particles, these movements in every direction will cancel out, resulting in an average displacement of zero for all time.

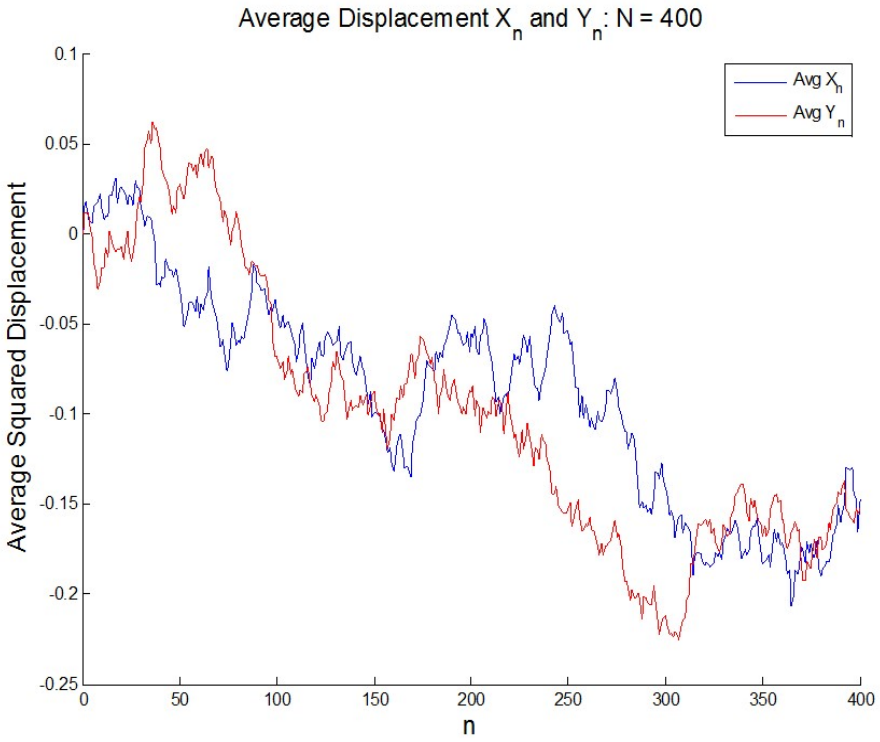

Figure 9: . Average displacements from the origin $\overline{X_n}$ and $\overline{Y_n}$. Notice the jagged fluctuations as result of random movement. Though the plots do not appear to converge to zero, they are close enough to zero relative to the container size.

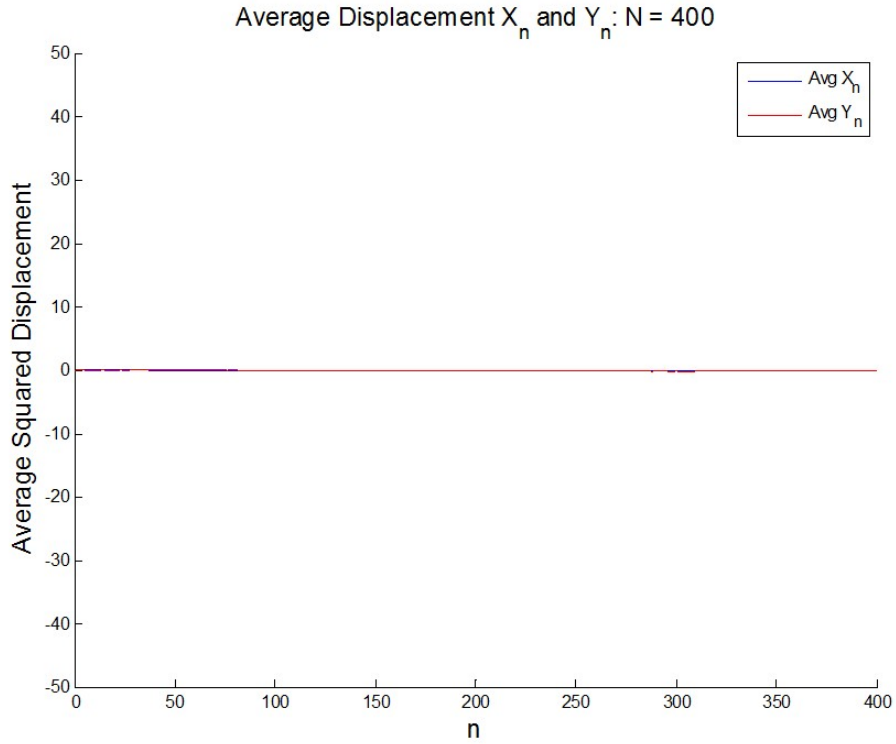

Figure 10: . Average displacements from the origin $\overline{X_n}$ and $\overline{Y_n}$ with y-axis containing the entire container. Notice how the average displacements are practically zero for all time.

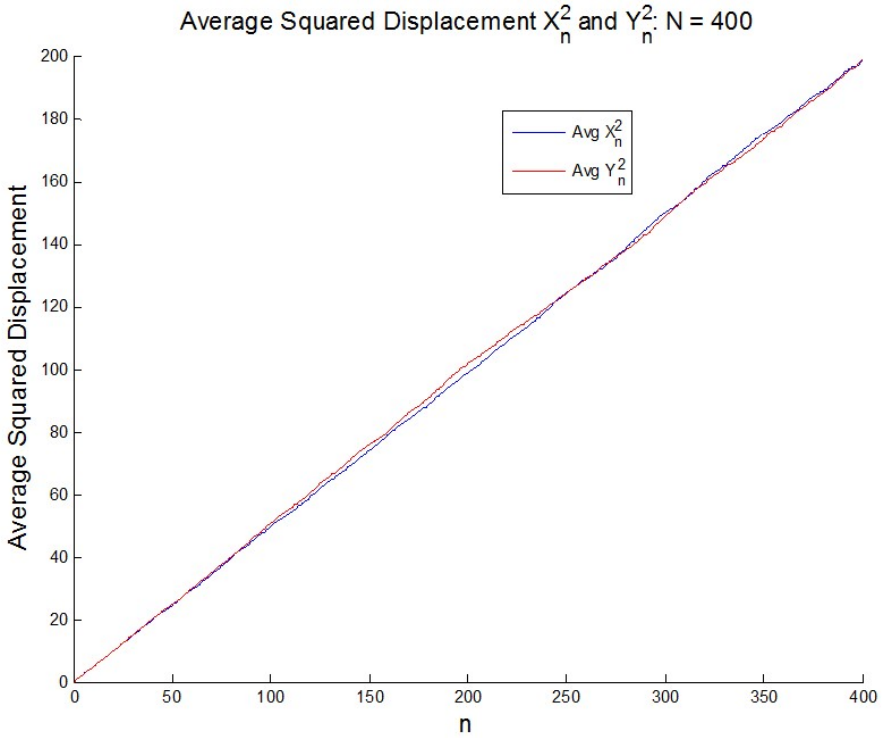

Figure 11: . Average squared displacements $\overline{X_n^2}$ and $\overline{Y_n^2}$. Notice the linear correspondence between the average squared displacements and the time steps n; $\overline{X_n^2}, \overline{Y_n^2} \propto n$.

Next, we plotted the average squared displacements, $\overline{X_n^2}$ and $\overline{Y_n^2}$ of our $N = 400$ time step system from Fig. 1. For this expectation value we expect a linear dependence of the time step n, $\overline{X_n^2}, \overline{Y_n^2} \propto n$. These values are plotted in Fig. 11 above. From Fig. 11 we do in fact confirm the linear correlation between the average squared displacement and the time step n. Because the average squared displacements squares negative terms, it is important because it provides information on the displacements of the particles whereas the average displacement could not due to canceling terms. The linear relationship of the average squared displacements with the time step once again confirms a point made earlier; particles have a tendency to travel away from the origin due to Brownian motion and the longer the run times the further they travel. This linear relationship is actually rather remarkable in the sense that many particles must experience backtracking towards the origin on many time steps simply because of the random nature of their movement yet they still, on average, move away from the origin and attempt to occupy all of the container. What this linear relationship between the average squared distance and the time step actually is, then, is a result of the Second Law of Thermodynamics, that the entropy of system must continue to increase. Because the initial state of all of the particles being concentrated at the origin was highly ordered and has minimum entropy, the entropy must increase from that state. The primary way in which the entropy can increase is movement of the particles away from the origin, which creates disorder and therefore increases entropy. This law is the source of the average square distance's linearly relationship with the time step, which demands that the particles must move with time. The actual linearity of the relationship is due to the random walk simulation of Brownian motion and the simple fact that there is one spatial step for every time step. This relationship is in fact enshrined in the for-loop, which are linear in n steps, used to generate the data for the random walk trajectories.

1.3.4 Optional i

In the previous section we plotted the average squared distance for system with maximum time steps $N \leq 400$. We now wish to plot the average squared distance versus the time step n for a very large number of time steps $N \geq 400$ in order to observe how the average squared displacement deviates from linearity. We chose as our maximum number of time steps $N = 2000$, to ensure that we captured this transition. Our plot is in Fig. 12 below.

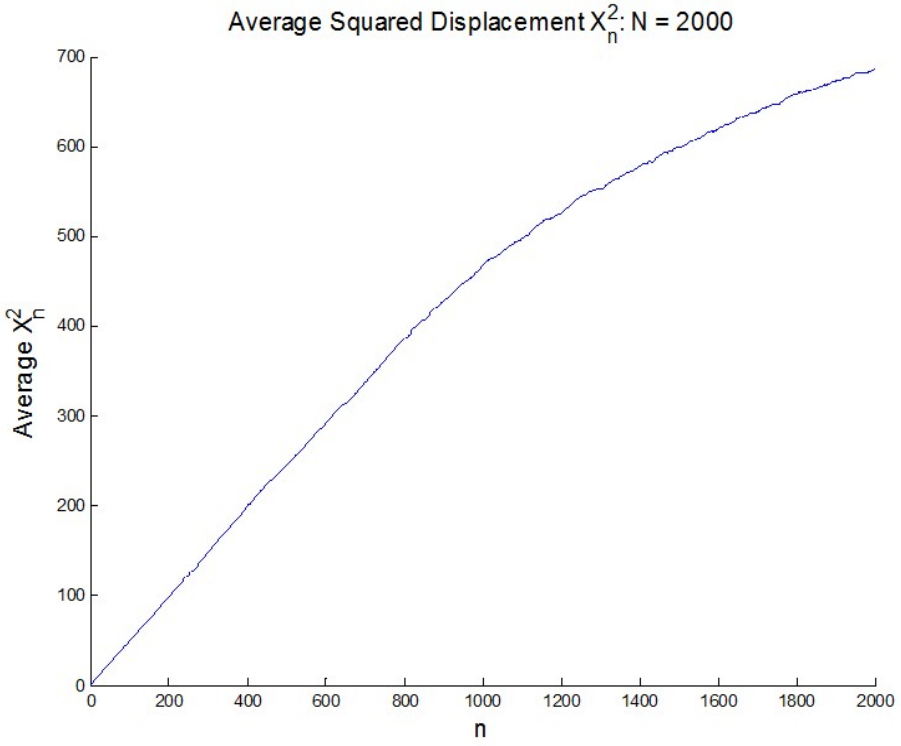

Figure 12: . Average squared displacement $\overline{X_n^2}$ versus time step n for a system of maximum time step $N = 2000$. Note that $\overline{X_n^2}$ is no longer linearly related to the time step around $n = 1000$ and appears to take on a square-root law behavior.

Figure 12 shows that $\overline{X_n^2}$ is no longer linearly related to the time step n around $n = 1000$. As mentioned in the problem, this is due to collision of the particles with the wall of the container. Once the particles reach the walls of the container, they can no move further away from the origin and simply bounce off the wall. As time progresses a maximum displacement will be reached, as shown by the leveling off of the average squared displacement, where the all particles have an equal probability of being anywhere in the container. This leveling off of the displacement also coincides with the entropy of the system reaching a maximum.

A simpler way to think of the nonlinear behavior of the average squared displacement past the time step $n = 1000$ is the fact that the particles *are colliding with the walls*. That is to say when a particle collides will a wall of the container, the particle is reflected and therefore ends up at a location closer to the origin than it was a moment ago. The more particles that reflect of the container walls, the less the average square displacement increases by its linear relationship, leading to the leveling off seen in Fig. 12.