PHY566 - Diffusion Equation

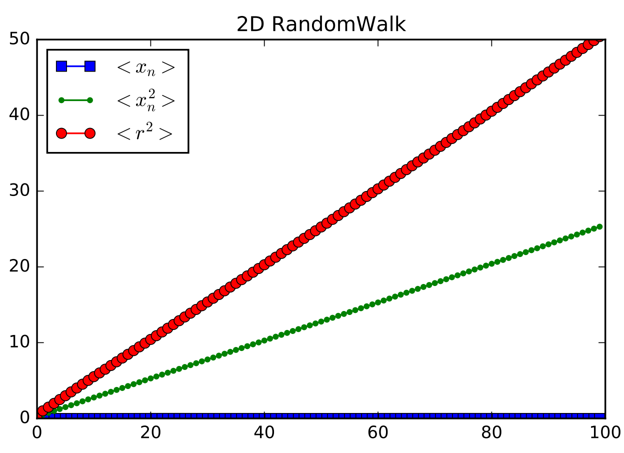
Tianyu Dai, Xiaoqing Li, Xuejian Ma, Yuheng Liao

1 Problem 1

To solve this problem, we first obtain x_n for one random walker. Put a random walker at the origin. Create a random number *movestep* in range (0,1,2,3), and these four numbers means moving one step right/left/up/down respectively.

We create a zero list to record the number of moving steps in every direction. After we know the moving direction of a step, we add the number of total steps in that certain direction by 1. If the total number of moving steps is n, we repeat the previous procedure n times. The number of total rightward steps minus the number of total leftward steps generates the x-component of the random walker's displacement, x_n. Likewise, the number of total upward steps minus the number of total downward steps generates the y-component of the random walker's displacement, y_n.

After that, x_n^2 and r_n^2 are easy to calculate. We use a function named random_walk to return the values of x_n, x_n^2, and r_n^2. Since our goal is averaging over 10^4 different walkers, we need a loop with 10^4 iterations to get the values of x_n, x_n^2, and r_n^2 of each walker, and then realize the average values, $\langle x_n \rangle$, $\langle x_n^2 \rangle$, and $\langle r_n^2 \rangle$.



2 Problem 2

2.1 Part A

To calculate $\left\langle x(t)^2 \right\rangle$, we can integrate it by part:

$$\begin{aligned}
\rho(x,t) &= \frac{1}{\sqrt{2\pi\sigma(t)^2}} exp\left(-\frac{x^2}{2\sigma(t)^2}\right) \\
\left\langle x(t)^2 \right\rangle &= \int_{-\infty}^{\infty} x^2 \frac{1}{\sqrt{2\pi\sigma(t)^2}} exp\left(-\frac{x^2}{2\sigma(t)^2}\right) dx \\
\left\langle x(t)^2 \right\rangle &= \int_{-\infty}^{\infty} \sigma(t)^2 x \frac{1}{\sqrt{2\pi\sigma(t)^2}} d\left(\exp\frac{-x^2}{2\sigma(t)^2}\right) \\
\left\langle x(t)^2 \right\rangle &= \sigma(t)^2 \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\sigma(t)^2}} exp\left(-\frac{x^2}{2\sigma(t)^2}\right) dx \\
\left\langle x(t)^2 \right\rangle &= \sigma(t)^2
\end{aligned}$$

Therefore,the spatial expectation value $\left\langle x(t)^2 \right\rangle$ of the 1D Normal Distribution equals $\sigma(t)^2$

2.2 Part B

The diffusion equation is:

$$\frac{\partial\phi(\vec{r},t)}{\partial t} = D\nabla^2\phi(\vec{r},t)$$

where $D = 2$ is a diffusion constant.
For a linear diffusion equation:

$$\frac{\partial\phi(\vec{r},t)}{\partial t} = D\frac{d^2\phi(\vec{r},t)}{dx^2}$$

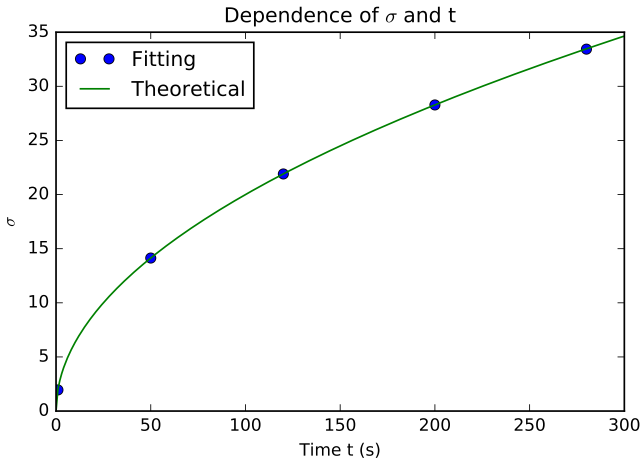
The numerical solution is:

$$\begin{aligned}
\frac{y_{j+1,i} - y_{j,i}}{\Delta t} &= D\frac{y_{j,i+1} + y_{j,i-1} - 2y_{j,i}}{\Delta x^2} \\
y_{j+1,i} &= y_{i,j} + \frac{D\Delta t}{\Delta x^2}(y_{j,i+1} + y_{j,i-1} - 2y_{j,i})
\end{aligned}$$

After getting y in each x for each time snapshot, we obtained $\sigma(t)$ by fitting it into equation:

$$\rho(x,t) = \frac{1}{\sqrt{2\pi\sigma(t)^2}} exp\left(-\frac{x^2}{2\sigma(t)^2}\right)$$

We choose 5 time snapshots [1,50,120,200,280]($\Delta t = 0.01$) to get $\sigma(t)$ and plot them in following figure.



The fitting points match the analytical function perfectly.