

SOUTHERN UNIVERSITY OF SCIENCE AND TECHNOLOGY

BIO304: SYSTEMS BIOLOGY

Project 3

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1 Simulate simple 2D Brownian motion of *E.coli*

1.1 Symbols

TABLE 1.1: The symbols used in the model of simulating simple 2D Brownian motion of *E.coli*

Symbol	Definition
$X(t)$	Stochastic processes
X_i	The direction of movement $X_i = 1, -1$
$B(t)$	Standard Brownian Motion
$N(\mu, \sigma)$	Normal distribution with mean μ and standard deviation σ
Δx	Space interval
Δt	Time interval
σ	$\sigma = \Delta x / \sqrt{\Delta t}$
(x, y)	Coordinates of <i>E.coli</i>
x_t	Coordinate in x axis at time t
y_t	Coordinate in y axis at time t
v	The speed of the movement of <i>E.coli</i>

1.2 Biological background

Escherichia coli is a Gram-negative, optional anaerobic, rod-shaped, coliform bacterium of the genus *Escherichia* that is commonly found in the lower intestine of warm-blooded organisms. *E.coli* are widely used in biological research, cells are typically rod-shaped, and are about $2.0 \mu m$ long and $0.25-1.0 \mu m$ in diameter, with a cell volume of $0.6-0.7 \mu m^3$. Strains that possess flagella are motile. The flagella have a peritrichous arrangement. It also attaches and effaces to the microvilli of the intestines via an adhesion molecule known as intimin. The thin straight filaments of bacteria called pili, that enable it to attach to specify substrate, and thicker longer helical filaments, called flagella, that enable it to swim.

Brownian motion is the random motion of microscopic particles suspended in a fluid resulting from their collision with the quick atoms or molecules in the liquid or gas. This phenomenon is named after British botanist Robert Brown. In 1827, while looking through a microscope at particles trapped in cavities inside pollen grains in water, Brown noted that the particles moved through the water randomly but failed to explain the mechanisms that caused this movement. He supposed that active molecules were inside those particles thus there was no relationship with the surrounded liquid.

The Brownian motion is a Gaussian process with time t , we can find that, for stochastic processes $\{X(t), t \geq 0\}$:

$$X(0) = 0$$

$$X(t) \sim N(0, \sigma^2 t)$$

$$X(t) = \Delta x (X_1 + \dots + X_{[t/\Delta t]})$$

$$\sigma^2 = \frac{(\Delta x)^2}{\Delta t}$$

Normally, we set $\sigma = 1$ and defines this kind of stochastic processes $\{X(t), t \geq 0\}$ as **Standard Brownian Motion** and they could be denote as $\{B(t), t \geq 0\}$, where :

$$B(0) = 0$$

$$B(t) \sim N(0, t)$$

1.3 Hypothesis for simulation

Assuming the *E.coli* here have no mitosis, so the number of cells maintain constant. I use (x, y) to define the location of each cell, assume all the cells start from origin $(0, 0)$. They have a random judging for each step in both x and y directions. Set the speed as $50\mu m/s$, so for each step,

$$\phi_x \sim N(0, 1)$$

$$\phi_y \sim N(0, 1)$$

$$x_{t+1} = x_t + \phi_x v$$

$$y_{t+1} = y_t + \phi_y v$$

The move on both x and y directions are random and it follows the Brownian motion.

So in theory, for a *E.coli* population large enough, we have:

$$\frac{1}{n} \sum_{i=1}^n x_i(t) \approx 0$$

$$\frac{1}{n} \sum_{i=1}^n y_i(t) \approx 0$$

$$\frac{1}{n} \sum_{i=1}^n x_i(t)^2 \approx v^2 t = 250t$$

$$\frac{1}{n} \sum_{i=1}^n y_i(t)^2 \approx v^2 t = 250t$$

1.4 Results of simulation

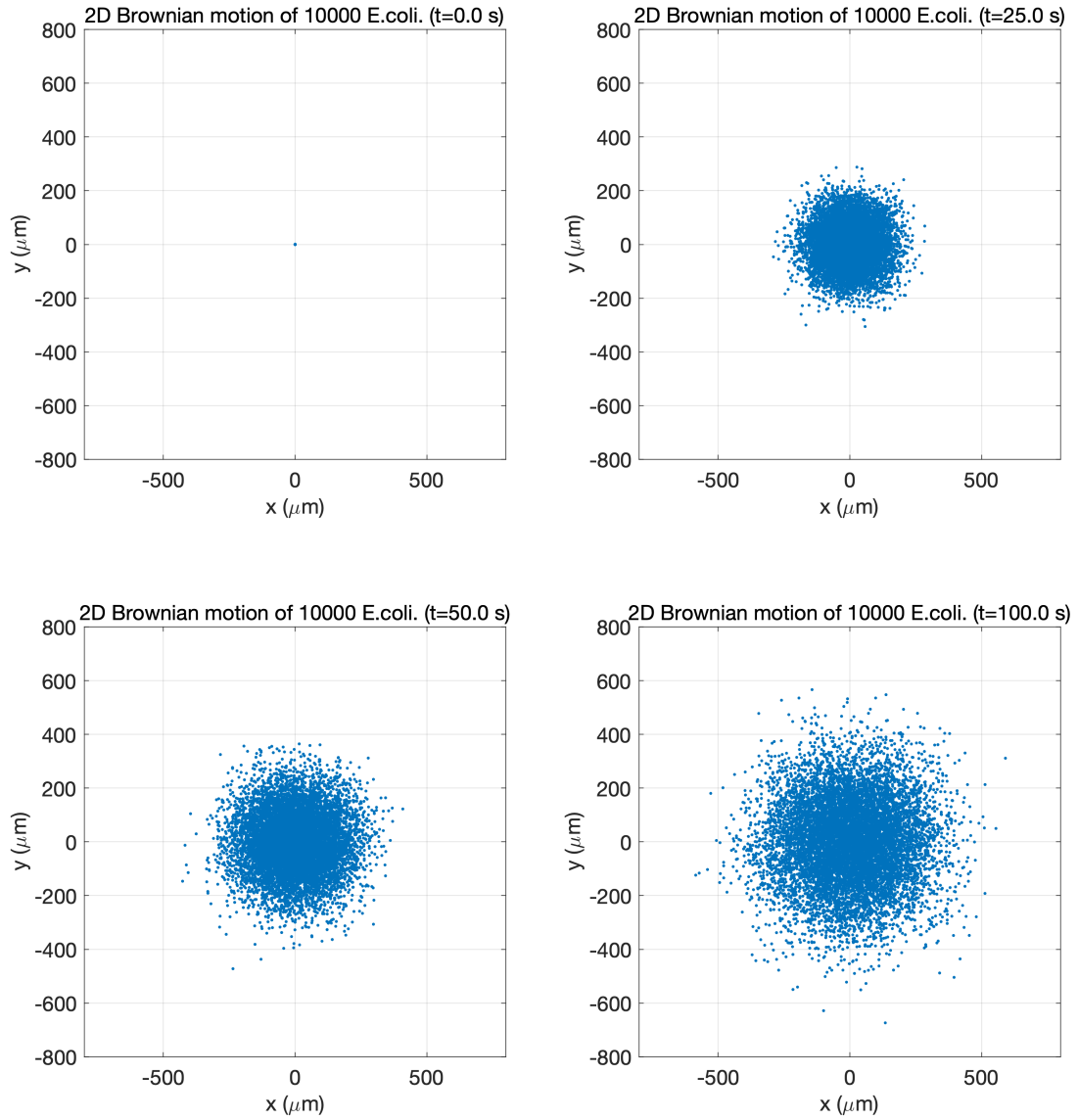


FIGURE 1.1: The simulation of 10000 *E. coli* cells for simple 2D Brownian motion from (0,0) after 100s

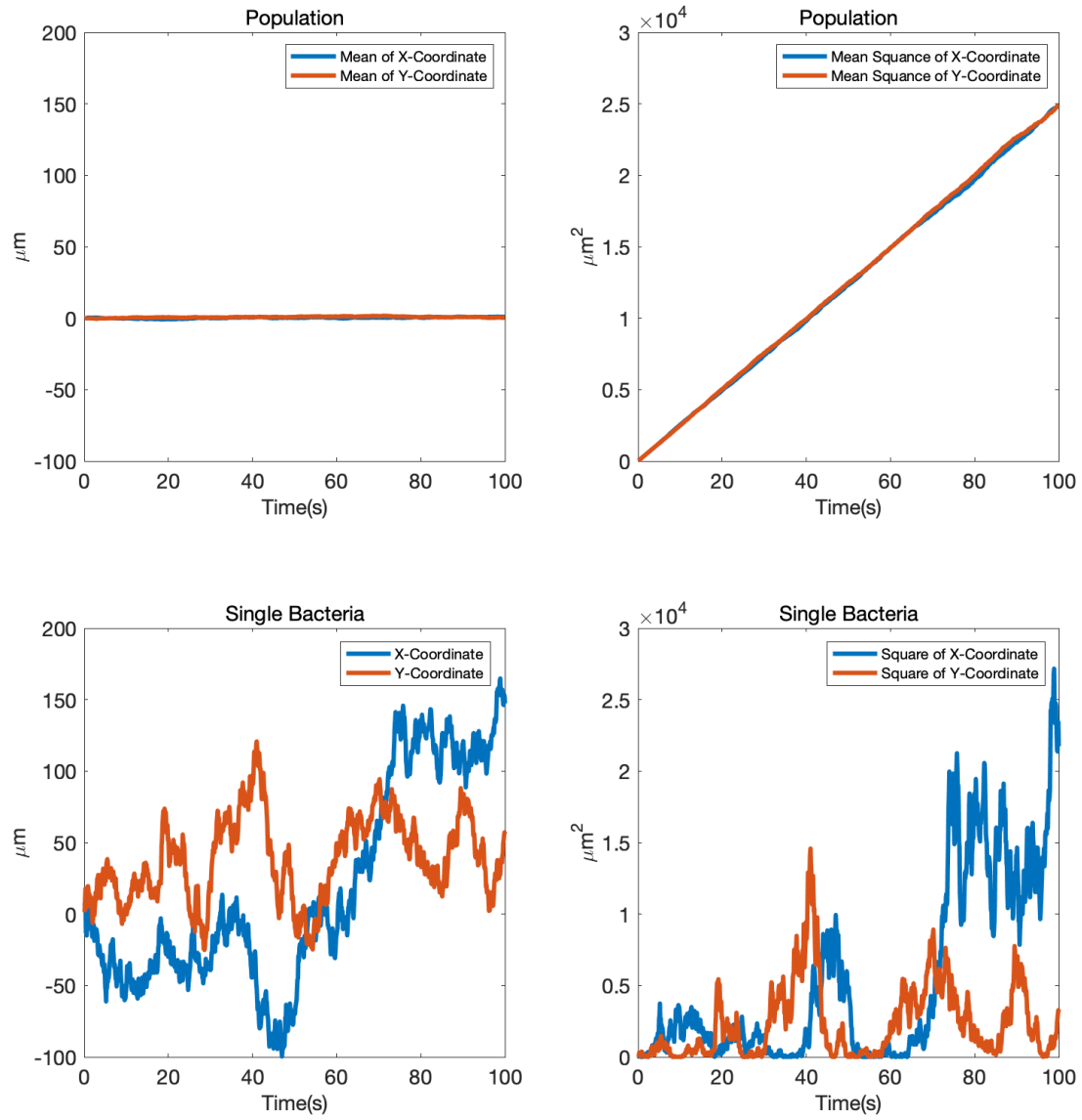


FIGURE 1.2: The "mean displacement" and "mean displacement-square" over-time for simple 2D brownic motion

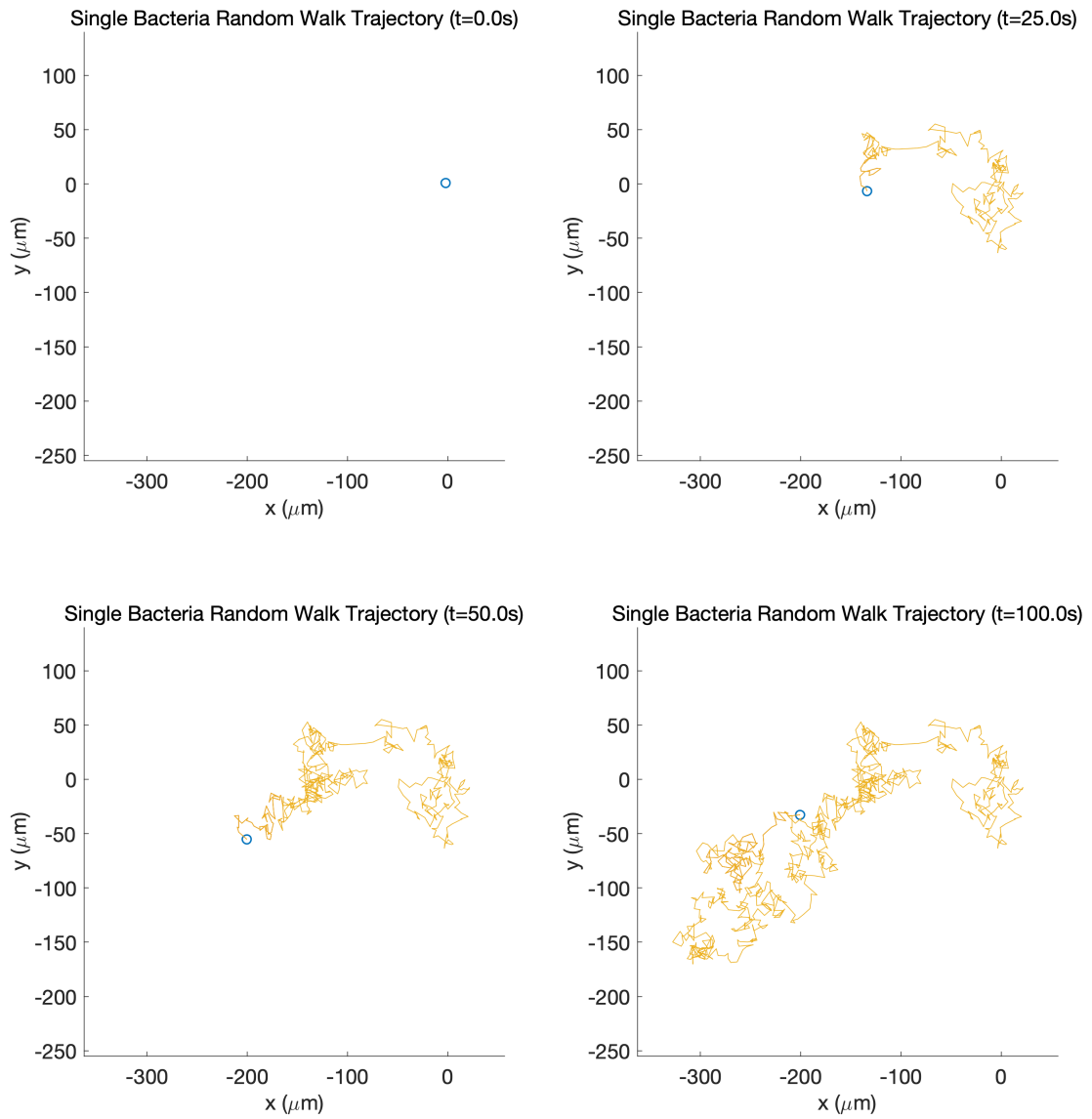


FIGURE 1.3: Single Bacteria Random Walk Trajectory

2 Simulate 2D Brownian motion of *E.coli* with constant chemoattractant(A) gradient along x-direction

2.1 Symbols

TABLE 2.1: The symbols used in the model of simulating simple 2D Brownian motion of *E.coli* with constant chemoattractant(A) gradient along x-direction

Symbol	Definition
$N(\mu, \sigma)$	Normal distribution with mean μ and standard deviation σ
Δx	Space interval
Δt	Time interval
σ	$\sigma = \Delta x / \sqrt{\Delta t}$
(x, y)	Coordinates of <i>E.coli</i>
x_t	Coordinate in x axis at time t
y_t	Coordinate in y axis at time t
v	The speed of the movement of <i>E.coli</i>
A	The chemoattractant
A_0	The chemoattractant at $x = 0$
k	Gradient of chemoattractant along x-direction

2.2 Hypothesize our own chemotaxis actions

$$A(x) = A_0 + kx$$

2.3 Hypothesis for simulation

Assuming the *E.coli* here have no mitosis, so the number of cells maintain constant. I use (x, y) to define the location of each cell, assume all the cells start from origin $(0, 0)$. They have a random judging for each step in both x and y directions. Set the speed as $50\mu m/s$, so for each step,

$$\phi_x \sim N(0, 1)$$

$$\phi_y \sim N(0, 1)$$

$$x_{t+1} = x_t + \phi_x v + \max[(A_0 + kx_t), 0]$$

$$y_{t+1} = y_t + \phi_y v$$

2.4 Results of simulation

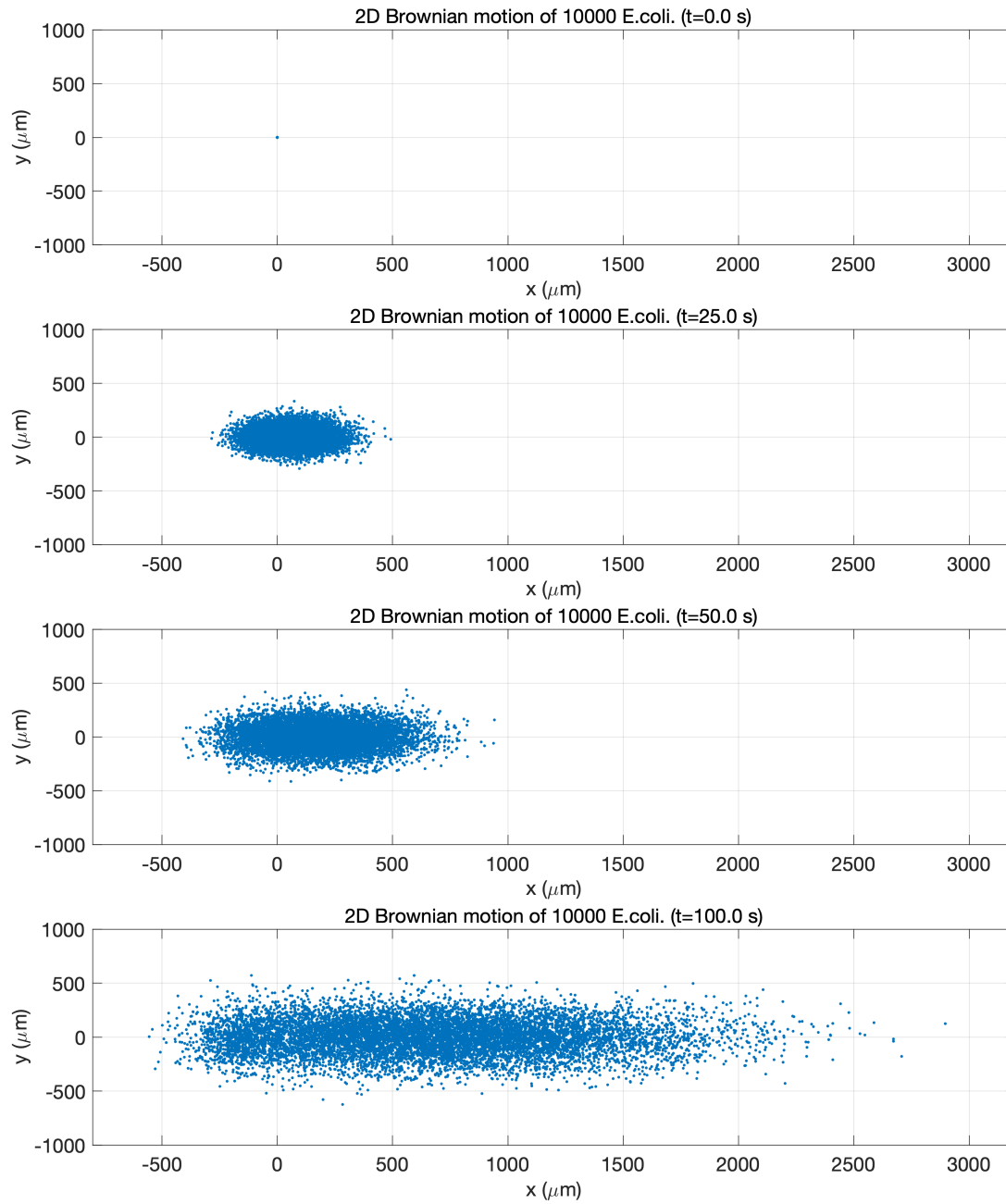


FIGURE 2.1: The simulation of 10000 *E.coli* cells for simple 2D Brownian motion with constant chemoattractant gradient along X-direction form (0,0) after 100s
 ** $A_0 = 2\mu\text{m}$ and $k = 0.02$

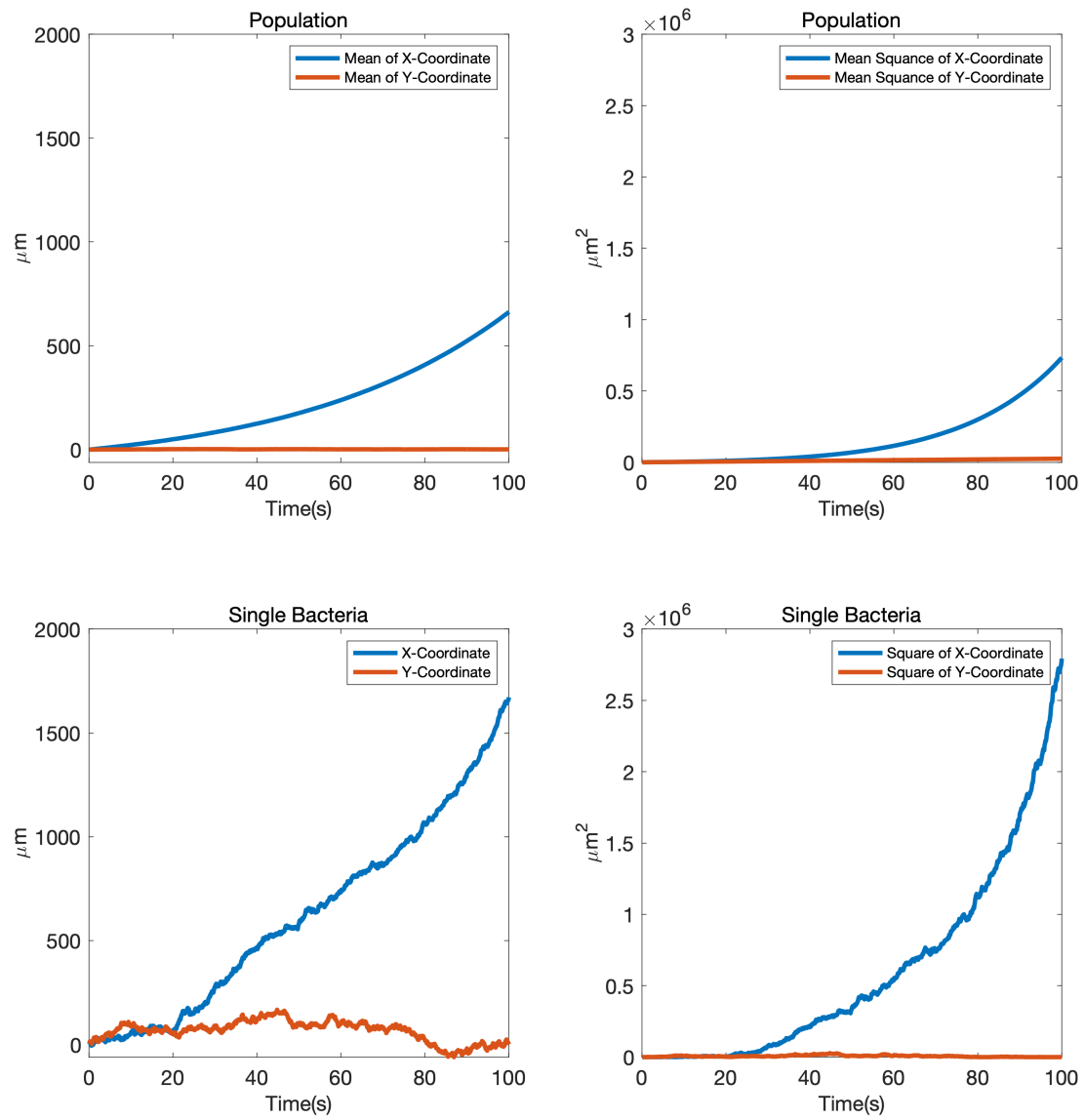


FIGURE 2.2: The "mean displacement" and "mean displacement-square" over-time for simple 2D brownic motion

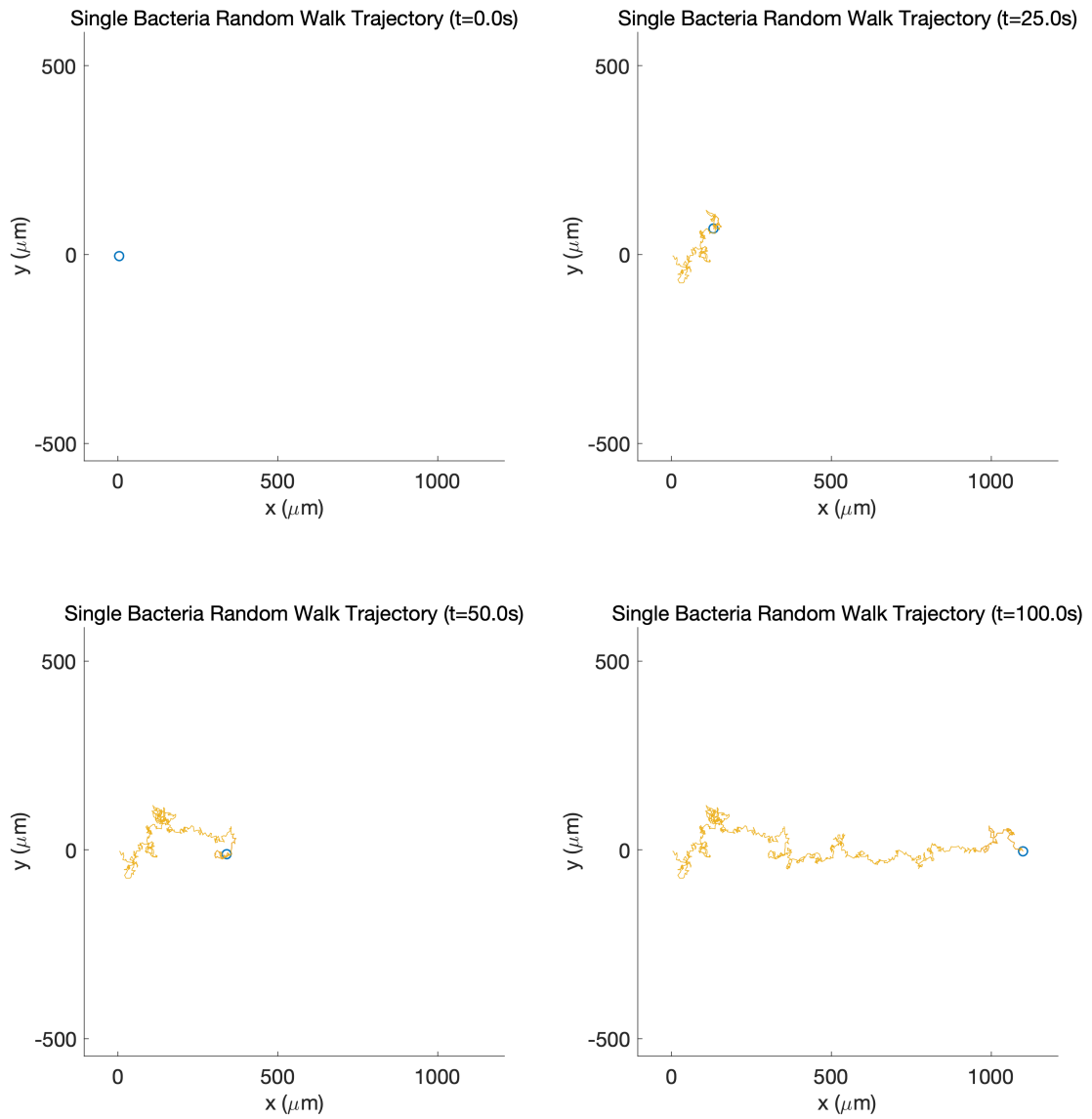


FIGURE 2.3: Single Bacteria Random Walk Trajectory

2.5 Comparing “simple Brownian motion” and “Brownian motion with chemotaxis in x-direction” for 10000 cells.

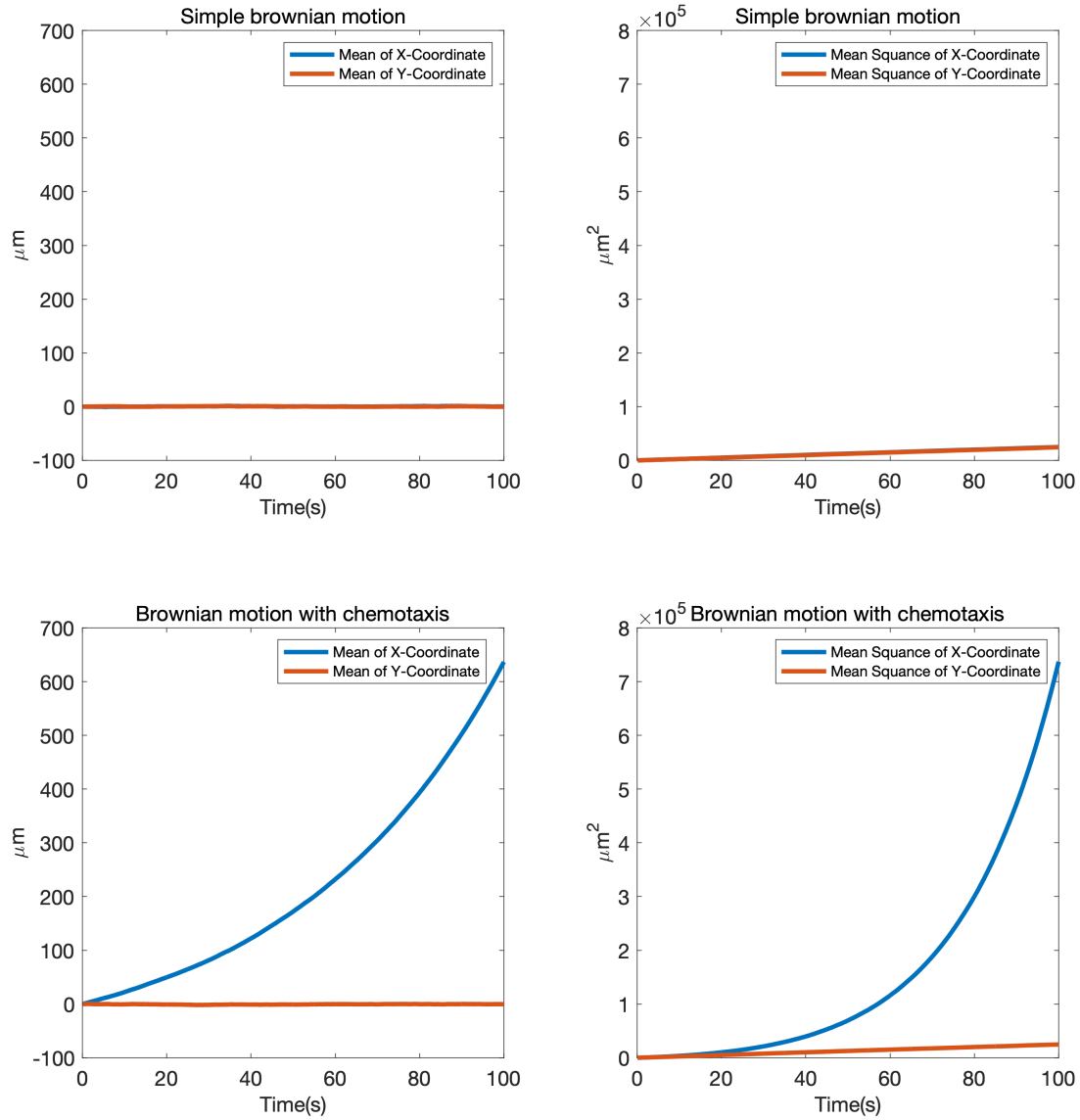


FIGURE 2.4: compare the “mean displacement” and “mean displacement-square” overtime between “simple Brownian motion” with “Brownian motion with chemotaxis in x-direction” for 10000 cells.

The simple 2D Brownian motion shows the random movement of the cells, both "mean displacement" and "mean displacement-square" show no distinct changes. While the simple model simulation shows the chemoattractant's influence on the E.coli motion, the "mean displacement" and "mean displacement-square" on X-direction are extremely increased. It really shows the chemotaxis's influence on the movement of E.coli, but it has no much biological meanings.

3 Image processing and tracking of all the cells in the given *E.coli* movie using u-track 2.0, and perform data analysis

3.1 Get data form movie

For the video: 1 pixel = $0.65\ \mu m$, 1 frame = 0.1 second.

The data were extracted by u-track to track the cell by method of Single-Particles and Gaussian Mixture-model Fitting. There are more than 14000 tracks.

3.2 Single bacteria trajectory

Form 14721 tracks, I choosed the track with the biggest number of un-NAN values and removed all of the NAN value to plot the movement of this single bacteria.

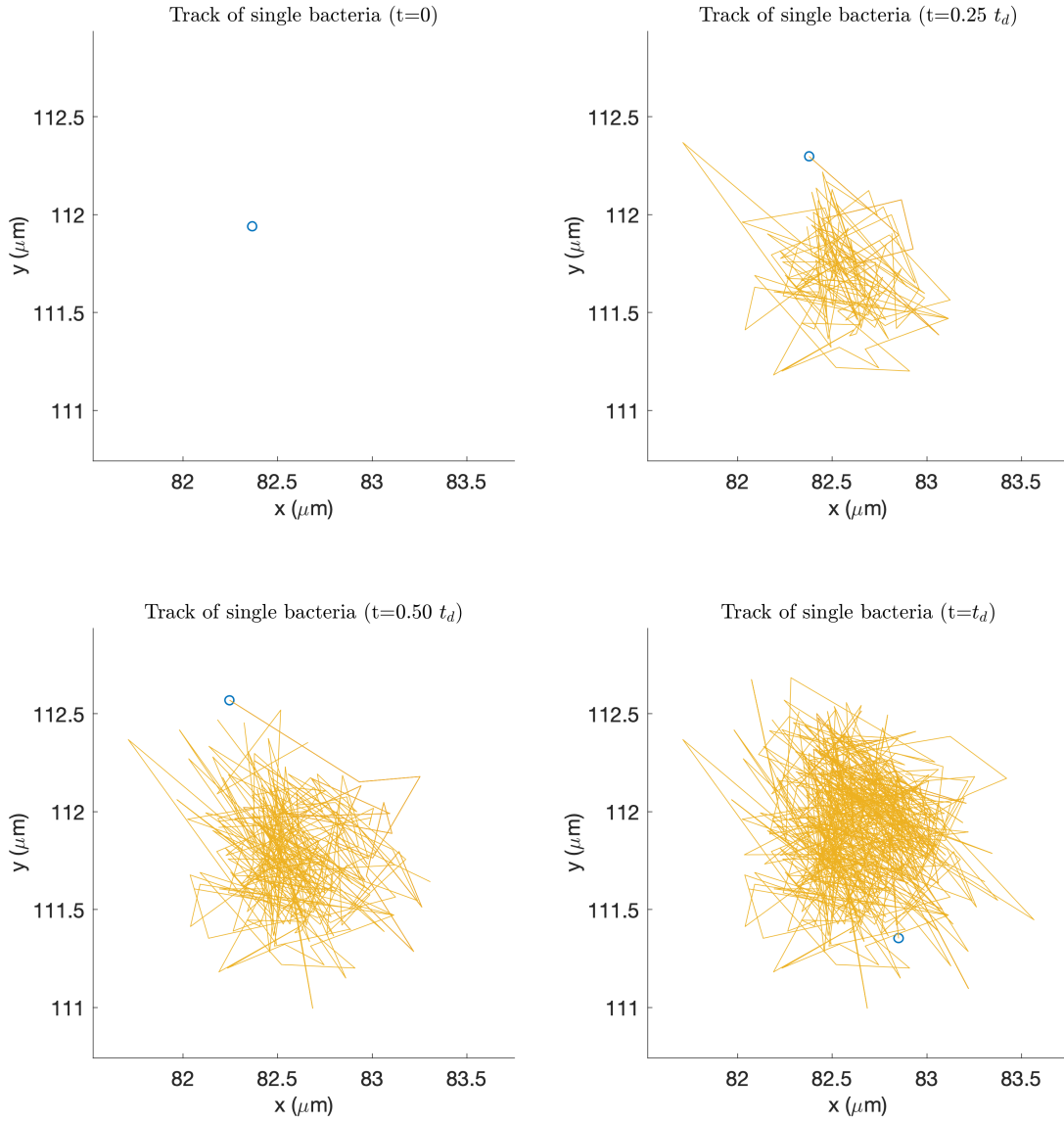


FIGURE 3.1: Single Bacteria Random Walk Trajectory

3.3 Bacteria population trajectory

Also track all the cells from the data, to calculate the population motions. The statistical results are shown in Figure 3.2.

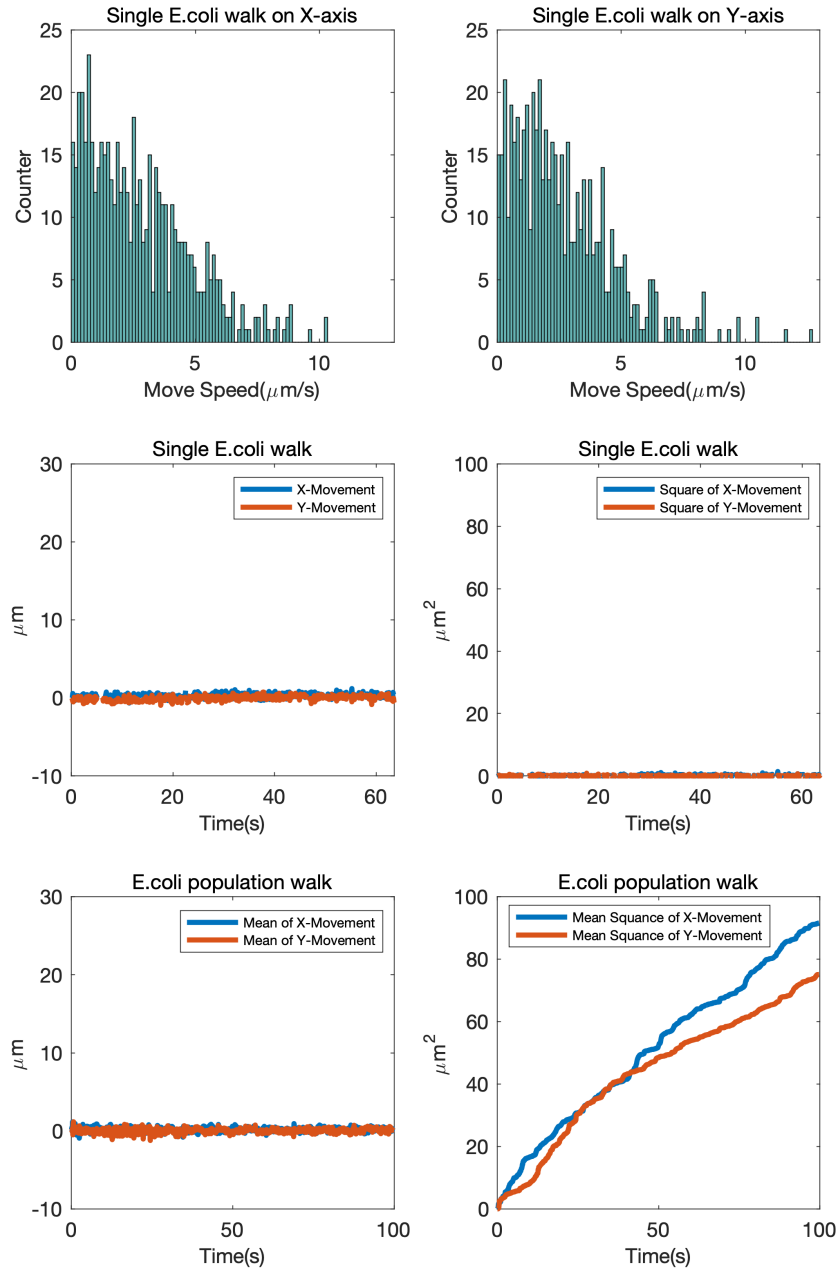


FIGURE 3.2: The “mean displacement” and “mean displacement-square” over-time for the cells in vedio

3.4 Fitting the Data with the Model

For a series of scatter points $(x_i, y_i) (i = 1, 2, \dots, n)$, if a direct proportional function was used to fit the data, we have:

$$y = \beta x$$

$$\beta = \sum_{i=1}^n x_i y_i / \sum_{i=1}^n x_i^2$$

As for our model:

$$\frac{1}{n} \sum_{i=1}^n x_i(t)^2 = v_x^2 t$$

$$\frac{1}{n} \sum_{i=1}^n y_i(t)^2 = v_y^2 t$$

So there are the fitting model:

$$\frac{1}{n} \sum_{i=1}^n x_i(t)^2 = \beta_x t = v_x^2 t$$

$$\frac{1}{n} \sum_{i=1}^n y_i(t)^2 = \beta_y t = v_y^2 t$$

$$\beta_x = \sum_{i=1}^n t_i x_i / \sum_{i=1}^n t_i^2$$

$$\beta_y = \sum_{i=1}^n t_i y_i / \sum_{i=1}^n t_i^2$$

We get:

$$\beta_x = 0.9862 \mu m^2 / s^2$$

$$v_x = 0.9931 \mu m / s$$

$$\beta_y = 0.8366 \mu m^2 / s^2$$

$$v_y = 0.9147 \mu m / s$$

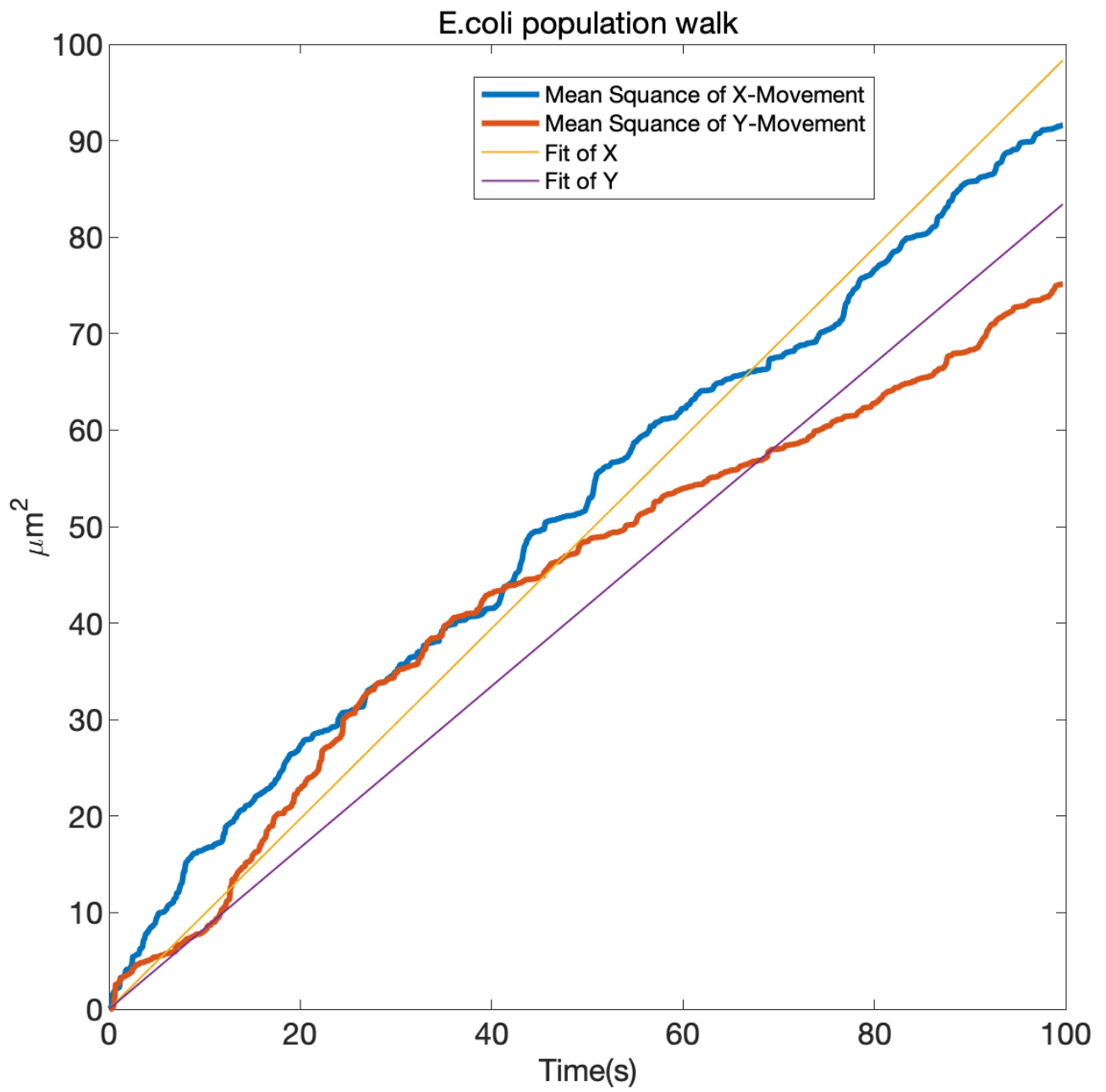


FIGURE 3.3: Fitting the Data by Model