Problem1-random_walkers

April 9, 2021

1 Random walks

Now we will look at Random walks in n dimensions. This will be the first Markov Chain Monte Carlo (MCMC) that we will utilize.

We will keep track of the paths of random walkers and use it to derive the conditions for diffusion in Brownian motion.

The "choice" and "cumsum" strategy here is adapted from here

[1]:
```
import numpy as np
import matplotlib.pyplot as plt
```

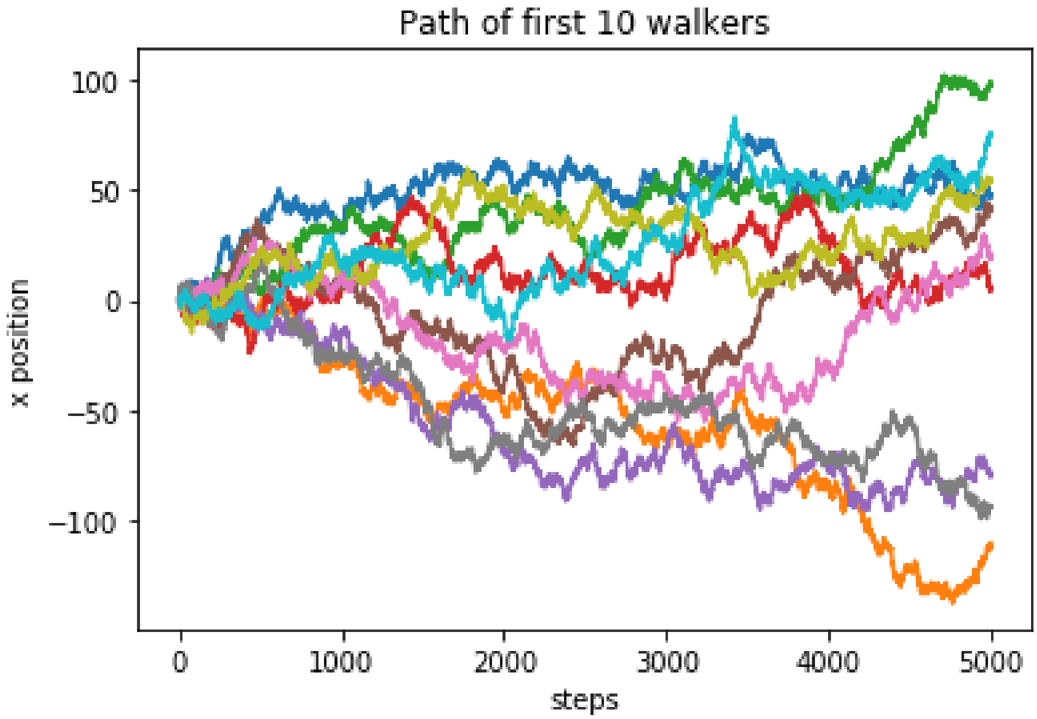
1.0.1 Run the walkers

[2]:
```
dims = 3
n_walkers = 1000
n_steps = 5000
t = np.arange(n_steps)
# Walkers can go in + direction, - direction, or stay still
step_set = [-1, 0, 1]
# The shape is for "n_walkers" taking "n_steps" in "dims" dimensions.
# So, in 1d if there are 10 walkers making 100 steps each,
# it will be (10, 100, 1)
step_shape = (n_walkers,n_steps,dims)
# These are the steps at each stage
steps = np.random.choice(a=step_set, size=step_shape)
# Now we add up the steps for each walker to get the x positions
x = steps.cumsum(axis=1)
```

1.0.2 Plot the x position of the first 10 walkers

[3]:
```
for i in range( min(10,n_walkers) ):
    plt.plot( x[i,:,0] )
plt.title("Path of first 10 walkers")
plt.xlabel("steps")
plt.ylabel("x position")
```

```
[3]: Text(0, 0.5, 'x position')
```



1.0.3 Accumulate statistics

Here, we now want to determine the relationship between diffusion and walks.

We know from lecture that after the nth step, each walker will have position

$$x_n = \sum_{i=1}^{n} s_i$$

where s_i is each walkers' step from the `steps` construct above. The average of s_i is zero because they are uniformly chosen from $(-1, 0, 1)$. However, the standard deviation for each walker is

$$\langle x_n^2 \rangle = \left\langle \sum_{i=1}^{n} \sum_{j=1}^{n} s_i s_j \right\rangle$$

$$\langle x_n^2 \rangle = \left\langle \sum_{i} s_i^2 \right\rangle + \left\langle \sum_{i} \sum_{j \neq i} s_i s_j \right\rangle$$

If there are m walkers each walking n steps, and the index k iterates over the walkers, then at each step n we have ensemble averages (in 1 dimension):

$$\langle x_n^4 \rangle = \sum_{k=1}^{m} \frac{x_{k,n}^4}{m}$$

$$\langle x_n^2 \rangle = \sum_{k=1}^{m} \frac{x_{k,n}^2}{m}$$

The overall diffusion width at the nth step, taking these ensemble averages, is therefore

$$\sigma_n^2 = \sqrt{\langle x_n^4 \rangle - \langle x_n^2 \rangle^2}$$

1.0.4 Homework assignment will go here:

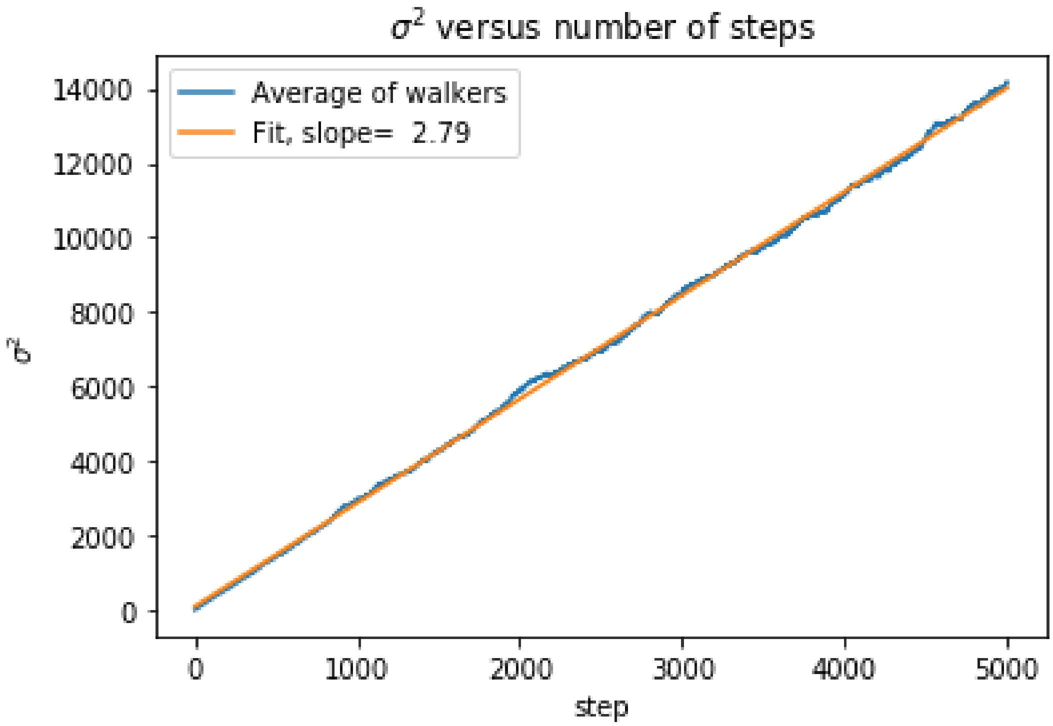
For 1d, 2d, and 3d:

- Calculate and plot σ^2 as a function of n.
- Compute a linear fit of σ^2 as a function of n, and also plot that.
- Compute the diffusion constant D in each of 1d,2d,3d

[4]:
```
# Now get the averages over the walkers
x2 = np.average( x**2, axis=0 )
x4 = np.average( x**4, axis=0 )
sigma2_nd = np.sqrt( x4 - x2**2 )
sigma2 = np.sum( sigma2_nd, axis=1 )
```

[5]:
```
plt.plot( sigma2,  label='Average of walkers' )
res = np.polyfit(t, sigma2,1 )
plt.plot( t, res[0]*t + res[1], label='Fit, slope=%6.2f' % res[0] )
plt.title(r"$\sigma^2$ versus number of steps")
plt.xlabel("step")
plt.ylabel(r"$\sigma^2$")
plt.legend()
```

[5]:
```
<matplotlib.legend.Legend at 0x7f79732438>
```



2 Problem 1

[6]:
```
import tensorflow as tf
```

2.1 1 Dimensions

2.1.1 Run the walkers

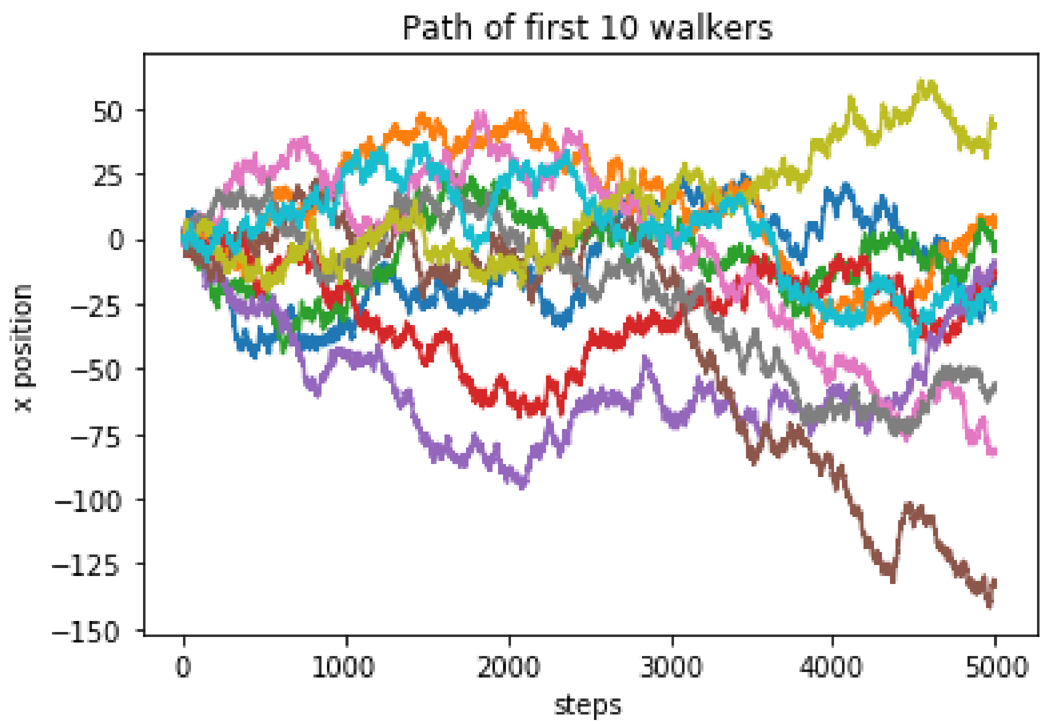
[7]:
```
g = tf.random.Generator.from_seed(1)

dims = 1
n_walkers = 1000
n_steps = 5000
t = np.arange(n_steps)
# Walkers can go in + direction, - direction, or stay still
step_set = [-1, 0, 1]
# The shape is for "n_walkers" taking "n_steps" in "dims" dimensions.
# So, in 1d if there are 10 walkers making 100 steps each,
# it will be (10, 100, 1)
step_shape = (n_walkers,n_steps,dims)
# These are the steps at each stage
steps = np.random.choice(a=step_set, size=step_shape)
steps = tf.random.stateless_uniform(
```

```
    step_shape, [0,1], minval=-1, maxval=2, dtype=tf.int32, name=None
)
# Now we add up the steps for each walker to get the x positions
steps = np.array(steps)
x = steps.cumsum(axis=1)
```

2.1.2 Plot the x position of the first 10 walkers

[8]:
```
for i in range( min(10,n_walkers) ):
    plt.plot( x[i,:,0] )
plt.title("Path of first 10 walkers")
plt.xlabel("steps")
plt.ylabel("x position")
```

[8]:
```
Text(0, 0.5, 'x position')
```



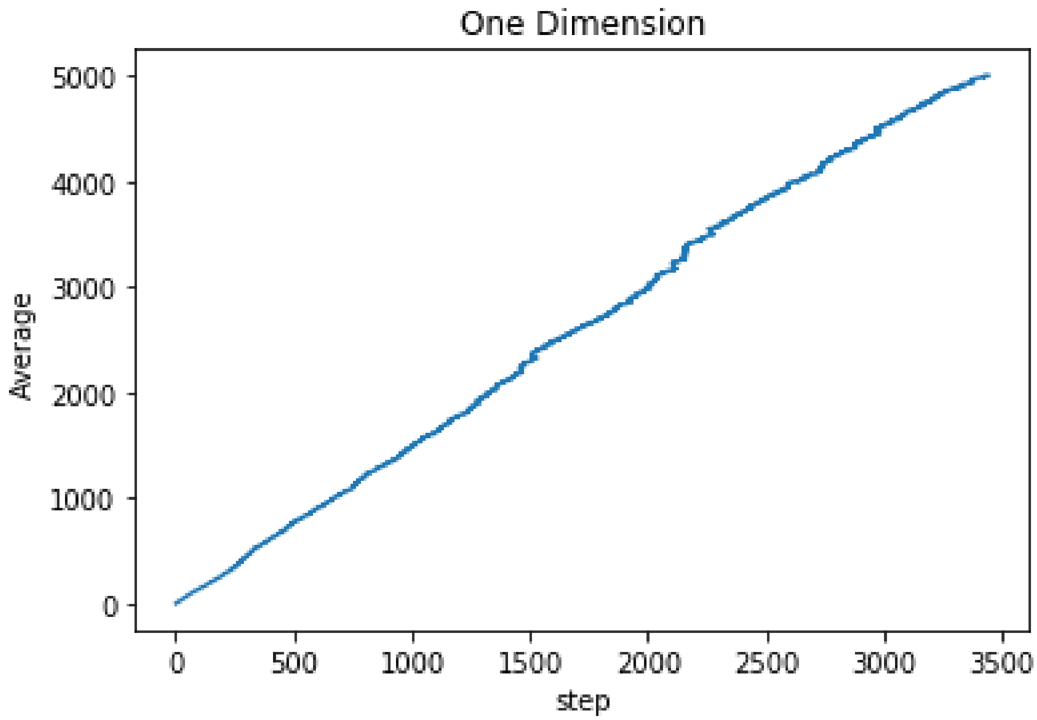
2.1.3 Compute the Averages

[9]:
```
# Now get the averages over the walkers
x2 = np.average( x**2, axis=0 )
x4 = np.average( x**4, axis=0 )
sigma2_nd = np.sqrt( x4 - x2**2 )
sigma2 = np.sum( sigma2_nd, axis=1 )
```

2.1.4 Plot the quantity $\langle |x_n|^2 \rangle$ vs n

[10]:
```
plt.plot( x2,t)
plt.title(r"One Dimension")
plt.xlabel("step")
plt.ylabel(r"Average")
```

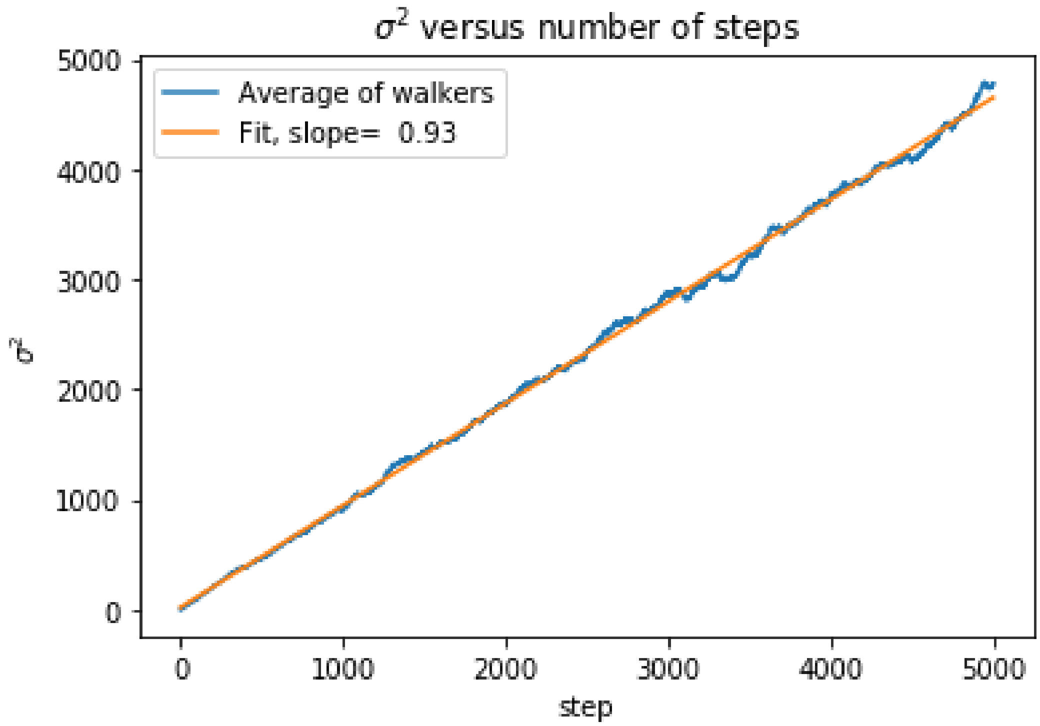
[10]: Text(0, 0.5, 'Average')



2.1.5 Calculate the Diffusion Constant and Compare to Theory

[11]:
```
plt.plot( sigma2,  label='Average of walkers' )
res = np.polyfit(t, sigma2,1 )
plt.plot( t, res[0]*t + res[1], label='Fit, slope=%6.2f' % res[0] )
plt.title(r"$\sigma^2$ versus number of steps")
plt.xlabel("step")
plt.ylabel(r"$\sigma^2$")
plt.legend()
```

[11]: <matplotlib.legend.Legend at 0x7f828f8f98>



[12]:
```
D = res[0]/(dims*2)
theoryD = 1/2
percentError = (abs(D-theoryD)/theoryD)*100
print("The value of the diffusion constant for " + str(dims) + " Dimensions is␣
↪" + str(D))
print("The theoretical value is " + str(theoryD))
print("The percent Error is: " +str(percentError) + " percent")
```

```
The value of the diffusion constant for 1 Dimensions is 0.46279260928789795
The theoretical value is 0.5
The percent Error is: 7.44147814242041 percent
```

2.2 2 Dimensions

2.2.1 Run the walkers

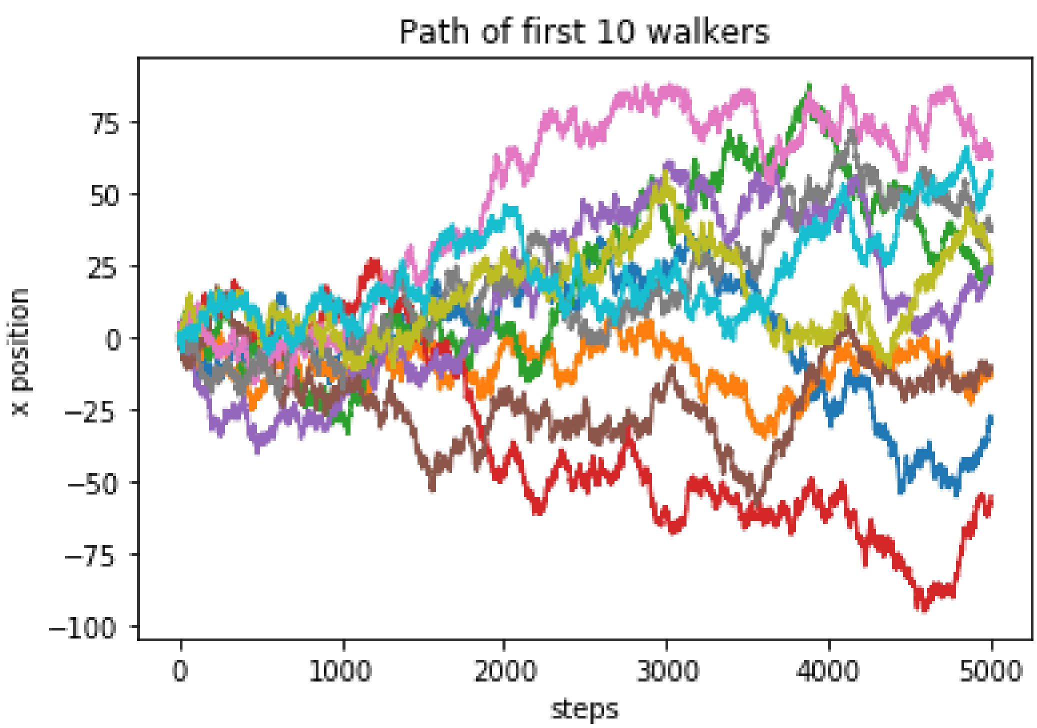
[13]:
```
g = tf.random.Generator.from_seed(1)

dims = 2
n_walkers = 1000
n_steps = 5000
t = np.arange(n_steps)
# Walkers can go in + direction, - direction, or stay still
step_set = [-1, 0, 1]
```

```
# The shape is for "n_walkers" taking "n_steps" in "dims" dimensions.
# So, in 1d if there are 10 walkers making 100 steps each,
# it will be (10, 100, 1)
step_shape = (n_walkers,n_steps,dims)
# These are the steps at each stage
steps = np.random.choice(a=step_set, size=step_shape)
steps = tf.random.stateless_uniform(
    step_shape, [0,1], minval=-1, maxval=2, dtype=tf.int32, name=None
)
# Now we add up the steps for each walker to get the x positions
steps = np.array(steps)
x = steps.cumsum(axis=1)
```

2.2.2 Plot the x position of the first 10 walkers

[14]:
```
for i in range( min(10,n_walkers) ):
    plt.plot( x[i,:,0] )
plt.title("Path of first 10 walkers")
plt.xlabel("steps")
plt.ylabel("x position")
```

[14]:
```
Text(0, 0.5, 'x position')
```



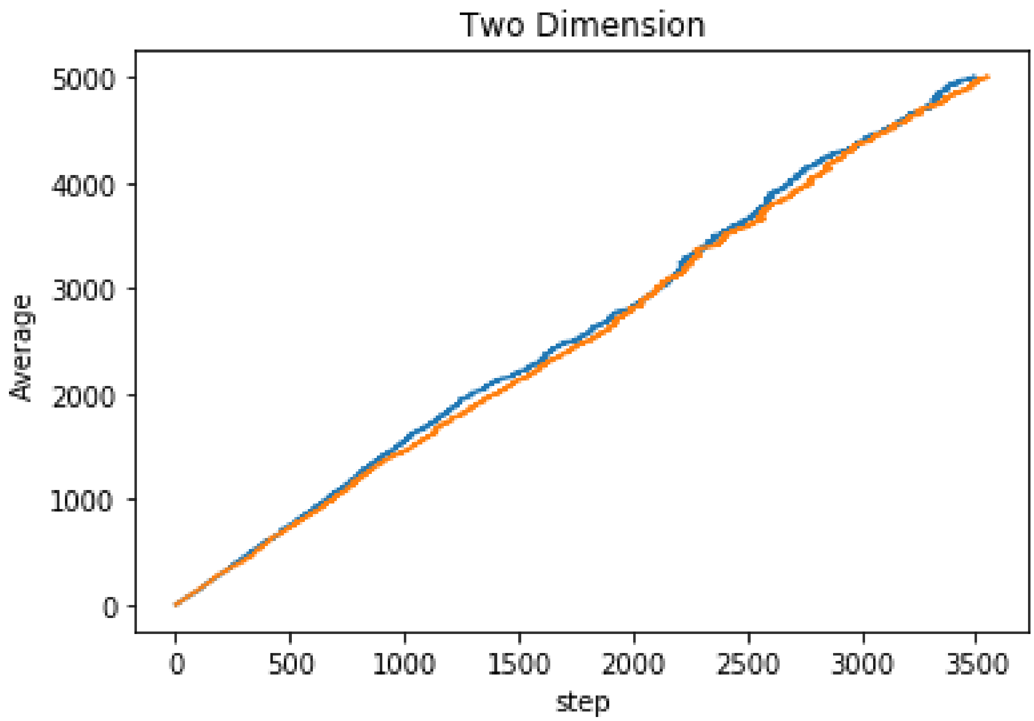
2.2.3 Compute the Averages

[15]:
```
# Now get the averages over the walkers
x2 = np.average( x**2, axis=0 )
x4 = np.average( x**4, axis=0 )
sigma2_nd = np.sqrt( x4 - x2**2 )
sigma2 = np.sum( sigma2_nd, axis=1 )
```

2.2.4 Plot the quantity $\langle |x_n|^2 \rangle$ vs n

[16]:
```
plt.plot( x2,t)
plt.title(r"Two Dimension")
plt.xlabel("step")
plt.ylabel(r"Average")
```

[16]: Text(0, 0.5, 'Average')

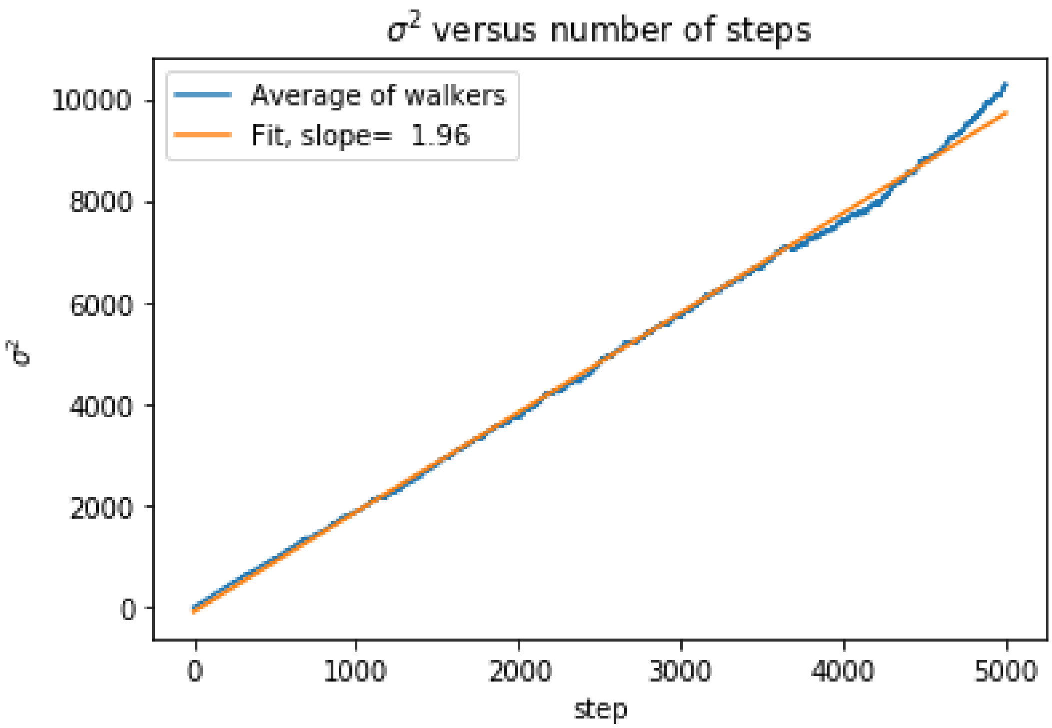


2.2.5 Calculate the Diffusion Constant and Compare to Theory

[17]:
```
plt.plot( sigma2,  label='Average of walkers' )
res = np.polyfit(t, sigma2,1 )
plt.plot( t, res[0]*t + res[1], label='Fit, slope=%6.2f' % res[0] )
plt.title(r"$\sigma^2$ versus number of steps")
```

```
plt.xlabel("step")
plt.ylabel(r"$\sigma^2$")
plt.legend()
```

[17]: <matplotlib.legend.Legend at 0x7f827c7198>



[18]:
```
D = res[0]/(dims*2)
theoryD = 1/2
percentError = (abs(D-theoryD)/theoryD)*100
print("The value of the diffusion constant for " + str(dims) + " Dimensions is␣
 ↪" + str(D))
print("The theoretical value is " + str(theoryD))
print("The percent Error is: " +str(percentError) + " percent")
```

```
The value of the diffusion constant for 2 Dimensions is 0.4904570667290827
The theoretical value is 0.5
The percent Error is: 1.908586654183464 percent
```

2.3 3 Dimensions

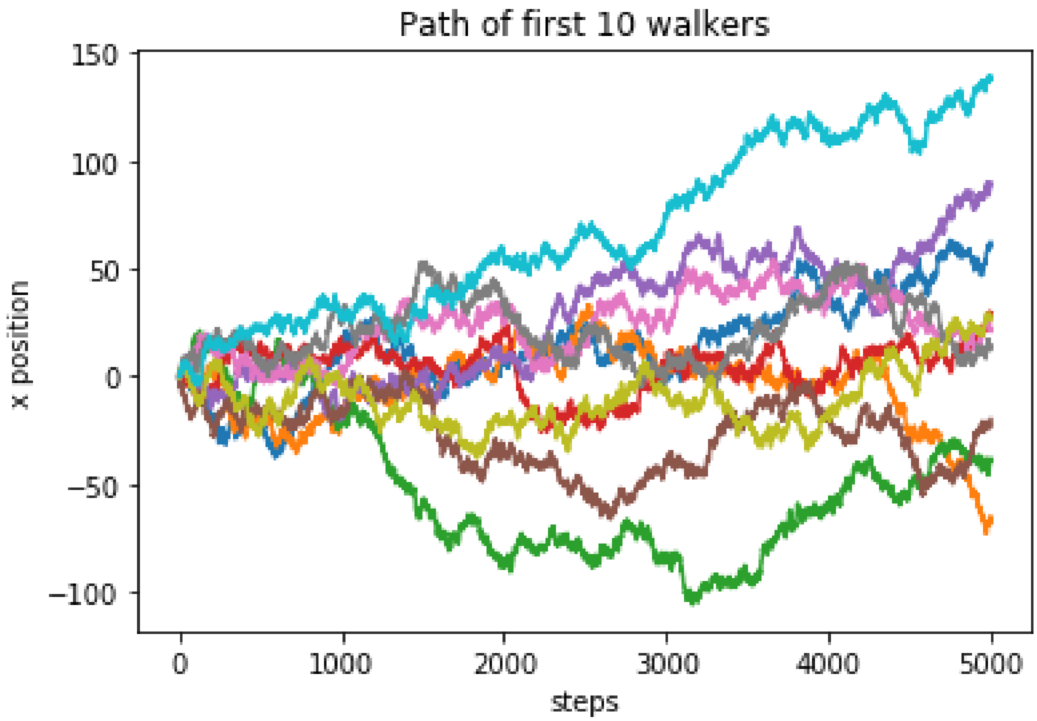
2.3.1 Run the walkers

[19]:
```
g = tf.random.Generator.from_seed(1)

dims = 3
n_walkers = 1000
n_steps = 5000
t = np.arange(n_steps)
# Walkers can go in + direction, - direction, or stay still
step_set = [-1, 0, 1]
# The shape is for "n_walkers" taking "n_steps" in "dims" dimensions.
# So, in 1d if there are 10 walkers making 100 steps each,
# it will be (10, 100, 1)
step_shape = (n_walkers,n_steps,dims)
# These are the steps at each stage
steps = np.random.choice(a=step_set, size=step_shape)
steps = tf.random.stateless_uniform(
    step_shape, [0,1], minval=-1, maxval=2, dtype=tf.int32, name=None
)
# Now we add up the steps for each walker to get the x positions
steps = np.array(steps)
x = steps.cumsum(axis=1)
```

2.3.2 Plot the x position of the first 10 walkers

[20]:
```
for i in range( min(10,n_walkers) ):
    plt.plot( x[i,:,0] )
plt.title("Path of first 10 walkers")
plt.xlabel("steps")
plt.ylabel("x position")
```

[20]:
```
Text(0, 0.5, 'x position')
```



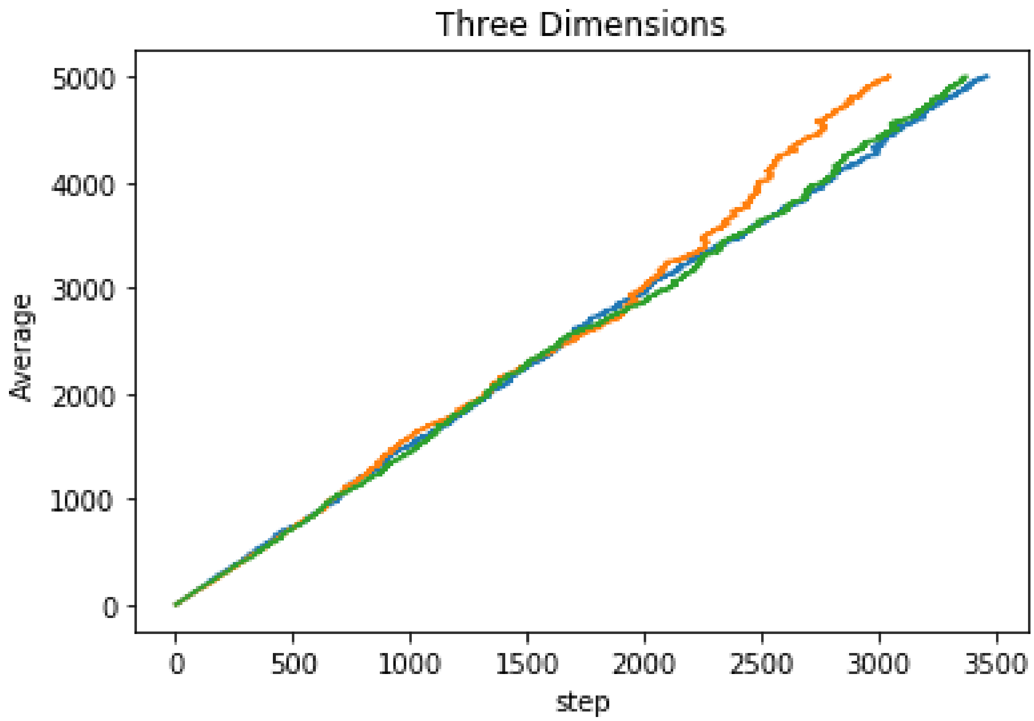
2.3.3 Compute the Averages

[21]:
```
# Now get the averages over the walkers
x2 = np.average( x**2, axis=0 )
x4 = np.average( x**4, axis=0 )
sigma2_nd = np.sqrt( x4 - x2**2 )
sigma2 = np.sum( sigma2_nd, axis=1 )
```

2.3.4 Plot the quantity $\langle |x_n|^2 \rangle$ vs n

[22]:
```
plt.plot( x2,t)
plt.title(r"Three Dimensions")
plt.xlabel("step")
plt.ylabel(r"Average")
```

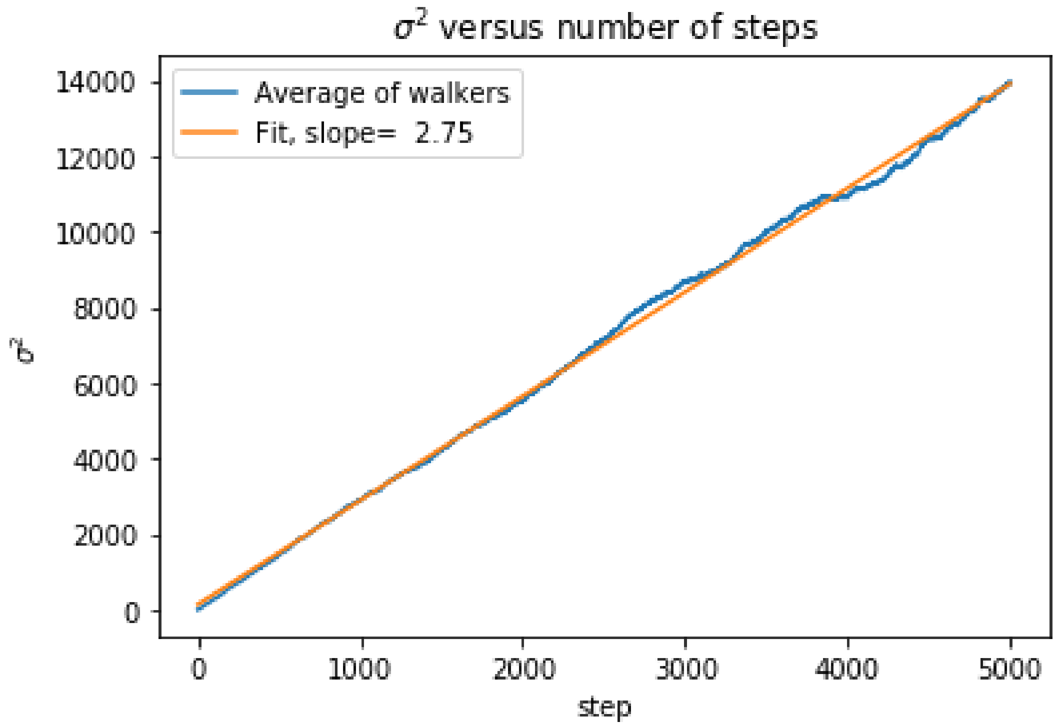
[22]: Text(0, 0.5, 'Average')



2.3.5 Calculate the Diffusion Constant and Compare to Theory

[23]:
```
plt.plot( sigma2,  label='Average of walkers' )
res = np.polyfit(t, sigma2,1 )
plt.plot( t, res[0]*t + res[1], label='Fit, slope=%6.2f' % res[0] )
plt.title(r"$\sigma^2$ versus number of steps")
plt.xlabel("step")
plt.ylabel(r"$\sigma^2$")
plt.legend()
```

[23]: <matplotlib.legend.Legend at 0x7f8268fda0>



[24]:
```
D = res[0]/(dims*2)
theoryD = 1/2
percentError = (abs(D-theoryD)/theoryD)*100
print("The value of the diffusion constant for " + str(dims) + " Dimensions is " + str(D))
print("The theoretical value is " + str(theoryD))
print("The percent Error is: " +str(percentError) + " percent")
```

```
The value of the diffusion constant for 3 Dimensions is 0.4591364281910324
The theoretical value is 0.5
The percent Error is: 8.17271436179352 percent
```

[ ]:
```
```