

Problem1

April 7, 2021

1 Problem 1: Tensorflow Random Walks

We implement the numpy Random Walks code from the [ubsuny/CompPhys](#) repository in 1D, 2D, and 3D. We also rewrite the code to use tensorflow functions instead of numpy. For each dimension, we plot $\langle |x_n|^2 \rangle$ and calculate the diffusion coefficient (or constant). We compare the diffusion coefficients calculated in the numpy and tensorflow methods.

The diffusion coefficient is calculated using the equation,

$$\sigma_n^2 = 2Dn$$

where,

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

is the diffusion width at the n^{th} step and D is the diffusion coefficient. In 1D, with m walkers, the equations for $\langle x_n^4 \rangle$ and $\langle x_n^2 \rangle^2$ are,

$$\begin{aligned}\langle x_n^2 \rangle &= \sum_{k=1}^m \frac{x_{k,n}^2}{m}, \text{ and} \\ \langle x_n^4 \rangle &= \sum_{k=1}^m \frac{x_{k,n}^4}{m}.\end{aligned}$$

For 2D and 3D, instead of using $\langle x_n^2 \rangle$ and $\langle x_n^4 \rangle$, we use,

$$\begin{aligned}\langle r_n^2 \rangle &= \sum_{i=1}^{dims} \sum_{k=1}^m \frac{u_{k,i,n}^2}{m}, \text{ and} \\ \langle r_n^4 \rangle &= \sum_{i=1}^{dims} \sum_{k=1}^m \frac{u_{k,i,n}^4}{m}.\end{aligned}$$

where $u_{k,i,n}$ is walker k 's position at step n in dimension i . Therefore, for 2 dimensions, we calculate the diffusion coefficient using the equations,

$$\begin{aligned}\sigma_n^2 &= \sigma_{n,1}^2 + \sigma_{n,2}^2, \\ &= 2Dn + 2Dn, \\ &= 4Dn,\end{aligned}$$

and for 3 dimensions we use,

$$\begin{aligned}\sigma_n^2 &= \sigma_{n,1}^2 + \sigma_{n,2}^2 + \sigma_{n,3}^2, \\ &= 2Dn + 2Dn + 2Dn, \\ &= 6Dn.\end{aligned}$$

Because σ_n^2 is a linear function of n , we can plot σ_n^2 vs. n and calculate D from the slope of a best fit line.

Tensorflow resources:

https://www.tensorflow.org/guide/random_numbers?hl=hr#setup

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

plt.rcParams['figure.figsize'] = [8.0, 6.0]
plt.rcParams['figure.dpi'] = 100
```

1.1 Numpy Method

In this method, taken from the `ubsuny/CompPhys` repository, the random selector is the numpy function `np.random.choice()`.

```
[2]: plot_num=1
```

```
[3]: n_walkers = 100
n_steps = 5000
t = np.arange(n_steps)
```

```
[4]: # Walkers can go in + direction, - direction, or stay still
step_set = [-1, 0, 1]
```

1.1.1 1D

```
[5]: # 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_1d = (n_walkers, n_steps, 1)
# These are the steps at each stage
start_time_1d_np = time.time()
steps_1d = np.random.choice(a=step_set, size=step_shape_1d)
time_1d_np = time.time() - start_time_1d_np

# Now we add up the steps for each walker to get the x positions
x_1d = steps_1d.cumsum(axis=1)
```

```

# Now get the averages over the walkers
x2_1d = np.average( x_1d**2, axis=0 )
x4_1d = np.average( x_1d**4, axis=0 )
sigma2_nd_1d = np.sqrt( x4_1d - x2_1d**2 )
sigma2_1d = np.sum( sigma2_nd_1d, axis=1 )

```

```

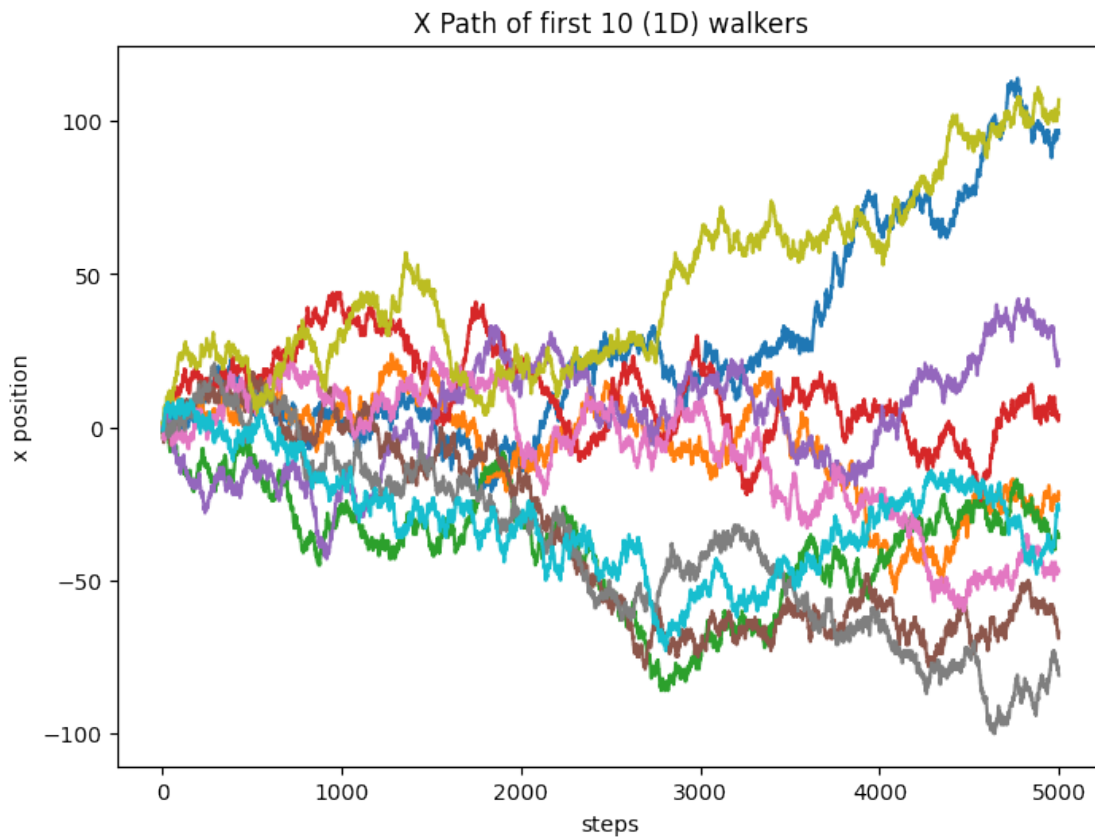
[6]: plt.figure(plot_num)
plot_num = plot_num + 1
for i in range( min(10,n_walkers) ):
    plt.plot( x_1d[i,:,0] )
plt.title("X Path of first 10 (1D) walkers")
plt.xlabel("steps")
plt.ylabel("x position")

```

```

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

```



1.1.2 2D

```
[7]: step_shape_2d = (n_walkers,n_steps,2)

start_time_2d_np = time.time()
steps_2d = np.random.choice(a=step_set, size=step_shape_2d)
time_2d_np = time.time() - start_time_2d_np

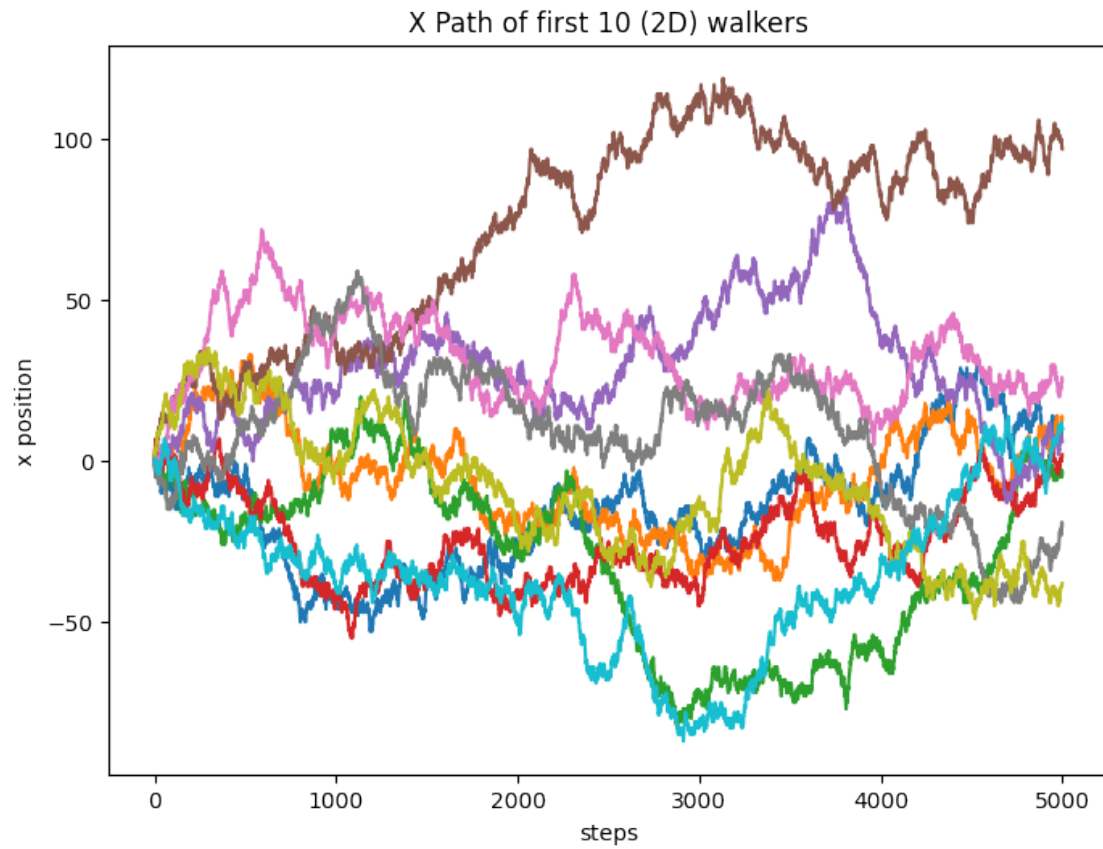
x_2d = steps_2d.cumsum(axis=1)

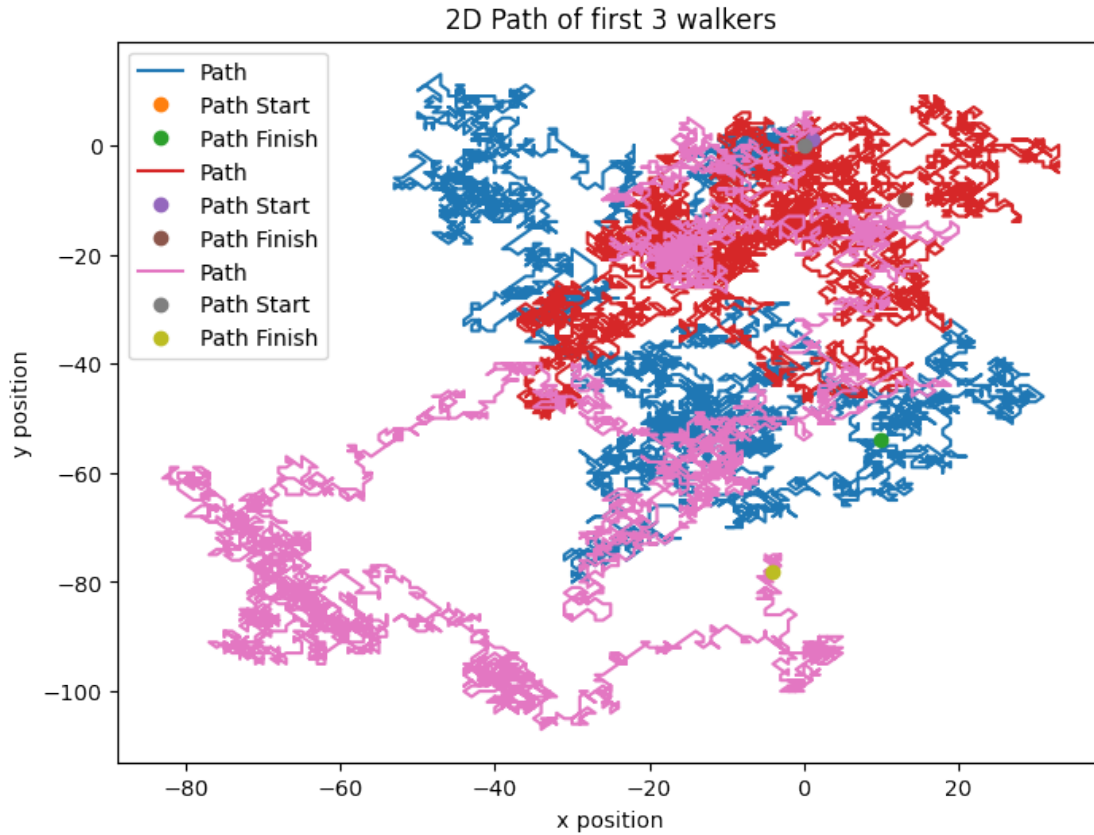
x2_2d = np.average( x_2d**2, axis=0 )
x4_2d = np.average( x_2d**4, axis=0 )
sigma2_nd_2d = np.sqrt( x4_2d - x2_2d**2 )
sigma2_2d = np.sum( sigma2_nd_2d, axis=1 )

[8]: plt.figure(plot_num)
plot_num = plot_num + 1
for i in range( min(10,n_walkers) ):
    plt.plot( x_2d[i,:,0] )
plt.title("X Path of first 10 (2D) walkers")
plt.xlabel("steps")
plt.ylabel("x position")

plt.figure(plot_num)
plot_num = plot_num + 1
for i in range( min(3,n_walkers) ):
    plt.plot( x_2d[i,:,0], x_2d[i,:,1], '-', label='Path' )
    plt.plot( x_2d[i,0,0], x_2d[i,0,1], 'o', label='Path Start' )
    plt.plot( x_2d[i,n_steps-1,0], x_2d[i,n_steps-1,1], 'o', label='Path_
↳Finish')
plt.title("2D Path of first 3 walkers")
plt.xlabel("x position")
plt.ylabel("y position")
plt.legend()

[8]: <matplotlib.legend.Legend at 0x7f8d3a3cf8>
```





1.1.3 3D

```
[9]: step_shape_3d = (n_walkers,n_steps,3)

start_time_3d_np = time.time()
steps_3d = np.random.choice(a=step_set, size=step_shape_3d)
time_3d_np = time.time() - start_time_3d_np

x_3d = steps_3d.cumsum(axis=1)

x2_3d = np.average( x_3d**2, axis=0 )
x4_3d = np.average( x_3d**4, axis=0 )
sigma2_nd_3d = np.sqrt( x4_3d - x2_3d**2 )
sigma2_3d = np.sum( sigma2_nd_3d, axis=1 )

[10]: plt.figure(plot_num)
plot_num = plot_num + 1
for i in range( min(10,n_walkers) ):
    plt.plot( x_3d[i,:,0] )
```

```

plt.title("X Path of first 10 (3D) walkers")
plt.xlabel("steps")
plt.ylabel("x position")

plt.figure(plot_num)
plot_num = plot_num + 1

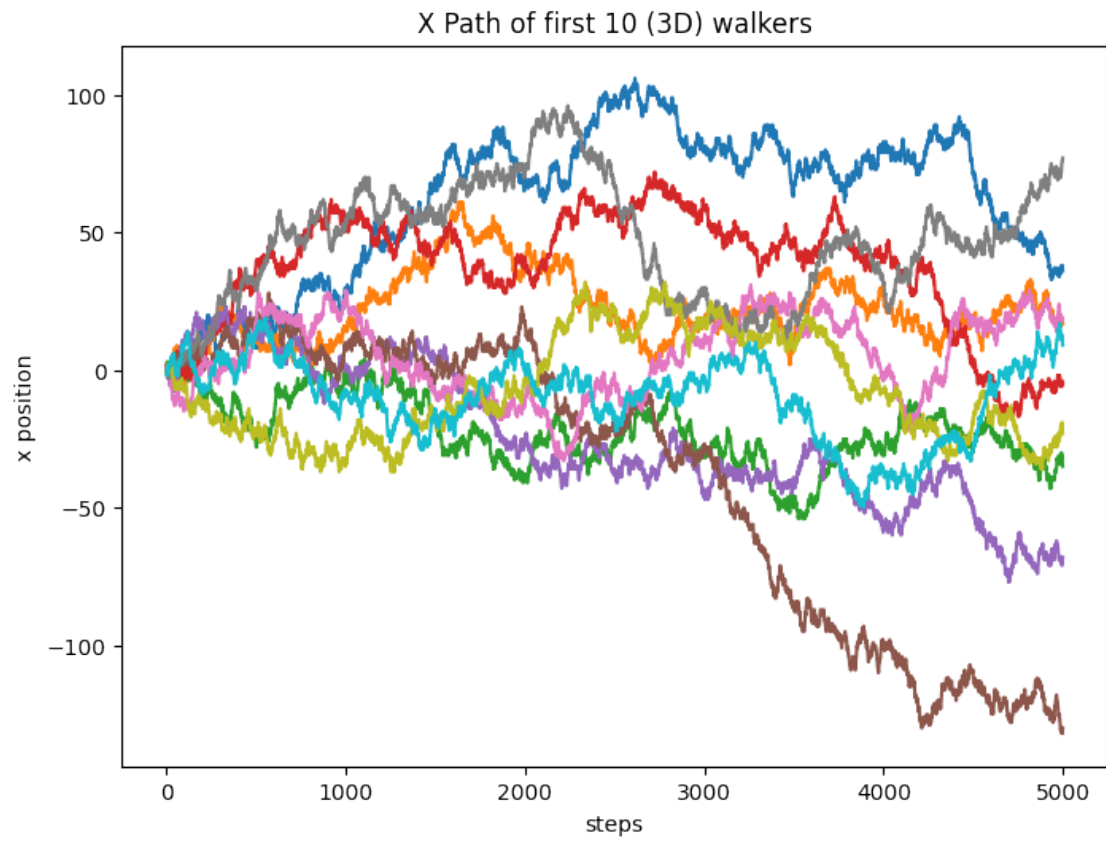
ax = plt.axes(projection='3d')
ax.grid(False)
ax.xaxis.pane.fill = ax.yaxis.pane.fill = ax.zaxis.pane.fill = False

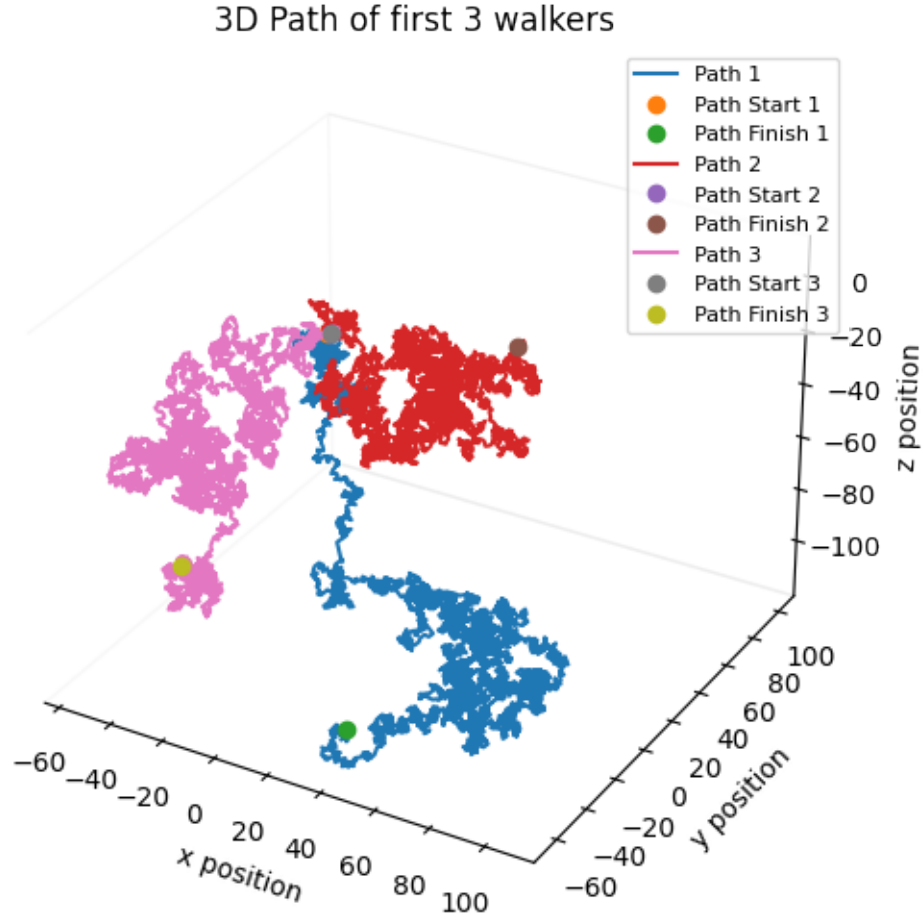
ax.set_xlabel("x position")
ax.set_ylabel("y position")
ax.set_zlabel("z position")

for i in range( min(3,n_walkers) ):
    ax.plot3D( x_3d[i,:,0], x_3d[i,:,1], x_3d[i,:,2], '-', label='Path %d' % (i+1) )
    ax.plot3D( x_3d[i,0,0], x_3d[i,0,1], x_3d[i,0,2], 'o', label='Path Start %d' % (i+1) )
    ax.plot3D( x_3d[i,n_steps-1,0], x_3d[i,n_steps-1,1], x_3d[i,n_steps-1,2], 'o', label='Path Finish %d' % (i+1) )
plt.title("3D Path of first 3 walkers")
plt.legend(fontsize=8)

```

[10]: <matplotlib.legend.Legend at 0x7f8d25b6a0>





1.1.4 Plot Statistics

From Random Walkers notebook: Each walker has 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 n th step, taking these ensemble averages, is therefore

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

```
[11]: plt.figure(plot_num)
      plot_num = plot_num + 1

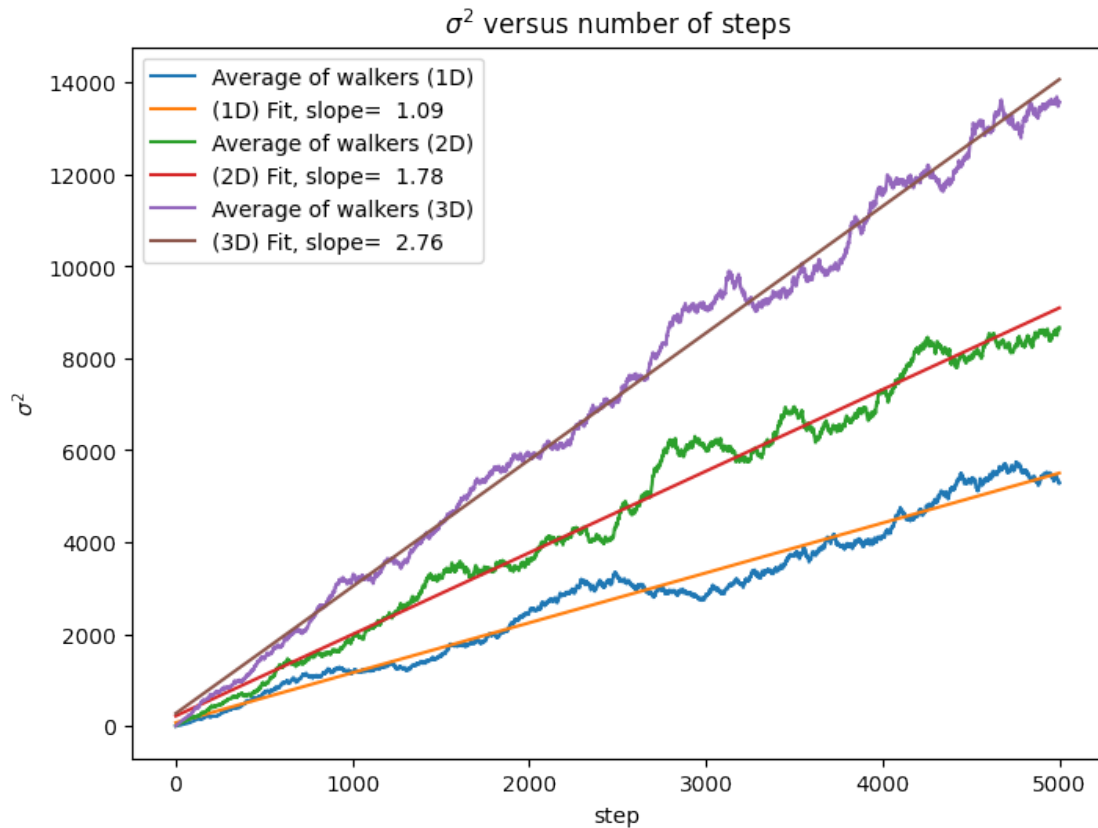
      plt.plot( sigma2_1d, label='Average of walkers (1D)' )
      res_1d = np.polyfit(t, sigma2_1d,1 )
      plt.plot( t, res_1d[0]*t + res_1d[1], label='(1D) Fit, slope=%6.2f' % res_1d[0],
      ↪)

      plt.plot( sigma2_2d, label='Average of walkers (2D)' )
      res_2d = np.polyfit(t, sigma2_2d,1 )
      plt.plot( t, res_2d[0]*t + res_2d[1], label='(2D) Fit, slope=%6.2f' % res_2d[0],
      ↪)

      plt.plot( sigma2_3d, label='Average of walkers (3D)' )
      res_3d = np.polyfit(t, sigma2_3d,1 )
      plt.plot( t, res_3d[0]*t + res_3d[1], label='(3D) Fit, slope=%6.2f' % res_3d[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 0x7f8a50aba8>
```



```
[12]: r2_1d = np.sum(x2_1d,1)
r2_2d = np.sum(x2_2d,1)
r2_3d = np.sum(x2_3d,1)

plt.figure(plot_num)
plot_num = plot_num + 1

plt.plot(r2_1d, label='1D data')
fit_1d = np.polyfit(t, r2_1d,1 )
plt.plot( t, fit_1d[0]*t + fit_1d[1], label='Fit (1D), slope=%6.2f' %_
↳(fit_1d[0]) )

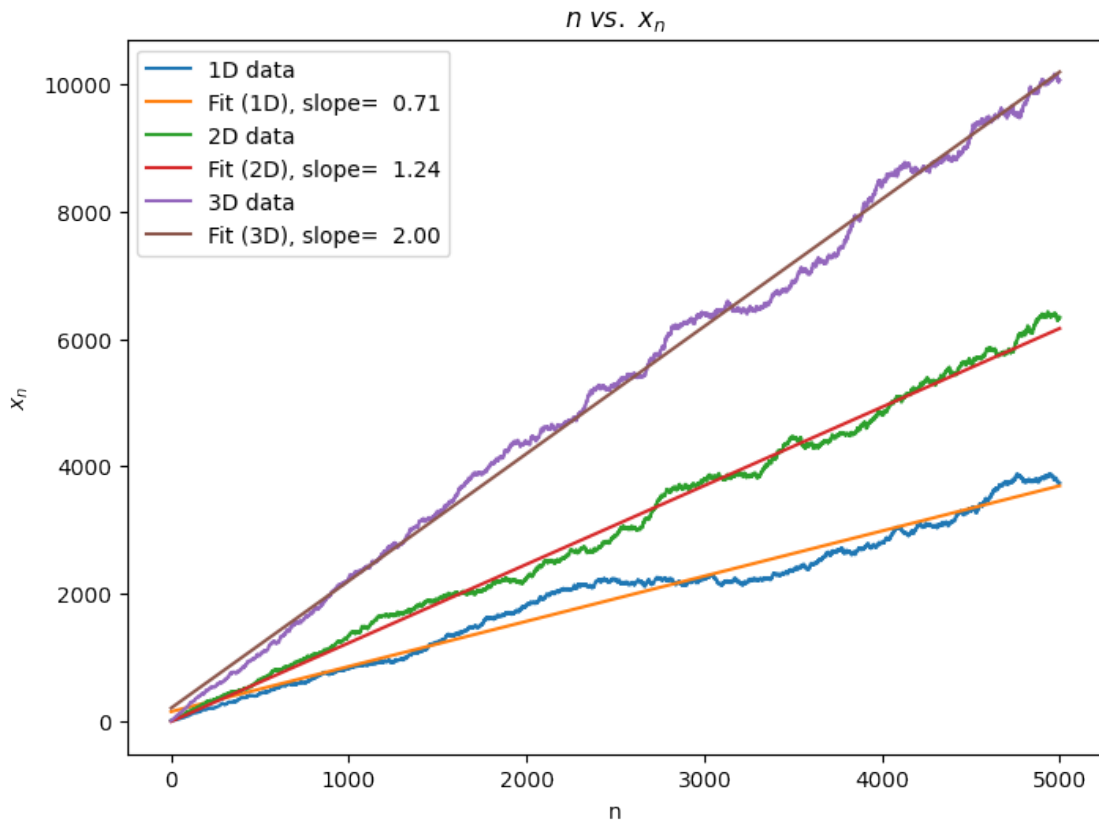
plt.plot(r2_2d, label='2D data')
fit_2d = np.polyfit(t, r2_2d,1 )
plt.plot( t, fit_2d[0]*t + fit_2d[1], label='Fit (2D), slope=%6.2f' %_
↳(fit_2d[0]) )

plt.plot(r2_3d, label='3D data')
fit_3d = np.polyfit(t, r2_3d,1 )
```

```
plt.plot( t, fit_3d[0]*t + fit_3d[1], label='Fit (3D), slope=%6.2f' %L
↪(fit_3d[0]) )

plt.xlabel("n")
plt.ylabel("$x_n$")
plt.title("$n$ \; vs. \; $x_n$")
plt.legend()
```

[12]: <matplotlib.legend.Legend at 0x7f8a48df28>



1.1.5 Calculate Diffusion Coefficients

```
[13]: D_numpy_1d = res_1d[0]/2
D_numpy_2d = res_2d[0]/4
D_numpy_3d = res_3d[0]/6

Df_numpy_1d = fit_1d[0]/2
Df_numpy_2d = fit_2d[0]/4
Df_numpy_3d = fit_3d[0]/6
```

1.2 Tensorflow Method

In tensorflow, the function `tensorflow.random.stateless_uniform()` is used to select the next step. `tensorflow.random.stateless_uniform()` outputs deterministic pseudorandom values from a uniform distribution [1].

```
[14]: import tensorflow as tf

tf.random.set_seed(0)
```

```
[15]: n_walkers_tf = 100
n_steps_tf = 5000

t_tf = np.arange(n_steps_tf)
```

1.2.1 1D

```
[16]: step_shape_tf_1d = (n_walkers_tf, n_steps_tf, 1)

start_time_1d_tf = time.time()
#steps_tf_1d = tf.random.stateless_uniform(shape=step_shape_tf_1d,
    ↪ minval=-1,maxval=2, seed=(2,3) , dtype=tf.int32)
steps_tf_1d = tf.random.uniform(shape=step_shape_tf_1d, minval=-1,maxval=2,
    ↪ seed=0 , dtype=tf.int32)
time_1d_tf = time.time() - start_time_1d_tf

x_tf_1d = tf.math.cumsum(steps_tf_1d, axis=1)

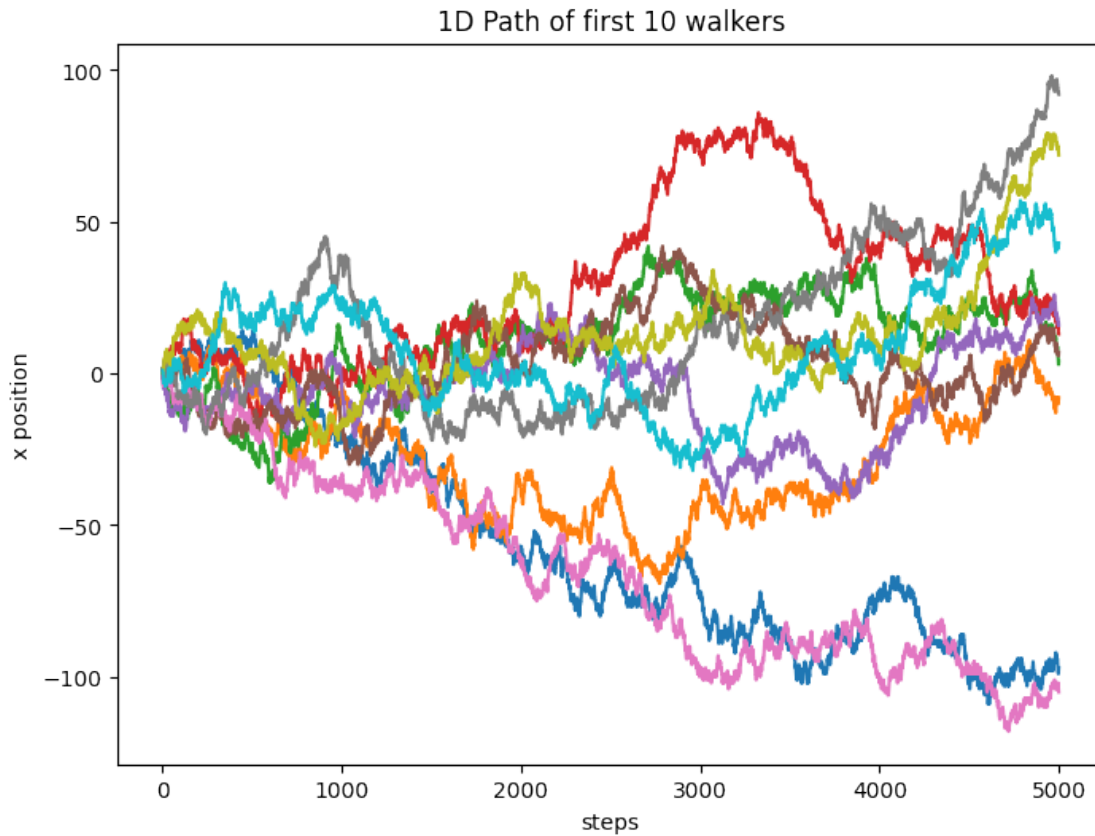
# Now get the averages over the walkers
x2_tf_1d = tf.math.reduce_mean( x_tf_1d**2, axis=0 )
x4_tf_1d = tf.math.reduce_mean( x_tf_1d**4, axis=0 )

r2_tf_1d = x2_tf_1d[:,0]
r4_tf_1d = x4_tf_1d[:,0]

sigma2_nd_tf_1d = tf.math.sqrt( tf.cast(x4_tf_1d, dtype=tf.float32) - tf.
    ↪ cast(x2_tf_1d, dtype=tf.float32)**2 )
sigma2_tf_1d = tf.reduce_sum(sigma2_nd_tf_1d, axis=1 )
```

```
[17]: plt.figure(plot_num)
plot_num = plot_num + 1
for i in range( min(10,n_walkers_tf) ):
    plt.plot( x_tf_1d[i,:,0] )
plt.title("1D Path of first 10 walkers")
plt.xlabel("steps")
plt.ylabel("x position")
```

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



1.2.2 2D

```
[18]: step_shape_tf_2d = (n_walkers_tf, n_steps_tf, 2)

start_time_2d_tf = time.time()
#steps_tf_2d = tf.random.stateless_uniform(shape=step_shape_tf_2d,
    ↳minval=-1,maxval=2, seed=(2,3), dtype=tf.int32)
steps_tf_2d = tf.random.uniform(shape=step_shape_tf_2d, minval=-1,maxval=2,
    ↳seed=0, dtype=tf.int32)
time_2d_tf = time.time() - start_time_2d_tf

x_tf_2d = tf.math.cumsum(steps_tf_2d, axis=1)

# Now get the averages over the walkers
x2_tf_2d = tf.math.reduce_mean( x_tf_2d**2, axis=0 )
x4_tf_2d = tf.math.reduce_mean( x_tf_2d**4, axis=0 )
```

```

r2_tf_2d = x2_tf_2d[:,0] + x2_tf_2d[:,1]
r4_tf_2d = x4_tf_2d[:,0] + x4_tf_2d[:,1]

sigma2_nd_tf_2d = tf.math.sqrt( tf.cast(x4_tf_2d, dtype=tf.float32) - tf.
    ↪cast(x2_tf_2d, dtype=tf.float32)**2 )
sigma2_tf_2d = tf.math.reduce_sum(sigma2_nd_tf_2d, axis=1 )

```

```

[19]: plt.figure(plot_num)
      plot_num = plot_num + 1
      for i in range( min(10,n_walkers_tf) ):
          plt.plot( x_tf_2d[i,:,0] )
      plt.title("X-Dimensional Path of first 10 2D walkers")
      plt.xlabel("steps")
      plt.ylabel("x position")

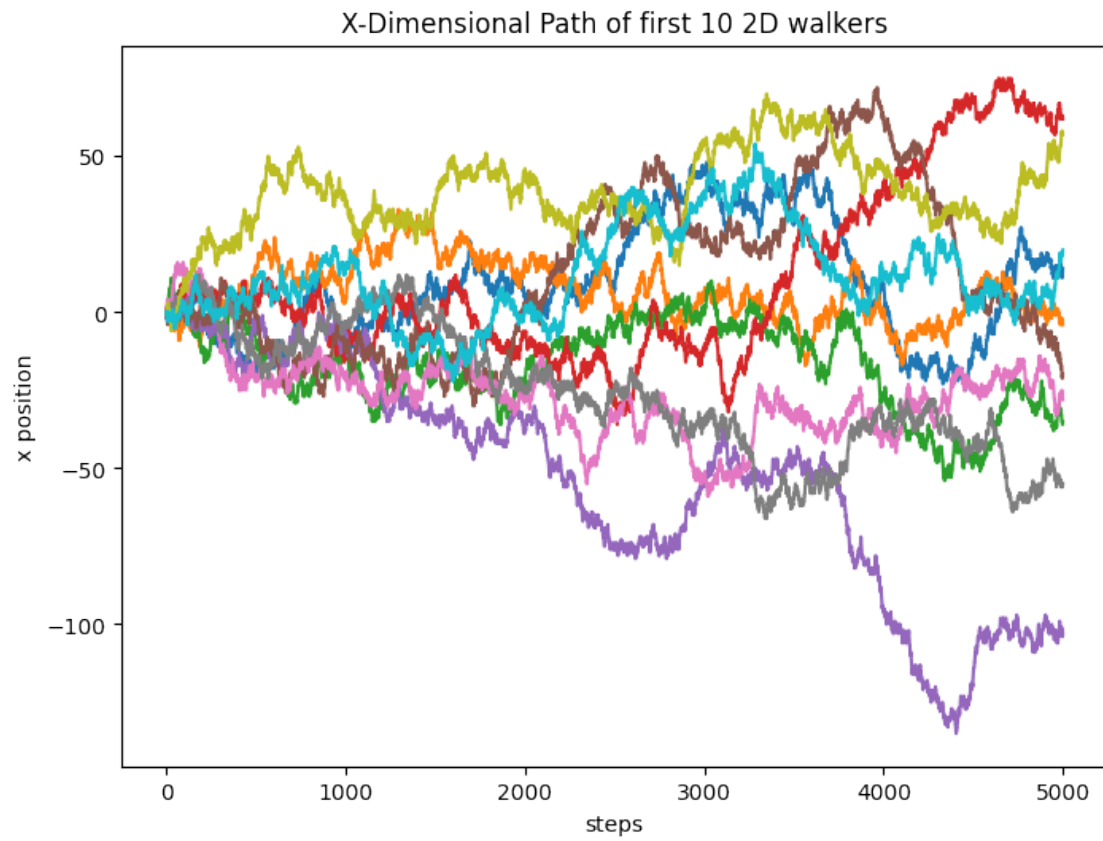
      plt.figure(plot_num)
      plot_num = plot_num + 1
      for i in range( min(3,n_walkers_tf) ):
          plt.plot( x_tf_2d[i,:,0], x_tf_2d[i,:,1], '-', label='Path' )
          plt.plot( x_tf_2d[i,0,0], x_tf_2d[i,0,1], 'o', label='Path Start' )
          plt.plot( x_tf_2d[i,n_steps-1,0], x_tf_2d[i,n_steps-1,1], 'o', label='Path_
          ↪Finish')
      plt.title("2D Path of first 3 walkers")
      plt.xlabel("x position")
      plt.ylabel("y position")
      plt.legend()

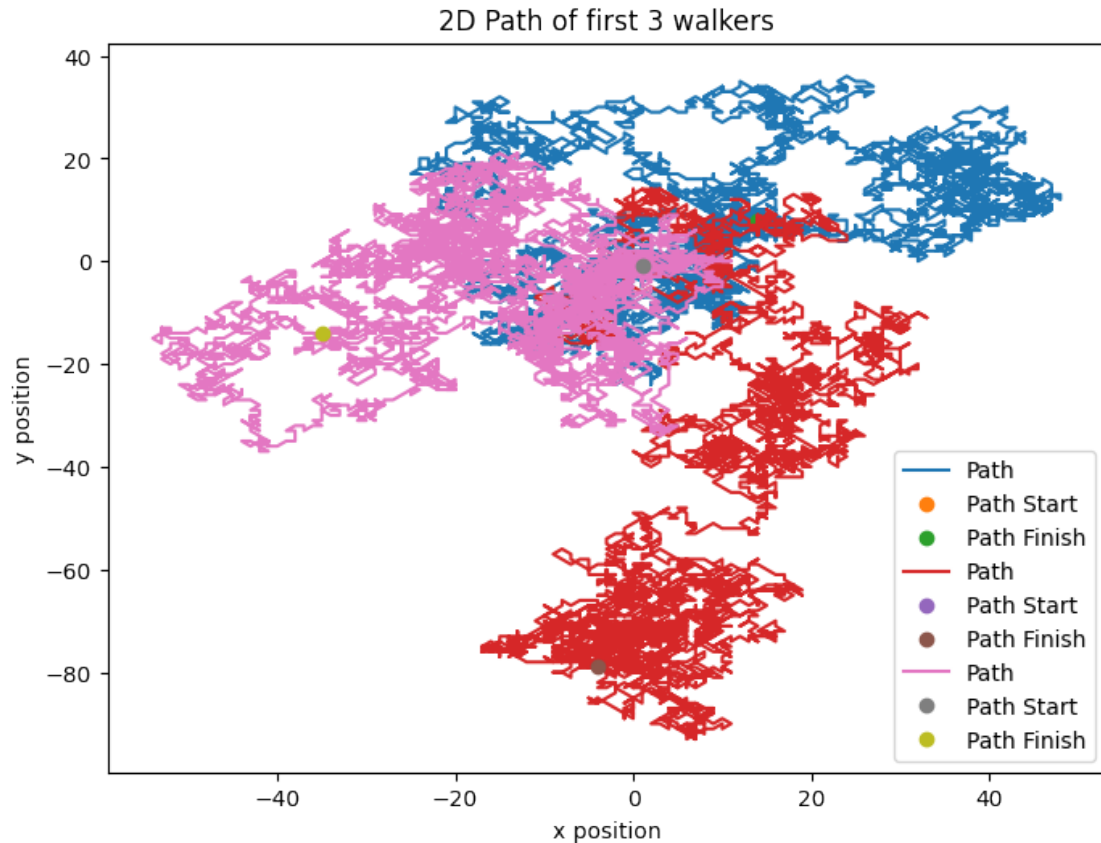
```

```

[19]: <matplotlib.legend.Legend at 0x7f0469a940>

```





1.2.3 3D

```
[20]: step_shape_tf_3d = (n_walkers_tf, n_steps_tf, 3)

start_time_3d_tf = time.time()
#steps_tf_3d = tf.random.stateless_uniform(shape=step_shape_tf_3d,
    ↳minval=-1,maxval=2, seed=(2,3), dtype=tf.int32)
steps_tf_3d = tf.random.uniform(shape=step_shape_tf_3d, minval=-1,maxval=2,
    ↳seed=0, dtype=tf.int32)
time_3d_tf = time.time() - start_time_3d_tf

x_tf_3d = tf.math.cumsum(steps_tf_3d, axis=1)

# Now get the averages over the walkers
x2_tf_3d = tf.math.reduce_mean( x_tf_3d**2, axis=0 )
x4_tf_3d = tf.math.reduce_mean( x_tf_3d**4, axis=0 )

r2_tf_3d = x2_tf_3d[:,0] + x2_tf_3d[:,1] + x2_tf_3d[:,2]
r4_tf_3d = x4_tf_3d[:,0] + x4_tf_3d[:,1] + x2_tf_3d[:,2]
```

```

sigma2_nd_tf_3d = tf.math.sqrt( tf.cast(x4_tf_3d, dtype=tf.float32) - tf.
    ↳ cast(x2_tf_3d, dtype=tf.float32)**2 )
sigma2_tf_3d = tf.math.reduce_sum(sigma2_nd_tf_3d, axis=1 )

```

```

[21]: plt.figure(plot_num)
      plot_num = plot_num + 1
      for i in range( min(10,n_walkers_tf) ):
          plt.plot( x_tf_2d[i,:,0] )
      plt.title("X-Dimensional Path of first 10 3D walkers")
      plt.xlabel("steps")
      plt.ylabel("x position")

      plt.figure(plot_num)
      plot_num = plot_num + 1

      ax = plt.axes(projection='3d')
      ax.grid(False)
      ax.xaxis.pane.fill = ax.yaxis.pane.fill = ax.zaxis.pane.fill = False

      ax.set_xlabel("x position")
      ax.set_ylabel("y position")
      ax.set_zlabel("z position")

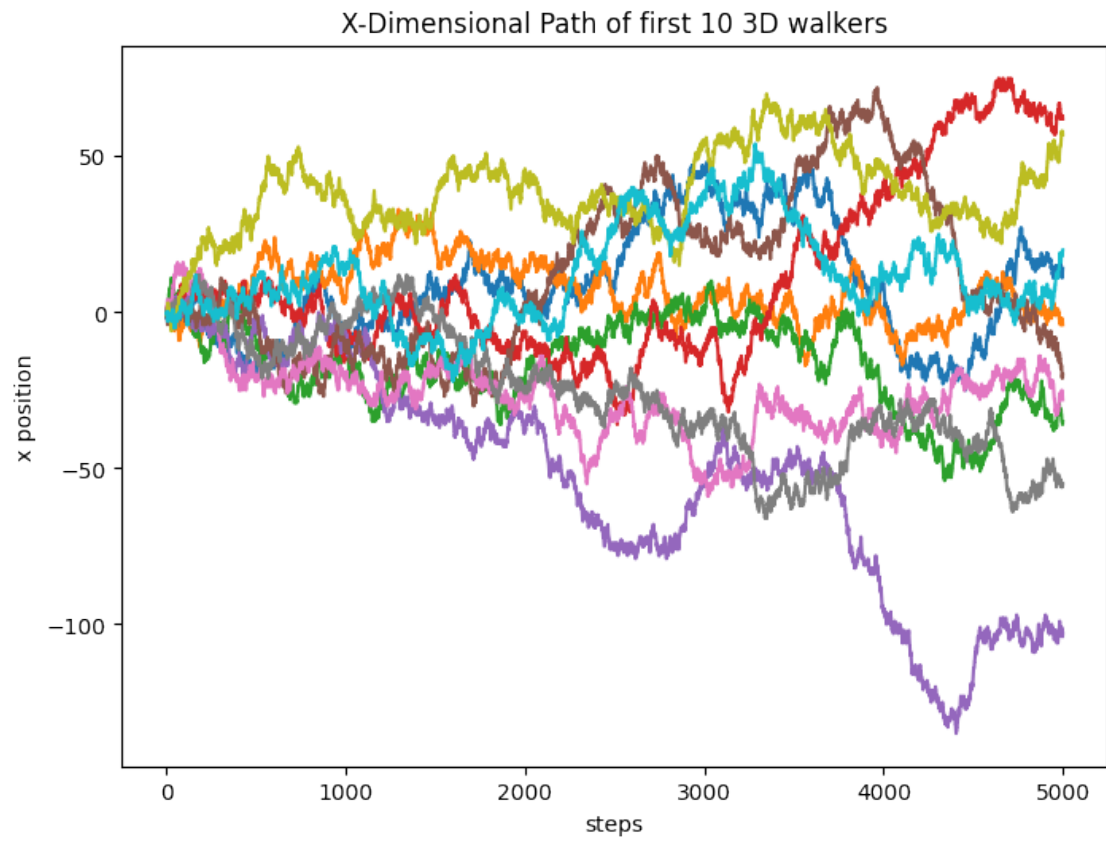
      for i in range( min(3,n_walkers_tf) ):
          ax.plot3D( x_tf_3d[i,:,0], x_tf_3d[i,:,1], x_tf_3d[i,:,2], '-', label='Path_
          ↳ %d' % (i+1) )
          ax.plot3D( x_tf_3d[i,0,0], x_tf_3d[i,0,1], x_tf_3d[i,0,2], 'o', label='Path_
          ↳ Start %d' % (i+1) )
          ax.plot3D( x_tf_3d[i,n_steps-1,0], x_tf_3d[i,n_steps-1,1],
          ↳ x_tf_3d[i,n_steps-1,2], 'o', label='Path Finish %d' % (i+1))
      plt.title("3D Path of first 3 walkers")
      plt.legend(fontsize=8)

```

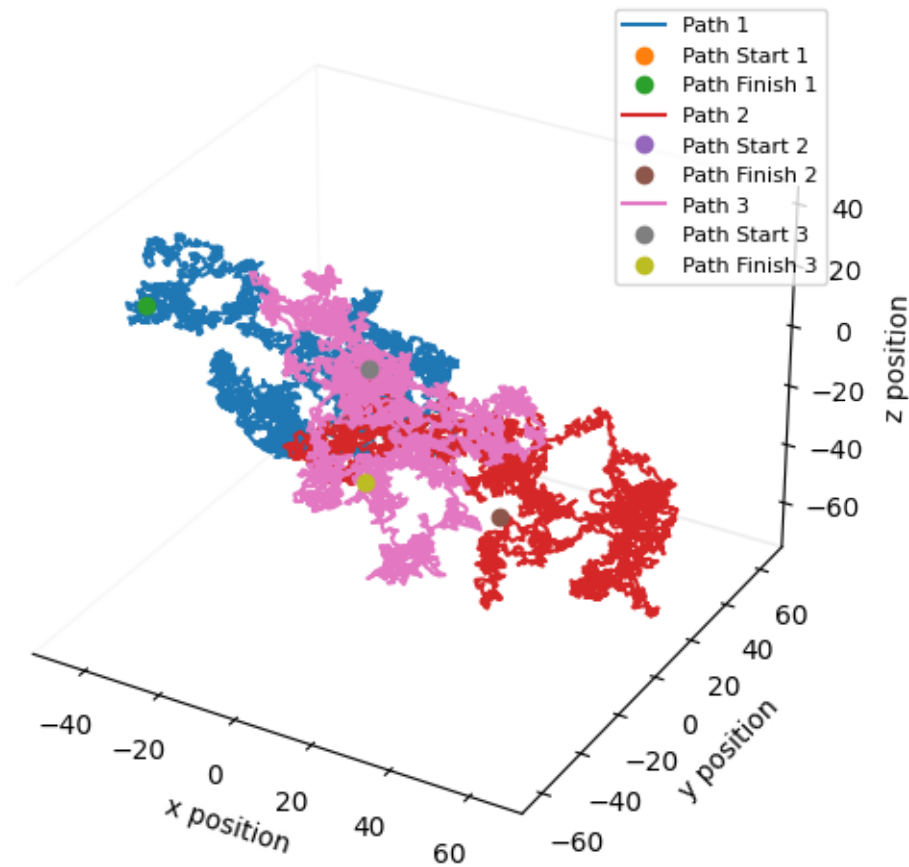
```

[21]: <matplotlib.legend.Legend at 0x7f045b3668>

```



3D Path of first 3 walkers



1.2.4 Statistical Plots

```
[22]: plt.figure(plot_num)
plot_num = plot_num + 1

plt.plot( sigma2_tf_1d, label='Average of walkers (1D)' )
res_1d = np.polyfit(t_tf, sigma2_tf_1d,1 )
plt.plot( t_tf, res_1d[0]*t_tf + res_1d[1], label='Fit (1D), slope=%6.2f' %_
↪res_1d[0] )

plt.plot( sigma2_tf_2d, label='Average of walkers (2D)' )
res_2d = np.polyfit(t_tf, sigma2_tf_2d,1 )
plt.plot( t_tf, res_2d[0]*t_tf + res_2d[1], label='Fit (2D), slope=%6.2f' %_
↪res_2d[0] )

plt.plot( sigma2_tf_3d, label='Average of walkers (3D)' )
```

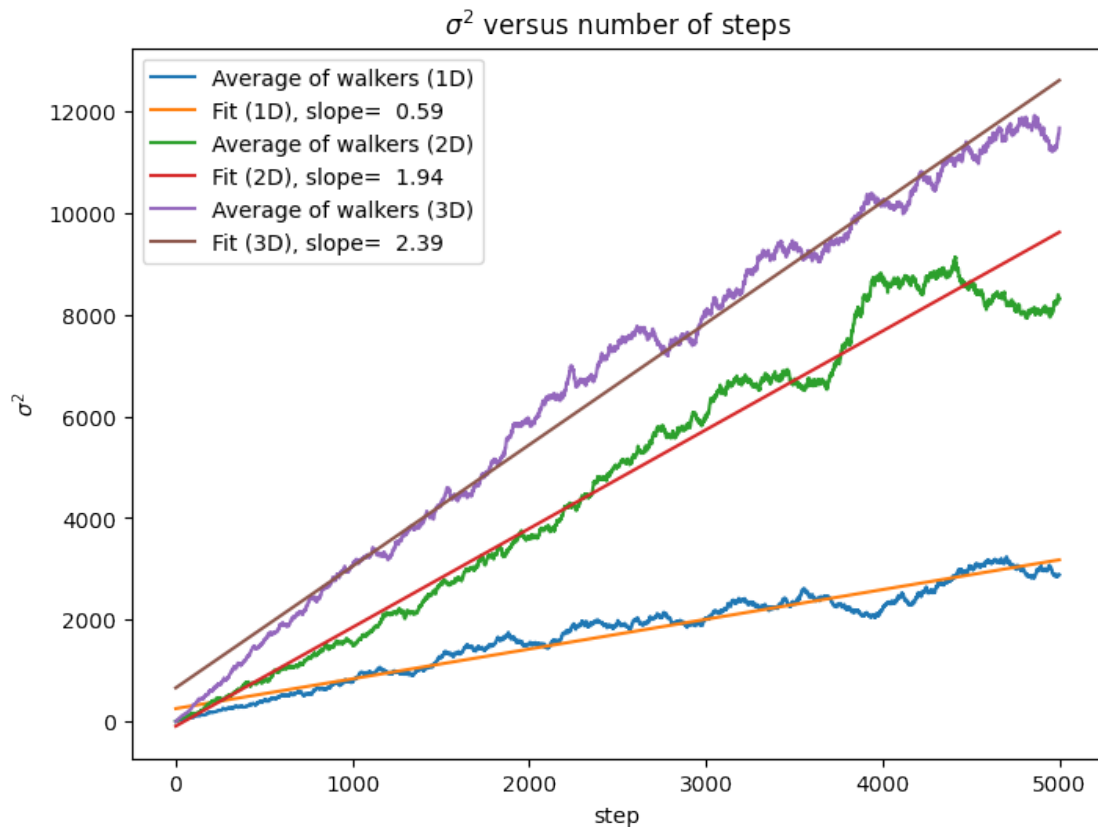
```

res_3d = np.polyfit(t_tf, sigma2_tf_3d,1 )
plt.plot( t_tf, res_3d[0]*t_tf + res_3d[1], label='Fit (3D), slope=%6.2f' %_
↳res_3d[0] )

plt.title(r"$\sigma^2$ versus number of steps")
plt.xlabel("step")
plt.ylabel(r"$\sigma^2$")
plt.legend()

```

[22]: <matplotlib.legend.Legend at 0x7f044b9320>



```

[23]: plt.figure(plot_num)
plot_num = plot_num + 1
plt.plot(x2_tf_1d, label='1D data')
fit_1d = np.polyfit(t_tf, x2_tf_1d,1 )
plt.plot( t_tf, fit_1d[0]*t_tf + fit_1d[1], label='Fit (1D), slope=%6.2f' %_
↳fit_1d[0] )

plt.plot(r2_tf_2d, label='2D data')

```

```

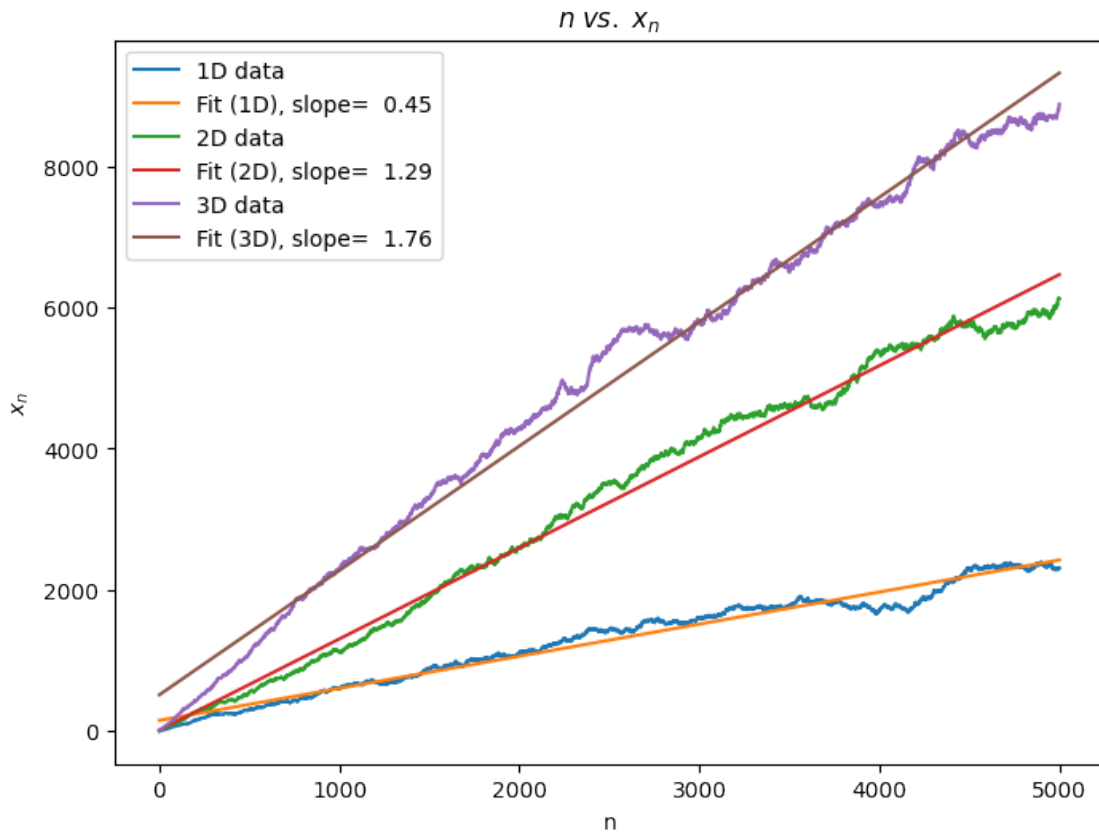
fit_2d = np.polyfit(t_tf, r2_tf_2d,1 )
plt.plot( t_tf, fit_2d[0]*t_tf + fit_2d[1], label='Fit (2D), slope=%6.2f' %_
    ↪fit_2d[0] )

plt.plot(r2_tf_3d, label='3D data')
fit_3d = np.polyfit(t_tf, r2_tf_3d,1 )
plt.plot( t_tf, fit_3d[0]*t_tf + fit_3d[1], label='Fit (3D), slope=%6.2f' %_
    ↪fit_3d[0] )

plt.xlabel("n")
plt.ylabel("$x_n$")
plt.title("$n$ \; vs. \; $x_n$")
plt.legend()

```

[23]: <matplotlib.legend.Legend at 0x7f04383dd8>



1.2.5 Calculate Diffusion Coefficients

```
[24]: D_tf_1d = res_1d[0]/2
      D_tf_2d = res_2d[0]/4
      D_tf_3d = res_3d[0]/6
```

```
[25]: err_tf_1d = abs((D_tf_1d - 0.5)/0.5)
      err_tf_2d = abs((D_tf_2d - 0.5)/0.5)
      err_tf_3d = abs((D_tf_3d - 0.5)/0.5)

      err_np_1d = abs((D_numpy_1d - 0.5)/0.5)
      err_np_2d = abs((D_numpy_2d - 0.5)/0.5)
      err_np_3d = abs((D_numpy_3d - 0.5)/0.5)

      err_tf = (err_tf_1d+err_tf_2d+err_tf_3d)/3
      err_np = (err_np_1d+err_np_2d+err_np_3d)/3
```

1.3 Compare Diffusion Coefficient Results

```
[48]: print("dim||Numpy\t|Error\t|Time [ms]\t||Tensorflow\t|Error\t|Time [ms]")
      print("-----")
      print("1D ||%0.3f\t|%0.3f\t|%1.3f\t\t||%0.3f\t\t|%0.3f\t\t|%1.3f" % (D_numpy_1d,
      ↪err_np_1d, time_1d_np*1000, D_tf_1d, err_tf_1d, time_1d_tf*1000))
      print("2D ||%0.3f\t|%0.3f\t|%1.3f\t\t||%0.3f\t\t|%0.3f\t\t|%1.3f" % (D_numpy_2d,
      ↪err_np_2d, time_2d_np*1000, D_tf_2d, err_tf_2d, time_2d_tf*1000))
      print("3D ||%0.3f\t|%0.3f\t|%1.3f\t\t||%0.3f\t\t|%0.3f\t\t|%1.3f" % (D_numpy_3d,
      ↪err_np_3d, time_3d_np*1000, D_tf_3d, err_tf_3d, time_3d_tf*1000))
      print("          avg. err: %0.3f\t\t\t\t          avg. err: %0.3f" % (err_np, err_tf))
```

dim Numpy	Error	Time [ms]	Tensorflow	Error	Time [ms]

1D 0.543	0.086	18.056	0.293	0.415	3178.035
2D 0.444	0.112	33.632	0.486	0.028	10.150
3D 0.460	0.080	46.800	0.398	0.203	8.902
avg. err: 0.084			avg. err: 0.344		

1.3.1 Comments

We expect the value of the diffusion coefficient to be $\frac{1}{2}$. The results are somewhat inconsistent between each run but, on average, the error for the tensorflow method is higher than the numpy method. Even when the 1D calculation, which is considerably worse than the other two, is excluded the error for the tensorflow method is higher than the numpy method. Each random selector function was also timed and the results are displayed in the table above. For 2D and 3D, tensorflow

is consistently faster but for 1D, the time to run the tensorflow selector is considerably longer than any other method.

[]: