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,

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

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

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

$$\langle r_n^2 \rangle = \sum_{i=1}^{dims} \sum_{k=1}^m \frac{u_{k,i,n}^2}{m}$$
, and

$$\langle r_n^4 \rangle = \sum_{i=1}^{dims} \sum_{k=1}^m \frac{u_{k,i,n}^4}{m}.$$

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,

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

1

and for 3 dimensions we use,

$$\sigma_n^2 = \sigma_{n,1}^2 + \sigma_{n,2}^2 + \sigma_{n,3}^2,$$

= $2Dn + 2Dn + 2Dn,$
= $6Dn.$

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 = 250
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

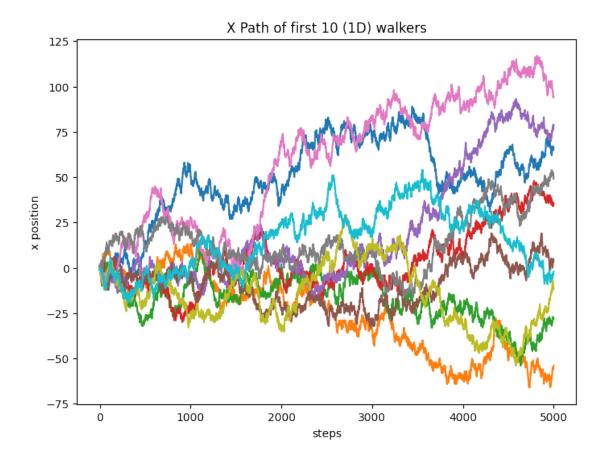
```
[5]: # The shape is for "n_walkers" taking "n_steps" in "dims" dimensions.
# So, in 1d if there are 10 walkers making 100 steps each,
# it will be (10, 100, 1)
step_shape_1d = (n_walkers,n_steps,1)
# These are the steps at each stage
start_time_1d_np = time.time()
steps_1d = np.random.choice(a=step_set, 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)

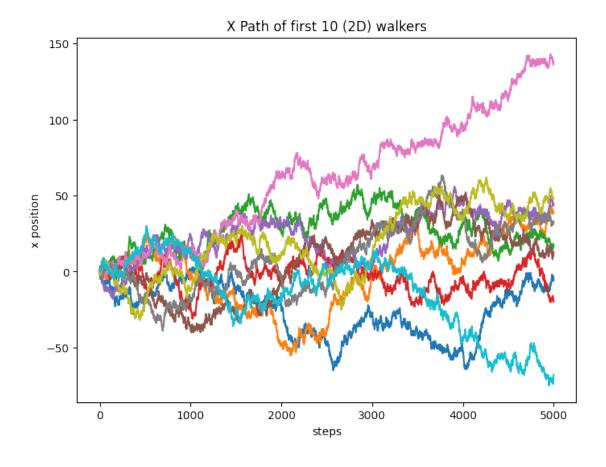
start_time_2d_np = time.time()
steps_2d = np.random.choice(a=step_set, size=step_shape_2d)
time_2d_np = time.time() - start_time_2d_np

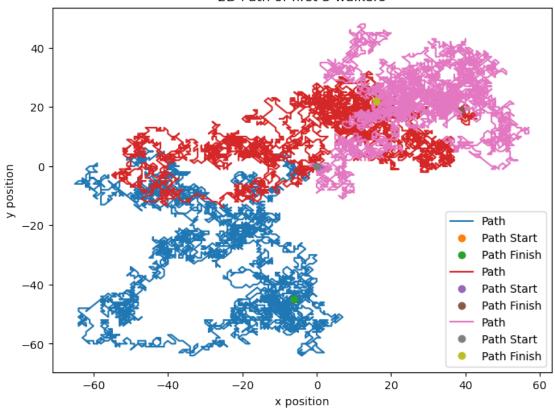
x_2d = steps_2d.cumsum(axis=1)

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 0x7f640fa400>





1.1.3 3D

plot_num = plot_num + 1

for i in range(min(10,n_walkers)):
 plt.plot(x_3d[i,:,0])

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

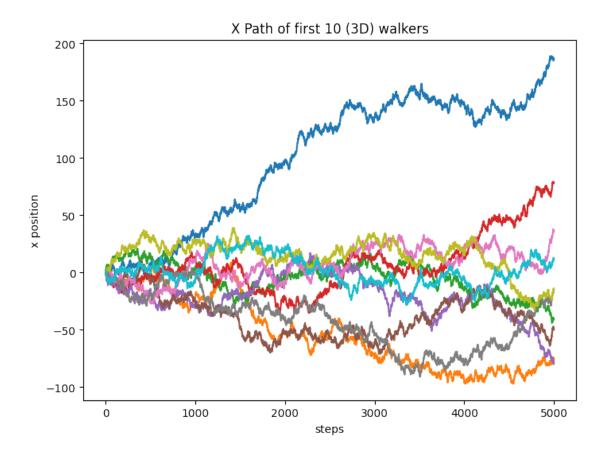
start_time_3d_np = time.time()
steps_3d = np.random.choice(a=step_set, size=step_shape_3d)
time_3d_np = time.time() - start_time_3d_np

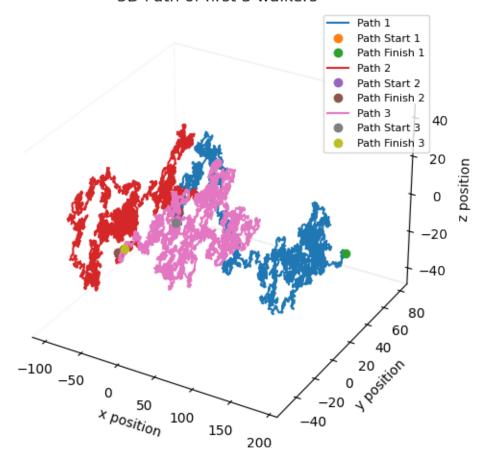
x_3d = steps_3d.cumsum(axis=1)

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)
```

```
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,0,0], 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 0x7f5ef7f748>





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

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

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

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):

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

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

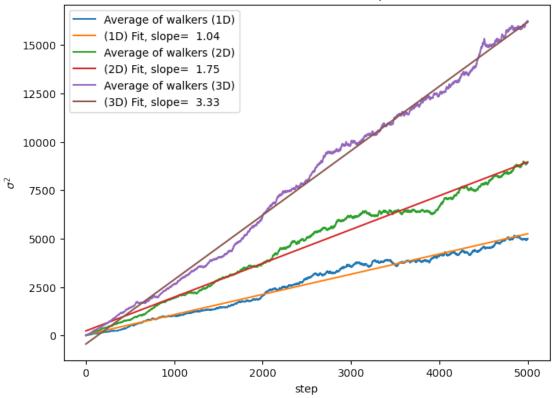
The overall diffusion width at the nth step, taking these ensemble averages, is therefore

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

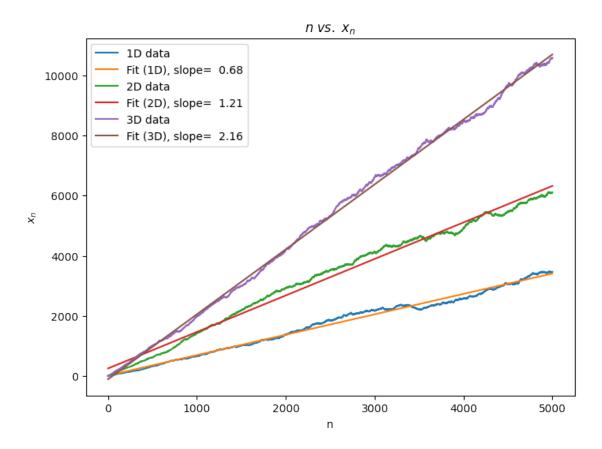
```
[11]: plt.figure(plot_num)
      plot_num = plot_num + 1
      plt.plot( sigma2_1d, label='Average of walkers (1D)' )
      res_1d = np.polyfit(t, sigma2_1d,1)
      plt.plot( t, res_1d[0]*t + res_1d[1], label='(1D) Fit, slope=%6.2f' % res_1d[0]_
      →)
      plt.plot( sigma2_2d, label='Average 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 0x7f5ee8ecc0>

σ^2 versus number of steps



[12]: <matplotlib.legend.Legend at 0x7f5ef19748>



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 = 250
n_steps_tf = 5000

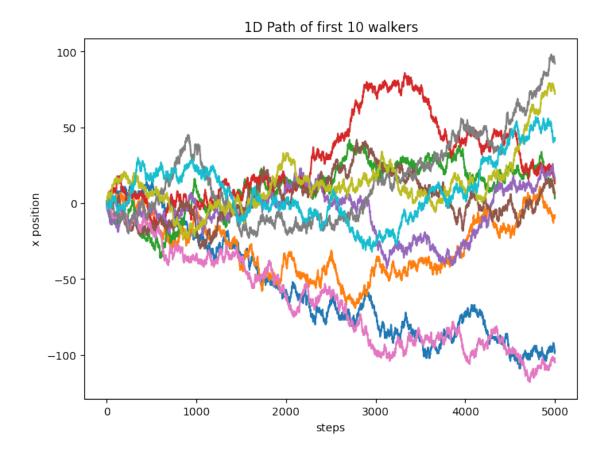
t_tf = np.arange(n_steps_tf)
```

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, \_
      \rightarrow 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.
      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")
```

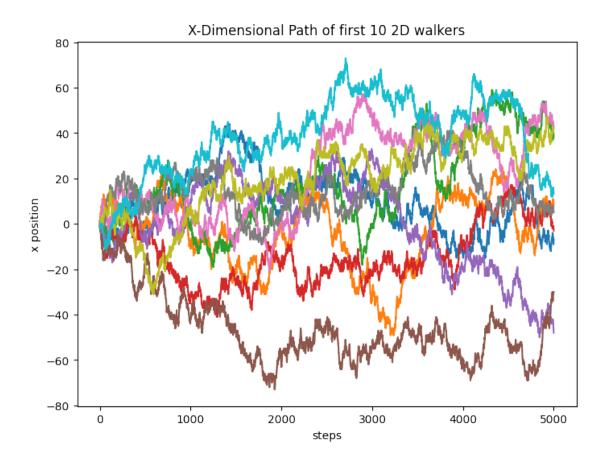
[17]: Text(0, 0.5, 'x position')

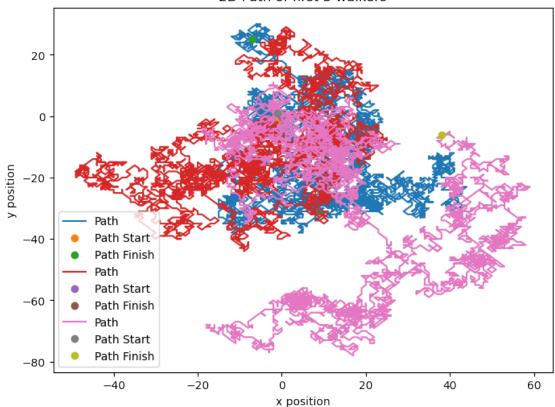


1.2.2 2D

```
[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 0x7ef00a3908>





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,u)

--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,u)

--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]
```

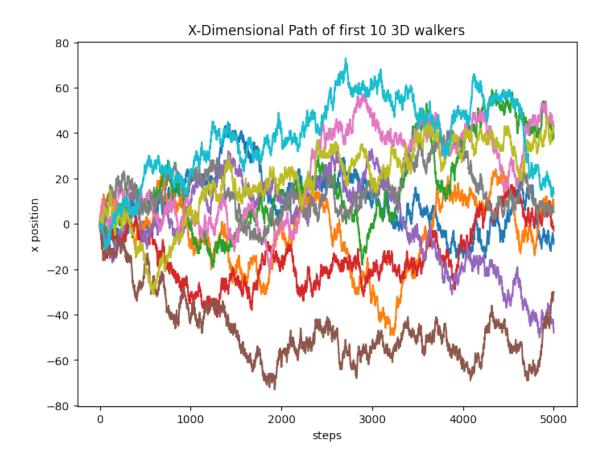
```
sigma2_nd_tf_3d = tf.math.sqrt( tf.cast(x4_tf_3d, dtype=tf.float32) - tf.

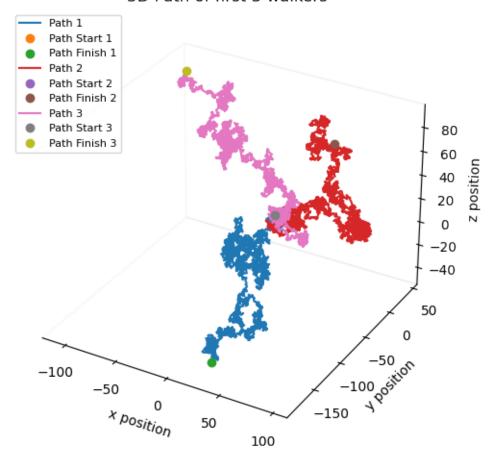
cast(x2_tf_3d, dtype=tf.float32)**2 )
sigma2_tf_3d = tf.math.reduce_sum(sigma2_nd_tf_3d, axis=1 )
```

```
[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_l'
      ax.plot3D(x_tf_3d[i,0,0], x_tf_3d[i,0,1], x_tf_3d[i,0,2], 'o', label='Path_u'

Start %d' % (i+1) )
         ax.plot3D( x_tf_3d[i,n_steps-1,0], x_tf_3d[i,n_steps-1,1],__
      plt.title("3D Path of first 3 walkers")
     plt.legend(fontsize=8)
```

[21]: <matplotlib.legend.Legend at 0x7ee8085f60>





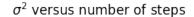
1.2.4 Statistical Plots

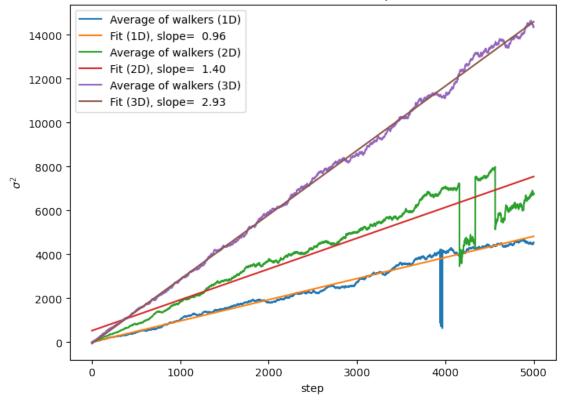
```
res_3d = np.polyfit(t_tf, sigma2_tf_3d,1 )
plt.plot( t_tf, res_3d[0]*t_tf + res_3d[1], label='Fit (3D), slope=%6.2f' %

→res_3d[0] )

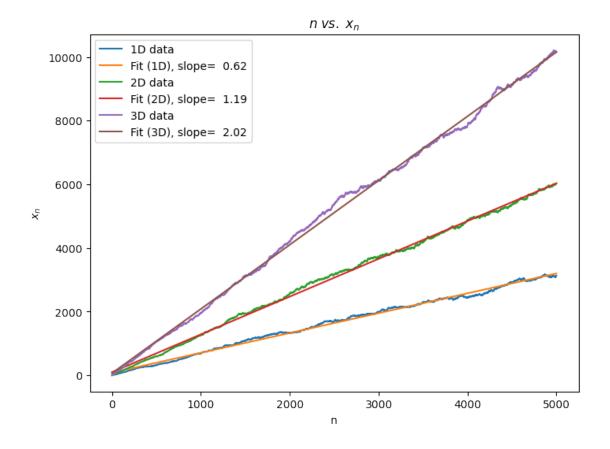
plt.title(r"$\sigma^2$ versus number of steps")
plt.xlabel("step")
plt.ylabel(r"$\sigma^2$")
plt.legend()
```

[22]: <matplotlib.legend.Legend at 0x7ed80fec18>





[23]: <matplotlib.legend.Legend at 0x7f38c38748>



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_np_6 = (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

dim Numpy	Error	Time [ms]	Tensorflow	Error	Time [ms]
1D 0.522	0.044	41.63	0.482	0.036	3294.80
2D 0.436	0.127	77.00	0.351	10.298	7.86
3D 0.554	0.109	116.33	0.489	10.022	18.44
avg. err: 0.093		avg. err: 0.119			

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. One thing to note is that the tensorflow method failed due to an apparent overworking of the NVIDIA Jetson for any $n_{walkers} > 250$. Each random selector function was also timed and the results are displayed in the table above. For 2D and 3D, tensorflow is consistenly faster but for 1D, the time to run the tensorflow selector is considerably longer than any other method. It is unclear why the 1D case behaves so differently for tensorflow.

[]:[