

# dataPlayground

July 24, 2023

```
[1]: import os
import numpy as np
import matplotlib.pyplot as plt
import torch
import torch
import copy
from scipy import stats
%matplotlib inline
import matplotlib.pyplot as plt
from sklearn import preprocessing
from dnaDataloader import experimentDataloader
import os
import random
import matplotlib.colors as mcolors
from IPython.core.interactiveshell import InteractiveShell
from dnaModelUtil import printStats
from dnaModelUtil import averageDiff
device = torch.device("cuda:1" if torch.cuda.is_available() else "cpu")
device
```

```
[1]: device(type='cuda', index=1)
```

## 1 Single-molecule experiment prediction model

This notebook is the step by step development process for making a SNN to predict the reactivity level and number of reactions in Single-molecule experiments Data is provided via the Kent State University chemistry department. The model development is provided by the Kent State University computer science department

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Working with data from Preprocessing/data/ should have folder for each experment setup (in terms of distance of magnet in mm). Each folder should have a list of events and their frame numbers as excel file. Events are recorded as events per 0.05 secs. The raw excel files are converted to CSV files with preprocess.py.

The processed file are shorted versions of the original files, i.e. its only the first X secs. These csv files have a 1 or a 0 for each 0.05 sec interval. 1 means event 0 means no event. The index file has the list of each processed file path and the target (total number of events) they are in.

- ran for 20 mins ~ 12000 frames
- folder
- total number of files
- 1.5mm\_35.14pN
- 27
- 2mm\_22.6pN
- 29
- 3mm\_9.24pN
- 16
- 5mm\_1.46pN
- 63
- 9mm\_0.002pN
- 21
- Total number of examples 156

```
[2]: datasetlow = expermentDataloader(
    "/home/khood/GitHub/SNN-DNA-project/Preprocessing/data/seperatedData/low/
    ↪index.csv",
    "/home/khood/GitHub/SNN-DNA-project/Preprocessing/data/seperatedData/low",
)
datasetmedium = expermentDataloader(
    "/home/khood/GitHub/SNN-DNA-project/Preprocessing/data/seperatedData/medium/
    ↪index.csv",
    "/home/khood/GitHub/SNN-DNA-project/Preprocessing/data/seperatedData/medium",
)
datasetHigh = expermentDataloader(
    "/home/khood/GitHub/SNN-DNA-project/Preprocessing/data/seperatedData/high/
    ↪index.csv",
    "/home/khood/GitHub/SNN-DNA-project/Preprocessing/data/seperatedData/high",
)

print(f"datasetlow:{len(datasetlow)}")
print(f"datasetmedium:{len(datasetmedium)}")
print(f"datasetHigh:{len(datasetHigh)}")
print(f"Total: {len(datasetlow) + len(datasetmedium) + len(datasetHigh)}")
```

```
datasetlow:56
datasetmedium:16
datasetHigh:84
Total: 156
```

```
[3]: highTargets = [i[1][0] for i in datasetHigh]
      mediumTargets = [i[1][0] for i in datasetmedium]
      lowTargets = [i[1][0] for i in datasetlow]
      highTargets
```

```
[3]: [339,
      296,
      303,
      283,
      337,
      301,
      305,
      342,
      310,
      321,
      321,
      298,
      392,
      328,
      379,
      340,
      340,
      285,
      274,
      285,
      282,
      105,
      51,
      297,
      191,
      352,
      238,
      80,
      303,
      167,
      103,
      107,
      184,
      379,
      55,
      89,
      484,
```

535,  
262,  
113,  
501,  
196,  
179,  
488,  
165,  
327,  
710,  
135,  
87,  
167,  
133,  
258,  
635,  
224,  
53,  
538,  
462,  
311,  
187,  
219,  
57,  
34,  
165,  
446,  
175,  
219,  
363,  
243,  
375,  
413,  
210,  
155,  
342,  
252,  
55,  
234,  
336,  
248,  
90,  
93,  
228,  
61,  
280,  
456]

```
[4]: # def averageDiff(data: list):
#     diffs = []
#     while data:
#         point = data.pop()
#         for i in data:
#             diffs.append(abs(point - i))
#     return np.sum(diffs)/len(diffs)
```

```
[5]: # def printStats(data: list):
#     print("+-----")
#     print(f"| total number of experments: {len(data)}")
#     print(f"| min: {np.min(data)}")
#     print(f"| max: {np.max(data)}")
#     print(f"| average: {np.average(data)}")
#     print(f"| median: {np.median(data)}")
#     print(f"| mode: {st.mode(data, keepdims=False)}")
#     print(f"| average difference: {averageDiff(data)}")
#     print("+-----")
```

```
[6]: plt.plot(list(range(len(highTargets))), highTargets, '.', color='red',
             ↪label="highTargets")
plt.plot(list(range(len(mediumTargets))), mediumTargets, 'x', color='green',
             ↪label="mediumTargets")
plt.plot(list(range(len(lowTargets))), lowTargets, '+', color='blue',
             ↪label="lowTargets")
plt.legend(numpoints=1)
print("High")
printStats(highTargets)
print("Medium")
printStats(mediumTargets)
print("Low")
printStats(lowTargets)
```

High

```
+-----
| total number of experments: 84
| min: 34
| max: 710
| average: 265.01190476190476
| median: 277.0
| mode: ModeResult(mode=55, count=2)
| std: 138.69695417121417
| average difference: 156.210843373494
+-----
```

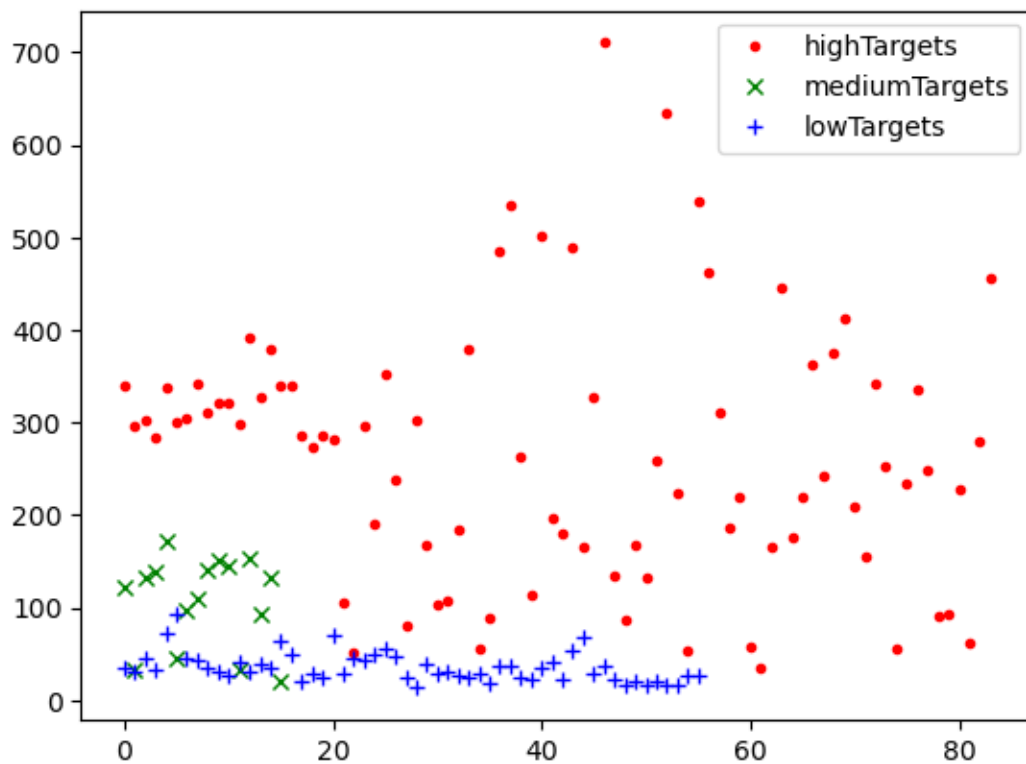
Medium

```
+-----
| total number of experments: 16
| min: 20
```

```

| max: 172
| average: 107.25
| median: 127.0
| mode: ModeResult(mode=132, count=2)
| std: 47.49144659830863
| average difference: 55.6
+-----
Low
+-----
| total number of experments: 56
| min: 13
| max: 93
| average: 35.42857142857143
| median: 30.5
| mode: ModeResult(mode=29, count=4)
| std: 15.76145517989234
| average difference: 16.967532467532468
+-----

```



## 1.1 Working with new data

- ran for 1 hour ~ 72000 frames  
folder

```

total number of files
50_nM_AR
640
100_nM_AR
499
400_nM_AR
477
800_nM_AR
564
1200_nM_AR
794
1800_nM_AR
888
Total number of examples 3862

```

```

[7]: datasetLarge = expermentDataloader(
    "/home/khood/GitHub/SNN-DNA-project/Preprocessing/large_dataset/allData/
    ↪index.csv",
    "/home/khood/GitHub/SNN-DNA-project/Preprocessing/large_dataset/allData/",
)
print(f"datasetLarge:{len(datasetLarge)}")

```

datasetLarge:3862

```

[8]: targets = [i[1][0] for i in datasetLarge]
plt.plot(list(range(len(targets))), targets, '.', color='black',
    ↪label="targets")
plt.legend(numpoints=1)
print("Large Dataset")
printStats(targets)

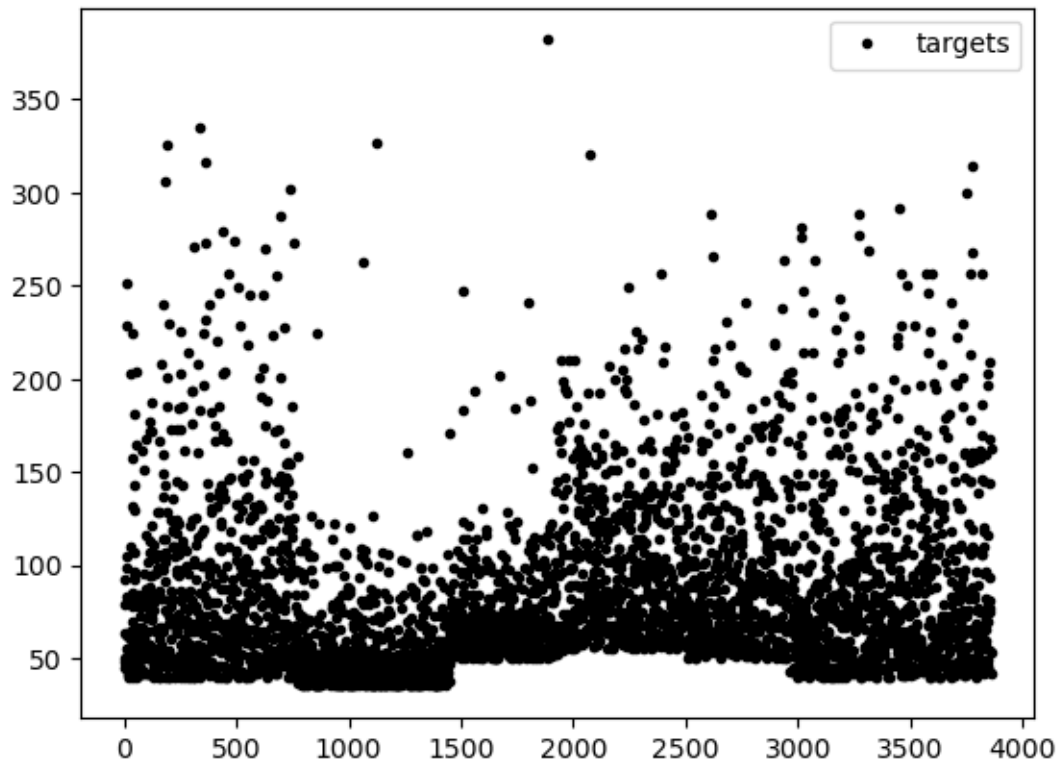
```

Large Dataset

```

+-----
| total number of experments: 3862
| min: 35
| max: 382
| average: 83.42050750906266
| median: 68.0
| mode: ModeResult(mode=51, count=83)
| std: 45.67206043130445
| average difference: 45.66128694559559
+-----

```



```
[9]: len(datasetLarge[0][0])
```

```
[9]: 12000
```

```
[10]: rawData = [datasetLarge[i] for i in list(range(len(datasetLarge)))]
def switchToDuration(expermentFrames):
    lastOne = 0
    for i in range(len(expermentFrames)):
        if expermentFrames[i]:
            expermentFrames[i] = i - lastOne if lastOne != 0 else 0
            lastOne = i
    return expermentFrames

for i in rawData:
    i = (switchToDuration(i[0]), i[1])
print(f"input: {rawData[0][0]}")
print(f"output: {rawData[0][1]}")
```

```
input: [0 0 0 ... 0 0 0]
```

```
output: [50]
```

```
[11]: np.max(rawData[0][0])
```

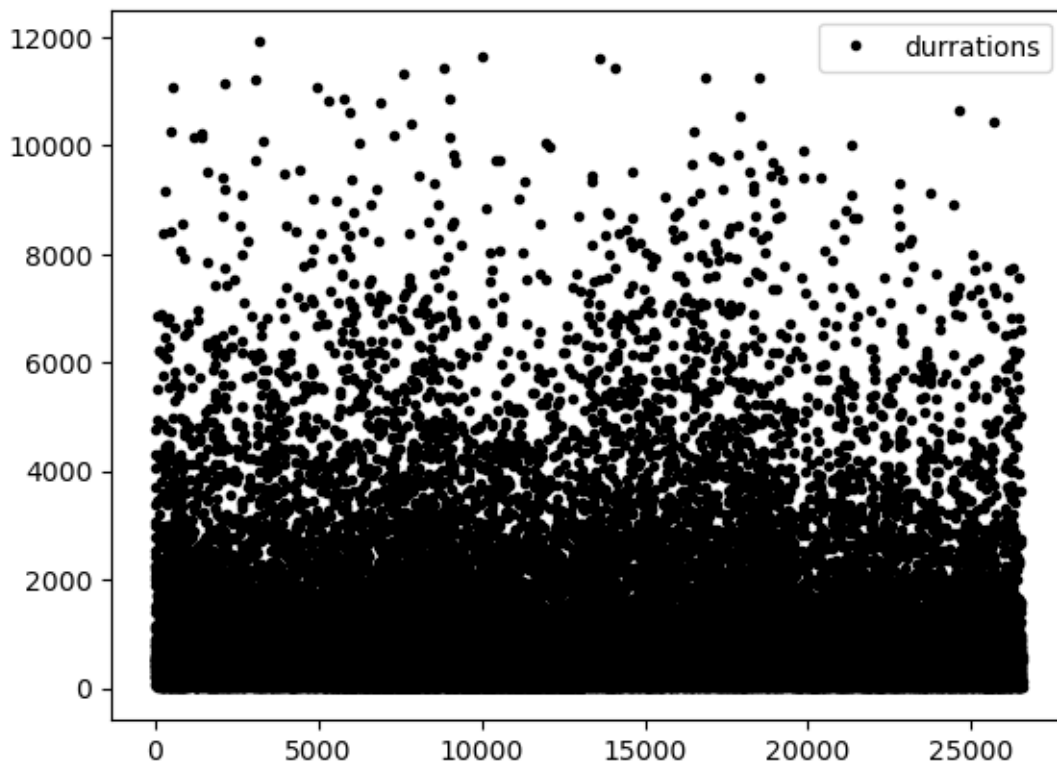


[11]: 2990

```
[12]: durations = []
      for i in rawData:
          for event in i[0]:
              if event:
                  durations.append(event)
      printStats(copy.deepcopy(durations))
      plt.plot(list(range(len(durations))), durations, '.', color='black',
               ↵label="durations")
      plt.legend(numpoints=1)
      len(durations)
```

```
+-----
| total number of experments: 26537
| min: 1
| max: 11904
| average: 1182.0039190564119
| median: 641.0
| mode: ModeResult(mode=2, count=319)
| std: 1494.0991292401238
| average difference: 1390.3879774224142
+-----
```

[12]: 26537



```
[13]: std_scale = preprocessing.StandardScaler().fit([[i] for i in durations])
normalized_durations = std_scale.transform([[i] for i in durations])
print(len(normalized_durations))
normalized_durations = [i[0] for i in normalized_durations]
normalized_durations
```

26537

```
[13]: [1.2100911148131834,
-0.44508687947273134,
-0.19744601498191514,
-0.018743012768272095,
-0.7596577073394438,
-0.5555213190429602,
-0.6545776648392867,
0.6572496173282802,
1.2689894825839723,
0.5407914810542207,
-0.4839062582307512,
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-0.5120168428486276,
0.5883117550511071,
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-0.03815270214728202,
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-0.3346524399025025,
-0.40559820108095257,
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-0.07563348163778393,
-0.4544570743453568,
-0.6431995710653843,
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```

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-0.649892567402974,  
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-0.4551263739791158,  
-0.6264670802214103,  
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-0.2563443827527039,  
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-0.1566187373226184,  
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-0.6030415930398465,  
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-0.1572880369563774,  
-0.07697208090530185,  
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-0.2523285849501501,  
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0.5113422971688264,  
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-0.5709152106194163,  
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-0.6746566538520555,  
-0.7804059959859717,  
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-0.7723744003808641,  
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-0.7583191080719259,  
-0.5749310084219701,

-0.42166139229116767,  
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-0.6646171593456711,  
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-0.6632785600781532,  
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1.060167996851176,  
-0.5642222142818267,  
-0.6017029937723286,  
-0.7589884077056849,  
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```

-0.6606013615431173,
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-0.34469193440888696,
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-0.4196534933898908,
-0.20681620985454063,
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-0.5160326406511814,
0.356064782136747,
-0.092365972481758,
-0.2523285849501501,
-0.7476103139317825,
-0.39823590510960394,
-0.5247335358900479,
-0.43906318276890066,
...]
```

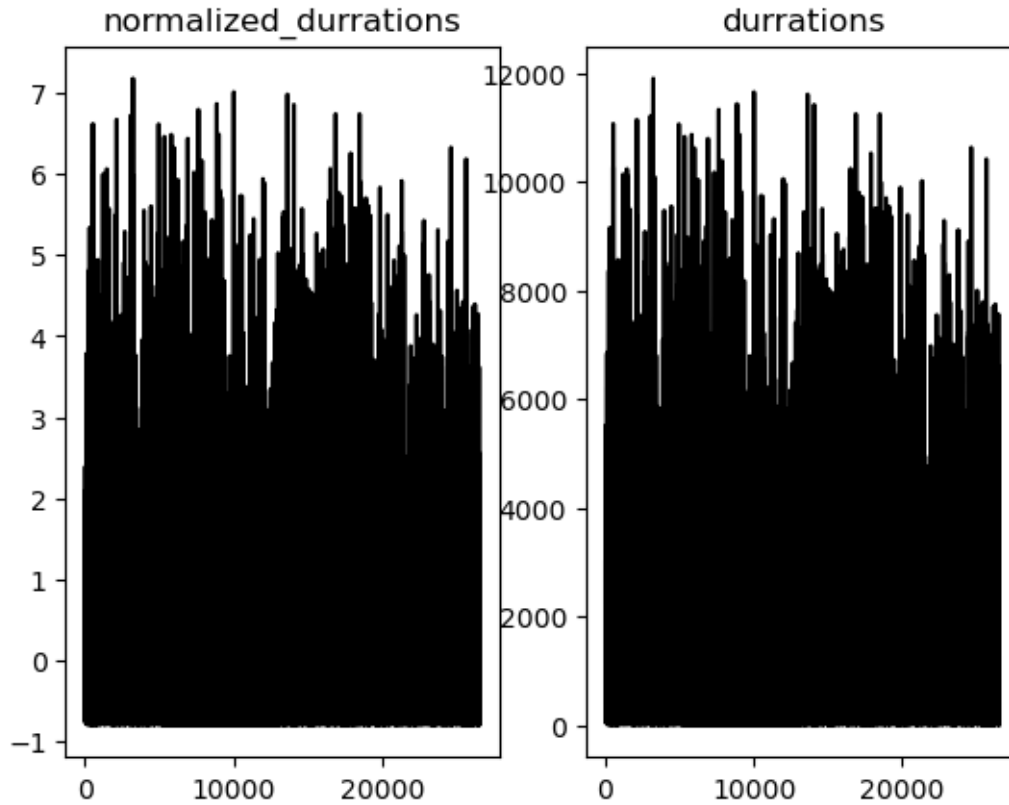
```

[14]: plt.plot(list(range(len(normalized_durations))), normalized_durations, '.',
             color='black', label="normalized_durations")
plt.legend(numpoints=1)

defultePlotSize = plt.rcParams['figure.figsize']
plt.rcParams['figure.figsize'] = [200, 5]
plt.subplot(1, 2, 1)
plt.title('normalized_durations')
plt.plot(list(range(len(normalized_durations))), normalized_durations, '-',
         color='black', )
plt.subplot(1, 2, 2)
plt.title('durations')
plt.plot(list(range(len(durations))), durations, '-', color='black')
plt.rcParams['figure.figsize'] = defultePlotSize
```

/tmp/ipykernel\_3054737/2366011641.py:6: MatplotlibDeprecationWarning: Auto-removal of overlapping axes is deprecated since 3.6 and will be removed two minor releases later; explicitly call `ax.remove()` as needed.

```
plt.subplot(1, 2, 1)
```



## 1.2 ## Baseline estimates via naive approach

Small data set

```
[15]: datasetlow = expermentDataloader(
    "/home/khood/GitHub/SNN-DNA-project/Preprocessing/data/seperatedData/low/
    ↪index.csv",
    "/home/khood/GitHub/SNN-DNA-project/Preprocessing/data/seperatedData/low",
)
datasetmedium = expermentDataloader(
    "/home/khood/GitHub/SNN-DNA-project/Preprocessing/data/seperatedData/medium/
    ↪index.csv",
    "/home/khood/GitHub/SNN-DNA-project/Preprocessing/data/seperatedData/medium",
)
datasetHigh = expermentDataloader(
    "/home/khood/GitHub/SNN-DNA-project/Preprocessing/data/seperatedData/high/
    ↪index.csv",
    "/home/khood/GitHub/SNN-DNA-project/Preprocessing/data/seperatedData/high",
)
print(f"datasetlow:{len(datasetlow)}")
```



```

print(f"datasetmedium:{len(datasetmedium)}")
print(f"datasetHigh:{len(datasetHigh)}")
print(f"Total: {len(datasetlow) + len(datasetmedium) + len(datasetHigh)}")
rawData = [i for i in datasetlow] + [i for i in datasetmedium] + [i for i in
    ↪datasetHigh]
print(len(rawData))
rawData[:3]

```

```

datasetlow:56
datasetmedium:16
datasetHigh:84
Total: 156
156

```

```

[15]: [(array([0, 0, 0, ..., 0, 0, 0]), array([34])),
      (array([0, 0, 0, ..., 0, 0, 0]), array([30])),
      (array([0, 0, 0, ..., 0, 0, 0]), array([45]))]

```

Dumb method is to just assume that the rate of events is constant (i.e. this data has the first half of the experment we will just double the sum of events)

```

[16]: predictions = [np.sum(i[0])*2 for i in rawData]
      predictions[:3]

```

```

[16]: [26, 40, 66]

```

```

[17]: targets = [i[1][0] for i in rawData]
      targets[:3]

```

```

[17]: [34, 30, 45]

```

```

[18]: for em in range(21):
      acc = np.isclose(predictions,targets, atol=em)
      print(f"accurate within {em} events {int((np.sum(acc)/len(acc))*100)}% of
    ↪the time")

```

```

accurate within 0 events 0% of the time
accurate within 1 events 7% of the time
accurate within 2 events 9% of the time
accurate within 3 events 10% of the time
accurate within 4 events 12% of the time
accurate within 5 events 14% of the time
accurate within 6 events 17% of the time
accurate within 7 events 19% of the time
accurate within 8 events 20% of the time
accurate within 9 events 25% of the time
accurate within 10 events 26% of the time
accurate within 11 events 30% of the time
accurate within 12 events 30% of the time

```

```

accurate within 13 events 34% of the time
accurate within 14 events 36% of the time
accurate within 15 events 39% of the time
accurate within 16 events 41% of the time
accurate within 17 events 44% of the time
accurate within 18 events 46% of the time
accurate within 19 events 49% of the time
accurate within 20 events 50% of the time

```

Large data set

```

[19]: datasetLarge = expermentDataLoader(
        "/home/khood/GitHub/SNN-DNA-project/Preprocessing/large_dataset/allData/
        ↪index.csv",
        "/home/khood/GitHub/SNN-DNA-project/Preprocessing/large_dataset/allData/",
    )
print(f"datasetLarge:{len(datasetLarge)}")
rowData = [i for i in datasetLarge]
print(len(rowData))
rowData[:3]

```

```

datasetLarge:3862
3862

```

```

[19]: [(array([0, 0, 0, ..., 0, 0, 0]), array([50])),
       (array([0, 0, 0, ..., 0, 0, 0]), array([79])),
       (array([0, 0, 0, ..., 0, 0, 0]), array([48]))]

```

```

[20]: predictions = [np.sum(i[0])*6 for i in rowData]
      predictions[:3]

```

```

[20]: [30, 42, 24]

```

```

[21]: targets = [i[1][0] for i in rowData]
      targets[:3]

```

```

[21]: [50, 79, 48]

```

```

[22]: for em in range(21):
        acc = np.isclose(predictions,targets, atol=em)
        print(f"accurate within {em} events {int((np.sum(acc)/len(acc))*100)}% of_
        ↪the time")

```

```

accurate within 0 events 0% of the time
accurate within 1 events 2% of the time
accurate within 2 events 3% of the time
accurate within 3 events 5% of the time
accurate within 4 events 6% of the time
accurate within 5 events 7% of the time
accurate within 6 events 9% of the time

```

```

accurate within 7 events 10% of the time
accurate within 8 events 11% of the time
accurate within 9 events 12% of the time
accurate within 10 events 14% of the time
accurate within 11 events 15% of the time
accurate within 12 events 16% of the time
accurate within 13 events 18% of the time
accurate within 14 events 19% of the time
accurate within 15 events 20% of the time
accurate within 16 events 22% of the time
accurate within 17 events 24% of the time
accurate within 18 events 25% of the time
accurate within 19 events 26% of the time
accurate within 20 events 27% of the time

```

### 1.3 ##### working with old data set expect its only the first 3.33 min (200sec)

```

[23]: datasetLarge = expermentDataloader(
        "/home/khood/GitHub/SNN-DNA-project/Preprocessing/smallData6min/allData/
        ↪index.csv",
        "/home/khood/GitHub/SNN-DNA-project/Preprocessing/smallData6min/allData",
    )
print(f"datasetLarge:{len(datasetLarge)}")
rawData = [i for i in datasetLarge]
len(rawData[0][0])

```

datasetLarge:156

[23]: 4000

### 1.4 ##### working with data in seprated folders

```

[24]: folders = [d[0] for d in os.walk("/home/khood/GitHub/SNN-DNA-project/
        ↪Preprocessing/sorted")][1:] # remove first one is it is "/home/khood/GitHub/
        ↪SNN-DNA-project/Preprocessing/sorted"
folders

```

```

[24]: [' /home/khood/GitHub/SNN-DNA-project/Preprocessing/sorted/1800_nM_AR_out',
        '/home/khood/GitHub/SNN-DNA-project/Preprocessing/sorted/800_nM_AR_out',
        '/home/khood/GitHub/SNN-DNA-project/Preprocessing/sorted/1200_nM_AR_out',
        '/home/khood/GitHub/SNN-DNA-project/Preprocessing/sorted/400_nM_AR_out',
        '/home/khood/GitHub/SNN-DNA-project/Preprocessing/sorted/50_nM_AR_out',
        '/home/khood/GitHub/SNN-DNA-project/Preprocessing/sorted/100_nM_AR_out']

```

```

[25]: datasets = []
for d in folders:
    datasets.append(expermentDataloader(
        f"{d}/index.csv",
    )

```

```
        f"{d}",
    ))
```

```
[26]: colors = []
      ↪ ['black', 'brown', 'red', 'darkred', 'olive', 'yellow', 'olivedrab', 'forestgreen', 'green', 'darksl
      # for c in list(mcolors.CSS4_COLORS.keys()):
      #     colors.append(c)
```

```
[27]: assert(len(colors) >= len(datasets))
```

```
[28]: defulte_ast_node_interactivity = InteractiveShell.ast_node_interactivity
      defultePlotSize = plt.rcParams['figure.figsize']
      InteractiveShell.ast_node_interactivity = 'all'
      InteractiveShell.ast_node_interactivity
```

```
[28]: 'all'
```

```
[29]: targets = []
      for d in datasets:
          targets.append([i[1] for i in d])

      plt.rcParams['figure.figsize'] = [20, 5]
      for i in range(len(targets)):
          c = colors.pop(random.randrange(len(colors)))
          plt.plot(list(range(len(targets[i]))), targets[i], '.', color=c,
          ↪ label=f"dataset {i}")
          print(f"dataset {i}")
          printStats(targets[i])
      plt.legend(numpoints=1)
```

```
[29]: [<matplotlib.lines.Line2D at 0x7f65d917b490>]
```

```
dataset 0
+-----+
| total number of experments: 888
| min: 40
| max: 314
| average: 90.42792792792793
| median: 72.0
| mode: ModeResult(mode=array([40]), count=array([22]))
| std: 51.60189983787117
| average difference: 53.028403262337875
+-----+
```

```
[29]: [<matplotlib.lines.Line2D at 0x7f65d917b700>]
```

```
dataset 1
+-----+
```

```

| total number of experments: 564
| min: 55
| max: 321
| average: 99.34219858156028
| median: 87.0
| mode: ModeResult(mode=array([56]), count=array([16]))
| std: 40.73101863266106
| average difference: 43.4588954814003
+-----

```

[29]: [<matplotlib.lines.Line2D at 0x7f65d917ba00>]

```

dataset 2
+-----
| total number of experments: 794
| min: 40
| max: 335
| average: 88.81863979848866
| median: 71.0
| mode: ModeResult(mode=array([40]), count=array([30]))
| std: 52.30042893384055
| average difference: 52.46033777924598
+-----

```

[29]: [<matplotlib.lines.Line2D at 0x7f65d917bd00>]

```

dataset 3
+-----
| total number of experments: 477
| min: 50
| max: 289
| average: 93.79874213836477
| median: 81.0
| mode: ModeResult(mode=array([53]), count=array([15]))
| std: 43.31442933681775
| average difference: 44.79590578369713
+-----

```

[29]: [<matplotlib.lines.Line2D at 0x7f65d917bf40>]

```

dataset 4
+-----
| total number of experments: 640
| min: 35
| max: 327
| average: 53.5765625
| median: 46.0
| mode: ModeResult(mode=array([35]), count=array([45]))
| std: 24.50172979982421

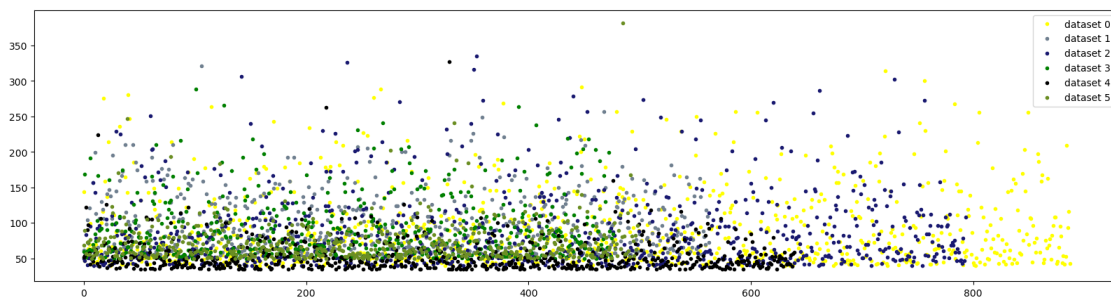
```

```
| average difference: 21.00057218309859
+-----
```

```
[29]: [<matplotlib.lines.Line2D at 0x7f65d91c8220>]
```

```
dataset 5
+-----
| total number of experiments: 499
| min: 50
| max: 382
| average: 72.72144288577154
| median: 64.0
| mode: ModeResult(mode=array([50]), count=array([23]))
| std: 28.88898939975788
| average difference: 24.575013480776814
+-----
```

```
[29]: <matplotlib.legend.Legend at 0x7f65d91bc1f0>
```



```
[30]: plt.rcParams['figure.figsize'] = defultePlotSize
InteractiveShell.ast_node_interactivity = defulte_ast_node_interactivity
```

## 1.5 ##### finding margin of error

```
[31]: folders = [d[0] for d in os.walk("/home/khood/GitHub/SNN-DNA-project/
↳Preprocessing/sorted")][1:] # remove first one is it is "/home/khood/GitHub/
↳SNN-DNA-project/Preprocessing/sorted"
targets = []
for d in folders:
    data = expermentDataloader(
        f"{d}/index.csv",
        f"{d}",
    )
    targets.append([d[1] for d in data])
```

```
[32]: print(len(targets))
      targets
```

6

```
[32]: [[array([144]),
        array([47]),
        array([58]),
        array([56]),
        array([64]),
        array([69]),
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```

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$$M.O.E. = z \times \frac{\sigma}{\sqrt{n}}$$

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