test_gd

April 17, 2022

[1]:

```python
## Abstractions
import numpy as np
import pandas as pd

## Plotting
from matplotlib import pyplot as plt
plt.style.use('seaborn')
import seaborn as sns
import pylab as pl

## Scalers
from sklearn.preprocessing import StandardScaler
from sklearn.preprocessing import MinMaxScaler

## Models
from sklearn.linear_model import LogisticRegression

## Model Selection
from sklearn.model_selection import GridSearchCV
from sklearn.model_selection import KFold
from sklearn.model_selection import StratifiedKFold

## Timing
import time

# Model
from MAPEstimator import MAPEstimator
```

Import Data

[2]:

```python
headers = ['molecule_name', 'conformation_name']
for i in range(1, 167):
    name = 'f%i' % i
    headers.append(name)
headers.append('class')
```

[3]:

```python
# headers = pd.read_csv('clean2.info')
df = pd.read_csv('src/clean2.data')
```

```
df.columns = headers
```

```
[4]: X = np.asarray(df.iloc[:,2:-1])
     y = np.asarray(df.iloc[:,-1])
```

Standard Scaler

```
[5]: X_std = StandardScaler().fit_transform(X)
```

Train and Test Model

```
[6]: clf = MAPEstimator(w_D = np.zeros(X.shape[1]), step_size=0.1, alpha=0.1,␣
      ↪max_iter = 10000000)
     clf.fit(X_std,y)
     predict_y = clf.predict_proba(X_std)
```

```
[7]: score = clf.score(X_std, y)
     score
```

```
[7]: 0.6296801576474155
```

```
[8]: (np.sum(y==0)) / len(y)
```

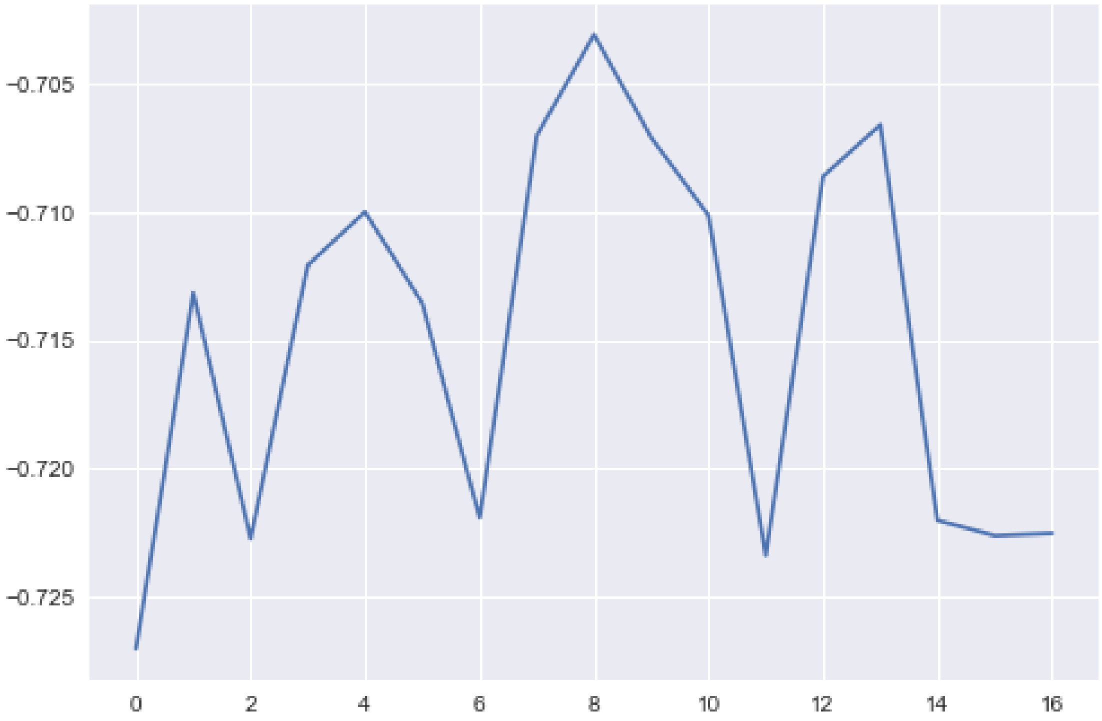
```
[8]: 0.8459906017886918
```

```
[10]: clf.iteration_count
```

```
[10]: 1700000
```

```
[11]: plt.plot(clf.loss_array)
```

```
[11]: [<matplotlib.lines.Line2D at 0x7fd71c99fee0>]
```



[17]:
```
clf = MAPEstimator(w_D = np.zeros(X.shape[1]), step_size=0.1, alpha=0.1,␣
 ↪max_iter = 10000000, step_size_type = 'differential')
clf.fit(X_std,y)
predict_y = clf.predict_proba(X_std)
```

[18]:
```
score = clf.score(X_std, y)
score
```

[18]:
```
0.6396847051690162
```

[19]:
```
(np.sum(y==0)) / len(y)
```

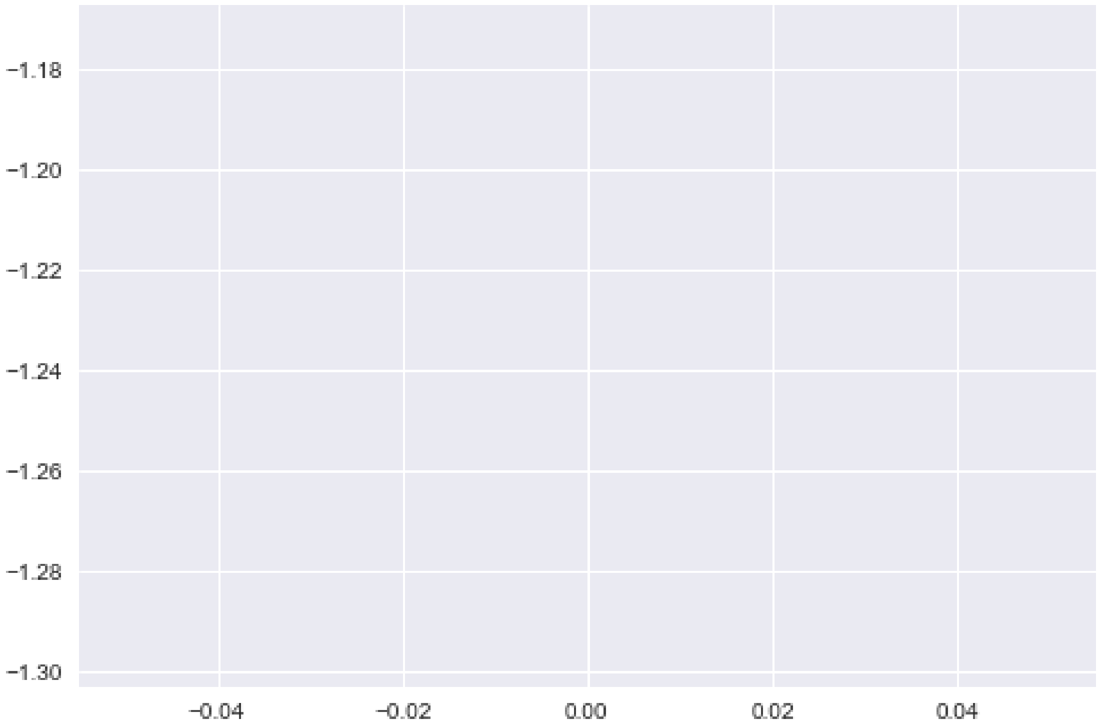
[19]:
```
0.8459906017886918
```

[20]:
```
clf.iteration_count
```

[20]:
```
300000
```

[21]:
```
plt.plot(clf.loss_array)
```

[21]:
```
[<matplotlib.lines.Line2D at 0x7fd71cb516a0>]
```



Model Evaluation

[6]:
```
kf = KFold(n_splits=10, shuffle = True, random_state = 136)
kf.get_n_splits(X_std, y)
```

[6]:
```
10
```

[7]:
```
iteration_counts = []
test_scores = []

for train_index, test_index in kf.split(X_std, y):
    X_train, X_test = X_std[train_index], X_std[test_index]
    y_train, y_test = y[train_index], y[test_index]
    clf = MAPEstimator(w_D = np.zeros(X.shape[1]), step_size=0.1, alpha=0.1, max_iter = 10000000)
    clf.fit(X_train,y_train)
    iteration_counts.append(clf.iteration_count)
    score = clf.score(X_test, y_test)
    test_scores.append(score)
```

[8]:
```
test_scores
```

[8]:

```
[0.6181818181818182,
 0.5409090909090909,
 0.6151515151515151,
 0.6439393939393939,
 0.5772727272727273,
 0.6,
 0.5590909090909091,
 0.575113808801214,
 0.6236722306525038,
 0.6585735963581184]
```

[9]:

```
iteration_counts
```

[9]:

```
[470000,
 2986000,
 155000,
 150000,
 1942000,
 4821000,
 352000,
 507000,
 1327000,
 260000]
```

[10]:

```
basic_test_scores = test_scores
```

[11]:

```
basic_iteration_counts = iteration_counts
```

[12]:

```
np.mean(basic_test_scores)
```

[12]:

```
0.6011905090357291
```

[13]:

```
np.mean(basic_iteration_counts)
```

[13]:

```
1297000.0
```

[14]:

```
kf = KFold(n_splits=10, shuffle = True, random_state = 136)
kf.get_n_splits(X_std, y)
```

[14]:

```
10
```

[15]:

```
iteration_counts = []
test_scores = []

for train_index, test_index in kf.split(X_std, y):
    X_train, X_test = X_std[train_index], X_std[test_index]
    y_train, y_test = y[train_index], y[test_index]
    clf = MAPEstimator(w_D = np.zeros(X.shape[1]), step_size=0.1, alpha=0.1,␣
↪max_iter = 10000000, step_size_type = 'differential')
    clf.fit(X_train,y_train)
    iteration_counts.append(clf.iteration_count)
    score = clf.score(X_test, y_test)
    test_scores.append(score)
```

```
/Users/nathanieldavis/Documents/tufts/2022spring/cs136/project/cs136_final_proje
ct/Checkpoint 2/MAPEstimator.py:141: RuntimeWarning: divide by zero encountered
in log
  L = train_y[example_num] * np.log(sig) + (1-train_y[example_num]) *
np.log(1-sig)
/Users/nathanieldavis/Documents/tufts/2022spring/cs136/project/cs136_final_proje
ct/Checkpoint 2/MAPEstimator.py:141: RuntimeWarning: invalid value encountered
in double_scalars
  L = train_y[example_num] * np.log(sig) + (1-train_y[example_num]) *
np.log(1-sig)
```

[16]:

```
test_scores
```

[16]:

```
[0.6393939393939394,
 0.6287878787878788,
 0.6272727272727273,
 0.696969696969697,
 0.6681818181818182,
 0.6106060606060606,
 0.5015151515151515,
 0.5386949924127465,
 0.5766312594840668,
 0.6176024279210925]
```

[17]:

```
iteration_counts
```

[17]:

```
[273000,
 889000,
 1997000,
 272000,
 301000,
 411000,
 1267000,
 2137000,
 434000,
 751000]
```

[18]:

```
differential_test_scores = test_scores
```

[19]:

```
differential_iteration_counts = iteration_counts
```

```
[20]: np.mean(differential_test_scores)
```

```
[20]: 0.6105655952545179
```

```
[21]: np.mean(differential_iteration_counts)
```

```
[21]: 873200.0
```

```
[22]: plot_test_scores = np.array([np.mean(basic_test_scores),np.
       ↪mean(differential_test_scores)])
```

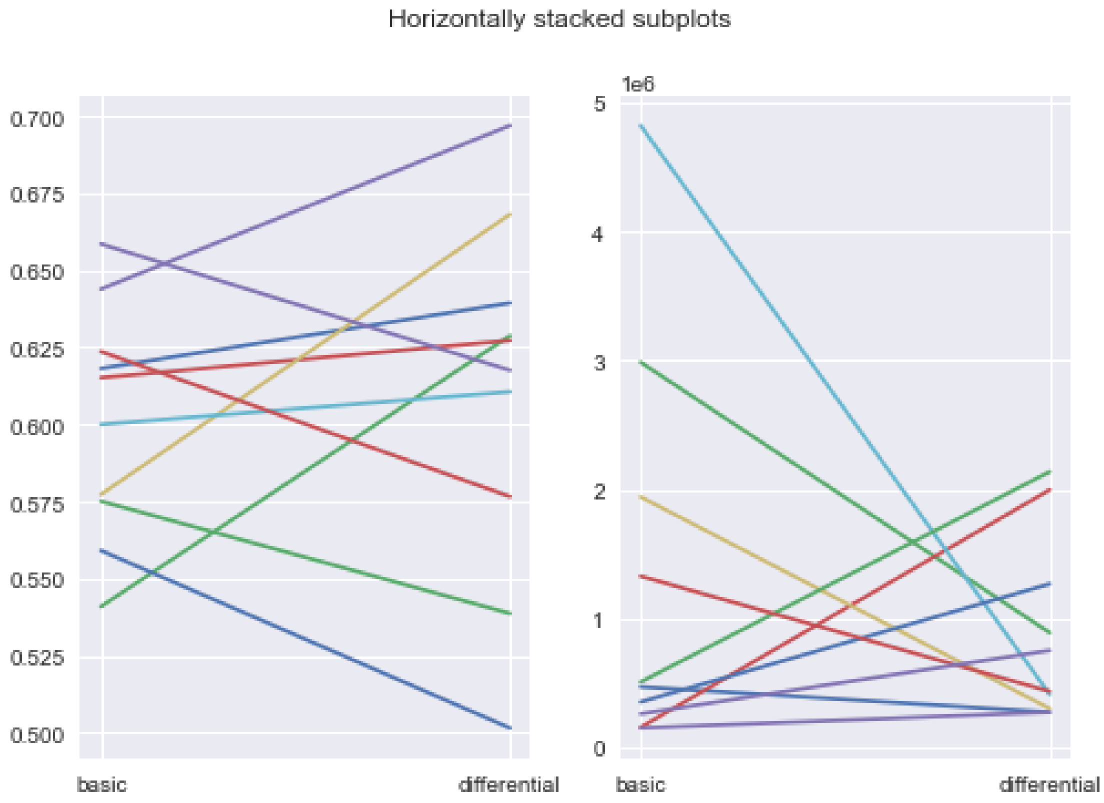
```
[23]: plot_iteration_counts = np.array([np.mean(basic_iteration_counts), np.
       ↪mean(differential_iteration_counts)])
```

```
[24]: plot_test_scores = np.array([basic_test_scores, differential_test_scores])
```

```
[25]: plot_iteration_counts = np.array([basic_iteration_counts,␣
       ↪differential_iteration_counts])
```

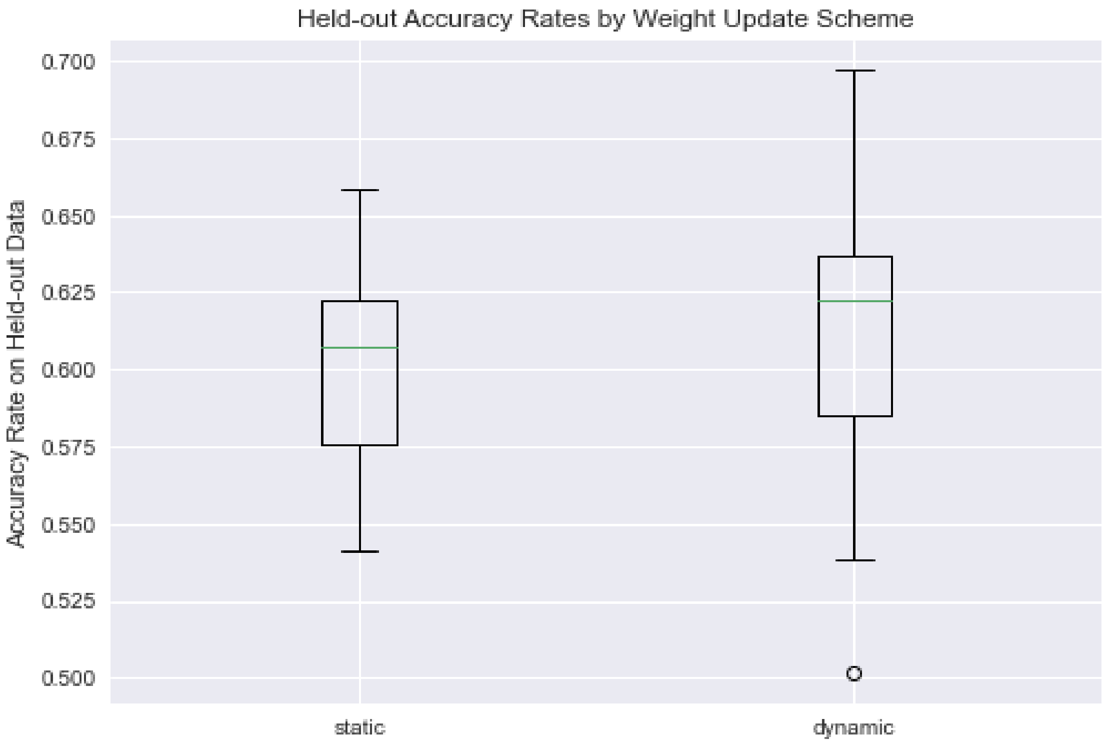
```
[26]: fig, (ax1, ax2) = plt.subplots(1, 2)
      fig.suptitle('Horizontally stacked subplots')
      ax1.plot(['basic','differential'],plot_test_scores)
      ax2.plot(['basic','differential'], plot_iteration_counts)
```

```
[26]: [<matplotlib.lines.Line2D at 0x7f9bf0f40c10>,
       <matplotlib.lines.Line2D at 0x7f9bf0f40bb0>,
       <matplotlib.lines.Line2D at 0x7f9bf0f40d60>,
       <matplotlib.lines.Line2D at 0x7f9bf0f40e80>,
       <matplotlib.lines.Line2D at 0x7f9bf0f40fa0>,
       <matplotlib.lines.Line2D at 0x7f9bf0f4e100>,
       <matplotlib.lines.Line2D at 0x7f9bf0f40c40>,
       <matplotlib.lines.Line2D at 0x7f9bf0f4e220>,
       <matplotlib.lines.Line2D at 0x7f9bf0f4e430>,
       <matplotlib.lines.Line2D at 0x7f9bf0f4e550>]
```



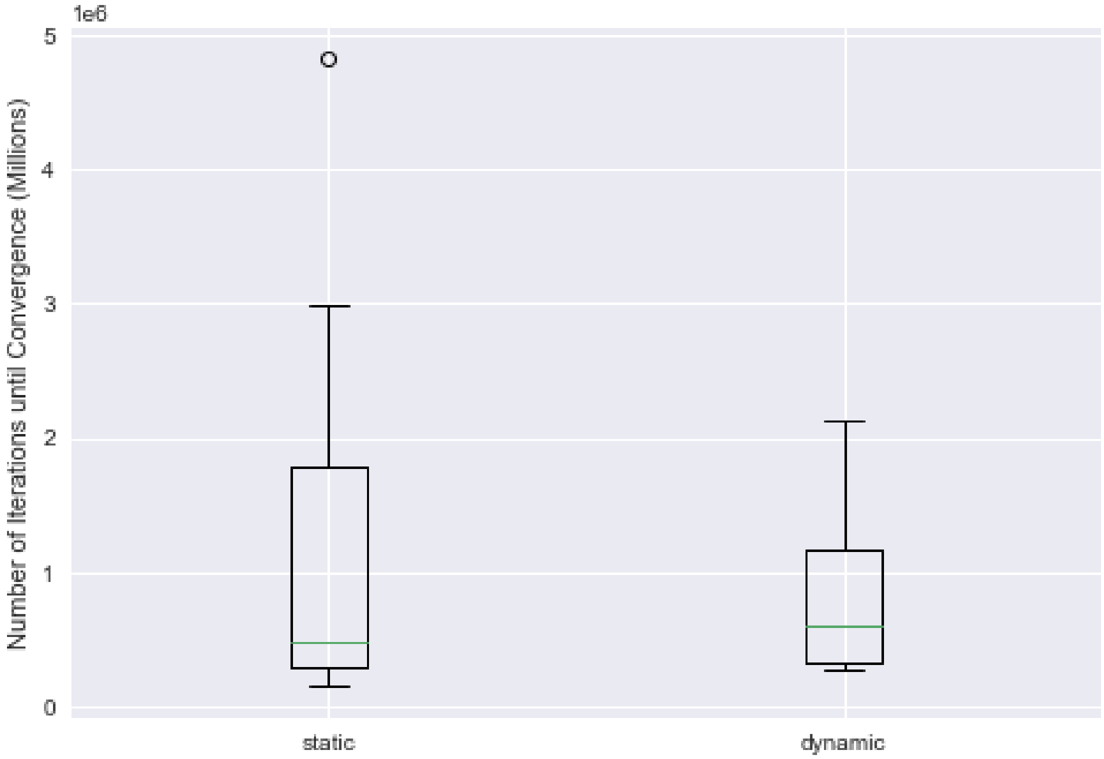
```
[35]: plt.boxplot(np.transpose(plot_test_scores), labels = ['static', 'dynamic'])
      plt.title('Held-out Accuracy Rates by Weight Update Scheme')
      plt.ylabel('Accuracy Rate on Held-out Data')
```

```
[35]: Text(0, 0.5, 'Accuracy Rate on Held-out Data')
```



```
[36]: plt.boxplot(np.transpose(plot_iteration_counts), labels = ['static', 'dynamic'])
      plt.ylabel('Number of Iterations until Convergence (Millions)')
```

```
[36]: Text(0, 0.5, 'Number of Iterations until Convergence (Millions)')
```

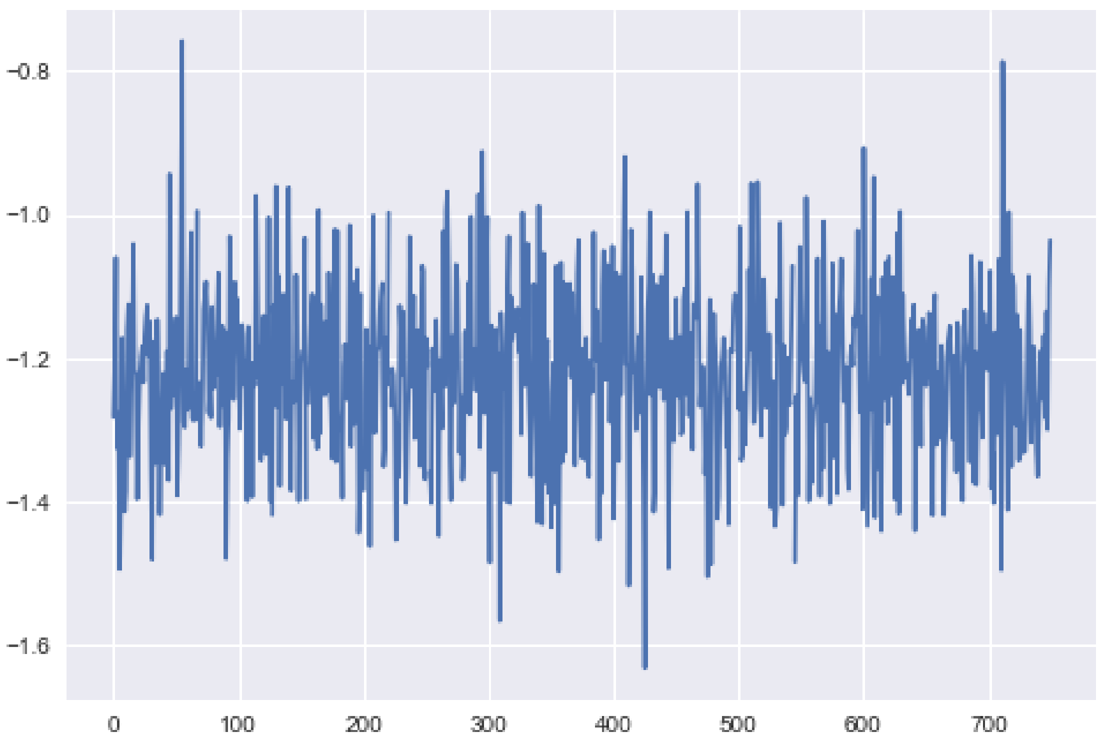


```
[51]: plot_test_scores
```

```
[51]: array([[0.61818182, 0.63787879, 0.61515152, 0.64393939, 0.59848485,
                0.5530303 , 0.55909091, 0.57511381, 0.53717754, 0.6585736 ],
               [0.63939394, 0.62878788, 0.63484848, 0.6969697 , 0.66818182,
                0.61060606, 0.65151515, 0.61001517, 0.57663126, 0.61760243]])
```

```
[39]: plt.plot(clf.loss_array)
```

```
[39]: [<matplotlib.lines.Line2D at 0x7f9bf15eed60>]
```


−0.8
−1.0
−1.2
−1.4
−1.6
0
100
200
300
400
500
600
700

```
[ ]:
```