Deepnote aasdasd / 👏 Welcome - Duplicate Published at Feb 7, 2023 Unlisted

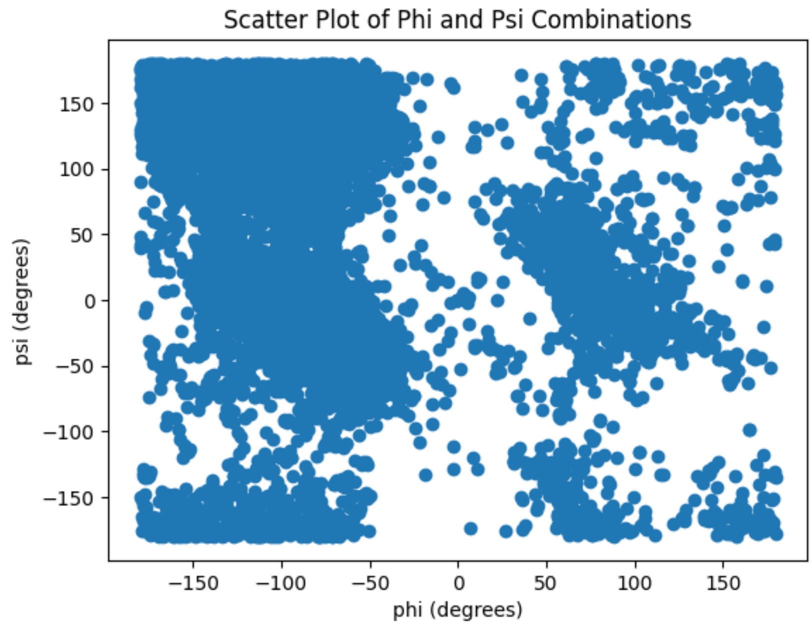
SQL Saved to variable df

```sql
SELECT *
FROM 'data_assignment3.csv'
```

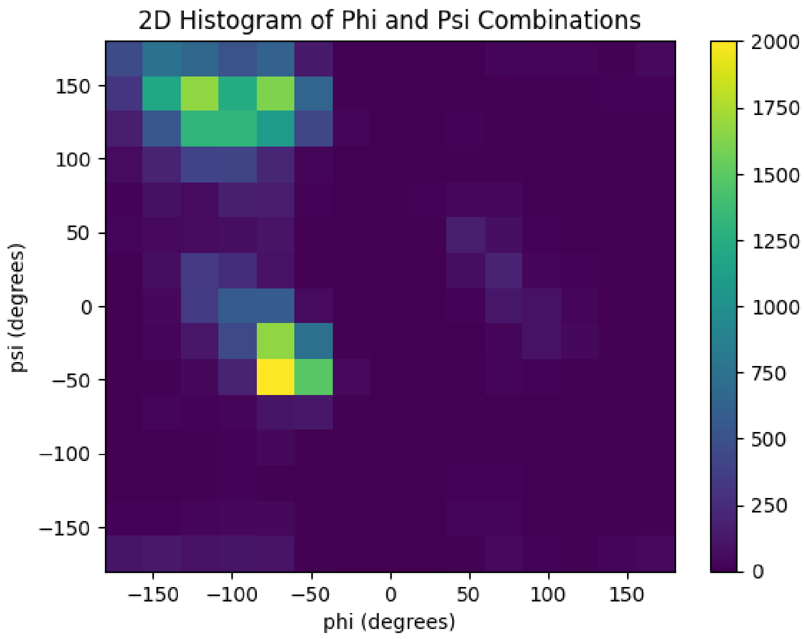
	residue name obj...	position int64	chain object	phi float64	psi float64
	LEU 8.6% GLY 7.4% 18 others 84%	1 - 772	A 33.2% B 17.5% 17 others 49.4%		
29140	ASP	144	B	63.913851	19.526092
29141	MET	145	B	-87.949329	-27.653868
29142	ILE	146	B	-124.307292	139.159315
29143	ASP	147	B	-152.104702	-176.079553
29144	ASN	148	B	48.898069	55.697055
29145	LEU	149	B	-74.15836	-43.500613
29146	LEU	150	B	-133.016846	147.535712
29147	SER	151	B	-130.258218	152.566267
29148	PRO	152	B	-52.371554	-33.945923
29149	ASP	153	B	-65.598604	-7.968961

```python
import matplotlib.pyplot as plt
import numpy as np
import warnings
warnings.filterwarnings("ignore")
from sklearn.cluster import KMeans
from sklearn.metrics import silhouette_score
from sklearn.cluster import DBSCAN
from sklearn import metrics
from sklearn import datasets
from sklearn.datasets import make_blobs
from sklearn.preprocessing import StandardScaler
```

```python
plt.scatter(df['phi'], df['psi'])
plt.xlabel('phi (degrees)')
plt.ylabel('psi (degrees)')
plt.title('Scatter Plot of Phi and Psi Combinations')
plt.show()
```

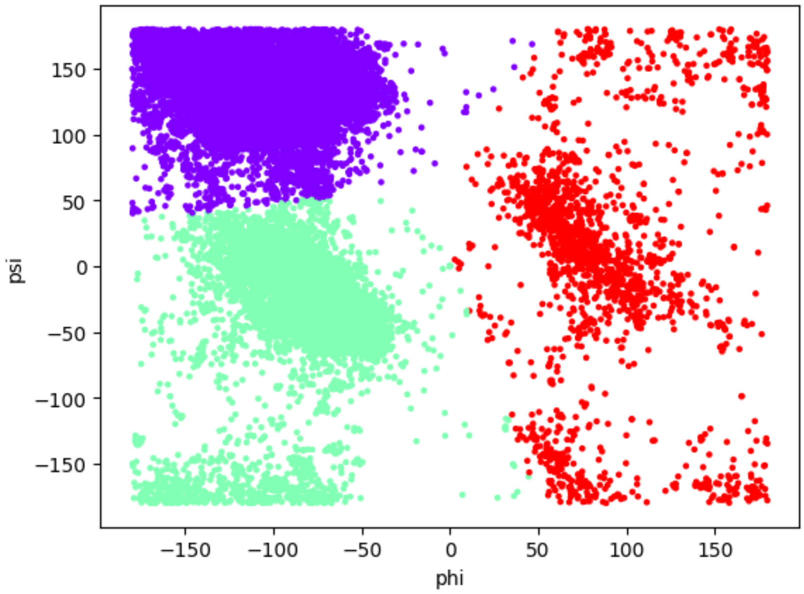



```
#Stugers Rule bins = log2(n) + 1
hist, xedges, yedges = np.histogram2d(df['phi'], df['psi'], bins=15)


plt.imshow(hist.T, origin='lower', extent=[xedges[0], xedges[-1], yedges[0], yedges[-1]], aspect='a
plt.xlabel('phi (degrees)')
plt.ylabel('psi (degrees)')
plt.title('2D Histogram of Phi and Psi Combinations')
plt.colorbar()
plt.show()
```

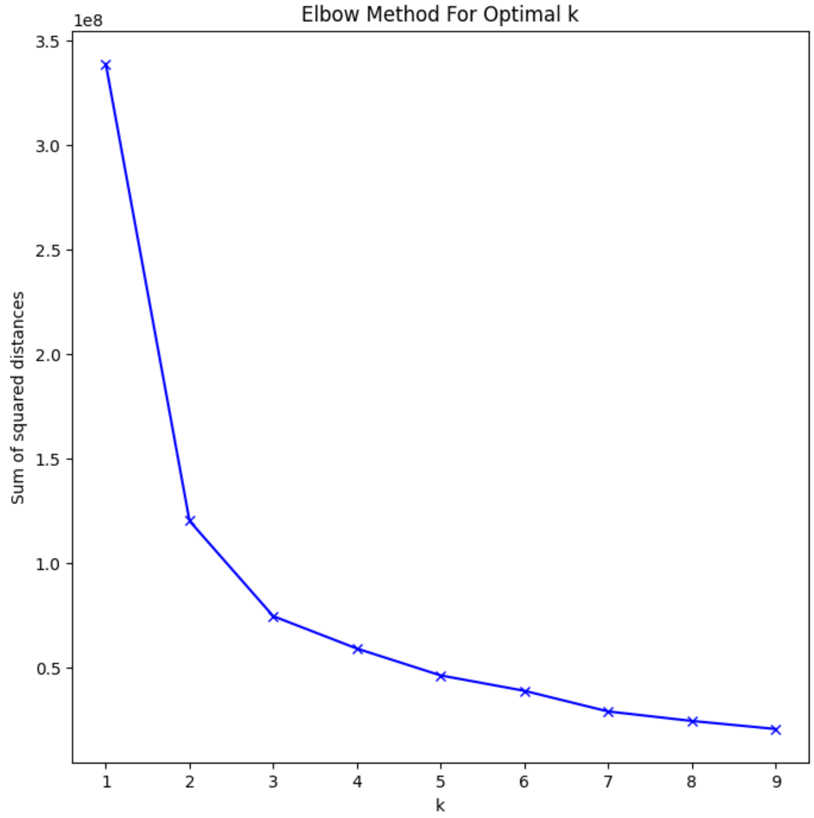



```
X = df[['phi', 'psi']].values

kmeans = KMeans(n_clusters=3, random_state=0).fit(X)

df['cluster'] = kmeans.labels_

plt.scatter(x=df['phi'], y=df['psi'], c = df['cluster'], cmap='rainbow', s = 5)
plt.rcParams['figure.figsize'] = (8,8)
plt.xlabel('phi')
plt.ylabel('psi')
plt.show
```

```
<function matplotlib.pyplot.show(close=None, block=None)>
```




```
sum_of_squared_distances = []
K = range(1, 10)

for k in K:
    kmeans = KMeans(n_clusters=k, random_state=0).fit(X)
    sum_of_squared_distances.append(kmeans.inertia_)

plt.plot(K, sum_of_squared_distances, 'bx-')
plt.xlabel('k')
plt.ylabel('Sum of squared distances')
plt.title('Elbow Method For Optimal k')
plt.rcParams['figure.figsize'] = (8,8)
plt.show()
```

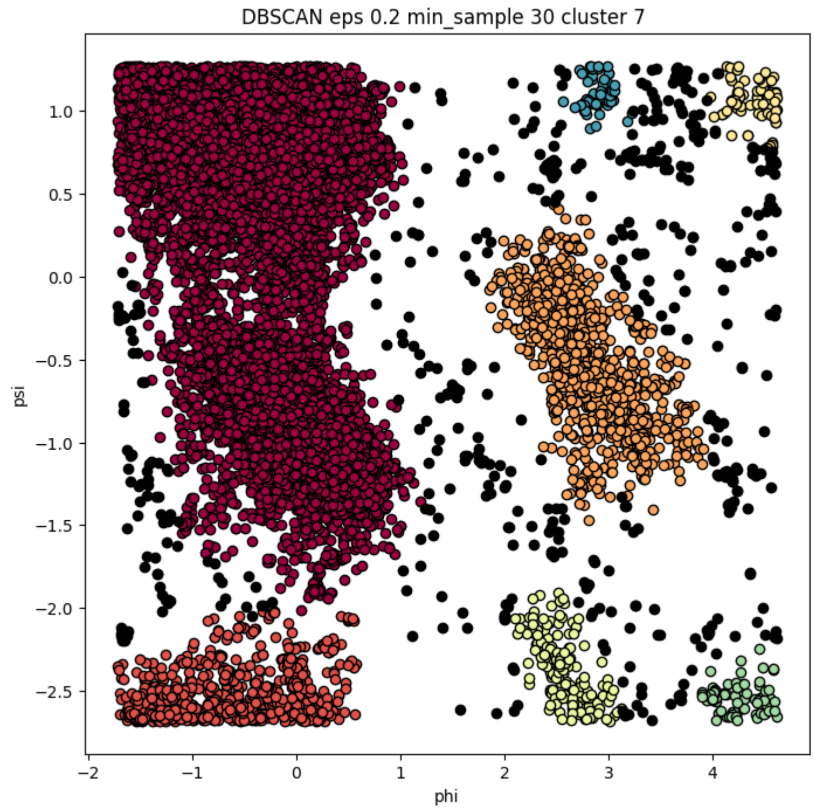



```
silhouette_score = silhouette_score(X, df['cluster'])
```

```
X = df.loc[:, ["phi", "psi"]].values.reshape(-1, 2)
X = StandardScaler().fit_transform(X)
X_with_res = df.loc[:, ["residue name", "phi", "psi"]].values.reshape(-1, 3)
X_outliers_clsuter = []

eps=0.20
min_samples=30
db = DBSCAN(eps = eps, min_samples=min_samples).fit(X)
labels = db.labels_


# Number of clusters in labels, ignoring noise if present.
n_clusters_ = len(set(labels)) - (1 if -1 in labels else 0)
n_noise_ = list(labels).count(-1)

core_samples_mask = np.zeros_like(labels, dtype=bool)
core_samples_mask[db.core_sample_indices_] = True

print("Estimated number of clusters: %d" % n_clusters_)
print("Estimated number of noise points: %d" % n_noise_)


unique_labels = set(labels)
####
```

```
colors = [plt.cm.Spectral(each) for each in np.linspace(0, 1, len(unique_labels))]

for k, col in zip(unique_labels, colors):
    if k == -1:
        #continue
        # Black used for noise.
        col = [0, 0, 0, 1]

        xy = X_with_res[class_member_mask & core_samples_mask]
        X_outliers_clsuter.append(xy)


    class_member_mask = (labels == k)
    xy = X[class_member_mask & core_samples_mask]
    plt.plot(xy[:, 0], xy[:, 1], 'o', markerfacecolor=tuple(col),
    markeredgecolor='k')

    xy = X[class_member_mask & ~core_samples_mask]
    plt.plot(xy[:, 0], xy[:, 1], 'o', markerfacecolor=tuple(col),
    markeredgecolor='k')

plt.title('DBSCAN eps {} min_sample {} cluster {} '.format(eps, min_samples, n_clusters_))
plt.xlabel('phi')
plt.ylabel('psi')
plt.figure().set_size_inches(30, 30, forward=True)
plt.show()
```

```
Estimated number of clusters: 7
Estimated number of noise points: 524
```




```
<Figure size 3000x3000 with 0 Axes>
```

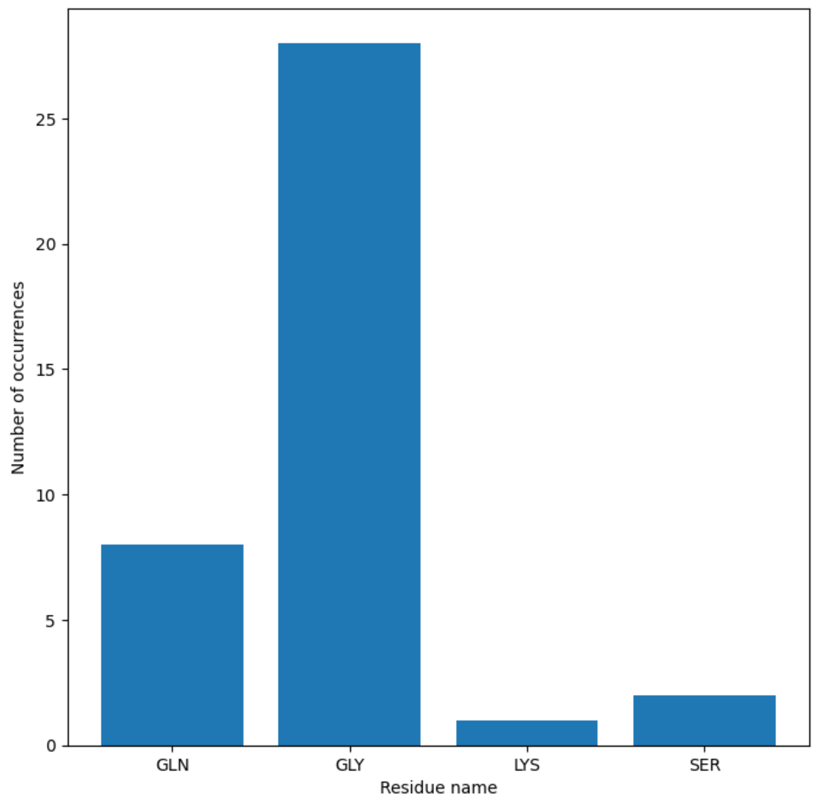
```python
X_outliers_clsuter
noise_array=X_outliers_clsuter[0]
print(noise_array)
```

```
 ['GLY' 88.304673 170.169727]
 ['GLY' 85.160294 170.342431]
 ['GLY' 79.476594 174.459781]
 ['GLY' 88.986741 165.176338]
 ['GLN' 77.407208 159.563241]
 ['GLY' 85.948045 161.685919]
 ['GLY' 89.295576 166.060984]
 ['GLN' 74.535132 159.897831]
 ['GLY' 90.581166 161.039301]
 ['GLN' 75.993735 161.650218]
 ['GLY' 85.324549 163.424606]
 ['GLN' 77.468888 161.26735]
 ['GLY' 86.009406 161.738911]
 ['GLY' 83.424989 162.79495]
 ['GLY' 88.584215 162.461663]
 ['GLN' 78.867345 159.250914]
 ['GLY' 89.318819 162.530689]
```

```
['GLN' 77.421884 159.619315]
['GLY' 83.764407 166.030142]
['GLY' 88.13937 160.726134]
['GLY' 89.465921 160.432265]
['GLN' 76.686336 160.668612]
['GLY' 80.913036 159.386764]
['GLN' 74.503777 158.280592]
['GLY' 88.639373 163.568616]
['GLY' 76.684997 171.135138]
['GLY' 88.030885 176.085544]
['GLY' 85.517131 173.051232]
['GLY' 83.547155 164.506545]
['GLY' 90.410669 166.17308]]
```

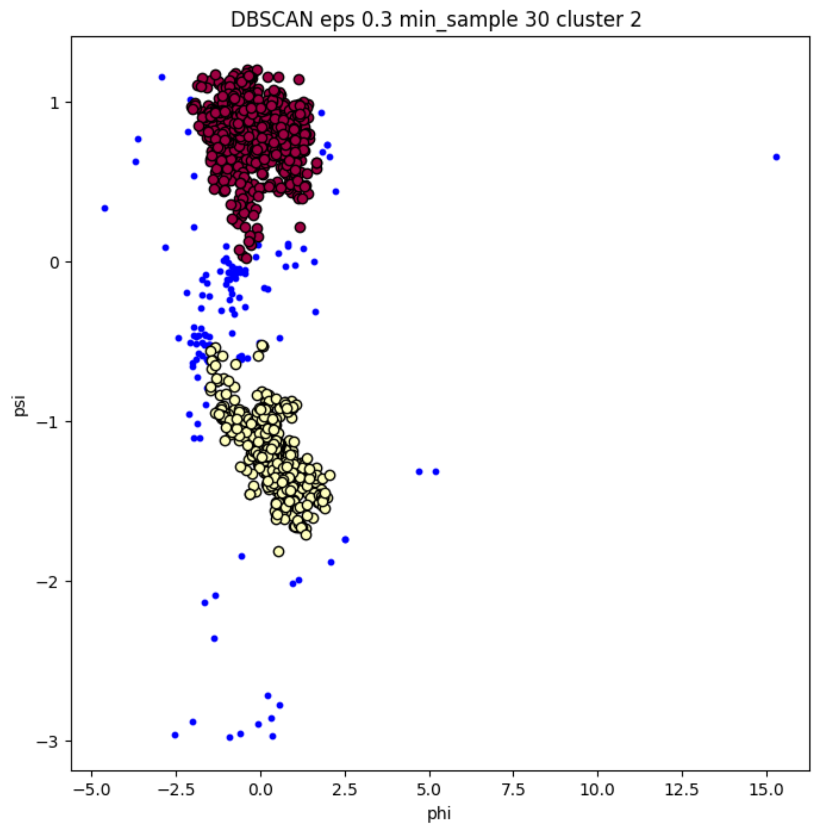
```
residue_types = np.array([i[0] for i in noise_array])
unique_residue_types, counts = np.unique(residue_types, return_counts=True)

plt.ylabel("Number of occurrences")
plt.xlabel("Residue name")
plt.bar(unique_residue_types, counts)
```

```
<BarContainer object of 4 artists>
```



```
#Filter only PRO residue
df_pro = df[df['residue name'] == 'PRO']
X = df_pro.loc[:, ['phi', 'psi']].values.reshape(-1,2)
X = StandardScaler().fit_transform(X)
eps=0.3
min_samples = 30

#Perform DBSCAN
plt.scatter(X[:, 0], X[:, 1], s=10, c='blue')
db = DBSCAN(eps = eps, min_samples=min_samples).fit(X)
labels = db.labels_


# Number of clusters in labels, ignoring noise if present.
n_clusters_ = len(set(labels)) - (1 if -1 in labels else 0)
n_noise_ = list(labels).count(-1)

core_samples_mask = np.zeros_like(labels, dtype=bool)
core_samples_mask[db.core_sample_indices_] = True

print("Estimated number of clusters: %d" % n_clusters_)
print("Estimated number of noise points: %d" % n_noise_)


unique_labels = set(labels)
####
colors = [plt.cm.Spectral(each) for each in np.linspace(0, 1, len(unique_labels))]

for k, col in zip(unique_labels, colors):
    if k == -1:
        continue
        # Black used for noise.
        col = [0, 0, 0, 1]

    class_member_mask = (labels == k)
    xy = X[class_member_mask & core_samples_mask]
    plt.plot(xy[:, 0], xy[:, 1], 'o', markerfacecolor=tuple(col),
    markeredgecolor='k')

    xy = X[class_member_mask & ~core_samples_mask]
    plt.plot(xy[:, 0], xy[:, 1], 'o', markerfacecolor=tuple(col),
    markeredgecolor='k')

plt.title('DBSCAN eps {} min_sample {} cluster {} '.format(eps, min_samples, n_clusters_))
plt.xlabel('phi')
plt.ylabel('psi')
plt.figure().set_size_inches(30, 30, forward=True)
plt.show()
```

```
Estimated number of clusters: 2
Estimated number of noise points: 128
```




```
<Figure size 3000x3000 with 0 Axes>
```

```python
print(df_pro)
```

```
      residue name  position chain        phi         psi  cluster
1              PRO        11     A -44.283210  136.002076        0
17             PRO        27     A -49.944645  -25.888991        1
68             PRO        79     A -76.452014   97.745207        0
110            PRO       121     A -53.054020  -27.254912        1
123            PRO       134     A -66.751364   94.099782        0
...            ...       ...   ...        ...         ...      ...
29284          PRO       288     B -54.565923  -42.141418        1
29339          PRO       349     B -66.803083  136.260650        0
29340          PRO       350     B -59.612140  160.048387        0
29347          PRO       357     B -48.679835  135.208297        0
29356          PRO       366     B -61.621274  -41.694960        1

[1596 rows x 6 columns]
```