# Brian Reppeto_DSC630_4_2_Clustering

September 22, 2024

### 0.0.1 DSC 630 Week : 4.2

**Clustering**

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**Load the libraries that will be used**

[47]:
```
# import libraries

import pandas as pd
from sklearn.preprocessing import StandardScaler
from sklearn.cluster import KMeans
from sklearn.metrics import silhouette_score
import matplotlib.pyplot as plt
from sklearn.decomposition import PCA
from sklearn.cluster import KMeans
from sklearn.metrics import silhouette_score
```

**Load the ALS data file**

[48]:
```
# load the file

als_df = pd.read_csv('als_data.csv')
```

**Display the first few rows to understand what is in the data**

[49]:
```
# display the first few rows

als_df.head()
```

[49]:

| | ID | Age_mean | Albumin_max | Albumin_median | Albumin_min | Albumin_range | \ |
|---|---|---|---|---|---|---|---|
| 0 | 1 | 65 | 57.0 | 40.5 | 38.0 | 0.066202 | |
| 1 | 2 | 48 | 45.0 | 41.0 | 39.0 | 0.010453 | |
| 2 | 3 | 38 | 50.0 | 47.0 | 45.0 | 0.008929 | |
| 3 | 4 | 63 | 47.0 | 44.0 | 41.0 | 0.012111 | |
| 4 | 5 | 63 | 47.0 | 45.5 | 42.0 | 0.008292 | |

| | ALSFRS_slope | ALSFRS_Total_max | ALSFRS_Total_median | ALSFRS_Total_min | … | \ |
|---|---|---|---|---|---|---|
| 0 | -0.965608 | 30 | 28.0 | 22 | … | |
| 1 | -0.921717 | 37 | 33.0 | 21 | … | |

```
2     -0.914787                24                  14.0                  10  …
3     -0.598361                30                  29.0                  24  …
4     -0.444039                32                  27.5                  20  …

   Sodium_min  Sodium_range  SubjectID  trunk_max  trunk_median  trunk_min  \
0       143.0      0.017422        533          8           7.0          7
1       136.0      0.010453        649          8           7.0          5
2       140.0      0.008929       1234          5           0.0          0
3       138.0      0.012469       2492          5           5.0          3
4       138.0      0.008292       2956          6           4.0          1

   trunk_range  Urine.Ph_max  Urine.Ph_median  Urine.Ph_min
0     0.002646           6.0              6.0           6.0
1     0.005386           7.0              5.0           5.0
2     0.008929           6.0              5.0           5.0
3     0.004988           7.0              6.0           5.0
4     0.008489           6.0              5.0           5.0

[5 rows x 101 columns]
```

**Print the columns so I can see if they are all needed and what they consist of**

[50]:
```
# get column names

columns = als_df.columns.tolist()

print(columns)
```

```
['ID', 'Age_mean', 'Albumin_max', 'Albumin_median', 'Albumin_min',
'Albumin_range', 'ALSFRS_slope', 'ALSFRS_Total_max', 'ALSFRS_Total_median',
'ALSFRS_Total_min', 'ALSFRS_Total_range', 'ALT.SGPT._max', 'ALT.SGPT._median',
'ALT.SGPT._min', 'ALT.SGPT._range', 'AST.SGOT._max', 'AST.SGOT._median',
'AST.SGOT._min', 'AST.SGOT._range', 'Bicarbonate_max', 'Bicarbonate_median',
'Bicarbonate_min', 'Bicarbonate_range', 'Blood.Urea.Nitrogen..BUN._max',
'Blood.Urea.Nitrogen..BUN._median', 'Blood.Urea.Nitrogen..BUN._min',
'Blood.Urea.Nitrogen..BUN._range', 'bp_diastolic_max', 'bp_diastolic_median',
'bp_diastolic_min', 'bp_diastolic_range', 'bp_systolic_max',
'bp_systolic_median', 'bp_systolic_min', 'bp_systolic_range', 'Calcium_max',
'Calcium_median', 'Calcium_min', 'Calcium_range', 'Chloride_max',
'Chloride_median', 'Chloride_min', 'Chloride_range', 'Creatinine_max',
'Creatinine_median', 'Creatinine_min', 'Creatinine_range', 'Gender_mean',
'Glucose_max', 'Glucose_median', 'Glucose_min', 'Glucose_range', 'hands_max',
'hands_median', 'hands_min', 'hands_range', 'Hematocrit_max',
'Hematocrit_median', 'Hematocrit_min', 'Hematocrit_range', 'Hemoglobin_max',
'Hemoglobin_median', 'Hemoglobin_min', 'Hemoglobin_range', 'leg_max',
'leg_median', 'leg_min', 'leg_range', 'mouth_max', 'mouth_median', 'mouth_min',
'mouth_range', 'onset_delta_mean', 'onset_site_mean', 'Platelets_max',
'Platelets_median', 'Platelets_min', 'Potassium_max', 'Potassium_median',
```

```
'Potassium_min', 'Potassium_range', 'pulse_max', 'pulse_median', 'pulse_min',
'pulse_range', 'respiratory_max', 'respiratory_median', 'respiratory_min',
'respiratory_range', 'Sodium_max', 'Sodium_median', 'Sodium_min',
'Sodium_range', 'SubjectID', 'trunk_max', 'trunk_median', 'trunk_min',
'trunk_range', 'Urine.Ph_max', 'Urine.Ph_median', 'Urine.Ph_min']
```

**Remove the columns that are not relavant to the ALS condition that we are testing for**

[51]:
```
# remove columns not relevant to pat ALS

als_rev_data = als_df.drop(columns=['ID','SubjectID'])
```

**Check the dataset for missing or NaN values to understand if they need to be corrected**

[52]:
```
# check for missing or NaN values in the dataset

missing_values = als_rev_data.isna().sum()

# display columns that have missing values along with the count of missing␣
 ↪values

missing_values = missing_values[missing_values > 0]
missing_values
```

[52]:
```
Series([], dtype: int64)
```

**Summarize the ALS data set and get descriptive stats about the data**

[53]:
```
# summary als

als_rev_data.describe()
```

[53]:

| | Age_mean | Albumin_max | Albumin_median | Albumin_min | Albumin_range | \ |
|---|---|---|---|---|---|---|
| count | 2223.000000 | 2223.000000 | 2223.000000 | 2223.000000 | 2223.000000 | |
| mean | 54.550157 | 47.011134 | 43.952542 | 40.766347 | 0.013779 | |
| std | 11.396546 | 3.233980 | 2.654804 | 3.193087 | 0.009567 | |
| min | 18.000000 | 37.000000 | 34.500000 | 24.000000 | 0.000000 | |
| 25% | 47.000000 | 45.000000 | 42.000000 | 39.000000 | 0.009042 | |
| 50% | 55.000000 | 47.000000 | 44.000000 | 41.000000 | 0.012111 | |
| 75% | 63.000000 | 49.000000 | 46.000000 | 43.000000 | 0.015873 | |
| max | 81.000000 | 70.300000 | 51.100000 | 49.000000 | 0.243902 | |

| | ALSFRS_slope | ALSFRS_Total_max | ALSFRS_Total_median | ALSFRS_Total_min | \ |
|---|---|---|---|---|---|
| count | 2223.000000 | 2223.000000 | 2223.000000 | 2223.000000 | |
| mean | -0.728274 | 31.692308 | 27.104926 | 19.877193 | |
| std | 0.622329 | 5.314228 | 6.633643 | 8.583509 | |
| min | -4.345238 | 11.000000 | 2.500000 | 0.000000 | |
| 25% | -1.086310 | 29.000000 | 23.000000 | 14.000000 | |
| 50% | -0.620748 | 33.000000 | 28.000000 | 20.000000 | |

```
75%       -0.283832          36.000000             32.000000          27.000000
max        1.207011          40.000000             40.000000          40.000000

       ALSFRS_Total_range  …  Sodium_median   Sodium_min  Sodium_range  \
count         2223.000000  …    2223.000000  2223.000000   2223.000000
mean             0.026035  …     140.145254   136.755061      0.015000
std              0.016156  …       1.789886     2.715247      0.009283
min              0.000000  …     128.000000   112.000000      0.000000
25%              0.014035  …     139.000000   135.000000      0.010582
50%              0.023297  …     140.000000   137.000000      0.013123
75%              0.034799  …     141.000000   138.000000      0.017278
max              0.117647  …     146.500000   145.000000      0.142857

         trunk_max  trunk_median    trunk_min  trunk_range  Urine.Ph_max  \
count  2223.000000   2223.000000  2223.000000  2223.000000   2223.000000
mean      6.203779      4.893387     2.955915     0.007136      6.820450
std       1.747660      2.146076     2.358095     0.004503      0.932141
min       0.000000      0.000000     0.000000     0.000000      5.000000
25%       5.000000      3.000000     1.000000     0.003643      6.000000
50%       7.000000      5.000000     3.000000     0.006920      7.000000
75%       8.000000      6.500000     5.000000     0.009639      7.000000
max       8.000000      8.000000     8.000000     0.042017      9.000000

       Urine.Ph_median  Urine.Ph_min
count      2223.000000   2223.000000
mean          5.710639      5.183221
std           0.625039      0.437222
min           5.000000      5.000000
25%           5.000000      5.000000
50%           6.000000      5.000000
75%           6.000000      5.000000
max           9.000000      8.000000

[8 rows x 99 columns]
```

**Apply the standard scaler to the data to scale to unit variance & convert to a Dataframe**

[54]:
```
# apply a standard scaler to the data

scaler = StandardScaler()
als_scaled_data = scaler.fit_transform(als_rev_data)

# convert scaled data to a df for ease of use

als_scaled_df = pd.DataFrame(als_scaled_data, columns=als_rev_data.columns)

# display the first few rows
```

```
als_scaled_df.head()
```

[54]:

| | Age_mean | Albumin_max | Albumin_median | Albumin_min | Albumin_range | \ |
|---|---|---|---|---|---|---|
| 0 | 0.917137 | 3.089417 | -1.300781 | -0.866550 | 5.480929 | |
| 1 | -0.574879 | -0.622016 | -1.112401 | -0.553303 | -0.347725 | |
| 2 | -1.452535 | 0.924415 | 1.148162 | 1.326179 | -0.507103 | |
| 3 | 0.741606 | -0.003443 | 0.017880 | 0.073191 | -0.174361 | |
| 4 | 0.741606 | -0.003443 | 0.583021 | 0.386438 | -0.573670 | |

| | ALSFRS_slope | ALSFRS_Total_max | ALSFRS_Total_median | ALSFRS_Total_min | \ |
|---|---|---|---|---|---|
| 0 | -0.381450 | -0.318520 | 0.134960 | 0.247368 | |
| 1 | -0.310907 | 0.998995 | 0.888863 | 0.130839 | |
| 2 | -0.299769 | -1.447819 | -1.975969 | -1.150976 | |
| 3 | 0.208801 | -0.318520 | 0.285741 | 0.480425 | |
| 4 | 0.456831 | 0.057913 | 0.059570 | 0.014311 | |

| | ALSFRS_Total_range | … | Sodium_median | Sodium_min | Sodium_range | \ |
|---|---|---|---|---|---|---|
| 0 | -0.301588 | … | 2.992342 | 2.300470 | 0.260968 | |
| 1 | 0.166537 | … | -1.198812 | -0.278144 | -0.489913 | |
| 2 | -0.064100 | … | 1.595291 | 1.195350 | -0.654169 | |
| 3 | -0.685524 | … | -0.639992 | 0.458603 | -0.272701 | |
| 4 | -0.350529 | … | -0.081171 | 0.458603 | -0.722774 | |

| | trunk_max | trunk_median | trunk_min | trunk_range | Urine.Ph_max | \ |
|---|---|---|---|---|---|---|
| 0 | 1.028018 | 0.981832 | 1.715365 | -0.997420 | -0.880376 | |
| 1 | 1.028018 | 0.981832 | 0.867032 | -0.388669 | 0.192665 | |
| 2 | -0.688950 | -2.280669 | -1.253800 | 0.398249 | -0.880376 | |
| 3 | -0.688950 | 0.049689 | 0.018699 | -0.477181 | 0.192665 | |
| 4 | -0.116627 | -0.416383 | -0.829634 | 0.300598 | -0.880376 | |

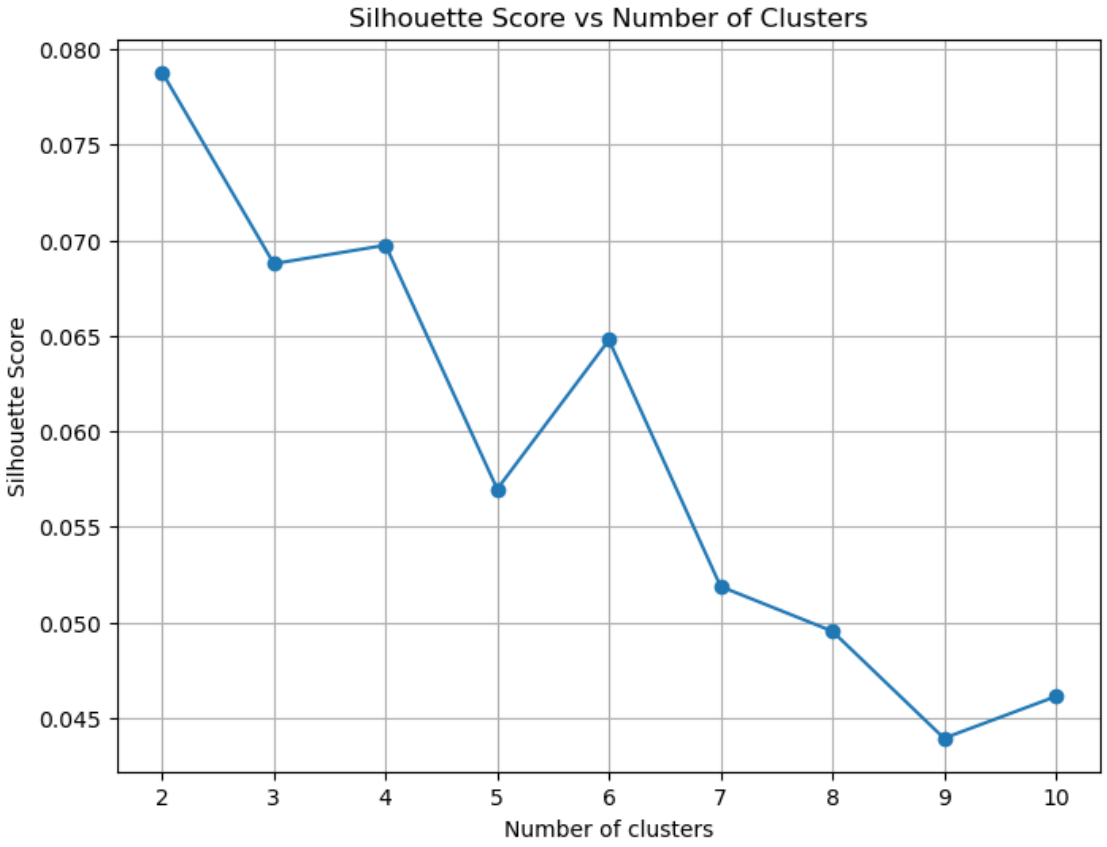
| | Urine.Ph_median | Urine.Ph_min |
|---|---|---|
| 0 | 0.463054 | 1.868532 |
| 1 | -1.137208 | -0.419151 |
| 2 | -1.137208 | -0.419151 |
| 3 | 0.463054 | -0.419151 |
| 4 | -1.137208 | -0.419151 |

[5 rows x 99 columns]

**Use the KMeans cluster to test diff numbers of clusters on the scaled data to find the best number of clusters**

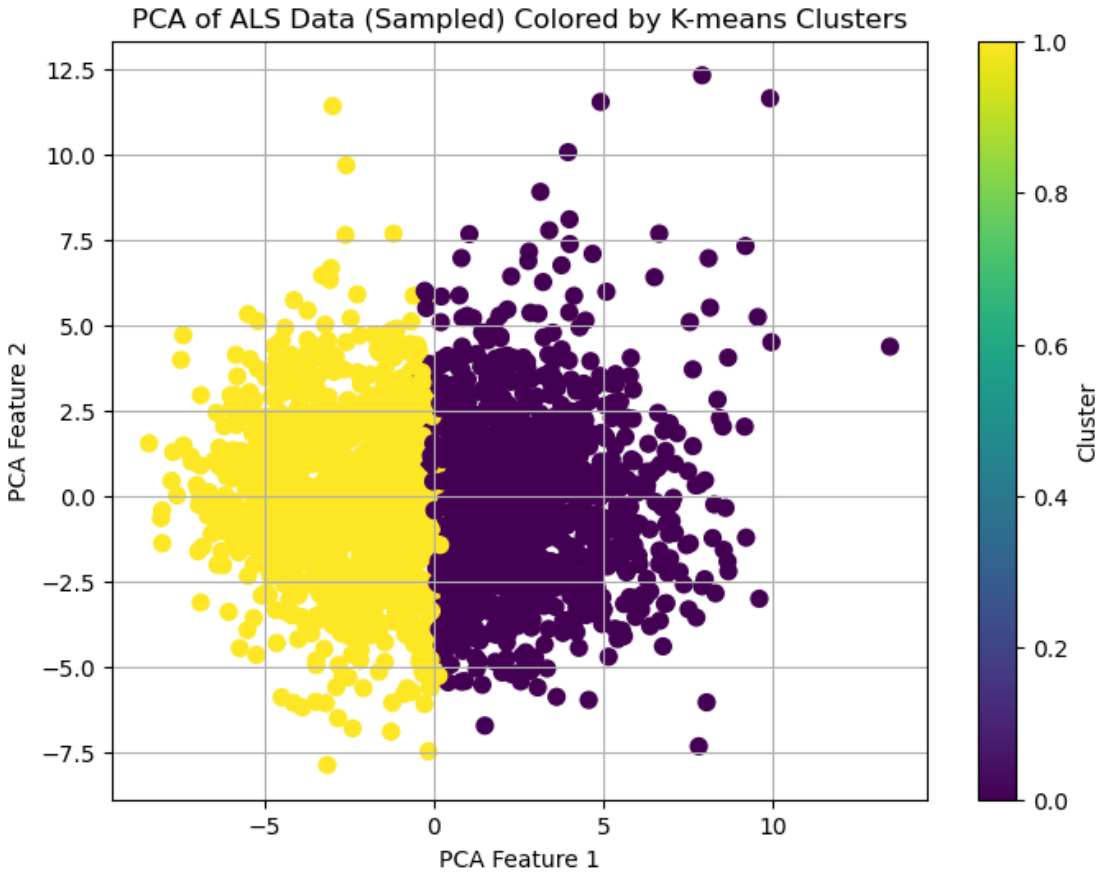
[55]:
```
# range for number of clusters to try

cluster_range = range(2,11)
# empy list for the scores
```

```
silhouette_scores = []

# interate over number in the cluster range

for n_clusters in cluster_range:
    kmeans = KMeans(n_clusters=n_clusters, random_state=42, n_init=10)
    cluster_labels = kmeans.fit_predict(als_scaled_df)
    silhouette_avg = silhouette_score(als_scaled_df, cluster_labels)
    silhouette_scores.append(silhouette_avg)

# plot the silhouette scores

plt.figure(figsize=(8, 6))
plt.plot(cluster_range, silhouette_scores, marker='o')
plt.title('Silhouette Score vs Number of Clusters')
plt.xlabel('Number of clusters')
plt.ylabel('Silhouette Score')
plt.grid(True)
plt.show()
```



**Fit a KMeans cluster model with 2 clusters to the ALS data, transforming with PCA and visualize the clusters**

[56]:
```
# k = 2 is the optimal number of clusters

optimal_n = 2

# K-means with the optimal number of clusters

kmeans_optimal = KMeans(n_clusters=optimal_n, random_state=42, n_init=10)
cluster_labels_optimal = kmeans_optimal.fit_predict(als_scaled_data)

# PCA transformation with two features

pca = PCA(n_components=2)
pca_data = pca.fit_transform(als_scaled_data)

# scatter plot of the PCA-transformed data

plt.figure(figsize=(8, 6))
plt.scatter(pca_data[:, 0], pca_data[:, 1], c=cluster_labels_optimal,␣
 ↪cmap='viridis', s=50)
plt.title('PCA of ALS Data (Sampled) Colored by K-means Clusters')
plt.xlabel('PCA Feature 1')
plt.ylabel('PCA Feature 2')
plt.colorbar(label='Cluster')
plt.grid(True)
plt.show()
```




### 0.0.2 Conclusion:

Using the ALS patient dataset, I applied K-means clustering and Principal Component Analysis (PCA) to determined the optimal number of clusters which is 2. The PCA analysis allowed me to visualize the two clusters. Moreover, the clustering approach provides an initial, unsupervised means of segmenting patients based on the available features. However, further investigation is necessary to understand the underlying characteristics and clinical relevance of these clusters. By exploring which features contribute most to the differentiation and examining how these clusters correlate with patient outcomes or treatment responses. Overall, clustering and dimensionality reduction proved to be effective techniques for uncovering potential structures within this complex dataset. However, further analysis is needed to understand the clinical or biological implications of these groupings fully.

[ ]: