MLS Clustering ML

June 30, 2024

[34]:
```
# Imports
import numpy as np
import pandas as pd
from IPython.display import display
```

[35]:
```
# Load
file_path = '/Users/nickblackford/Desktop/Python/als_data.csv'
df = pd.read_csv(file_path)
```

[36]:
```
# Preview df
df.head()
```

[36]:

	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]
```

[37]:
```
# Temporarily display all columns
pd.set_option('display.max_columns', None)

# Display the DataFrame
print(df)

# Reset to default (optional)
pd.reset_option('display.max_columns')
```

```
        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
…      …        …          …               …            …          …
2218  2419        33         50.0            49.0         45.0       0.008772
2219  2420        61         47.0            45.0         42.0       0.009074
2220  2421        47         46.0            44.0         41.0       0.012111
2221  2422        37         49.0            44.0         39.0       0.017857
2222  2424        48         48.0            45.0         40.0       0.018476

      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
…              …                  …                    …                 …
2218     -0.239501                35                 32.5                30
2219     -0.388711                31                 26.0                17
2220     -0.108631                26                 23.0                20
2221     -0.855880                34                 29.5                21
2222     -2.050562                37                 34.0                11

      ALSFRS_Total_range  ALT.SGPT._max  ALT.SGPT._median  ALT.SGPT._min  \
0               0.021164           24.0              22.0           18.0
1               0.028725           25.0              13.0            8.0
2               0.025000           25.0              20.0           14.0
3               0.014963           62.0              60.0           41.0
4               0.020374           38.0              26.5           22.0
…                    …              …                 …              …
```

```
2218           0.009107          46.0             27.0          18.0
2219           0.025408          23.0             18.0          15.0
2220           0.010949         129.0             76.5          62.0
2221           0.023214          95.0             51.0          42.0
2222           0.059908          37.0             32.0          13.0

      ALT.SGPT._range  AST.SGOT._max  AST.SGOT._median  AST.SGOT._min  \
0            0.020906             31              27.5           23.0
1            0.029617             31              17.0           14.0
2            0.019643             24              19.0           18.0
3            0.052369             46              40.0           33.0
4            0.026534             35              26.5           20.0
…                 …              …                 …              …
2218         0.049123             38              27.0           23.0
2219         0.014519             27              22.0           18.0
2220         0.047619             62              46.0           41.0
2221         0.094643             63              44.0           36.0
2222         0.055427             38              28.0           11.0

      AST.SGOT._range  Bicarbonate_max  Bicarbonate_median  Bicarbonate_min  \
0            0.027875             30.0                28.0             25.0
1            0.029617             32.0                28.0             25.0
2            0.010714             35.0                29.0             24.0
3            0.032419             23.0                20.0             20.0
4            0.024876             32.0                28.0             23.0
…                 …                …                   …                …
2218         0.026316             31.0                28.0             23.0
2219         0.016334             31.0                27.8             24.0
2220         0.035016             31.0                28.0             21.0
2221         0.048214             32.0                29.0             21.0
2222         0.062356             31.0                27.0             22.0

      Bicarbonate_range  Blood.Urea.Nitrogen..BUN._max  \
0              0.017422                         8.0322
1              0.012195                         8.3973
2              0.019643                         5.4765
3              0.007481                         8.0322
4              0.014925                         5.1114
…                 …                              …
2218           0.014035                         5.4765
2219           0.012704                         6.0700
2220           0.014925                         7.8500
2221           0.019643                         6.2067
2222           0.020785                         7.5000

      Blood.Urea.Nitrogen..BUN._median  Blood.Urea.Nitrogen..BUN._min  \
0                              7.11945                        6.57180
1                              4.74630                        4.01610
```

```
2                              4.38120                        3.65100
3                              8.03220                        6.57180
4                              4.19865                        3.65100
…                                …                              …
2218                           3.65100                        2.92080
2219                           5.00000                        3.57000
2220                           6.43000                        4.53000
2221                           4.01610                        3.28590
2222                           5.36000                        1.27785

      Blood.Urea.Nitrogen..BUN._range  bp_diastolic_max  bp_diastolic_median  \
0                            0.005089                90                 83.0
1                            0.007633                80                 78.0
2                            0.003260                86                 76.0
3                            0.003642                90                 80.0
4                            0.002422               100                 80.0
…                               …                    …                    …
2218                         0.004484                85                 78.0
2219                         0.004537                95                 90.0
2220                         0.005817               102                 86.0
2221                         0.005216                90                 77.0
2222                         0.014370                90                 80.0

      bp_diastolic_min  bp_diastolic_range  bp_systolic_max  \
0                   69            0.055556              160
1                   64            0.028725              140
2                   58            0.050000              120
3                   70            0.049875              150
4                   68            0.053068              160
…                 …                 …                …
2218                70            0.027322              150
2219                80            0.027223              155
2220                76            0.045694              140
2221                70            0.035714              150
2222                70            0.046083              150

      bp_systolic_median  bp_systolic_min  bp_systolic_range  Calcium_max  \
0                  139.0              129           0.082011      2.49500
1                  132.5              104           0.064632      2.32035
2                  110.0               90           0.053571      2.47005
3                  130.0              120           0.074813      2.47005
4                  130.0              104           0.092869      2.42015
…                  …                …                …          …
2218               115.0              100           0.091075      2.39520
2219               140.0              130           0.045372      2.50000
2220               120.0              102           0.066784      2.58000
2221               122.0              100           0.089286      2.47005
2222               130.0              110           0.092166      2.65000
```

	Calcium_median	Calcium_min	Calcium_range	Chloride_max	\
0	2.220550	2.22055	0.000956	109.0	
1	2.170650	2.02095	0.000522	108.0	
2	2.295400	2.19560	0.000490	108.0	
3	2.345300	2.23000	0.000474	109.0	
4	2.257975	2.17065	0.000414	107.0	
…	…	…	…	…	
2218	2.320350	2.17065	0.000394	111.0	
2219	2.300000	2.13000	0.000672	111.0	
2220	2.340000	2.30000	0.000474	111.0	
2221	2.320350	2.22055	0.000446	105.0	
2222	2.430000	2.33000	0.000739	108.0	

	Chloride_median	Chloride_min	Chloride_range	Creatinine_max	\
0	108.0	103.0	0.020906	79.560	
1	102.0	100.0	0.013937	61.880	
2	106.0	104.0	0.007143	88.400	
3	107.0	106.0	0.007481	70.720	
4	104.0	100.0	0.011609	61.880	
…	…	…	…	…	
2218	104.0	102.0	0.015789	88.400	
2219	106.0	101.0	0.018149	72.000	
2220	105.0	99.0	0.015873	82.000	
2221	102.0	98.0	0.012500	61.880	
2222	107.0	99.0	0.020785	93.704	

	Creatinine_median	Creatinine_min	Creatinine_range	Gender_mean	\
0	79.56	70.72	0.030801	1	
1	53.04	44.20	0.030801	1	
2	79.56	70.72	0.031571	2	
3	61.88	53.04	0.044090	2	
4	48.62	26.52	0.058640	1	
…	…	…	…	…	
2218	70.72	61.88	0.046526	2	
2219	55.00	41.00	0.056261	1	
2220	54.00	45.00	0.048654	2	
2221	44.20	26.52	0.063143	2	
2222	76.00	68.00	0.059363	2	

	Glucose_max	Glucose_median	Glucose_min	Glucose_range	hands_max	\
0	7.4370	4.4955	4.2180	0.011216	8	
1	6.7710	4.9950	4.0515	0.004738	8	
2	5.6610	5.1060	4.2180	0.002577	4	
3	5.1060	4.7730	4.6620	0.001107	6	
4	7.4925	5.7165	5.0505	0.004050	8	
…	…	…	…	…	…	
2218	5.4390	4.8285	3.9960	0.002532	6	

```
2219      11.3000          6.5000       4.8000       0.011797          6
2220       7.4000          5.7000       4.8000       0.004695          5
2221       6.8820          4.8840       4.1070       0.004955          8
2222       6.3000          5.5500       4.9000       0.003333          8

      hands_median  hands_min  hands_range  Hematocrit_max  Hematocrit_median  \
0              7.5          6     0.005291            44.6              43.15
1              6.0          6     0.003591            41.9              39.60
2              1.0          0     0.007143            49.1              46.20
3              5.5          4     0.004988            46.3              43.00
4              6.5          3     0.008489            44.0              42.85
…              …          …           …                …                 …
2218           4.0          3     0.005464            51.6              48.20
2219           4.0          1     0.009074            42.0              40.00
2220           2.0          2     0.005474            46.0              45.00
2221           6.5          4     0.007143            51.5              48.05
2222           7.0          0     0.018433            54.0              51.00

      Hematocrit_min  Hematocrit_range  Hemoglobin_max  Hemoglobin_median  \
0               40.7          0.013589           156.0              146.0
1               37.7          0.007317           138.0              132.0
2               44.0          0.009107           161.0              154.0
3               41.7          0.011471           154.0              145.0
4               39.5          0.007463           152.0              146.5
…               …                …                …                  …
2218            45.6          0.010526           172.0              161.0
2219            38.0          0.007260           137.0              132.0
2220            43.0          0.009701           157.0              151.0
2221            45.2          0.012186           171.0              162.5
2222            46.6          0.017090           178.0              167.0

      Hemoglobin_min  Hemoglobin_range  leg_max  leg_median  leg_min  \
0              143.0          0.045296        8         6.5        4
1              128.0          0.017422        8         7.5        3
2              151.0          0.017857        4         3.0        2
3              144.0          0.024938        4         3.5        2
4              138.0          0.023217        2         2.0        0
…              …                …       …         …       …
2218           153.0          0.033333        8         8.0        8
2219           127.0          0.018149        8         8.0        6
2220           147.0          0.031056        3         2.0        2
2221           155.0          0.030948        3         3.0        2
2222           161.0          0.039261        8         8.0        6

      leg_range  mouth_max  mouth_median  mouth_min  mouth_range  \
0      0.010582          5           3.5          0     0.013228
1      0.008977          9           8.0          4     0.008977
2      0.003571         10           7.0          4     0.010714
```

```
3      0.004988          12           12.0          12     0.000000
4      0.003396          12           12.0          12     0.000000
…         …         …            …          …           …
2218   0.000000          12           11.0          10     0.003643
2219   0.003630           8            6.0           4     0.007260
2220   0.001825          10           10.0           9     0.001825
2221   0.001786          12           12.0          10     0.003571
2222   0.004608          10            8.0           3     0.016129

      onset_delta_mean  onset_site_mean  Platelets_max  Platelets_median  \
0                -1023                1            172             169.0
1                 -341                1            286             264.0
2                -1181                1            233             213.0
3                 -365                2            275             233.0
4                -1768                2            313             283.5
…                    …              …            …                …
2218              -817                2            242             202.0
2219              -527                1            260             217.0
2220             -1589                2            246             222.0
2221              -558                2            271             237.0
2222              -204                1            357             299.0

      Platelets_min  Potassium_max  Potassium_median  Potassium_min  \
0             152.0            4.5              4.25            4.0
1             230.0            5.0              4.30            3.9
2             167.0            4.1              4.00            3.9
3             204.0            4.3              4.20            4.0
4             268.0            4.6              3.75            3.5
…                 …              …                 …              …
2218          176.0            4.4              4.10            3.9
2219          196.0            4.8              4.25            3.9
2220          187.0            4.4              3.95            3.7
2221          187.0            4.8              4.20            3.9
2222          248.0            5.3              4.60            4.2

      Potassium_range  pulse_max  pulse_median  pulse_min  pulse_range  \
0            0.001742         79          68.0         61     0.047619
1            0.001916         90          76.0         64     0.046679
2            0.000357         82          73.0         60     0.039286
3            0.000748         84          72.0         68     0.039900
4            0.001824        101          96.0         74     0.044776
…               …          …             …           …           …
2218         0.000877         80          67.5         56     0.043716
2219         0.001633         86          78.0         72     0.025408
2220         0.001425        102          86.0         62     0.070299
2221         0.001607        104          90.0         85     0.033929
2222         0.002949         98          84.0         64     0.078341
```

```
      respiratory_max  respiratory_median  respiratory_min  respiratory_range  \
0                   4                 3.0                3           0.002646
1                   4                 4.0                3           0.001795
2                   4                 4.0                4           0.000000
3                   3                 3.0                3           0.000000
4                   4                 4.0                3           0.001698
…                 …                   …                …                 …
2218                4                 4.0                4           0.000000
2219                4                 4.0                3           0.001815
2220                4                 4.0                3           0.001825
2221                4                 4.0                2           0.003571
2222                4                 4.0                1           0.006912

      Sodium_max  Sodium_median  Sodium_min  Sodium_range  SubjectID  \
0          148.0          145.5       143.0      0.017422        533
1          142.0          138.0       136.0      0.010453        649
2          145.0          143.0       140.0      0.008929       1234
3          143.0          139.0       138.0      0.012469       2492
4          143.0          140.0       138.0      0.008292       2956
…          …              …           …          …              …
2218       144.0          141.0       136.0      0.014035     997136
2219       146.0          143.0       141.0      0.009074     998047
2220       144.0          141.0       135.0      0.013123     998773
2221       140.0          139.0       136.0      0.007143     998908
2222       145.0          141.0       137.0      0.018476     999482

      trunk_max  trunk_median  trunk_min  trunk_range  Urine.Ph_max  \
0             8           7.0          7     0.002646          6.00
1             8           7.0          5     0.005386          7.00
2             5           0.0          0     0.008929          6.00
3             5           5.0          3     0.004988          7.00
4             6           4.0          1     0.008489          6.00
…           …             …          …           …               …
2218          7           5.0          5     0.003643          7.00
2219          5           4.0          3     0.003630          7.41
2220          5           4.0          4     0.001825          9.00
2221          8           4.5          2     0.010714          6.00
2222          8           8.0          1     0.016129          5.00

      Urine.Ph_median  Urine.Ph_min
0                 6.0           6.0
1                 5.0           5.0
2                 5.0           5.0
3                 6.0           5.0
4                 5.0           5.0
…                 …             …
2218              6.0           5.0
2219              5.5           5.0
```

```
2220              6.0           5.0
2221              5.0           5.0
2222              5.0           5.0

[2223 rows x 101 columns]
```

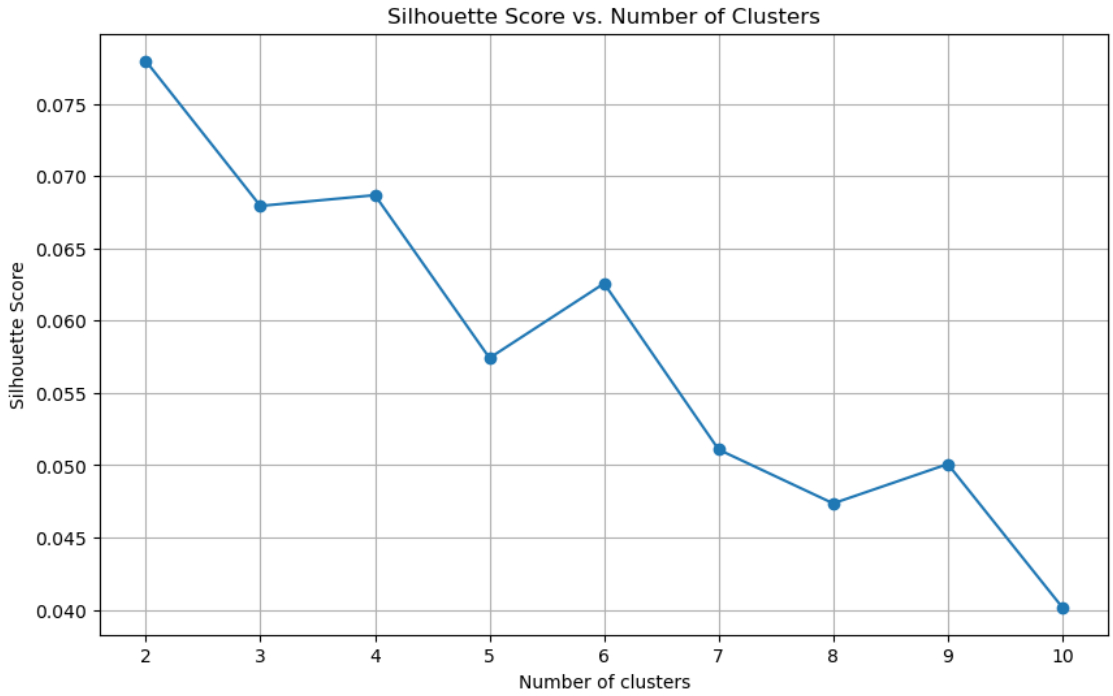
[38]:
```
# Remove any data that is not relevant to the patient's ALS condition
df = df.drop(columns=['ID'])
```

[39]:
```
# Apply standard scaler
from sklearn.preprocessing import StandardScaler

# Initialize scaler
scaler = StandardScaler()

# Fit the scaler on the data and transform it
df_scaled = scaler.fit_transform(df)

# Convert the scaled data back to a DataFrame
X_scaled = pd.DataFrame(df_scaled, columns=df.columns)
```

[40]:
```
import matplotlib.pyplot as plt
from sklearn.cluster import KMeans
from sklearn.metrics import silhouette_score

# Calculate silhouette scores for different numbers of clusters
silhouette_scores = []
cluster_range = range(2, 11)

for k in cluster_range:
    kmeans = KMeans(n_clusters=k,n_init=10,random_state=10)
    y_kmeans = kmeans.fit_predict(X_scaled)
    score = silhouette_score(X_scaled, y_kmeans)
    silhouette_scores.append(score)

# Print silhouette scores for debugging
for k, score in zip(cluster_range, silhouette_scores):
    print(f'Number of clusters: {k}, Silhouette Score: {score}')
```

```
Number of clusters: 2, Silhouette Score: 0.0779489418382482
Number of clusters: 3, Silhouette Score: 0.06792675217846486
Number of clusters: 4, Silhouette Score: 0.06867177357095701
Number of clusters: 5, Silhouette Score: 0.05740976392457452
Number of clusters: 6, Silhouette Score: 0.06256617707910656
Number of clusters: 7, Silhouette Score: 0.051075921419424526
Number of clusters: 8, Silhouette Score: 0.04735394077311848
Number of clusters: 9, Silhouette Score: 0.050075176240459866
Number of clusters: 10, Silhouette Score: 0.04016513650091586
```

[41]:
```
# Plot silhouette scores vs. number of clusters
plt.figure(figsize=(10, 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.xticks(cluster_range)
plt.grid(True)
plt.show()
```



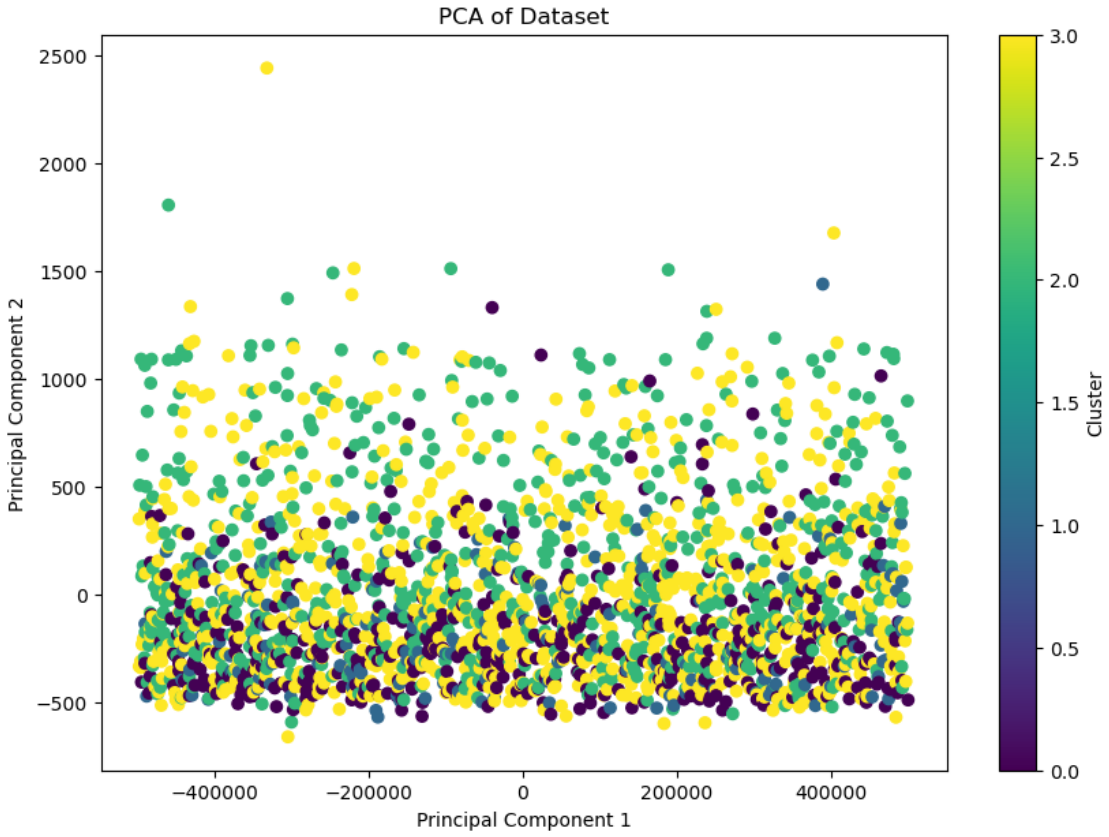
Analyzing the Silhouette Score vs. Number of clusters plot, we are going to select 4 as an optimal number of clusters. 4 clusters has the second highest silhouette score only to 2. Given the data we are working with, selecting 4 clusters as opposed to 2 will likely give us more insights when conducting analysis on ALS patients.

[48]:
```
# Create and fit the K-means model
kmeans = KMeans(n_clusters=4, n_init=10, random_state=10)
kmeans.fit(X_scaled)

# Predict the clusters for the data points
df['Cluster'] = kmeans.labels_
```

[49]:
```
from sklearn.decomposition import PCA

# Fit PCA with 2 components
```

```
pca = PCA(n_components=2)
X_pca = pca.fit_transform(df)

# Create a df with the PCA results
df_pca = pd.DataFrame(data=X_pca, columns=['Principal Component 1', 'Principal␣
 ↪Component 2'])
df_pca['Cluster'] = df['Cluster']
```

[50]:
```
# Make a scatterplot of the PCA transformed data
plt.figure(figsize=(10, 7))
scatter = plt.scatter(df_pca['Principal Component 1'], df_pca['Principal␣
 ↪Component 2'], c=df_pca['Cluster'], cmap='viridis')
plt.xlabel('Principal Component 1')
plt.ylabel('Principal Component 2')
plt.title('PCA of Dataset')
plt.colorbar(scatter, label='Cluster')
plt.show()
```



0.1 Conclusion

0.1.1 Objective

The goal of this analysis was to cluster ALS (Amyotrophic Lateral Sclerosis) patient health metrics using K-means clustering and evaluate the clustering performance to gain insights into potential patterns or subgroups within the patient population.

0.1.2 Steps Taken

1. **Data Preparation**:
   - Loaded the dataset containing 100 different health metrics for ALS patients.
   - Scaled the data to standardize the features, ensuring each feature contributes equally to the clustering process.
2. **Optimal Number of Clusters**:
   - Utilized the Silhouette Score to determine the optimal number of clusters.
   - The Silhouette Score indicated that 4 clusters provided the highest sihlouette score second to 2 clusters, suggesting a well-defined clustering structure.
3. **K-means Clustering**:
   - Fitted the K-means model with 4 clusters.
   - Assigned cluster labels to each data point (patient).
4. **PCA Transformation and Visualization**:
   - Applied PCA to reduce the dimensionality of the data to two principal components.
   - Created a scatter plot to visualize the clustering results, coloring each point by its cluster label.

0.1.3 Conclusion

Based on the clustering analysis and performance evaluation, we can draw the following conclusions:

1. **Distinct Subgroups**:
   - The analysis identified four distinct subgroups within the ALS patient population based on the 100 health metrics.
   - This suggests that there may be underlying patterns or characteristics that differentiate these four groups, which could be related to disease progression, response to treatment, or other health-related factors.
2. **Clinical Implications**:
   - These subgroups could potentially inform clinical decisions, such as tailoring treatment plans to specific patient profiles or identifying patients who may benefit from more intensive monitoring.
   - Further analysis is needed to understand the specific health metrics that contribute most significantly to the clustering, which could highlight critical factors in ALS management.
3. **Future Research**:
   - This preliminary clustering analysis provides a foundation for more detailed studies. Future research could involve investigating the specific characteristics of each cluster, exploring correlations with clinical outcomes, and validating the findings with larger datasets.

- Additionally, integrating other data sources (e.g., genetic data, lifestyle factors) could provide a more comprehensive understanding of the patient subgroups.

4. **Limitations**:
   - The current analysis is exploratory and should be interpreted with caution. The clustering results depend on the selected features and the scaling method used.

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