ALS Condition of ALS Patient (K-means and PCA)

In [ ]:

In [1]:
```
# Import packages
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
import numpy as np
from sklearn.preprocessing import StandardScaler
from sklearn.metrics import silhouette_score
from sklearn.datasets import make_blobs
from sklearn.cluster import KMeans
from sklearn.decomposition import PCA
```

In [2]:
```
# Upload data
data = pd.read_csv('/Users/Malloryh5/Downloads/als_data.csv')
```

Remove any data that is not relevant to the patient's ALS condition.

In [3]:
```
# Review the different columns
data.info(1)
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 2223 entries, 0 to 2222
Data columns (total 101 columns):
 #    Column                              Dtype
---   ------                              -----
 0    ID                                  int64
 1    Age_mean                            int64
 2    Albumin_max                         float64
 3    Albumin_median                      float64
 4    Albumin_min                         float64
 5    Albumin_range                       float64
 6    ALSFRS_slope                        float64
 7    ALSFRS_Total_max                    int64
 8    ALSFRS_Total_median                 float64
 9    ALSFRS_Total_min                    int64
 10   ALSFRS_Total_range                  float64
 11   ALT.SGPT._max                       float64
 12   ALT.SGPT._median                    float64
 13   ALT.SGPT._min                       float64
 14   ALT.SGPT._range                     float64
 15   AST.SGOT._max                       int64
 16   AST.SGOT._median                    float64
 17   AST.SGOT._min                       float64
 18   AST.SGOT._range                     float64
 19   Bicarbonate_max                     float64
 20   Bicarbonate_median                  float64
 21   Bicarbonate_min                     float64
 22   Bicarbonate_range                   float64
 23   Blood.Urea.Nitrogen..BUN._max       float64
 24   Blood.Urea.Nitrogen..BUN._median    float64
 25   Blood.Urea.Nitrogen..BUN._min       float64
 26   Blood.Urea.Nitrogen..BUN._range     float64
 27   bp_diastolic_max                    int64
 28   bp_diastolic_median                 float64
 29   bp_diastolic_min                    int64
 30   bp_diastolic_range                  float64
 31   bp_systolic_max                     int64
 32   bp_systolic_median                  float64
 33   bp_systolic_min                     int64
 34   bp_systolic_range                   float64
 35   Calcium_max                         float64
 36   Calcium_median                      float64
 37   Calcium_min                         float64
 38   Calcium_range                       float64
 39   Chloride_max                        float64
 40   Chloride_median                     float64
 41   Chloride_min                        float64
 42   Chloride_range                      float64
 43   Creatinine_max                      float64
 44   Creatinine_median                   float64
 45   Creatinine_min                      float64
 46   Creatinine_range                    float64
 47   Gender_mean                         int64
 48   Glucose_max                         float64
 49   Glucose_median                      float64
 50   Glucose_min                         float64
 51   Glucose_range                       float64
 52   hands_max                           int64
 53   hands_median                        float64
 54   hands_min                           int64
 55   hands_range                         float64
 56   Hematocrit_max                      float64
 57   Hematocrit_median                   float64
 58   Hematocrit_min                      float64
 59   Hematocrit_range                    float64
 60   Hemoglobin_max                      float64
 61   Hemoglobin_median                   float64
 62   Hemoglobin_min                      float64
 63   Hemoglobin_range                    float64
 64   leg_max                             int64
 65   leg_median                          float64
 66   leg_min                             int64
 67   leg_range                           float64
 68   mouth_max                           int64
 69   mouth_median                        float64
 70   mouth_min                           int64
 71   mouth_range                         float64
 72   onset_delta_mean                    int64
 73   onset_site_mean                     int64
 74   Platelets_max                       int64
```

```
 75   Platelets_median                float64
 76   Platelets_min                   float64
 77   Potassium_max                   float64
 78   Potassium_median                float64
 79   Potassium_min                   float64
 80   Potassium_range                 float64
 81   pulse_max                       int64
 82   pulse_median                    float64
 83   pulse_min                       int64
 84   pulse_range                     float64
 85   respiratory_max                 int64
 86   respiratory_median              float64
 87   respiratory_min                 int64
 88   respiratory_range               float64
 89   Sodium_max                      float64
 90   Sodium_median                   float64
 91   Sodium_min                      float64
 92   Sodium_range                    float64
 93   SubjectID                       int64
 94   trunk_max                       int64
 95   trunk_median                    float64
 96   trunk_min                       int64
 97   trunk_range                     float64
 98   Urine.Ph_max                    float64
 99   Urine.Ph_median                 float64
 100  Urine.Ph_min                    float64
dtypes: float64(75), int64(26)
memory usage: 1.7 MB
```

In [4]:
```
# Drop all columns with slope, range, min and max
data = data.loc[:,~data.columns.str.contains('slope|range|min|max', case=False)]
```

I do not know enough about ALS to know what is important and what is not. I also do not even know what some of these columns mean.I will run a correlation matrix to determine what can be removed.

Correlation Matrix

In [5]:
```
# Make a correlation of the data
cor_data = data.corr()
```

In [6]:
```
# Heat map will be too large to understand. Remove any correlations below .2
## Set correlation threshold
threshold = .2
## Set the self correlation to na to remove the columns that correlates with its self
np.fill_diagonal(cor_data.values, np.nan)
## Remove the lower correlations columns
cor_remove = cor_data.columns[(cor_data.abs() > threshold).any()]
## Save these columns
data_f = data[cor_remove]
```

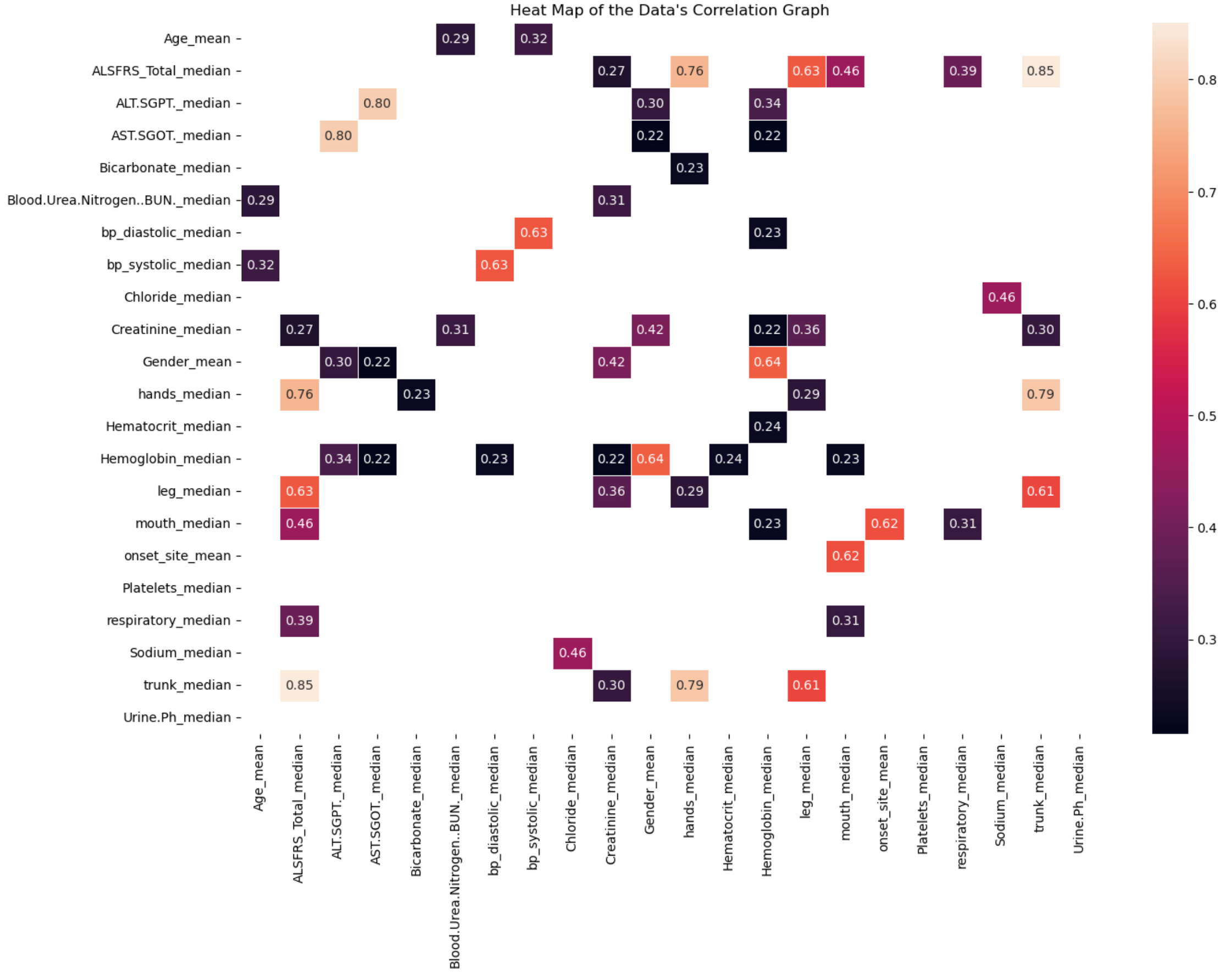
In [7]:
```
# Drop repeat ID column
data_f = data_f.drop(columns = ['SubjectID', 'ID'])
```

In [8]:
```
data_f.columns
```

Out[8]:
```
Index(['Age_mean', 'ALSFRS_Total_median', 'ALT.SGPT._median',
       'AST.SGOT._median', 'Bicarbonate_median',
       'Blood.Urea.Nitrogen..BUN._median', 'bp_diastolic_median',
       'bp_systolic_median', 'Chloride_median', 'Creatinine_median',
       'Gender_mean', 'hands_median', 'Hematocrit_median', 'Hemoglobin_median',
       'leg_median', 'mouth_median', 'onset_site_mean', 'Platelets_median',
       'respiratory_median', 'Sodium_median', 'trunk_median',
       'Urine.Ph_median'],
      dtype='object')
```

In [9]:
```
# Make a correlation graph of these columns
cor_check = data_f.corr()
# Only highlight the important columns
cor_import = cor_check.mask((cor_check < threshold) | (cor_check < -threshold))
# Drop the self-correlation
np.fill_diagonal(cor_import.values, np.nan)
```

In [10]:
```
# Use seaborn to make a heatmap
# Figure size
plt.figure(figsize=(15,10))
# Make heatmap
sns.heatmap(cor_import, annot=True, linewidth=.5, fmt='.2f')
# Title
plt.title("Heat Map of the Data's Correlation Graph")
# Print graph
plt.show()
```



I do not know anything about ASL. Instead of just picking columns to remove, I used a correlation matrix to remove any column with a correlation below .2. I set the threshold to .2 for two reasons: one, 23 is not many columns, and two because it mainly shows correlations of things that are obviously correlated, like both the bp columns. Or the leg and truck column. However, I did not remove them because I am not sure how important they are. I had to remove the columns with self-correlation for it to work. I drop the SubjectID and ID.

Apply a standard scalar to the data.

In [11]:
```
# Allow scaler
scale = StandardScaler()
```

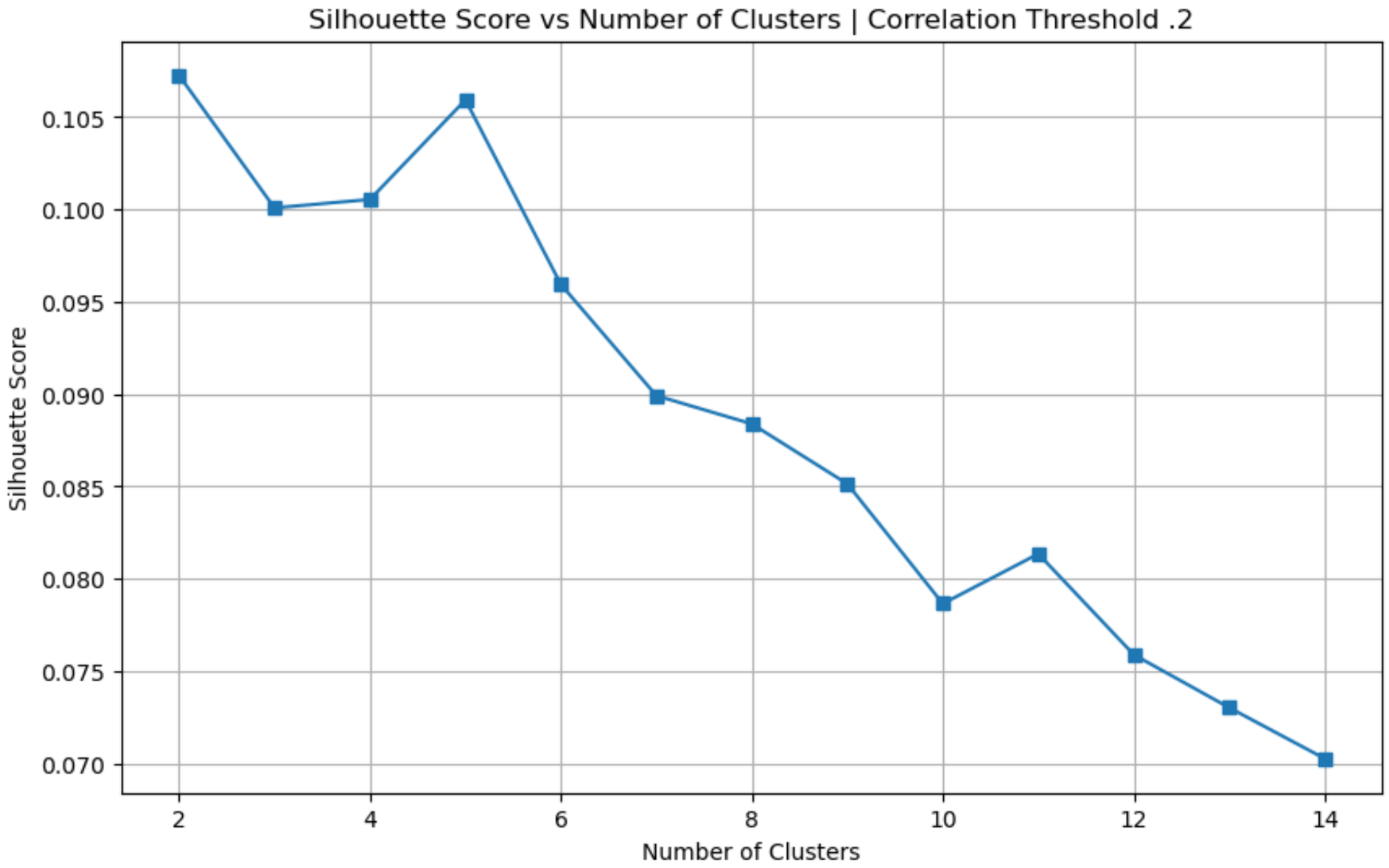
In [12]:
```
# Fit transform the data
data_ft = scale.fit_transform(data_f)
```

Plot of the cluster silhouette score versus the number of clusters in a K-means cluster.

In [13]:
```
# Empty list
scores = []
# Cluster range
c_range = range(2,15)
```

In [14]:
```
# For loop to find clusters
for n_clusters in c_range:
    #find kmeans
    kmeans = KMeans(n_clusters=n_clusters, n_init=10, random_state=42)
    # predict the labels
    labels = kmeans.fit_predict(data_ft)
    # find the silhouette score
    silhouette_avg = silhouette_score(data_ft, labels)
    # Append it to the list
    scores.append(silhouette_avg)
```

In [15]:
```
# Plotting
# Plot size
plt.figure(figsize=(10, 6))
# Plot graph
plt.plot(c_range, scores, marker='s')
# Title
plt.title('Silhouette Score vs Number of Clusters | Correlation Threshold .2')
# X-axis label
plt.xlabel('Number of Clusters')
# Y-axis label
plt.ylabel('Silhouette Score')
# Add grid
plt.grid()
# Show plot
plt.show()
```



Use the plot created to choose optimal number of clusters for K-means.

Using the silhouette score to predict the clusters, the optimal number of clusters is 2. Four clusters for K-means have a silhouette score of about .1. However, this might not be the best method to predict because the silhouette score is so low. The higher the score, the more defined the clusters become.

Fit a K-means model to the data with the optimal number of clusters chosen.

In [16]:
```
# Optimal cluster
o_cluster = 2
```

In [17]:
```
# K-means
k_m = KMeans(n_clusters=o_cluster, n_init=10, random_state=42)
```

In [18]:
```
# Fit the data.
fit_k_m = k_m.fit(data_ft)
# Show Kmeans
fit_k_m;
```

Out[18]:
```
KMeans(n_clusters=2, n_init=10, random_state=42)
```

Fit a PCA transformation with two features to the scaled data.

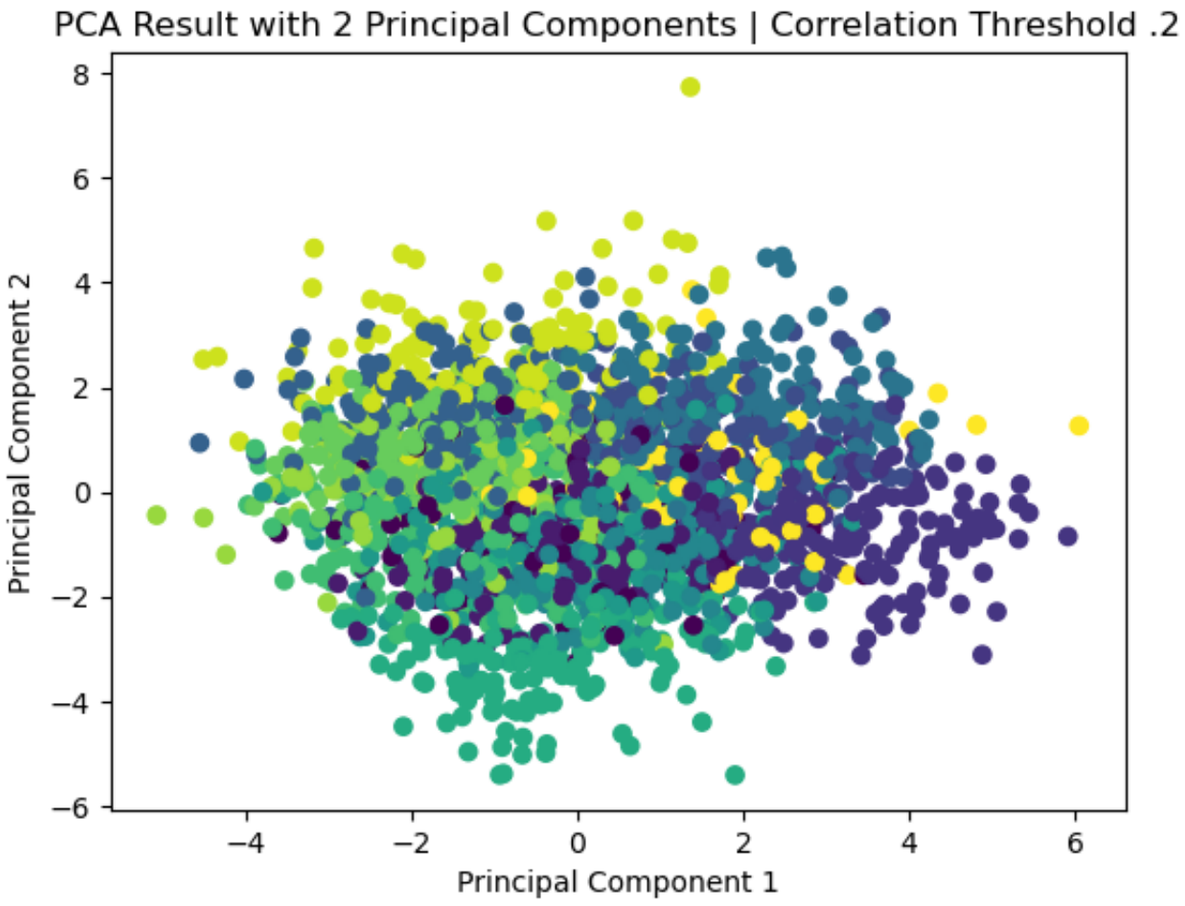
In [19]:
```
# PCA with two features
pca = PCA(n_components=2)
# Show OCA
pca;
```

Out[19]:
```
PCA(n_components=2)
```

In [20]:
```
# Fit and transform the data based on scatter plot
pca_data = pca.fit_transform(data_ft)
```

Make a scatterplot the PCA transformed data coloring each point by its cluster value.

In [21]:
```
# Scatter plot... I am not sure this is right
plt.scatter(pca_data[:, 0],pca_data[:, 1], c=labels)
# Add tile
plt.title('PCA Result with 2 Principal Components | Correlation Threshold .2')
# Add X-axis label
plt.xlabel('Principal Component 1')
# Add y-axis label
plt.ylabel('Principal Component 2')
# Show
plt.show()
```

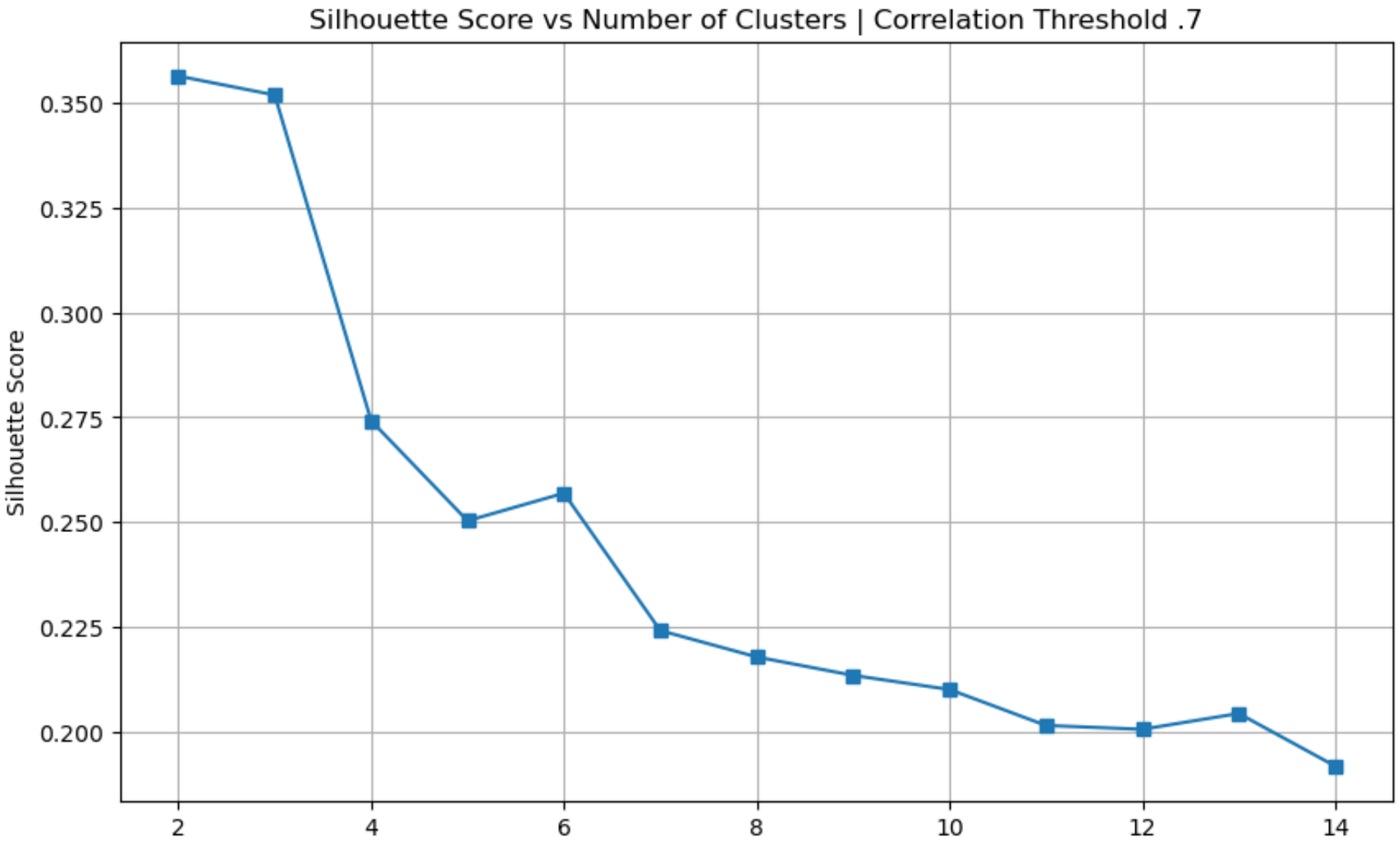


The graph is hard to read. It has clustered the points, but it is too difficult to differentiate between the groups.

Add a threshold = .7 to model

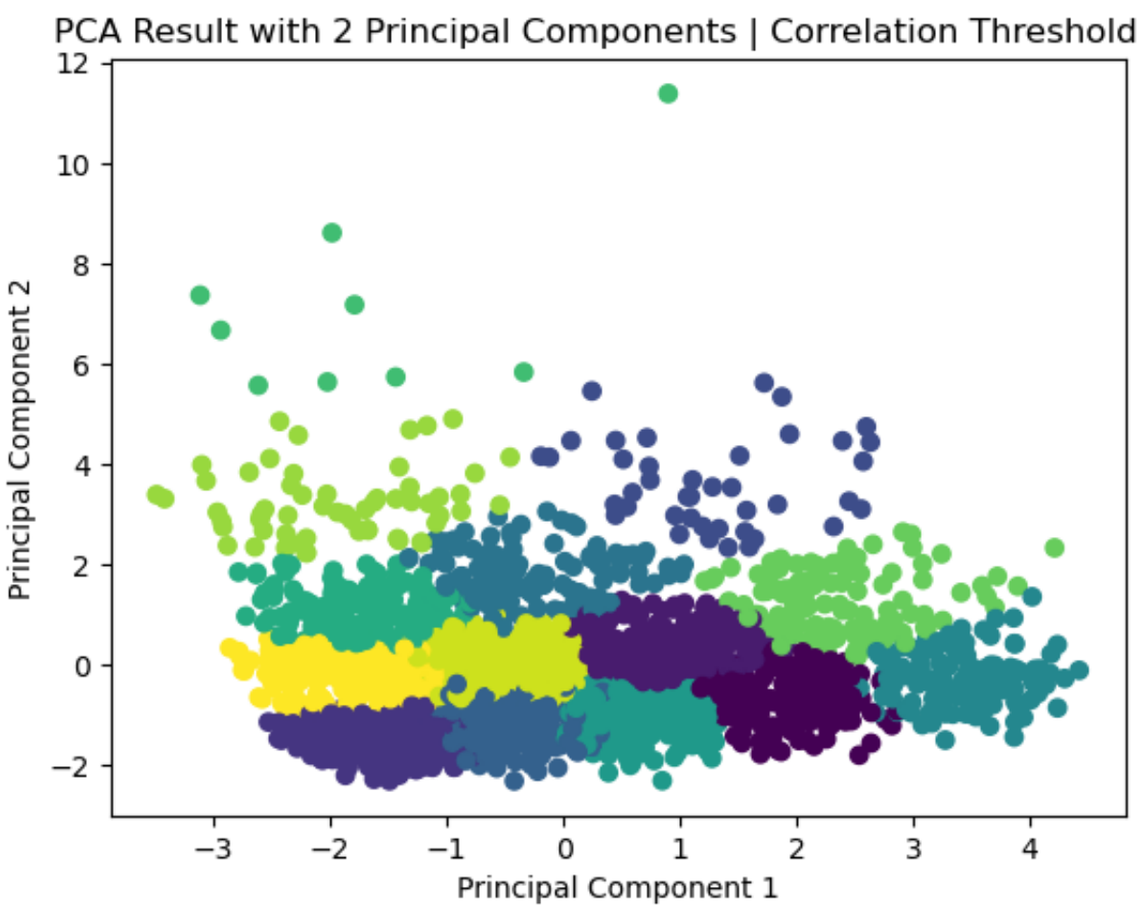
In [28]:
```
# Remove any correlations below .7
## Set correlation threshold
threshold = .7
## Set the self correlation to na to remove the columns that correlates with its self
np.fill_diagonal(cor_data.values, np.nan)
## Remove the lower correlations columns
cor_remove = cor_data.columns[(cor_data.abs() > threshold).any()]
## Save these columns
data_f = data[cor_remove]

# Drop repeat ID column
data_f = data_f.drop(columns = ['SubjectID', 'ID'])

# Allow scaler
scale = StandardScaler()

# Fit transform the data
data_ft = scale.fit_transform(data_f)

# Empty list
scores = []
# Cluster range
c_range = range(2,15)

# For loop to find clusters
for n_clusters in c_range:
    #find kmeans
    kmeans = KMeans(n_clusters=n_clusters, n_init=10, random_state=42)
    # predict the labels
    labels = kmeans.fit_predict(data_ft)
    # find the silhouette score
    silhouette_avg = silhouette_score(data_ft, labels)
    # Append it to the list
    scores.append(silhouette_avg)
```

In [30]:
```
# Plotting
# Plot size
plt.figure(figsize=(10, 6))
# Plot graph
plt.plot(c_range, scores, marker='s')
# Title
plt.title('Silhouette Score vs Number of Clusters | Correlation Threshold .7')
# X-axis label
plt.xlabel('Number of Clusters')
# Y-axis label
plt.ylabel('Silhouette Score')
# Add grid
plt.grid()
# Show plot
plt.show()
```



In [31]:
```
# Fit and transform the data based on scatter plot
pca_data = pca.fit_transform(data_ft)
```

In [32]:
```
# Scatter plot... I am not sure this is right
plt.scatter(pca_data[:, 0],pca_data[:, 1], c=labels)
# Add tile
plt.title('PCA Result with 2 Principal Components | Correlation Threshold .7')
# Add X-axis label
plt.xlabel('Principal Component 1')
# Add y-axis label
plt.ylabel('Principal Component 2')
# Show
plt.show()
```



Conclusion.

I ran the test multiple times and changed the threshold each time. However, I only included two of the tests. Only including columns that correlate more than .2 allows the prediction to consider more things when making predictions to ensure the model does not overfit, but the clusters are not as good. If .2 is used to decide what columns to keep, I believe a different model would be best.

Raising the threshold for the correlation to .7 in regards to whether or not to include the column improves the clusters, but this can cause the model to overfit. Not that it has caused overfitting, but it can. I did .2 in the beginning because I did not want to exclude so much information. If .7 is used as a threshold to decide what columns to keep, it is better but not great. It might still be better to use a different model, but it does not have to be. It is at a reasonable level. The Silhouette Score to around .35, which is even better, but preferable the score should be around .5 or more.

In [27]:
```
# Show everything to print PDF
pd.set_option('display.max_colwidth', None)
pd.set_option('display.max_rows', None)
pd.set_option('display.max_columns', None)
```