STATS 3DA3

Homework Assignment 6

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```
import pandas as pd

import numpy as np

import seaborn as sns

import matplotlib.pyplot as plt

import matplotlib.cm as cm


from sklearn.preprocessing import StandardScaler

from sklearn.model_selection import train_test_split, GridSearchCV

from sklearn import neighbors

from sklearn.neighbors import KNeighborsClassifier

from sklearn.linear_model import LinearRegression

from sklearn.linear_model import LogisticRegression

from sklearn import metrics

from sklearn.model_selection import cross_val_score

from sklearn.decomposition import PCA

from sklearn.cluster import KMeans

from sklearn.cluster import AgglomerativeClustering

from sklearn.metrics import silhouette_samples, silhouette_score

from sklearn.metrics import confusion_matrix, classification_report, roc_curve, roc_auc_score

from sklearn.metrics import accuracy_score

from mlxtend.feature_selection import ExhaustiveFeatureSelector as EFS

from sklearn import svm
```

(1)

The goal is to predict whether a patient has heart disease based on 13 explanatory variables. The response variable which is categorical is expected to be binary (0-no heart disease, 1-presence of heart disease). However, there are 4 levels of presence of heart disease (1, 2, 3, 4) for the response variable. This causes the supervised classification problem, meaning that the classifiers are overfitting.

(2)

```
df=pd.read_csv('https://archive.ics.uci.edu/static/public/45/data.csv')
```

```
df.head(10)
```

	age	sex	cp	trestbps	chol	fbs	restecg	thalach	exang	oldpeak	slope	ca	thal	num
0	63	1	1	145	233	1	2	150	0	2.3	3	0.0	6.0	0
1	67	1	4	160	286	0	2	108	1	1.5	2	3.0	3.0	2
2	67	1	4	120	229	0	2	129	1	2.6	2	2.0	7.0	1
3	37	1	3	130	250	0	0	187	0	3.5	3	0.0	3.0	0
4	41	0	2	130	204	0	2	172	0	1.4	1	0.0	3.0	0
5	56	1	2	120	236	0	0	178	0	0.8	1	0.0	3.0	0
6	62	0	4	140	268	0	2	160	0	3.6	3	2.0	3.0	3
7	57	0	4	120	354	0	0	163	1	0.6	1	0.0	3.0	0
8	63	1	4	130	254	0	2	147	0	1.4	2	1.0	7.0	2
9	53	1	4	140	203	1	2	155	1	3.1	3	0.0	7.0	1

```
# drop the missing data
df_dropnan=df.dropna()
```

The categorical variables such as num have already been used one-hot coding. We do not need to transform the response variable which is categorical.

(3)

```
df.shape
```

```
(303, 14)
```

```
df.isnull().sum()
```

```
age         0
sex         0
```

```
cp          0
trestbps    0
chol        0
fbs         0
restecg     0
thalach     0
exang       0
oldpeak     0
slope       0
ca          4
thal        2
num         0
dtype: int64
```

```
df.columns
```

```
Index(['age', 'sex', 'cp', 'trestbps', 'chol', 'fbs', 'restecg', 'thalach',
       'exang', 'oldpeak', 'slope', 'ca', 'thal', 'num'],
      dtype='object')
```

```
df.dtypes
```

```
age           int64
sex           int64
cp            int64
trestbps      int64
chol          int64
fbs           int64
restecg       int64
thalach       int64
exang         int64
oldpeak     float64
```

```
slope         int64
ca          float64
thal        float64
num           int64
dtype: object
```

```
# drop the categorical variables to analyze the distributions
df_num=df.drop(columns=['sex', 'cp', 'fbs', 'restecg', 'exang', 'slope', 'thal', 'num'])
```

```
df_num.describe()
```

	age	trestbps	chol	thalach	oldpeak	ca
count	303.000000	303.000000	303.000000	303.000000	303.000000	299.000000
mean	54.438944	131.689769	246.693069	149.607261	1.039604	0.672241
std	9.038662	17.599748	51.776918	22.875003	1.161075	0.937438
min	29.000000	94.000000	126.000000	71.000000	0.000000	0.000000
25%	48.000000	120.000000	211.000000	133.500000	0.000000	0.000000
50%	56.000000	130.000000	241.000000	153.000000	0.800000	0.000000
75%	61.000000	140.000000	275.000000	166.000000	1.600000	1.000000
max	77.000000	200.000000	564.000000	202.000000	6.200000	3.000000

```
# describe the categorical variables
df['sex'].value_counts()
```

```
sex
1    206
0     97
Name: count, dtype: int64
```

```
df['cp'].value_counts()
```

```
cp
```

```
4    144
3     86
2     50
1     23
Name: count, dtype: int64
```

```
df['fbs'].value_counts()
```

```
fbs
0    258
1     45
Name: count, dtype: int64
```

```
df['restecg'].value_counts()
```

```
restecg
0    151
2    148
1      4
Name: count, dtype: int64
```

```
df['exang'].value_counts()
```

```
exang
0    204
1     99
Name: count, dtype: int64
```

```
df['slope'].value_counts()
```

```
slope
1    142
```

```
2    140
3     21
Name: count, dtype: int64
```

```python
df['thal'].value_counts()
```

```
thal
3.0    166
7.0    117
6.0     18
Name: count, dtype: int64
```

```python
df['num'].value_counts()
```

```
num
0    164
1     55
2     36
3     35
4     13
Name: count, dtype: int64
```

Numerical attributes: age, trestbps, chol, thalach, oldpeak, ca

Categorical attributes: sex, cp, fbs, restecg, exang, slope, thal, num (response variable)

There are 303 observations and 13 features in the dataset, while there are 4 missing values in ca and 2 missing values in thal. The variable chol has the largest variance and widest range. The variable which has the high variance can dominate clustering results, making other variables less influential.

(4)

```
df['num']=df['num'].apply(lambda x: 1 if x>0 else 0)
```

```
df.head(10)
```

	age	sex	cp	trestbps	chol	fbs	restecg	thalach	exang	oldpeak	slope	ca	thal	num
0	63	1	1	145	233	1	2	150	0	2.3	3	0.0	6.0	0
1	67	1	4	160	286	0	2	108	1	1.5	2	3.0	3.0	1
2	67	1	4	120	229	0	2	129	1	2.6	2	2.0	7.0	1
3	37	1	3	130	250	0	0	187	0	3.5	3	0.0	3.0	0
4	41	0	2	130	204	0	2	172	0	1.4	1	0.0	3.0	0
5	56	1	2	120	236	0	0	178	0	0.8	1	0.0	3.0	0
6	62	0	4	140	268	0	2	160	0	3.6	3	2.0	3.0	1
7	57	0	4	120	354	0	0	163	1	0.6	1	0.0	3.0	0
8	63	1	4	130	254	0	2	147	0	1.4	2	1.0	7.0	1
9	53	1	4	140	203	1	2	155	1	3.1	3	0.0	7.0	1

(5)

```
correlation=df.corr()
correlation
```

	age	sex	cp	trestbps	chol	fbs	restecg	thalach	exang
age	1.000000	-0.097542	0.104139	0.284946	0.208950	0.118530	0.148868	-0.393806	0.09166
sex	-0.097542	1.000000	0.010084	-0.064456	-0.199915	0.047862	0.021647	-0.048663	0.14620
cp	0.104139	0.010084	1.000000	-0.036077	0.072319	-0.039975	0.067505	-0.334422	0.38406
trestbps	0.284946	-0.064456	-0.036077	1.000000	0.130120	0.175340	0.146560	-0.045351	0.06476
chol	0.208950	-0.199915	0.072319	0.130120	1.000000	0.009841	0.171043	-0.003432	0.06131
fbs	0.118530	0.047862	-0.039975	0.175340	0.009841	1.000000	0.069564	-0.007854	0.02566
restecg	0.148868	0.021647	0.067505	0.146560	0.171043	0.069564	1.000000	-0.083389	0.08486
thalach	-0.393806	-0.048663	-0.334422	-0.045351	-0.003432	-0.007854	-0.083389	1.000000	-0.3781
exang	0.091661	0.146201	0.384060	0.064762	0.061310	0.025665	0.084867	-0.378103	1.00000

	age	sex	cp	trestbps	chol	fbs	restecg	thalach	exang
oldpeak	0.203805	0.102173	0.202277	0.189171	0.046564	0.005747	0.114133	-0.343085	0.28822
slope	0.161770	0.037533	0.152050	0.117382	-0.004062	0.059894	0.133946	-0.385601	0.25774
ca	0.362605	0.093185	0.233214	0.098773	0.119000	0.145478	0.128343	-0.264246	0.14557
thal	0.127389	0.380936	0.265246	0.133554	0.014214	0.071358	0.024531	-0.279631	0.32968
num	0.223120	0.276816	0.414446	0.150825	0.085164	0.025264	0.169202	-0.417167	0.43189

```
correlation['num'].sort_values(ascending=False)
```

```
num         1.000000
thal        0.525689
ca          0.460442
exang       0.431894
oldpeak     0.424510
cp          0.414446
slope       0.339213
sex         0.276816
age         0.223120
restecg     0.169202
trestbps    0.150825
chol        0.085164
fbs         0.025264
thalach    -0.417167
Name: num, dtype: float64
```

The variable thal has the most positive correlation with the response variable num. The variable thalach has the only negative correlation with the response variable num. The variables such as thal, ca, oldpeak, and thalach have the strong relationship with the response variable num since they have the large absolute correlation. The variables such as fbs and chol have the weak correlation with the response variable num. For the feature selection, the variables have the strong correlation are considered to keep, while the variables have the weak correlation are considered to remove.

(6)

```
df.isnull().sum()
```

```
age         0
sex         0
cp          0
trestbps    0
chol        0
fbs         0
restecg     0
thalach     0
exang       0
oldpeak     0
slope       0
ca          4
thal        2
num         0
dtype: int64
```

```
# drop the missing data
df=df.dropna()
```

There are 4 missing values in ca and 2 missing values in thal.

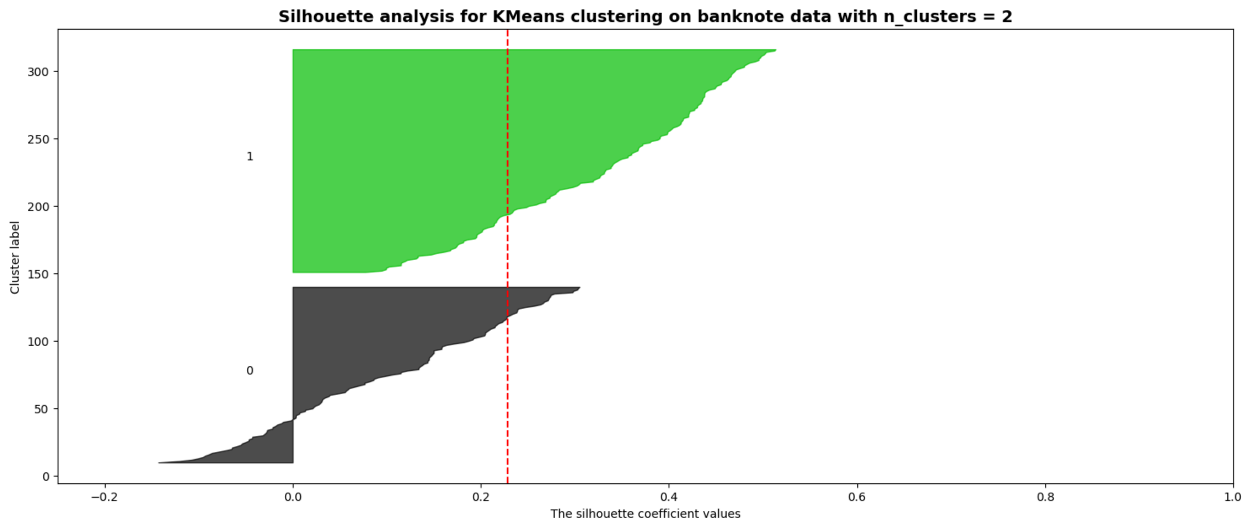
(7)

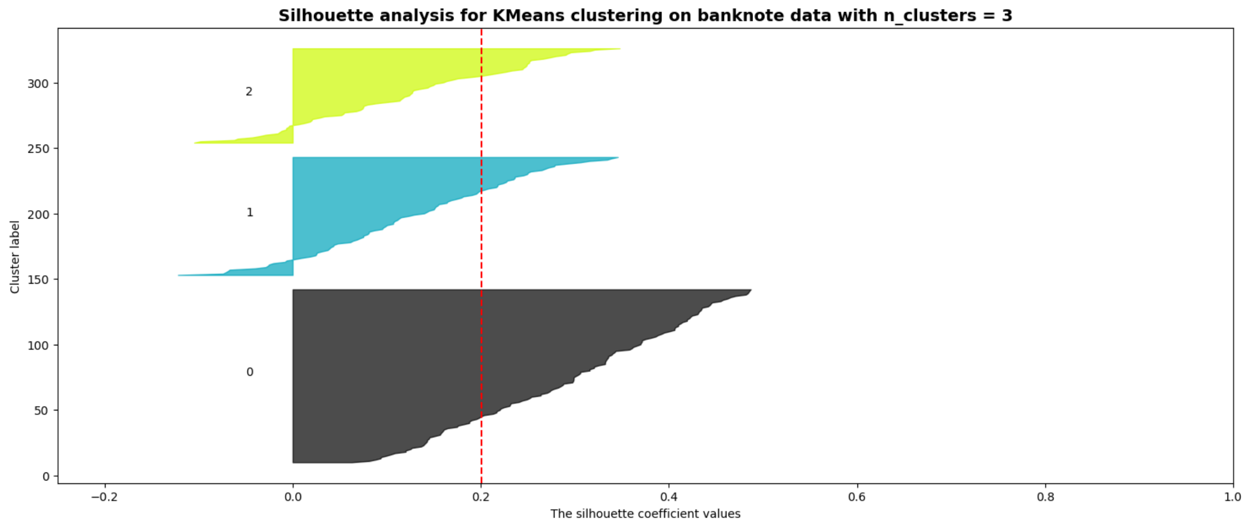
```
# drop the categorical variables to analyze the distributions
df_num=df.drop(columns=['sex', 'cp', 'fbs', 'restecg', 'exang', 'slope', 'thal', 'num'])
```

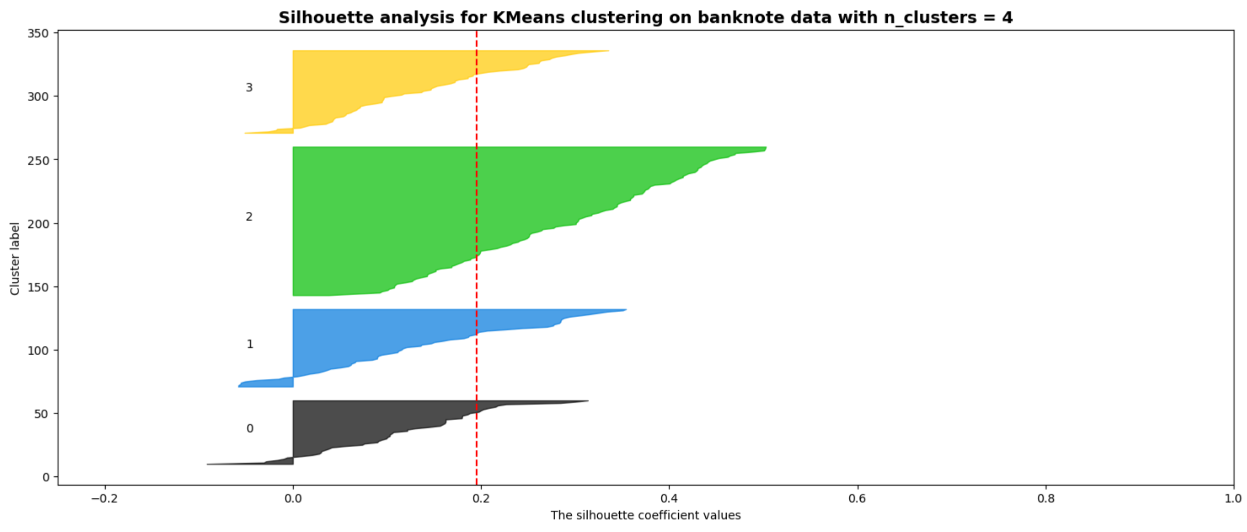
```
scaler=StandardScaler()


df_num_sc=pd.DataFrame(scaler.fit_transform(df_num), columns=df_num.columns)
df_num_sc
```

	age	trestbps	chol	thalach	oldpeak	ca
0	0.936181	0.750380	-0.276443	0.017494	1.068965	-0.721976
1	1.378929	1.596266	0.744555	-1.816334	0.381773	2.478425
2	1.378929	-0.659431	-0.353500	-0.899420	1.326662	1.411625
3	-1.941680	-0.095506	0.051047	1.633010	2.099753	-0.721976
4	-1.498933	-0.095506	-0.835103	0.978071	0.295874	-0.721976
...	...	...	...	...	...	...
292	0.272059	0.468418	-0.122330	-1.161395	-0.734914	-0.721976
293	-1.056185	-1.223355	0.320744	-0.768432	0.124076	-0.721976
294	1.489615	0.693988	-1.047008	-0.375469	2.013854	1.411625
295	0.272059	-0.095506	-2.241384	-1.510696	0.124076	0.344824
296	0.272059	-0.095506	-0.218651	1.065396	-0.906712	0.344824

```
range_n_clusters = range(2, 5)
for n_clusters in range_n_clusters:
    km = KMeans(n_clusters = n_clusters, n_init = 20, random_state=0)
    cluster_labels_km = km.fit_predict(df_num_sc)
    silhouette_avg_km = silhouette_score(df_num_sc, cluster_labels_km)
    # Compute the silhouette scores for each sample
    sample_silhouette_values = silhouette_samples(df_num_sc, cluster_labels_km)
    fig, ax1 = plt.subplots(1, 1)
    fig.set_size_inches(18, 7)
    ax1.set_xlim([-0.25, 1])# change this based on the silhouette range

    y_lower = 10

    for i in range(n_clusters):
        # Aggregate the silhouette scores for samples belonging to
        # cluster i, and sort them
        ith_cluster_silhouette_values = sample_silhouette_values[cluster_labels_km == i]
        ith_cluster_silhouette_values.sort()

        size_cluster_i = ith_cluster_silhouette_values.shape[0]
        y_upper = y_lower + size_cluster_i

        color = cm.nipy_spectral(float(i) / n_clusters)
        ax1.fill_betweenx(
            np.arange(y_lower, y_upper),
            0,
            ith_cluster_silhouette_values,
            facecolor=color,
            edgecolor=color,
            alpha=0.7,
        )

        # Label the silhouette plots with their cluster numbers at the middle
        ax1.text(-0.05, y_lower + 0.5 * size_cluster_i, str(i))

        # Compute the new y_lower for next plot
        y_lower = y_upper + 10

    ax1.set_title("The silhouette plot for various cluster")
    ax1.set_xlabel("The silhouette coefficient values")
    ax1.set_ylabel("Cluster label")

    # The vertical line for average silhouette score of all the values
    ax1.axvline(x=silhouette_avg_km, color="red", linestyle="--")
    plt.title(
        "Silhouette analysis for KMeans clustering on banknote data with n_clusters = %d"
        % n_clusters,
        fontsize=14,
        fontweight="bold",
    )
```







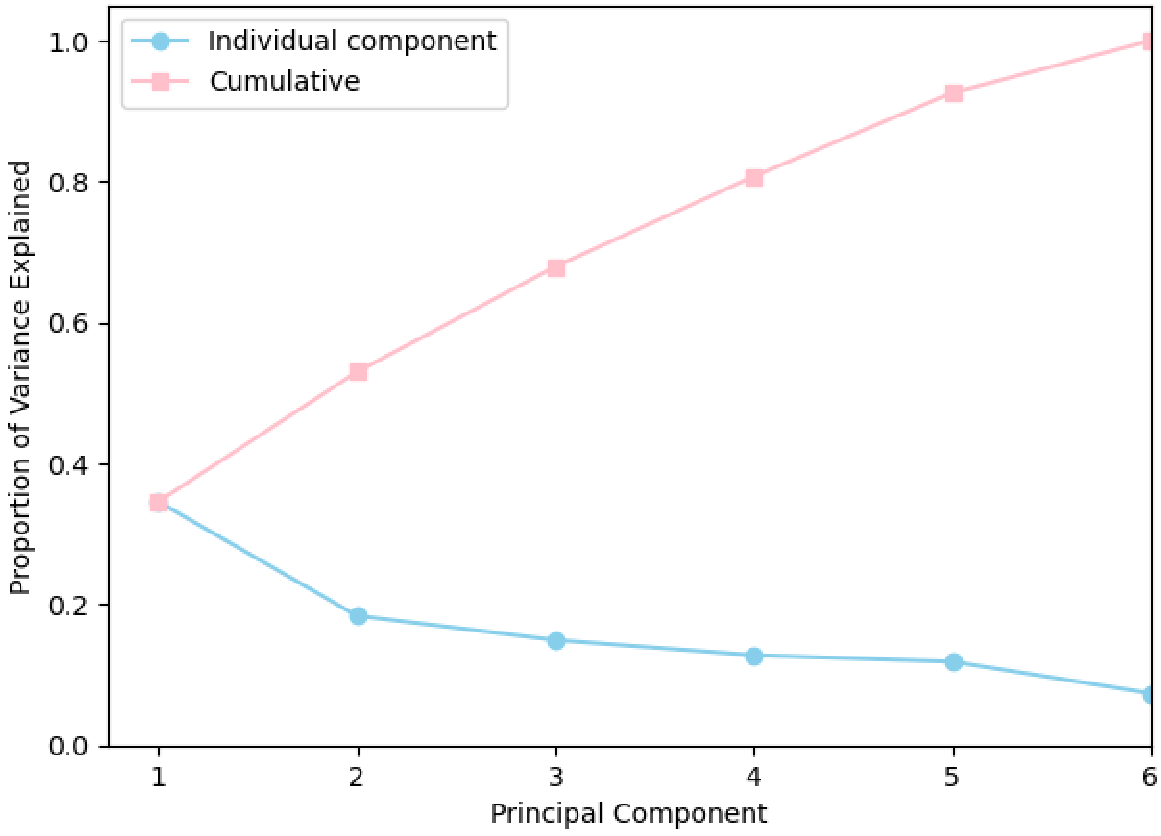
```
# choose n_clusters=2
kmeans_optimal=KMeans(n_clusters=2, n_init=20, random_state=42)
cluster_labels_optimal=kmeans_optimal.fit_predict(df_num_sc)
```

```
pca=PCA()
```

```
pca.fit(df_num_sc)
```

```
PCA()
```

```
# scree plot
plt.figure(figsize=(7, 5))

plt.plot([1,2,3,4,5,6], pca.explained_variance_ratio_, '-o', label='Individual component',
         color='skyblue')
plt.plot([1,2,3,4,5,6], np.cumsum(pca.explained_variance_ratio_), '-s', label='Cumulative',
         color='pink')

plt.ylabel('Proportion of Variance Explained')
plt.xlabel('Principal Component')
plt.xlim(0.75, 4.25)
plt.ylim(0, 1.05)
plt.xticks([1,2,3,4,5,6])
plt.legend(loc=2);
```

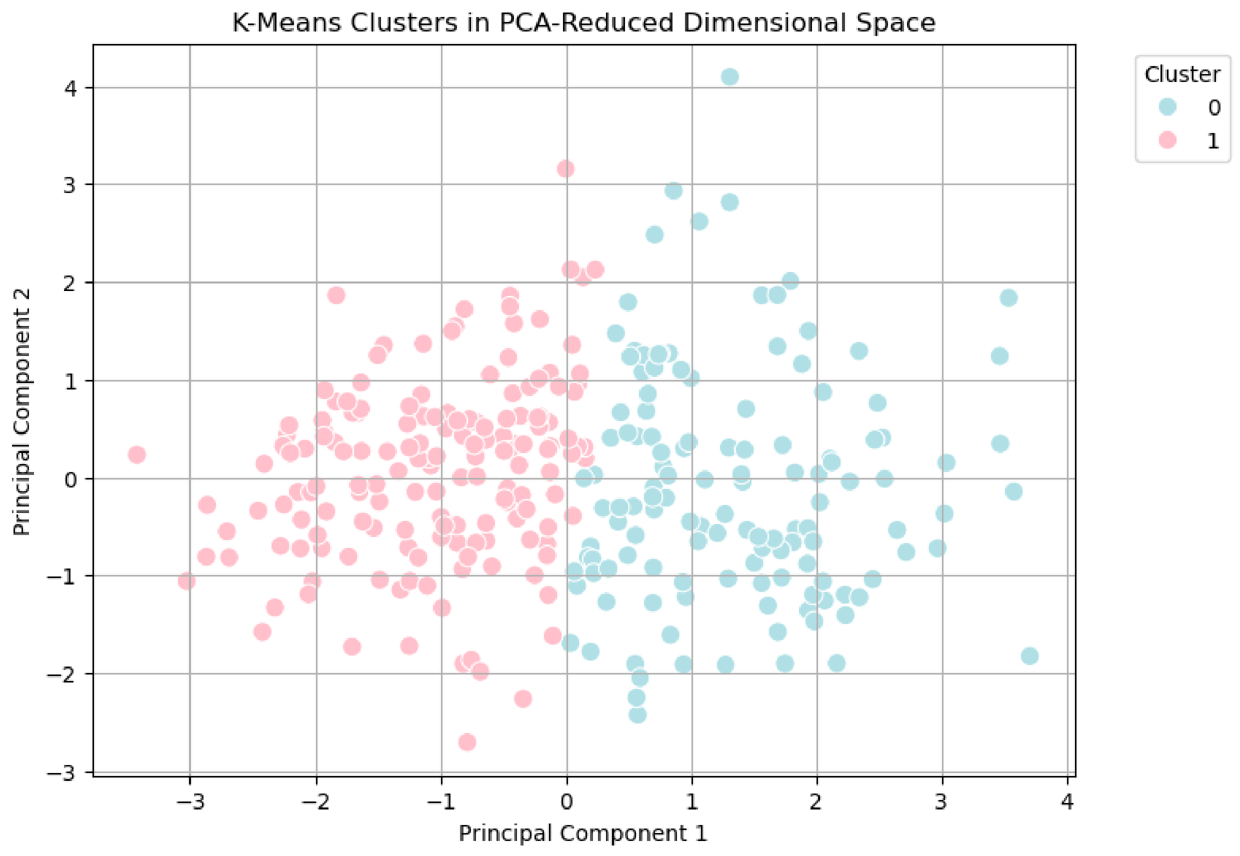


```
pca_2=PCA(n_components=2)
```

```
pca_2.fit(df_num_sc)
```

```
PCA(n_components=2)
```

```
pca_2.fit_transform(df_num_sc)


plt.figure(figsize=(8, 6))
sns.scatterplot(
    x=pca_2.fit_transform(df_num_sc)[:, 0],
    y=pca_2.fit_transform(df_num_sc)[:, 1],
    hue=cluster_labels_optimal,
    palette=['powderblue', 'pink'],
    s=80
)

plt.xlabel('Principal Component 1')
plt.ylabel('Principal Component 2')
plt.title('K-Means Clusters in PCA-Reduced Dimensional Space')
plt.legend(title='Cluster', bbox_to_anchor=(1.05, 1), loc='upper left')
plt.grid()
plt.show()
```



(8)

```python
df_drop=df.drop(columns=['num'])
```

```python
scaler=StandardScaler()


df_sc=pd.DataFrame(scaler.fit_transform(df_drop), columns=df_drop.columns)
df_sc
```

	age	sex	cp	trestbps	chol	fbs	restecg	thalach	exang
0	0.936181	0.691095	-2.240629	0.750380	-0.276443	2.430427	1.010199	0.017494	-0.696419
1	1.378929	0.691095	0.873880	1.596266	0.744555	-0.411450	1.010199	-1.816334	1.435916
2	1.378929	0.691095	0.873880	-0.659431	-0.353500	-0.411450	1.010199	-0.899420	1.435916
3	-1.941680	0.691095	-0.164289	-0.095506	0.051047	-0.411450	-1.003419	1.633010	-0.696419
4	-1.498933	-1.446980	-1.202459	-0.095506	-0.835103	-0.411450	1.010199	0.978071	-0.696419
...	...	...	...	...	...	...	...	...	...
292	0.272059	-1.446980	0.873880	0.468418	-0.122330	-0.411450	-1.003419	-1.161395	1.435916
293	-1.056185	0.691095	-2.240629	-1.223355	0.320744	-0.411450	-1.003419	-0.768432	-0.696419
294	1.489615	0.691095	0.873880	0.693988	-1.047008	2.430427	-1.003419	-0.375469	-0.696419
295	0.272059	0.691095	0.873880	-0.095506	-2.241384	-0.411450	-1.003419	-1.510696	1.435916
296	0.272059	-1.446980	-1.202459	-0.095506	-0.218651	-0.411450	1.010199	1.065396	-0.696419

```python
X=df_sc
y=df['num']
```

```python
X_train, X_test, y_train, y_test = train_test_split(
    X,
    y,
    test_size=0.3,
    random_state=1,
    stratify=y
    )
```

(9)

1. Logistic Regression: We refer the coefficients to indicate the feature influence and see how each feature affects the probability of heart disease.

2. KNN: We refer the similarity to nearby data points to predict classes of presence of heart disease.

(10)

1. Accuracy: It is computed by the proportion of correctly predicted observations out of the total observations using confusion matrix.

2. ROC-AUC: We plot True Positive Rate vs. False Positive Rate for ROC curve and calculate AUC which is the area under the ROC curve to see how well the model can distinguish between classes across all classification thresholds.

(11)

```
# logistic regression
log_param_grid={'C': [0.01, 0.1, 1, 10, 100],}
```

```
log_grid_search=GridSearchCV(LogisticRegression(),
                             log_param_grid,
                             cv=5,
                             scoring='accuracy')

log_grid_search.fit(X_train, y_train)
```

```
GridSearchCV(cv=5, estimator=LogisticRegression(),
             param_grid={'C': [0.01, 0.1, 1, 10, 100]}, scoring='accuracy')
```

```
log_grid_search.best_estimator_
```

```
LogisticRegression(C=0.01)
```

```
# optimal tuning parameters - best C
log_grid_search.best_params_
```

```
{'C': 0.01}
```

```
# knn
knn_param_grid={'n_neighbors': list(range(1, 20))}
```

```
knn_grid_search=GridSearchCV(KNeighborsClassifier(),
                             knn_param_grid,
                             cv=5,
                             scoring='accuracy')

knn_grid_search.fit(X_train, y_train)
```

```
GridSearchCV(cv=5, estimator=KNeighborsClassifier(),
             param_grid={'n_neighbors': [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12,
                                         13, 14, 15, 16, 17, 18, 19]},
             scoring='accuracy')
```

```
knn_grid_search.best_estimator_
```

```
KNeighborsClassifier(n_neighbors=7)
```

```
# optimal tuning parameters - best n_neighbors
knn_grid_search.best_params_
```

```
{'n_neighbors': 7}
```

(12)

```
# feature selection
efs=EFS(
    LogisticRegression(),
    min_features=1,
    max_features=5,
    scoring='accuracy',
    cv=5)

efs.fit(X_train, y_train)
```

```
Features: 2379/2379
```

```
ExhaustiveFeatureSelector(estimator=LogisticRegression(),
                          feature_groups=[[0], [1], [2], [3], [4], [5], [6],
                                          [7], [8], [9], [10], [11], [12]],
                          max_features=5)
```

```
best_features=list(efs.best_feature_names_)
best_features
```

```
['sex', 'exang', 'ca', 'thal']
```

```
X_train_efs=X_train[best_features]
X_test_efs=X_test[best_features]
```

```
efs_log_grid_search=GridSearchCV(LogisticRegression(),
                                 log_param_grid,
                                 cv=5,
                                 scoring='accuracy')

efs_log_grid_search.fit(X_train_efs, y_train)
```

```
GridSearchCV(cv=5, estimator=LogisticRegression(),
             param_grid={'C': [0.01, 0.1, 1, 10, 100]}, scoring='accuracy')
```

```
efs_log_grid_search.best_estimator_
```

```
LogisticRegression(C=0.1)
```

```
# optimal tuning parameters - best C
efs_log_grid_search.best_params_
```

```
{'C': 0.1}
```

(13)

```
best_log=log_grid_search.best_estimator_


log_pred_prob=best_log.predict_proba(X_test)[:, 1]


log_y_pred=best_log.predict(X_test)
```

```
accuracy_score(y_test, log_y_pred)
```

```
0.8555555555555555
```

```
best_knn=knn_grid_search.best_estimator_


knn_pred_prob=best_knn.predict_proba(X_test)[:, 1]


knn_y_pred=best_knn.predict(X_test)
```

```
accuracy_score(y_test, knn_y_pred)
```

```
0.8222222222222222
```

```
best_efs_log=efs_log_grid_search.best_estimator_

efs_log_pred_prob=best_efs_log.predict_proba(X_test_efs)[:, 1]

efs_log_y_pred=best_efs_log.predict(X_test_efs)
```

```
accuracy_score(y_test, efs_log_y_pred)
```

```
0.7444444444444445
```

```
roc_auc_score(y_test, log_pred_prob)
```

```
0.9136904761904763
```

```
roc_auc_score(y_test, knn_pred_prob)
```

```
0.8973214285714285
```

```
roc_auc_score(y_test, efs_log_pred_prob)
```

```
0.8591269841269841
```

Among the three classifiers tested — Logistic Regression, K-Nearest Neighbors (KNN), and Logistic Regression with feature selection, all perform well in terms of accuracy and ROC-AUC. Logistic Regression achieves the highest accuracy score and ROC-AUC score, suggesting it has the most efficiency of distinguishing between patients with and without heart disease.

The accuracy score and ROC-AUC score of Logistic Regression get lower after applying EFS. While EFS helps reduce dimensionality and may prevent over-fitting in high-dimensional settings in the dataset. Over-simplifying can actually hurt performance, suggesting all features contribute meaningfully.

(14)

```
m_log=LogisticRegression()
m_log.fit(X_train, y_train)
```

```
LogisticRegression()
```

```
coefficient=pd.DataFrame(m_log.coef_, columns=df_drop.columns)
coefficient
```

	age	sex	cp	trestbps	chol	fbs	restecg	thalach	exang	oldpeak
0	-0.098968	0.783227	0.553553	0.332895	0.38974	-0.412099	0.041425	-0.439762	0.529723	0.19436

```
# Question 12
best_features=list(efs.best_feature_names_)
best_features
```

```
['sex', 'exang', 'ca', 'thal']
```

The top important variables are: ca, sex, thal, exang since they have the highest absolute value of coefficients. These features are strongly associated with the presence of heart disease.

(15)

```
# the fourth classifier
clf=svm.SVC(kernel="linear")
```

```
svm_param_grid={'C': [0.1, 1, 10, 100, 1000]}
```

```
svm_grid_search=GridSearchCV(
    estimator=clf,
    param_grid=svm_param_grid,
    cv=5,
    scoring='accuracy'
    )


svm_grid_search.fit(X_train, y_train)
```

```
GridSearchCV(cv=5, estimator=SVC(kernel='linear'),
             param_grid={'C': [0.1, 1, 10, 100, 1000]}, scoring='accuracy')
```

```
svm_grid_search.best_estimator_
```

```
SVC(C=0.1, kernel='linear')
```

```
# optimal tuning parameters - best C
svm_grid_search.best_params_
```

```
{'C': 0.1}
```

```
clf_best_c=svm_grid_search.best_estimator_
```

```
best_clf=svm.SVC(kernel="linear", C=clf_best_c.C, probability=True)
```

```
best_clf.fit(X_train, y_train)
```

```
SVC(C=0.1, kernel='linear', probability=True)
```

```
clf_pred_prob=best_clf.predict_proba(X_test)[:, 1]
clf_y_pred=best_clf.predict(X_test)
```

```
accuracy_score(y_test, clf_y_pred)
```

```
0.8666666666666667
```

```
roc_auc_score(y_test, clf_pred_prob)
```

```
0.898809523809524
```

The accuracy score for the fourth classifier slightly increases, and the ROC-AUC score almost keeps the same for the fourth classifier, showing a better performance. This suggests that sub-groups have distinct characteristics.

References

Janosi, A., Steinbrunn, W., Pfisterer, M., & Detrano, R. (1989). Heart Disease [Dataset]. UCI Machine Learning Repository. https://doi.org/10.24432/C52P4X.