

# **STATS 3DA3**

## **Homework Assignment 6**

Ashley Chen, Jasmine Ho, JC Abanto

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## Question

1)

Our target variable measure the severity of heart disease which can be defined as binary classification problem. Our goal would then to be able to predict the probability of heart disease. This means we can carry out a logistic regression and a random forest classifier to predict the presence and absence of heart disease.

2)

```
from ucimlrepo import fetch_ucirepo
from sklearn.preprocessing import StandardScaler

heart_disease = fetch_ucirepo(id=45)

X = heart_disease.data.features
y = heart_disease.data.targets

scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X)
```

3)

We have 13 features and 1 target variable. Starting with our features, we have age (age in years), sex (1 = male; 0 = female), cp (1: typical angina, 2: atypical angina, 3: non-anginal pain, 4: asymptomatic), trestbps (resting blood pressure in mm Hg on admission to the hospital), chol (serum cholestoral in mg/dl), fbs (fasting blood sugar > 120 mg/dl where 1 = true; 0 = false), restecg (resting electrocardiographic results), exang (exercise induced angina), oldpeak (ST depression induced by exercise relative to rest), slope (1 = upsloping, 2 = flat, 3 = downsloping), ca (number of major vessels colored by floursopy), thal (3 = normal; 6 = fixed defect; 7 = reversable defect). Finally our target variable, 'num', is the diagnosis of heart disease.

```
print(f"Observations in X: {len(X)}")
print(f"Summary of X:\n{X.describe()}")
print(f"Summary of y:\n{y.describe()}")
```

Observations in X: 303

Summary of X:

	age	sex	cp	trestbps	chol	fbs \
count	303.000000	303.000000	303.000000	303.000000	303.000000	303.000000
mean	54.438944	0.679868	3.158416	131.689769	246.693069	0.148515
std	9.038662	0.467299	0.960126	17.599748	51.776918	0.356198
min	29.000000	0.000000	1.000000	94.000000	126.000000	0.000000
25%	48.000000	0.000000	3.000000	120.000000	211.000000	0.000000
50%	56.000000	1.000000	3.000000	130.000000	241.000000	0.000000
75%	61.000000	1.000000	4.000000	140.000000	275.000000	0.000000
max	77.000000	1.000000	4.000000	200.000000	564.000000	1.000000

	restecg	thalach	exang	oldpeak	slope	ca \
count	303.000000	303.000000	303.000000	303.000000	303.000000	299.000000
mean	0.990099	149.607261	0.326733	1.039604	1.600660	0.672241
std	0.994971	22.875003	0.469794	1.161075	0.616226	0.937438
min	0.000000	71.000000	0.000000	0.000000	1.000000	0.000000
25%	0.000000	133.500000	0.000000	0.000000	1.000000	0.000000
50%	1.000000	153.000000	0.000000	0.800000	2.000000	0.000000
75%	2.000000	166.000000	1.000000	1.600000	2.000000	1.000000
max	2.000000	202.000000	1.000000	6.200000	3.000000	3.000000

	thal
count	301.000000
mean	4.734219
std	1.939706
min	3.000000
25%	3.000000

```
50%      3.000000
75%      7.000000
max       7.000000
```

Summary of y:

```
          num
count  303.000000
mean    0.937294
std     1.228536
min     0.000000
25%     0.000000
50%     0.000000
75%     2.000000
max     4.000000
```

We find that the average age of patients is 54.4 years old, with a standard deviation of 9.1 years.

```
print(f"Data Types of X: \n{X.dtypes}")
print(f"\nData Types of y: \n{y.dtypes}")
```

Data Types of X:

```
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
dtype: object
```

Data Types of y:

```
num          int64
dtype: object
```

All of our data types in X are numerical but some representing categorical variables.

4)

```
print(f"y before transformation: {y['num'].value_counts()}")
y['num'] = y['num'].apply(lambda x: 1 if x > 0 else 0)
print(f"y before transformation: {y['num'].value_counts()}")
```

```
y before transformation: num
```

```
0    164
1     55
2     36
3     35
4     13
```

```
Name: count, dtype: int64
```

```
y before transformation: num
```

```
0    164
1    139
```

```
Name: count, dtype: int64
```

```
/var/folders/5q/w2pw9gp90mldwv2xvm9ml_jc0000gn/T/ipykernel_88054/2854447611.py:2: SettingWithCopyWarning: 
```

A value is trying to be set on a copy of a slice from a DataFrame.

Try using `.loc[row_indexer,col_indexer] = value` instead

See the caveats in the documentation: [https://pandas.pydata.org/pandas-docs/stable/user\\_guide/](https://pandas.pydata.org/pandas-docs/stable/user_guide/)

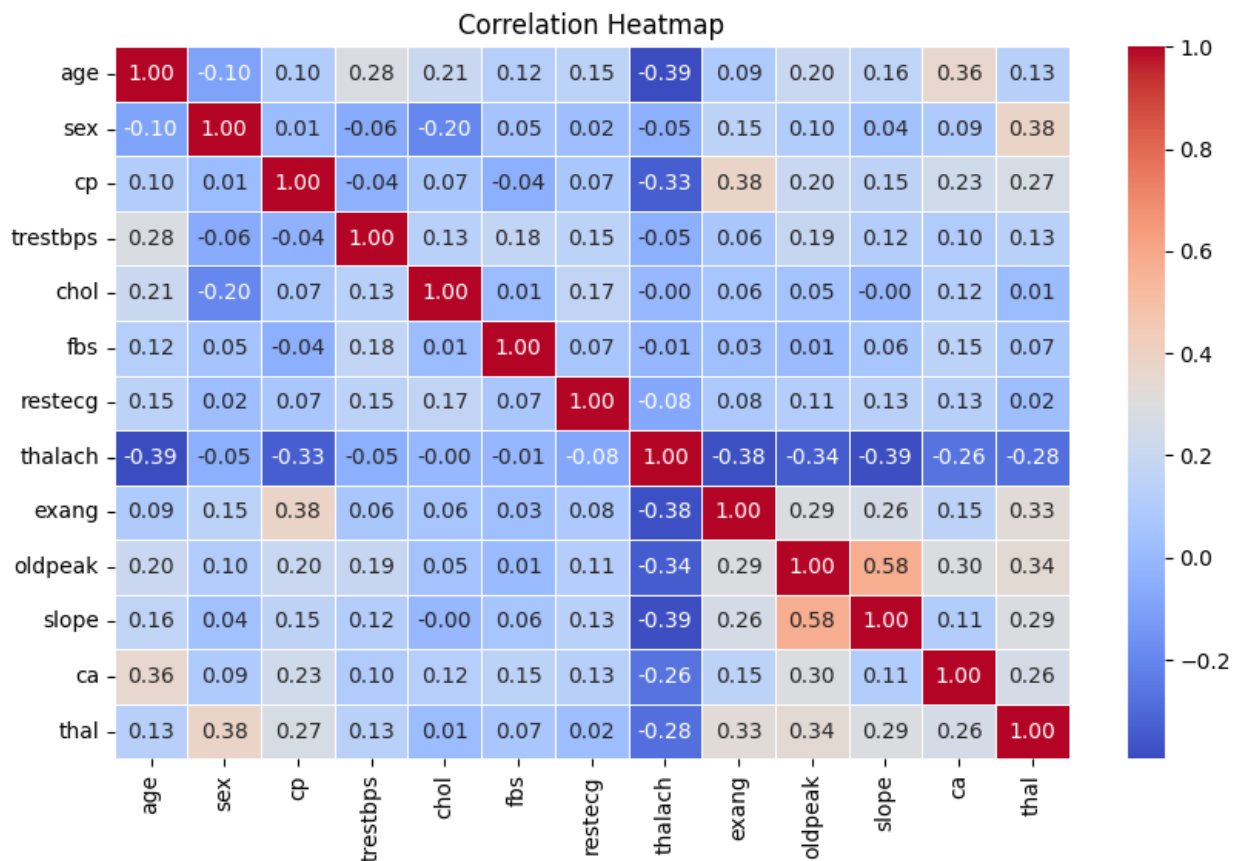
```
y['num'] = y['num'].apply(lambda x: 1 if x > 0 else 0)
```

5)

```
import seaborn as sns
import matplotlib.pyplot as plt

corr_matrix = X.corr()

plt.figure(figsize=(10, 6))
sns.heatmap(corr_matrix, annot=True, cmap='coolwarm', fmt=".2f", linewidths=0.5)
plt.title("Correlation Heatmap")
plt.show()
```



From this correlation matrix, we can conclude that thalach (max heart rate) has a strong negative correlation (-0.39) with age and oldpeak. We can assume that younger individuals tend to have a higher heart rate, while those with more severe heart disease (higher oldpeak) have lower thalach.

We also found that ca (number of major vessels) has a strong positive correlation (0.36) with age. We can say that older individuals are more likely to have more blocked vessels.

6)

```
X = X.dropna()
y = y.loc[X.index]

print(f"Length of X after transformations: {len(X)}")
print(f"Length of y after transformations: {len(y)}")
```

Length of X after transformations: 297

Length of y after transformations: 297

7)

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

categorical_columns = ['sex', 'cp', 'fbs', 'restecg', 'exang', 'slope', 'thal']
X_cleaned = X.drop(columns=categorical_columns)

scaler = StandardScaler()
X_scaled = scaler.fit_transform(X_cleaned)
```

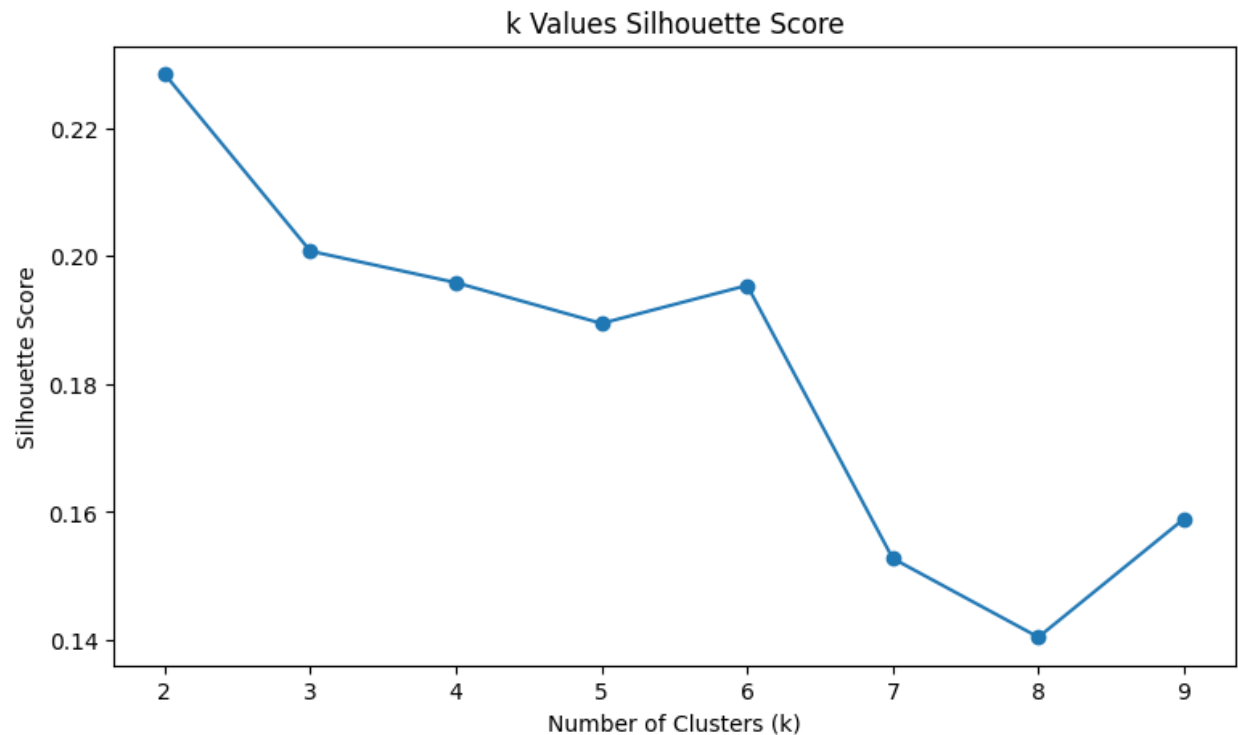
```

k_range = range(2,10)
silhouette_scores = []

for k in k_range:
    kmeans = KMeans(n_clusters = k, n_init = 20, random_state = 0)
    cluster_labels = kmeans.fit_predict(X_scaled)
    silhouette_avg = silhouette_score(X_scaled, cluster_labels)
    silhouette_scores.append(silhouette_avg)

plt.figure(figsize=(9, 5))
plt.plot(k_range, silhouette_scores, marker='o')
plt.ylabel("Silhouette Score")
plt.xlabel("Number of Clusters (k)")
plt.title("k Values Silhouette Score")
plt.show()

```





```

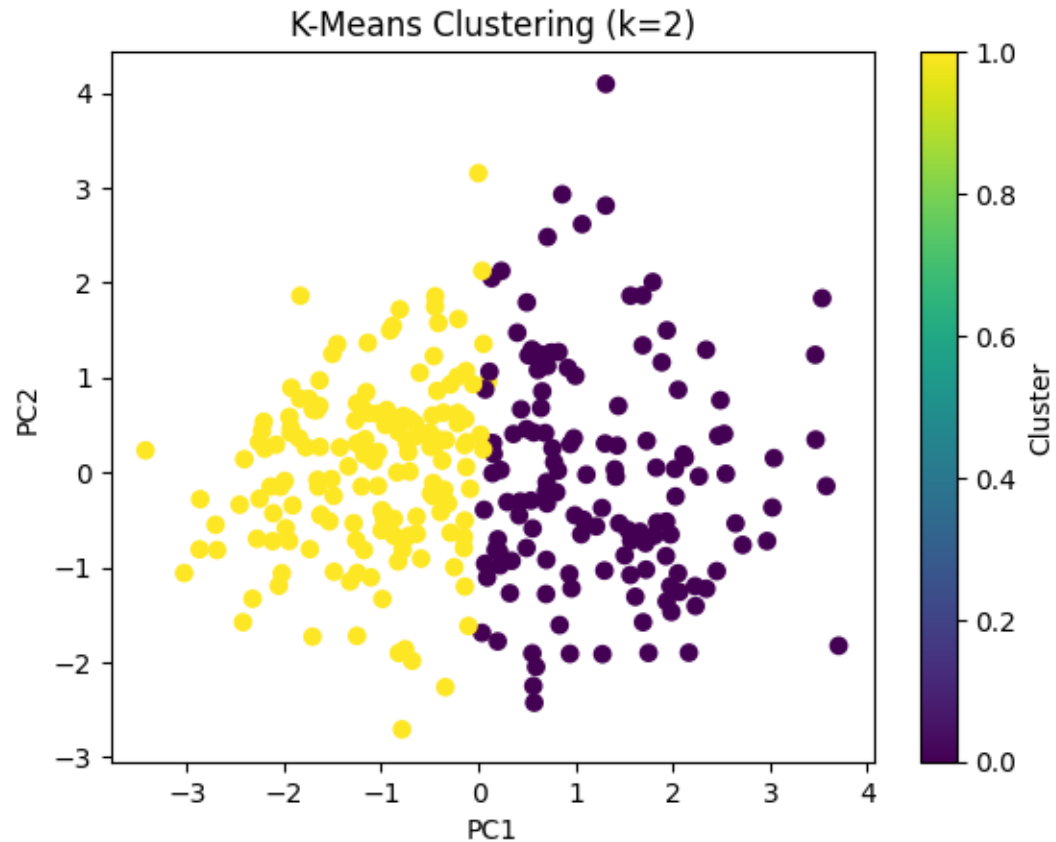
pca = PCA(n_components=2)
X_pca = pca.fit_transform(X_scaled)

kmeans = KMeans(n_clusters=2, random_state=1)
clusters = kmeans.fit_predict(X_scaled)

plt.scatter(X_pca[:, 0], X_pca[:, 1], c=clusters, cmap='viridis')
plt.title("K-Means Clustering (k=2)")
plt.xlabel("PC1")
plt.ylabel("PC2")
plt.colorbar(label="Cluster")
plt.show()

X_scaled_df = pd.DataFrame(X_scaled, columns=X_cleaned.columns)
X_scaled_df['cluster'] = clusters

```



8)

```
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.30, random_state=1)
```

9)

We are going to use logistic regression and random forest. Logistic regression is suitable for this assignment because it predicts a binary outcome, in which case, the target variable is 0 or 1. Random forest is also a good classifier to use because it has high predictive accuracy and does not depend on linear relationships, which is good for this dataset as there are both numerical and categorical variables.

10)

We are going to use accuracy and F1 scores to compare the classifier performance between logistic regression and random forest. We can create the confusion matrix from the predictions to calculate the accuracy and F1 scores. Accuracy scores are calculated by the number of correct predictions over the total number of predictions.

$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}$$

Where:

$TP$  = True Positives

$TN$  = True Negatives

$FP$  = False Positives

$FN$  = False Negatives

To obtain the F1 score, we will need to use precision and recall that are derived from the confusion matrix. Once we calculate that, the F1 score can be calculated by:

$$\text{Precision} = \frac{TP}{TP + FP}$$

$$\text{Recall} = \frac{TP}{TP + FN}$$

$$F_1 = \frac{2 \times \text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

Using these metrics, we can compare the overall accuracy and balance between the two classifiers to determine which classifier most optimal for predicting heart disease.

11)

```
import numpy as np
from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.preprocessing import StandardScaler
from sklearn.linear_model import LogisticRegression
from sklearn.metrics import accuracy_score, confusion_matrix, classification_report

scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train)
X_test_scaled = scaler.transform(X_test)

log_reg = LogisticRegression(solver='liblinear', max_iter=1000, random_state=42)

param_grid = {
    'penalty': ['l1', 'l2'],
    'C': [0.001, 0.01, 0.1, 1, 10, 100, 1000] # test this out to see if accuracy improves
}

grid_search = GridSearchCV(estimator=log_reg, param_grid=param_grid, cv=5, scoring='accuracy',
grid_search.fit(X_train_scaled, y_train)
```

```

print("Optimal parameters: ", grid_search.best_params_)
print("Cross-validation accuracy: {:.4f}".format(grid_search.best_score_))

best_log_reg = grid_search.best_estimator_
y_pred = best_log_reg.predict(X_test_scaled)
y_pred2 = best_log_reg.predict(X_train_scaled)

accuracy = accuracy_score(y_test, y_pred)
train_accuracy = accuracy_score(y_train, y_pred2)
cm = confusion_matrix(y_test, y_pred)
report = classification_report(y_test, y_pred, target_names=['No Heart Disease', 'Heart Disease'])

print(f"Test set accuracy: {accuracy:.4f}")
print(f"Train set accuracy: {train_accuracy:.4f}")
print("Confusion Matrix:")
print(cm)
print("Classification Report:")
print(report)

```

Fitting 5 folds for each of 14 candidates, totalling 70 fits

Optimal parameters: {'C': 0.01, 'penalty': 'l2'}

Cross-validation accuracy: 0.8456

Test set accuracy: 0.8556

Train set accuracy: 0.8454

Confusion Matrix:

```

[[45  6]
 [ 7 32]]

```

Classification Report:

	precision	recall	f1-score	support
No Heart Disease	0.87	0.88	0.87	51

Heart Disease	0.84	0.82	0.83	39
accuracy			0.86	90
macro avg	0.85	0.85	0.85	90
weighted avg	0.86	0.86	0.86	90

```

/Users/jasmineho/Library/Python/3.9/lib/python/site-packages/sklearn/utils/validation.py:1408:
  y = column_or_1d(y, warn=True)
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```





[illegible]



```

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/Users/jasmineho/Library/Python/3.9/lib/python/site-packages/sklearn/utils/validation.py:1408:
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```

```

from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.preprocessing import StandardScaler
from sklearn.ensemble import RandomForestClassifier, GradientBoostingClassifier
from sklearn.metrics import accuracy_score, confusion_matrix, classification_report

rf_clf = RandomForestClassifier(random_state=42)
rf_param_grid = {
    'n_estimators': [100, 200, 300],
    'max_depth': [None, 10, 20, 30],
    'min_samples_split': [2, 5, 10],

```

```

    'max_features': ['sqrt', 'log2', None],
    'criterion': ['gini', 'entropy']
}

rf_grid_search = GridSearchCV(estimator=rf_clf, param_grid=rf_param_grid, cv=5, scoring='accuracy')
rf_grid_search.fit(X_train_scaled, y_train)

print("Optimal Parameters:", rf_grid_search.best_params_)
print("Cross-Validation Accuracy:", rf_grid_search.best_score_)

best_rf_clf = rf_grid_search.best_estimator_
rf_y_pred = best_rf_clf.predict(X_test_scaled)

rf_accuracy = accuracy_score(y_test, rf_y_pred)
rf_cm = confusion_matrix(y_test, rf_y_pred)
rf_report = classification_report(y_test, rf_y_pred, target_names=['No Heart Disease', 'Heart Disease'])

print(f"Test Accuracy: {rf_accuracy:.4f}")
print("Confusion Matrix:")
print(rf_cm)
print("Classification Report:")
print(rf_report)

```

Fitting 5 folds for each of 216 candidates, totalling 1080 fits

```

/Users/jasmineho/Library/Python/3.9/lib/python/site-packages/sklearn/base.py:1389: DataConversionWarning:
    return fit_method(estimator, *args, **kwargs)
/Users/jasmineho/Library/Python/3.9/lib/python/site-packages/sklearn/base.py:1389: DataConversionWarning:
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```



















































[illegible]























































[illegible]











































```

    return fit_method(estimator, *args, **kwargs)
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    return fit_method(estimator, *args, **kwargs)

```

Optimal Parameters: {'criterion': 'gini', 'max\_depth': None, 'max\_features': 'sqrt', 'min\_samples': 10}

Cross-Validation Accuracy: 0.8166085946573751

Test Accuracy: 0.8444

Confusion Matrix:

```

[[44  7]
 [ 7 32]]

```

Classification Report:

	precision	recall	f1-score	support
No Heart Disease	0.86	0.86	0.86	51
Heart Disease	0.82	0.82	0.82	39
accuracy			0.84	90
macro avg	0.84	0.84	0.84	90
weighted avg	0.84	0.84	0.84	90

```

/Users/jasmineho/Library/Python/3.9/lib/python/site-packages/sklearn/base.py:1389: DataConversionWarning:
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```

## 15. (Bonus)

We are using the sub-groups from KMeans as a feature to improve the logistic regression model. After adding this feature and retraining the model, the classifier showed improved performance

compared to the original model. We see that the test set accuracy improved from 0.8556 to 0.9000 and the F1-score also increased for both classes.

```
categorical_columns = ['sex', 'cp', 'fbs', 'restecg', 'exang', 'slope', 'thal']
numerical_columns = [col for col in X.columns if col not in categorical_columns]
X_num = X[numerical_columns]

pca = PCA(n_components=2)
X_pca = pca.fit_transform(X_num)

kmeans = KMeans(n_clusters=2, random_state=42)
clusters = kmeans.fit_predict(X_pca)

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, random_state=42)

X_train_num = X_train[numerical_columns]
X_test_num = X_test[numerical_columns]

X_train_pca = pca.transform(X_train_num)
X_test_pca = pca.transform(X_test_num)

train_clusters = kmeans.predict(X_train_pca).reshape(-1, 1)
test_clusters = kmeans.predict(X_test_pca).reshape(-1, 1)

X_train_num = np.hstack((X_train.values, train_clusters))
X_test_num = np.hstack((X_test.values, test_clusters))

scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train_num)
X_test_scaled = scaler.transform(X_test_num)

log_reg = LogisticRegression(solver='liblinear', max_iter=1000, random_state=42)
```

```

param_grid = {
    'penalty': ['l1', 'l2'],
    'C': [0.001, 0.01, 0.1, 1, 10, 100, 1000]
}

grid_search = GridSearchCV(
    estimator=log_reg,
    param_grid=param_grid,
    cv=5,
    scoring='accuracy',
    n_jobs=-1,
    verbose=1
)
grid_search.fit(X_train_scaled, y_train)

print("Optimal parameters: ", grid_search.best_params_)
print("Cross-validation accuracy: {:.4f}".format(grid_search.best_score_))

best_log_reg = grid_search.best_estimator_
y_pred = best_log_reg.predict(X_test_scaled)
y_pred2 = best_log_reg.predict(X_train_scaled)

accuracy = accuracy_score(y_test, y_pred)
train_accuracy = accuracy_score(y_train, y_pred2)
cm = confusion_matrix(y_test, y_pred)
report = classification_report(y_test, y_pred, target_names=['No Heart Disease', 'Heart Disease'])

print(f"\nTest set accuracy: {accuracy:.4f}")
print(f"Train set accuracy: {train_accuracy:.4f}")
print("Confusion Matrix:")
print(cm)

```



```
print("Classification Report:")
print(report)
```

Fitting 5 folds for each of 14 candidates, totalling 70 fits

Optimal parameters: {'C': 0.01, 'penalty': 'l2'}

Cross-validation accuracy: 0.8211

Test set accuracy: 0.9000

Train set accuracy: 0.8309

Confusion Matrix:

```
[[47  2]
 [ 7 34]]
```

Classification Report:

	precision	recall	f1-score	support
No Heart Disease	0.87	0.96	0.91	49
Heart Disease	0.94	0.83	0.88	41
accuracy			0.90	90
macro avg	0.91	0.89	0.90	90
weighted avg	0.90	0.90	0.90	90

```
/Users/jasmineho/Library/Python/3.9/lib/python/site-packages/sklearn/utils/validation.py:1408:
```

```
y = column_or_1d(y, warn=True)
```

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```

## References

Stack Overflow. (2014, February 16). Fine-tuning parameters in logistic regression. Stack Overflow. <https://stackoverflow.com/questions/21816346/fine-tuning-parameters-in-logistic-regression>

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