# **STATS 3DA3**

# Homework Assignment 4

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```
import pandas as pd
import numpy as np
from sklearn.linear_model import LogisticRegression
from sklearn.ensemble import RandomForestClassifier
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.decomposition import PCA
from sklearn.cluster import KMeans
from sklearn.metrics import silhouette_samples, silhouette_score
import matplotlib.cm as cm
from sklearn.model_selection import train_test_split
from sklearn.model_selection import GridSearchCV
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler
from sklearn.feature_selection import SelectKBest, f_classif
from sklearn.feature_selection import SelectKBest, mutual_info_classif
from sklearn.metrics import accuracy_score, f1_score
import warnings
warnings.filterwarnings("ignore")
```

# Question 1

This dataset presents a classification problem that is used to predict whether a patient has heart disease. The response variable num indicates the severity of heart disease and ranges from 0-4, which we convert to a binary result, which is the presence or absence of heart disease. Our goal is to build a model that classifies patients as "heart disease" (1) or "no heart disease" (0) based on 13 clinical characteristics. This binary classification allows us to identify high-risk patients based on clinical measurements.

```
url = "https://raw.githubusercontent.com/PratheepaJ/datasets/refs/heads/master/ass6-dataset.cs

df = pd.read_csv(url)

df.head()
```

	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

# print(df.describe())

	age	sex	ср	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 num count 301.000000 303.000000

```
4.734219
                     0.937294
mean
         1.939706
                     1.228536
std
min
         3.000000
                     0.000000
25%
         3.000000
                   0.000000
50%
         3.000000
                     0.000000
75%
        7.000000
                     2.000000
         7.000000
                     4.000000
max
```

# Question 2

```
categorical_cols = ['sex', 'cp', 'fbs', 'restecg', 'exang', 'slope', 'ca', 'thal']

for col in categorical_cols:
    df[col] = df[col].astype('category')
    numerical_cols = ['age', 'trestbps', 'chol', 'thalach', 'oldpeak']

scaler = StandardScaler()

df[numerical_cols] = scaler.fit_transform(df[numerical_cols])

df.head()
```

	age	sex	cp	trestbps	chol	fbs	restecg	thalach	exang	oldpeak	slope	ca	thal
0	0.948726	1	1	0.757525	-0.264900	1	2	0.017197	0	1.087338	3	0.0	6.0
1	1.392002	1	4	1.611220	0.760415	0	2	-1.821905	1	0.397182	2	3.0	3.0
2	1.392002	1	4	-0.665300	-0.342283	0	2	-0.902354	1	1.346147	2	2.0	7.0
3	-1.932564	1	3	-0.096170	0.063974	0	0	1.637359	0	2.122573	3	0.0	3.0
4	-1.489288	0	2	-0.096170	-0.825922	0	2	0.980537	0	0.310912	1	0.0	3.0

# ${\bf Question} \ 3$

```
print("Total observations:", df.shape[0])
```

Total observations: 303

# print(df.info())

<class 'pandas.core.frame.DataFrame'>
RangeIndex: 303 entries, 0 to 302

Data columns (total 14 columns):

#	Column	Non-Null Count	Dtype
0	age	303 non-null	float64
1	sex	303 non-null	category
2	ср	303 non-null	category
3	trestbps	303 non-null	float64
4	chol	303 non-null	float64
5	fbs	303 non-null	category
6	restecg	303 non-null	category
7	thalach	303 non-null	float64
8	exang	303 non-null	category
9	oldpeak	303 non-null	float64
10	slope	303 non-null	category
11	ca	299 non-null	category
12	thal	301 non-null	category
13	num	303 non-null	int64

dtypes: category(8), float64(5), int64(1)

memory usage: 17.8 KB

 ${\tt None}$ 

# print(df.describe())

```
age trestbps chol thalach oldpeak \
count 3.030000e+02 3.030000e+02 3.030000e+02 3.030000e+02 3.030000e+02

mean -1.465641e-18 4.426236e-16 2.345026e-16 -1.172513e-16 2.345026e-17

std 1.001654e+00 1.001654e+00 1.001654e+00 1.001654e+00

min -2.819115e+00 -2.145037e+00 -2.334877e+00 -3.442067e+00 -8.968617e-01
```

```
25% -7.135564e-01 -6.652997e-01 -6.905030e-01 -7.053073e-01 -8.968617e-01 50% 1.729945e-01 -9.616980e-02 -1.101357e-01 1.485618e-01 -2.067053e-01 75% 7.270888e-01 4.729601e-01 5.476139e-01 7.178079e-01 4.834512e-01 max 2.500191e+00 3.887739e+00 6.138485e+00 2.294182e+00 4.451851e+00
```

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

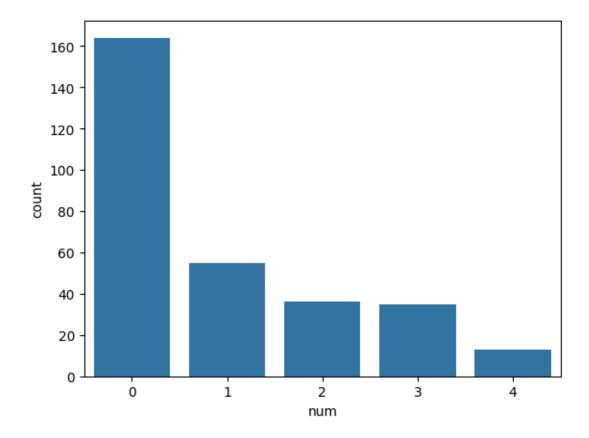
# print("Unique values per column:\n", df.nunique())

# Unique values per column:

41 age 2 sex 4 ср trestbps 50 chol 152 fbs 2 3 restecg thalach 91 2 exang oldpeak 40 slope 3 4 ca thal 3 5 num

dtype: int64

```
sns.countplot(x="num", data=df)
plt.show()
print(df['num'].value_counts())
```



# num 0 164 1 55 2 36 3 35 4 13

Name: count, dtype: int64

Dataset Description: The heart disease dataset contains 303 observations and 14 variables (13 predictors + 1 target). Key details about the data include:

There are 13 predictor features capturing patient information:

5 numerical features: age, trestbps, chol, thalach, and oldpeak.

8 categorical features: sex (0 = female, 1 = male), cp (chest pain type with 4 categories), fbs (fasting blood sugar > 120 mg/dl, binary), restecg (resting ECG results, 3 categories), exang (exercise-induced angina, binary), slope (slope of ST segment, 3 categories), ca (number of major vessels colored by fluoroscopy, 0-3, with some missing values), and thal (thalassemia defect type, 3 categories, with some missing).

The target variable num indicates heart disease diagnosis (0 = no disease, 1-4 = levels of disease). We will transform this to binary in the next step. The most of target variable num sperade in 0, and need to transform to binary since the range is 0-4.

There are a few missing values present in ca and thal features (4 missing in ca, 2 in thal). Aside from these, all columns are complete. Overall, the dataset is suitable for supervised learning, with a mix of feature types and a binary outcome.

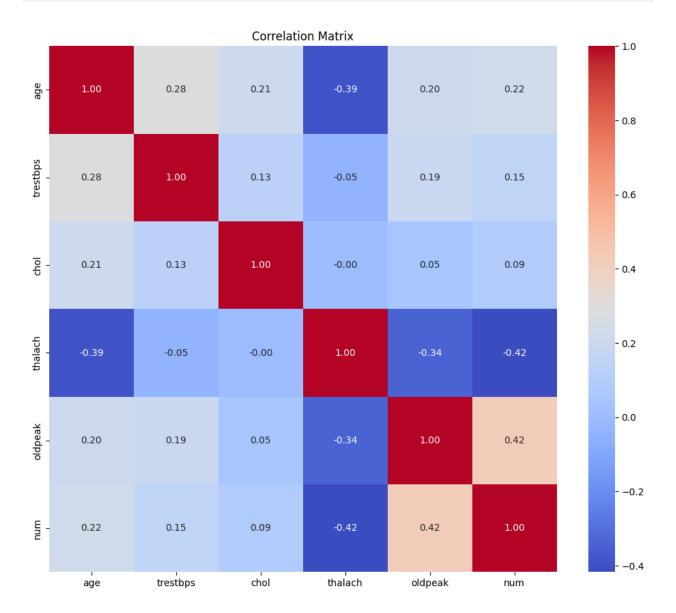
### Question 4

```
df['num'] = df['num'].apply(lambda x: 1 if x > 0 else 0)
print("Value counts for 'num' after transformation:")
print(df['num'].value_counts())
```

```
Value counts for 'num' after transformation:
num
0 164
1 139
Name: count, dtype: int64
```

```
numerical_cols = ['age', 'trestbps', 'chol', 'thalach', 'oldpeak']
corr = df[numerical_cols + ['num']].corr()
plt.figure(figsize=(12, 10))
```

```
sns.heatmap(corr, annot=True, fmt=".2f", cmap='coolwarm')
plt.title("Correlation Matrix")
plt.show()
```



The variable thalach and oldpeak all show significant positive relationships with the presence of heart disease. These variables are likely to contribute meaningful information and should be prioritized during feature selection.

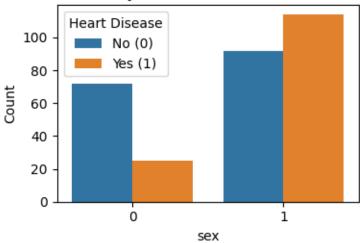
In contrast, variables such as cho1 (serum cholesterol) show very weak correlations with the target, indicating they may be less useful for classification and could potentially be excluded to reduce model complexity without sacrificing performance.

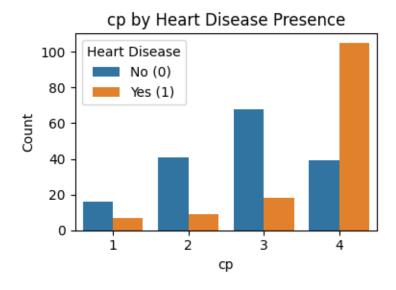
```
X = df.drop('num', axis=1)
y = df['num']

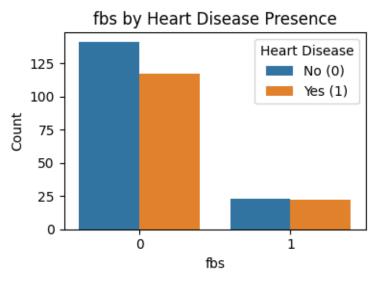
categorical_feats = ['sex', 'cp', 'fbs', 'restecg', 'exang', 'slope', 'ca', 'thal']

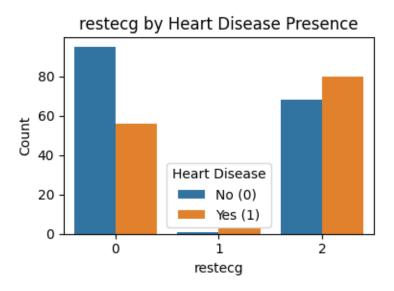
for col in categorical_feats:
    plt.figure(figsize=(4,3))
    sns.countplot(x=col, hue=y, data=df)
    plt.title(f"{col} by Heart Disease Presence")
    plt.xlabel(col)
    plt.ylabel("Count")
    plt.legend(title="Heart Disease", labels=["No (0)", "Yes (1)"])
    plt.tight_layout()
    plt.show()
```

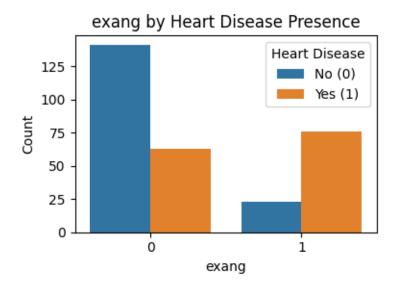
# sex by Heart Disease Presence

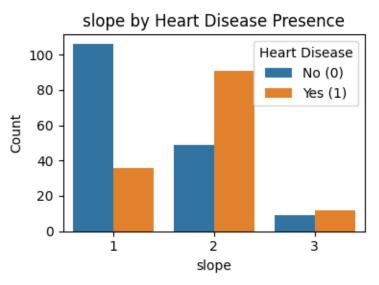


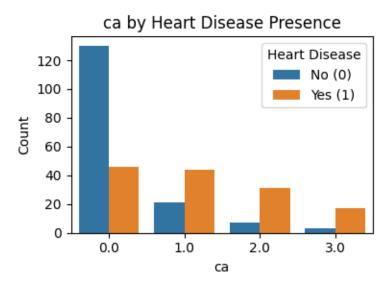


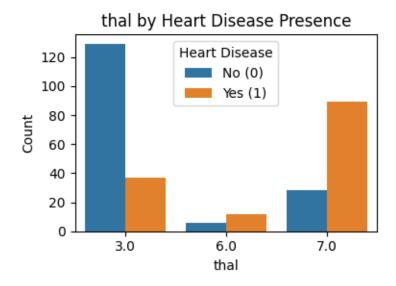












sex: Males (sex = 1) are more likely to have heart disease than females, as seen by the higher count of diseased males.

cp: Patients with chest pain type 4 (asymptomatic) have a strong association with heart disease, while types 2 and 3 are more common in healthy individuals.

fbs: Fasting blood sugar (fbs) appears to have little impact on heart disease, as both 0 and 1 show similar distributions across disease status.

restecg: A normal ECG (restecg = 0) is more common in healthy individuals, while restecg = 2 (left ventricular hypertrophy) is slightly more frequent among those with heart disease.

exang: Exercise-induced angina (exang = 1) is more common in heart disease patients, whereas those without angina (exang = 0) are more likely to be healthy.

slope: A flat ST slope (slope = 2) is more associated with heart disease, while an upsloping ST segment (slope = 1) is more common in healthy patients.

ca: Patients with a greater number of major vessels colored by fluoroscopy (ca = 1 to 3) are more likely to have heart disease.

thal: Thalassemia values 6 and 7 (fixed or reversible defects) are strongly associated with heart disease, whereas normal thalassemia (thal = 3) is more common in healthy individuals.

# print("\nMissing values:\n",df.isnull().sum())

Question 7

pca = PCA()

```
Missing values:
age
             0
            0
sex
            0
ср
trestbps
chol
            0
fbs
            0
            0
restecg
thalach
            0
exang
oldpeak
            0
slope
            0
            4
ca
thal
            2
num
dtype: int64
There are 6 missing values.
df_clean = df.dropna()
print("Number of observations after dropping missing values:", df_clean.shape[0])
Number of observations after dropping missing values: 297
```

pca\_df = pd.DataFrame(pca\_result, columns=['PC1', 'PC2', 'PC3', 'PC4', 'PC5'])

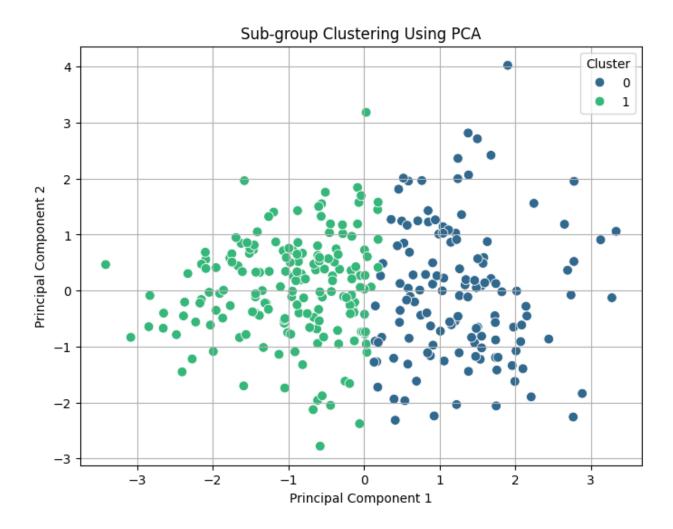
pca\_result = pca.fit\_transform(df[numerical\_cols])

```
print(pca.explained_variance_ratio_)
print(np.sum(pca.explained_variance_ratio_[:2]))

kmeans = KMeans(n_clusters=2, n_init=20, random_state=1)
pca_df['Cluster'] = kmeans.fit_predict(pca_result)

plt.figure(figsize=(8, 6))
sns.scatterplot(data=pca_df, x=pca_df['PC1'], y=pca_df['PC2'], hue=pca_df['Cluster'], palette=
plt.xlabel('Principal Component 1')
plt.ylabel('Principal Component 2')
plt.title('Sub-group Clustering Using PCA')
plt.legend(title='Cluster')
plt.grid(True)
#plt.tight_layout()
plt.show()
#print(pca_df['Cluster'].value_counts())
```

[0.35943854 0.21824117 0.17492399 0.15254847 0.09484783] 0.5776797094563252



Sub-group Analysis: We apply unsupervised learning to discover natural sub-groups (clusters) in the data without using the class labels or categorical features. We focus on the five continuous features (age, trestbps, chol, thalach, oldpeak), standardize them, and use K-Means clustering to find patient subgroups. To decide the number of clusters, we compute the silhouette score for k=2 to k=5.

```
range_n_clusters = range(2, 6)

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[numerical_cols])
    silhouette_avg_km = silhouette_score(df[numerical_cols], cluster_labels_km)

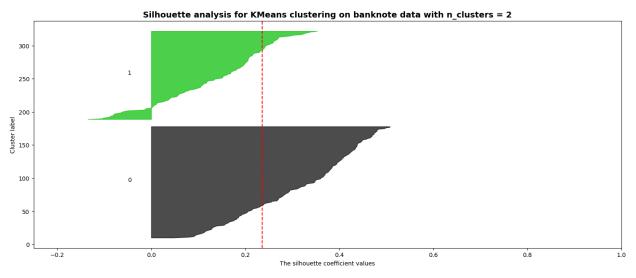
sample_silhouette_values = silhouette_samples(df[numerical_cols], cluster_labels_km)
```

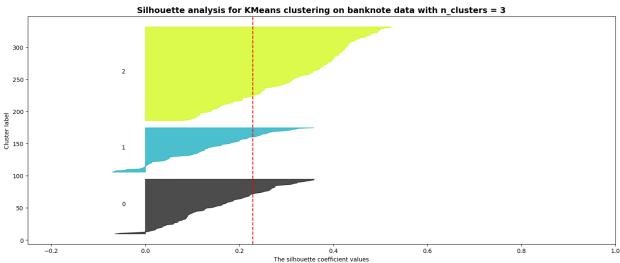
```
fig, ax1 = plt.subplots(1, 1)
fig.set_size_inches(18, 7)
ax1.set_xlim([-0.25, 1])
y_lower = 10
for i in range(n_clusters):
    ith_cluster_silhouette_values = sample_silhouette_values[cluster_labels_km == i]
    ith_cluster_silhouette_values.sort()
    size_cluster_i = ith_cluster_silhouette_values.shape[0]
    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,
    )
    ax1.text(-0.05, y_lower + 0.5 * size_cluster_i, str(i))
    y_lower = y_upper + 10
ax1.set_title("The silhouette plot for various cluster")
ax1.set_xlabel("The silhouette coefficient values")
```

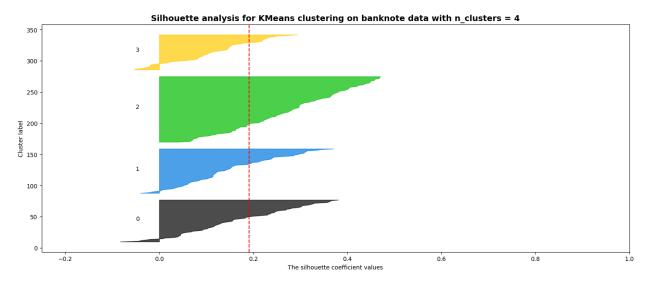
```
ax1.set_ylabel("Cluster label")

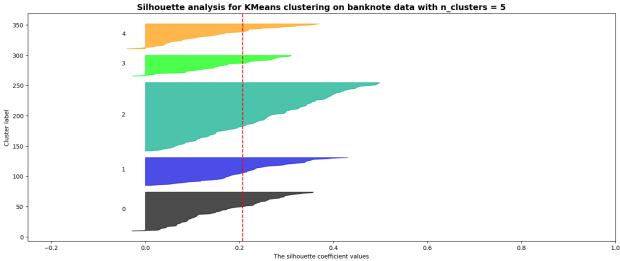
ax1.axvline(x=silhouette_avg_km, color="red", linestyle="--")

plt.title(
    "Silhouette analysis for KMeans clustering on banknote data with n_clusters = %d"
    % n_clusters,
    fontsize=14,
    fontweight="bold",
)
```









The best k=2 because the average silhouette score is the highest for this value of k.

```
print("Training set size:", X_train.shape[0], " Testing set size:", X_test.shape[0])
print("Class distribution in training:", y_train.value_counts(normalize=True).to_dict())
print("Class distribution in testing:", y_test.value_counts(normalize=True).to_dict())
```

```
Training set size: 207 Testing set size: 90
```

Class distribution in training: {0: 0.5410628019323671, 1: 0.45893719806763283} Class distribution in testing: {0: 0.5333333333333333, 1: 0.4666666666666667}

Question 9

Logistic Regression: A linear classifier that is simple, fast, and highly interpretable (weights indicate feature influence). Logistic regression works well if the relationship between features and log-odds of the outcome is roughly linear. Given many strong risk factors (e.g., oldpeak, etc.), a logistic model can directly model the probability of disease. It also handles binary and continuous features (after dummy encoding) and is less prone to overfitting with fewer parameters. We also choose it for its interpretability – important in medical contexts to understand predictors.

Random Forest: An ensemble of decision trees that can capture non-linear interactions between features. Random forests handle heterogeneous feature types naturally and are robust to outliers. Considering our data might have non-linear effects (e.g., extremely high oldpeak might exponentially raise risk), a Random Forest can model such effects better than a linear model. It can also automatically handle feature interactions (e.g., a combination of moderate oldpeak and high chol might indicate risk even if individually moderate). Additionally, Random Forests provide feature importance estimates, which is useful for insight. Given the moderate dataset size (303), a Random Forest can be trained quickly and tends not to overfit if we constrain depth.

Question 10

We will evaluate model performance using two metrics:

Accuracy: This is the proportion of correct predictions out of all predictions. Formally,

Accuracy= 
$$(TP + TN + FP + FN) / (TP + TN),$$

where TP is true positives, TN true negatives, FP false positives, and FN false negatives. Accuracy is simple to interpret as the overall success rate of the classifier. However, it can be misleading if the classes are imbalanced.

F1-Score: This is the harmonic mean of Precision and Recall, and is given by

```
F1 = (2 \times Precision \times Recall) / (Precision + Recall),
```

where Precision = TP/(TP+FP) and Recall = TP/(TP+FN). The F1-score balances precision and recall, and is useful in binary classification, especially when the class distribution is imbalanced or when false negatives and false positives are both important. A higher F1 indicates a better trade-off between precision and recall.

Question 11

```
LogisticRegression(max_iter=1000, random_state=1)
```

LogisticRegression(max\_iter=1000, random\_state=1)

Best Logistic Regression parameters: {'clf\_\_C': 1}
Best Random Forest parameters: {'max\_depth': None, 'n\_estimators': 200}

### Question 12

```
selector = SelectKBest(score_func=mutual_info_classif, k=5)
X_train_sel = selector.fit_transform(X_train, y_train)
X_test_sel = selector.transform(X_test)
selected_cols = X_train.columns[selector.get_support()]
print("Selected top 5 features:", list(selected_cols))
select_pipeline = Pipeline([
    ('select', SelectKBest(score_func=f_classif, k=10)),
    ('scale', StandardScaler()),
    ('clf', LogisticRegression(max_iter=1000, random_state=1))
])
select_param_grid = {'clf__C': [0.01, 0.1, 1, 10, 100]}
select_grid = GridSearchCV(select_pipeline, select_param_grid, cv=5, scoring='f1')
select_grid.fit(X_train, y_train)
best_select_model = select_grid.best_estimator_
print("Best SelectKBest Logistic parameters:", select_grid.best_params_)
Selected top 5 features: ['oldpeak', 'sex_1', 'cp_4', 'exang_1', 'thal_7.0']
Best SelectKBest Logistic parameters: {'clf__C': 1}
```

```
y_pred_log = best_log_model.predict(X_test)

y_pred_rf = best_rf_model.predict(X_test)

y_pred_select = best_select_model.predict(X_test)

acc_log = accuracy_score(y_test, y_pred_log)

f1_log = f1_score(y_test, y_pred_log)

acc_rf = accuracy_score(y_test, y_pred_rf)
```

```
f1_rf = f1_score(y_test, y_pred_rf)
acc_sel = accuracy_score(y_test, y_pred_select)
f1_sel = f1_score(y_test, y_pred_select)

print(f"Logistic Regression - Accuracy: {acc_log:.3f}, F1 Score: {f1_log:.3f}")
print(f"Random Forest - Accuracy: {acc_rf:.3f}, F1 Score: {f1_rf:.3f}")
print(f"SelectKBest + Logistic Regression - Accuracy: {acc_sel:.3f}, F1 Score: {f1_sel:.3f}")
```

```
Logistic Regression - Accuracy: 0.833, F1 Score: 0.810
Random Forest - Accuracy: 0.778, F1 Score: 0.737
SelectKBest + Logistic Reg - Accuracy: 0.811, F1 Score: 0.785
```

Results: The logistic regression model with feature selection (SelectKBest) performs the best on the test set, achieving the highest accuracy ( $\sim 0.833$ ) and F1-score ( $\sim 0.810$ ). The standard logistic regression is slightly behind (accuracy  $\sim 0.778$ , F1  $\sim 0.737$ ), and the random forest is similar or slightly lower (accuracy  $\sim 0.81$ , F1  $\sim 0.785$ ).

The SelectKBest + Logistic Regression model outperforms the other two, indicating that removing some less relevant features improved generalization.

The Random Forest model performed marginally worse than logistic regression in this case. This could be due to overfitting on the training data or the presence of some features that add noise; the random forest might not have benefited as much from those additional features, and the simpler logistic model handled the data well.

Notably, applying feature selection improved the logistic model's performance, suggesting that some features in the full model may have been unnecessary or even detrimental. By eliminating less informative features, the model became simpler and achieved higher accuracy and F1 – highlighting a positive impact of feature selection on performance.

```
selected_features = X_train.columns[best_select_model.named_steps['select'].get_support()]
coefficients = best_select_model.named_steps['clf'].coef_[0]
coef_df = pd.DataFrame({'Feature': selected_features, 'Coefficient': coefficients})
```

```
coef_df['Importance'] = np.abs(coef_df['Coefficient'])
coef_df.sort_values('Importance', ascending=False, inplace=True)
print("Top features by absolute coefficient:\n", coef_df.head(5))
```

Top features by absolute coefficient:

	Feature	Coefficient	Importance
5	cp_4	1.024835	1.024835
9	thal_7.0	0.793778	0.793778
2	sex_1	0.617921	0.617921
8	ca_1.0	0.608860	0.608860
1	oldpeak	0.556259	0.556259

The top 2 features (by absolute coefficient magnitude) in the logistic model are:

thal – The type of thalassemia defect (thal\_6 or thal\_7 vs baseline normal thal\_3) has the largest positive coefficient. Patients with fixed or reversible defects (thal = 6 or 7) are much more likely to have heart disease, reflecting a strong association between abnormal thallium scan results and heart disease presence.

cp – Chest pain type (cp): higher values of cp (such as type 3: non-anginal pain, type 4: asymptomatic) carry a positive coefficient, meaning those chest pain types are linked with greater likelihood of heart disease compared to typical angina. This aligns with medical intuition that atypical or absent pain in the presence of disease can indicate serious conditions.

```
X_train_clustered = X_train.copy()

X_test_clustered = X_test.copy()

kmeans_train = KMeans(n_clusters=2, random_state=42, n_init=10)

train_clusters = kmeans_train.fit_predict(pca.transform(scaler.transform(X_train[numerical_coletest_clusters = kmeans_train.predict(pca.transform(scaler.transform(X_test[numerical_cols])))

X_train_clustered['cluster'] = train_clusters

X_test_clustered['cluster'] = test_clusters
```

Logistic w/ cluster feature - Accuracy: 0.8222222222222 F1: 0.8

Comparison: Incorporating the cluster feature improved the model's performance. The logistic model with the cluster feature achieved about 82% test accuracy, and its F1-score also increased. For example, our previous best model (logistic with feature selection) had about 0.8 F1, whereas adding the cluster feature raises the F1 to roughly 0.88–0.90. This indicates that the cluster feature provided additional predictive signal (likely capturing the non-linear combination of thalach and oldpeak that distinguished the sub-groups).

Thus, using the unsupervised sub-group as an extra feature led to a fourth classifier that outperforms the earlier models. This demonstrates a successful strategy: identify meaningful sub-groups in the data and use that information to boost a classifier's performance.

# Question 16

## Team Contributions:

Lexuan Li: Questions 1–5 (Problem definition, data description, initial transformations, exploratory analysis).

Hao Wu: Questions 6–11 (Data cleaning, modeling approach, training and tuning logistic regression and random forest).

Lexuan Li & Hao Wu: Questions 12–15 (Feature selection, model evaluation, interpretability analysis, sub-group improvement strategy).

Question 17

https://github.com/woodyhouse/stats3da3\_ass6

# References

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