Ensemble Learning Architectures for Heart Disease Prediction

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2 Author

Sergio Sanz

3 GitHub Repository

https://github.com/sergio-sanz-rodriguez/Heart-Disease-Prediction-ML

4 Introduction

4.1 Objective

The goal of this project is to investigate the potential of ensemble architectures to improve prediction in binary classification problems. We will utilize a heart disease database in order to detect, using machine-learning models, the presence of heart disease in patients.

The evaluated models include: **Logistic Regression**, **Support Vector Machine (SVM)**, **Random Forest**, **Soft-Voting**, and **Stacking**. The last three correspond to ensemble architectures.

4.2 Data Overview

Column	Additional Information
age	The age of the patient.
sex	The gender of the patient (0 = female, 1 = male).
cp	Chest pain type (1 = typical angina, 2 = atypical angina, 3 = non-anginal pain, 4 = asymptomatic).
trestbps	Resting blood pressure (in mm Hg).
chol	Serum cholesterol level (in mg/dl).
fbs	Fasting blood sugar (> 120 mg/dl) (1 = true, 0 = false).
restecg	Resting electrocardiographic results (0 = normal, 1 = having ST-T wave abnormality, 2 = probable or definite left ventricular hypertrophy).
thalach	Maximum heart rate achieved.
exang	Exercise-induced angina (1 = yes, 0 = no).
oldpeak	ST depression induced by exercise relative to rest.
slope	Slope of the peak exercise ST segment (1 = upsloping, 2 = flat, 3 = downsloping)
caa	Number of major vessels colored by fluoroscopy.
thall	Thalassemia (a type of blood disorder) results (3 = normal, 6 = fixed defect, 7 = reversible defect).
output	0 = little risk of heart attack, 1 = high risk of heart attack

More information about this dataset can be found here: https://www.kaggle.com/datasets/johnsmith88/heart-disease-dataset

5 Packages and Import

[1]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import missingno as msno
import seaborn as sns
import itertools

from sklearn.compose import ColumnTransformer
from sklearn.pipeline import make_pipeline, Pipeline
from sklearn.preprocessing import OneHotEncoder, KBinsDiscretizer,␣
↪FunctionTransformer, StandardScaler, MinMaxScaler, RobustScaler,␣
↪PowerTransformer
from sklearn.model_selection import train_test_split, cross_val_score,␣
↪GridSearchCV, cross_val_predict
from sklearn.linear_model import LogisticRegression
from sklearn.metrics import confusion_matrix, accuracy_score, recall_score,␣
↪precision_score, roc_curve, roc_auc_score, f1_score, fbeta_score
from sklearn.feature_selection import SelectKBest, chi2, f_classif
```

```
from sklearn.svm import SVC
from sklearn.ensemble import RandomForestClassifier, VotingClassifier,␣
↪StackingClassifier

# Set plotting style
sns.set_style('whitegrid')
plt.rcParams['font.size'] = 14
plt.rcParams['figure.figsize'] = (8, 6)

RSEED=42
```

[2]:
```
df_heart = pd.read_csv("./data/heart.csv")
df = df_heart.copy()
```

6 Evaluation Functions

[3]:
```
def predict_and_print_scores(model,
                             X_train,
                             y_train,
                             X_test,
                             y_test,
                             training=True,
                             test=True,
                             accuracy=True,
                             recall=True,
                             precision=True,
                             fbeta=[True, 1.0],
                             roc_auc=True,
                             matrix=True,
                             figsize=(3,2),
                             cmap='YlGn'):

    '''
    Given an already trained model, this function predicts and print some␣
↪performance scores training and/or testing data.
    The supported metrics are: accuracy, recall, precision, fbeta_score (and␣
↪f1_score if beta = 1.0), roc_auc.
    If the input parameter "matrix" is set to True, the function plot the␣
↪confusion matrix with a color map given in "cmap".

    model                Trained model
    X_train              Training data with features
    y_train              Training data with labels or targets
    X_test               Testing data with features
    y_test               Testing data with labels or targets                ␣
↪
```

```
    training=True     True: print scores on the training set
    test=True         True: print scores on the testing set
    accuracy=True     True: print accuracy_score()
    recall=True       True: print recall_score()
    precision=True    True: print precision_score()
    fbeta=[True, 1.0] [True, beta]: print fbeta_score. If beta = 1.0: f1_score
    roc_auc=True      True: print roc_auc_score()
    matrix=True       True: plot confusion matrix
    figsize=(3,2)     Figure size for the confusion matrix
    cmap='YlGn')      Color map for the confusion matrix

    Possible color maps: 'Greys', 'Purples', 'Blues', 'Greens', 'Oranges',␣
↪'Reds',
                         'YlOrBr', 'YlOrRd', 'OrRd', 'PuRd', 'RdPu', 'BuPu',
                         'GnBu', 'PuBu', 'YlGnBu', 'PuBuGn', 'BuGn', 'YlGn'

    Returns: fig, ax: the figure objects of the confusion matrix (if enabled)
    '''

    # Prediction
    y_pred_train = model.predict(X_train)
    y_pred_test = model.predict(X_test)

    # Scores
    if accuracy:
        if training:
            print("Accuracy on training set:", round(accuracy_score(y_train,␣
↪y_pred_train), 2))
        if test:
            print("Accuracy on test set:", round(accuracy_score(y_test,␣
↪y_pred_test), 2))
        print("--------"*5)

    if recall:
        if training:
            print("Recall on training set:", round(recall_score(y_train,␣
↪y_pred_train), 2))
        if test:
            print("Recall on test set:", round(recall_score(y_test,␣
↪y_pred_test), 2))
        print("--------"*5)

    if precision:
        if training:
            print("Precision on training set:", round(precision_score(y_train,␣
↪y_pred_train), 2))
```

```
        if test:
            print("Precision on test set:", round(precision_score(y_test,
 ↪y_pred_test), 2))
        print("--------"*5)

    if fbeta[0]:
        if training:
            print("fbeta_score on training set:", round(fbeta_score(y_train,
 ↪y_pred_train, beta=fbeta[1]), 2))
        if test:
            print("fbeta_score on test set:", round(fbeta_score(y_test,
 ↪y_pred_test, beta=fbeta[1]), 2))
        print("--------"*5)

    if roc_auc:
        y_pred_train_p = model.predict_proba(X_train)[:,1]
        y_pred_test_p = model.predict_proba(X_test)[:,1]
        if training:
            print('roc_auc_score on trainig set: ',
 ↪round(roc_auc_score(y_train, y_pred_train_p), 2))
        if test:
            print('roc_auc_score on test set: ', round(roc_auc_score(y_test,
 ↪y_pred_test_p), 2))
        print("--------"*5)

    # Plot confusion matrix
    if matrix:
        fig = plt.figure(figsize=figsize)
        ax = fig.add_subplot()
        sns.heatmap(confusion_matrix(y_test, y_pred_test), annot=True,
 ↪cmap=cmap);
        plt.title('Test Set')
        plt.ylabel('True label')
        plt.xlabel('Predicted label')

def train_crossval_predict_score(model,
                                 hyperparams,
                                 X_train,
                                 y_train,
                                 X_test,
                                 y_test,
                                 cv=5,
                                 scoring='accuracy',
                                 verbose=0,
                                 n_jobs=-1,
                                 cross_val='full',
```

```
                                random_state='None',
                                training=True,
                                test=True,
                                accuracy=True,
                                recall=True,
                                precision=True,
                                fbeta=[True, 1.0],
                                roc_auc=True,
                                matrix=True,
                                figsize=(3,2),
                                cmap='YlGn'):

    '''
    Given an instantiated model, this function trains, cross-validate,␣
↪predicts, and prints some performance scores training and/or testing data.
    The cross-validation strategy is selected with the input parameters␣
↪"cross_val".
    The supported metrics are: accuracy, recall, precision, fbeta_score (and␣
↪f1_score if beta = 1.0), roc_auc.
    If the input parameter "matrix" is set to True, the function plot the␣
↪confusion matrix with a color map given in "cmap".

    model                   #Instantiated model
    hyperparams             #Dictionary including hyperparameters
    X_train                 #Training data with features
    y_train                 #Training data with labels or targets
    X_test                  #Testing data with features
    y_test                  #Testing data with labels or targets
    cv=5                    #Number of cross-validation folds
    scoring='accuracy'      #Scoring method
    verbose=0               #Verbose
    n_jobs=-1               #Number of jobs in parallel
    cross_val='full'        #'Full'/'full': Apply GridSearchCV. 'Random'/'random':
↪ Apply RandomSearchCV
    random_state            #Random state parameter for RandomSearchCV: 'None' or␣
↪an integer
    training=True           #True: print scores on the training set
    test=True               #True: print scores on the testing set
    accuracy=True           #True: print accuracy_score()
    recall=True             #True: print recall_score()
    precision=True          #True: print precision_score()
    fbeta=[True, 1.0]       #[True, beta]: print fbeta_score. If beta = 1.0:␣
↪f1_score
    roc_auc=True            #True: print roc_auc_score()
    matrix=True             #True: plot confusion matrix
    figsize=(3,2)           #Figure size for the confusion matrix
```

```
    cmap='YlGn'):         #Color map for the confusion matrix

    Possible color maps: 'Greys', 'Purples', 'Blues', 'Greens', 'Oranges',␣
↪'Reds',
                         'YlOrBr', 'YlOrRd', 'OrRd', 'PuRd', 'RdPu', 'BuPu',
                         'GnBu', 'PuBu', 'YlGnBu', 'PuBuGn', 'BuGn', 'YlGn'

    Returns:
    - best_model: object of the best model after cross-validation
    - best_params: hyperparameters of the best model
    - fig, ax: the figure objects of the confusion matrix (if enabled)
'''

    # Cross-validation
    if cross_val == 'Full' or cross_val == 'full':
        grid_model = GridSearchCV(model, param_grid=hyperparams, cv=cv,␣
↪scoring=scoring, verbose=verbose, n_jobs=n_jobs)
    elif cross_val == 'Random' or cross_val == 'random':
        grid_model = RandomizedSearchCV(model, param_distributions=hyperparams,␣
↪cv=cv, scoring=scoring, random_state=random_state, verbose=verbose,␣
↪n_jobs=n_jobs)

    # Fit
    grid_model.fit(X_train, y_train)
    best_model = grid_model.best_estimator_
    best_params = grid_model.best_params_
    print('Best params:', grid_model.best_params_)
    print("--------"*5)

    # Predict and print results
    predict_and_print_scores(best_model,
                             X_train,
                             y_train,
                             X_test,
                             y_test,
                             training=training,
                             test=test,
                             accuracy=accuracy,
                             recall=recall,
                             precision=precision,
                             fbeta=fbeta,
                             roc_auc=roc_auc,
                             matrix=matrix,
                             figsize=figsize,
                             cmap=cmap)

    return best_model, best_params
```

```python
def find_roc_threshold_tpr(model, X, y, value_target):
    """
    This function calculates the threshold and false positive rate␣
 ↪corresponding to a true positive rate of value_target (from 0 to 1).

    model                   # Trained model
    X                       # Feature dataset
    y                       # Target dataset
    value_target            # True positive rate value

    Returns:
    threshold               # Threshold value
    false_positive_rate     # False positive rate value
    """

    fpr, tpr, thr = roc_curve(y, model.predict_proba(X)[:,1])
    old_diff = 100000000
    for index, value in enumerate(tpr):
        new_diff = abs(value_target - value)
        if new_diff < old_diff:
            false_pos_rate = fpr[index]
            threshold = thr[index]
            old_diff = new_diff

    return threshold, false_pos_rate

def find_roc_threshold_f1(model, X, y):
    """
    This function calculates the threshold in the ROC curve that maximizes the␣
 ↪f1 score.
    model                   # Trained model
    X                       # Feature dataset
    y                       # Target dataset

    Returns:
    best_threshold          # Threshold value
    best_f1_score           # False positive rate value
    """

    pred_ = model.predict_proba(X)[:,1]
    best_threshold = 0.5
    best_f1_score = 0.0
    for value in np.arange(1, 10, 0.5):
        pred_tmp = np.where(pred_ >= float(value/10), 1, 0)
        cost = f1_score(y, pred_tmp)
```

```python
        if cost > best_f1_score:
            best_f1_score = cost
            best_threshold = float(value/10)

    return best_threshold, best_f1_score

def plot_confusion_matrix(cm, classes,
                          normalize=False,
                          title='Confusion matrix',
                          cmap=plt.cm.Oranges,
                          figsize=(10,10)):
    """
    This function prints and plots the confusion matrix.
    Normalization can be applied by setting `normalize=True`.
    Source: http://scikit-learn.org/stable/auto_examples/model_selection/
 ↪plot_confusion_matrix.html
    """
    # Confusion matrix
    #cm = confusion_matrix(test_labels, rf_predictions)
    #plot_confusion_matrix(cm, classes = ['Poor Health', 'Good Health'],
    #                      title = 'Health Confusion Matrix')

    if normalize:
        cm = cm.astype('float') / cm.sum(axis=1)[:, np.newaxis]

    # Plot the confusion matrix
    plt.figure(figsize = figsize)
    plt.imshow(cm, interpolation='nearest', cmap=cmap)
    plt.title(title, size = 18)
    plt.colorbar(aspect=4)
    tick_marks = np.arange(len(classes))
    plt.xticks(tick_marks, classes, rotation=45, size = 14)
    plt.yticks(tick_marks, classes, size = 14)

    fmt = '.2f' if normalize else 'd'
    thresh = cm.max() / 2.

    # Labeling the plot
    for i, j in itertools.product(range(cm.shape[0]), range(cm.shape[1])):
        plt.text(j, i, format(cm[i, j], fmt), fontsize = 18,
                 horizontalalignment="center",
                 color="white" if cm[i, j] > thresh else "black")

    plt.tight_layout()
    plt.grid(False)
    plt.ylabel('True label', size = 18)
    plt.xlabel('Predicted label', size = 18)
```

```
    plt.show()

def plot_roc_curves(model_dic, X_test, y_test, figsize=(6,5)):
    """
    This function plots the ROC curves of the models defined in model_dic.
    The model_dic format is {'model_label' : [model_object, color-line'], ...}.␣
 ↪Example:
    model_dic = {['model_1' : [model_1, 'r-'], 'model_2' : [model_2, 'b-']}
    """

    fig = plt.figure(figsize=figsize)
    ax = fig.add_subplot()
    for key, _ in model_dic.items():
        model = model_dic[key][0]
        fpr, tpr, _ = roc_curve(y_test, model.predict_proba(X_test)[:,1])
        plt.plot(fpr, tpr, model_dic[key][1], label=key)
    plt.plot([0,1],[0,1],'k:',label='Random')
    plt.plot([0,0,1,1],[0,1,1,1],'k--',label='Perfect')
    ax.set_xlabel('False Positive Rate')
    ax.set_ylabel('True Positive Rate (Recall)')
    ax.legend()
    plt.grid(True)
    plt.show()
    return fig, ax
```

7 Data Analysis

[4]:
```
df.head(2)
```

[4]:
```
   age  sex  cp  trtbps  chol  fbs  restecg  thalachh  exng  oldpeak  slp  \
0   63    1   3     145   233    1        0       150     0      2.3    0
1   37    1   2     130   250    0        1       187     0      3.5    0

   caa  thall  output
0    0      1       1
1    0      2       1
```

[5]:
```
print(f"Number of inputs: {df.shape[0]}")
print(f"Number of features: {df.shape[1]}")
```

```
Number of inputs: 303
Number of features: 14
```

[6]:
```
# All the features are int64 and float64, but some of them are, in fact,␣
 ↪categorical
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    int64
 1   sex       303 non-null    int64
 2   cp        303 non-null    int64
 3   trtbps    303 non-null    int64
 4   chol      303 non-null    int64
 5   fbs       303 non-null    int64
 6   restecg   303 non-null    int64
 7   thalachh  303 non-null    int64
 8   exng      303 non-null    int64
 9   oldpeak   303 non-null    float64
 10  slp       303 non-null    int64
 11  caa       303 non-null    int64
 12  thall     303 non-null    int64
 13  output    303 non-null    int64
dtypes: float64(1), int64(13)
memory usage: 33.3 KB
```

[7]:
```
# Change the name of the columns
dict = {'age' : 'age', # numerical OK!
        'sex' : 'sex', # categorical (binary) OK!
        'cp' : 'chest_pain_type', # categorical OK!
        'trtbps' : 'resting_blood_pressure', # numerical OK!
        'chol' : 'serum_cholestoral', # numerical OK!
        'fbs' : 'fasting_blood_sugar', # categorical (binary) OK!
        'restecg' : 'resting_electrocard_results', # categorical OK!
        'thalachh' : 'maximum_heartrate', # numerical OK!
        'exng' : 'exercise_induced_angina', # categorical (binary) OK!
        'oldpeak' : 'oldpeak', # numerical OK!
        'slp' : 'slope_peak_exercise_segment', # categorical OK!
        'caa' : 'no_major_vessels_col', # numerical OK!
        'thall' : 'thal', # categorical (3 values according to description, but
 ↪4!)
        'output' : 'output'} # binary
df = df.rename(columns=dict)
```

[8]:
```
df.describe().T
```

[8]:
```
                              count        mean        std   min    25%
age                           303.0   54.366337   9.082101  29.0   47.5  \
sex                           303.0    0.683168   0.466011   0.0    0.0
chest_pain_type               303.0    0.966997   1.032052   0.0    0.0
resting_blood_pressure        303.0  131.623762  17.538143  94.0  120.0
```

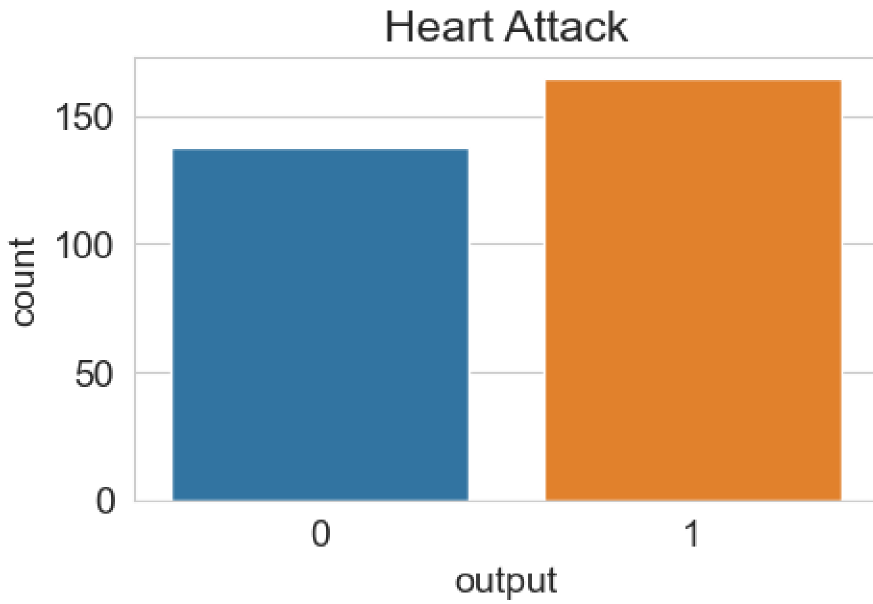
```
serum_cholestoral            303.0  246.264026  51.830751  126.0  211.0
fasting_blood_sugar          303.0    0.148515   0.356198    0.0    0.0
resting_electrocard_results  303.0    0.528053   0.525860    0.0    0.0
maximum_heartrate            303.0  149.646865  22.905161   71.0  133.5
exercise_induced_angina      303.0    0.326733   0.469794    0.0    0.0
oldpeak                      303.0    1.039604   1.161075    0.0    0.0
slope_peak_exercise_segment  303.0    1.399340   0.616226    0.0    1.0
no_major_vessels_col         303.0    0.729373   1.022606    0.0    0.0
thal                         303.0    2.313531   0.612277    0.0    2.0
output                       303.0    0.544554   0.498835    0.0    0.0

                               50%    75%    max
age                           55.0   61.0   77.0
sex                            1.0    1.0    1.0
chest_pain_type                1.0    2.0    3.0
resting_blood_pressure       130.0  140.0  200.0
serum_cholestoral            240.0  274.5  564.0
fasting_blood_sugar            0.0    0.0    1.0
resting_electrocard_results    1.0    1.0    2.0
maximum_heartrate            153.0  166.0  202.0
exercise_induced_angina        0.0    1.0    1.0
oldpeak                        0.8    1.6    6.2
slope_peak_exercise_segment    1.0    2.0    2.0
no_major_vessels_col           0.0    1.0    4.0
thal                           2.0    3.0    3.0
output                         1.0    1.0    1.0
```

[9]:
```
df.nunique()
```

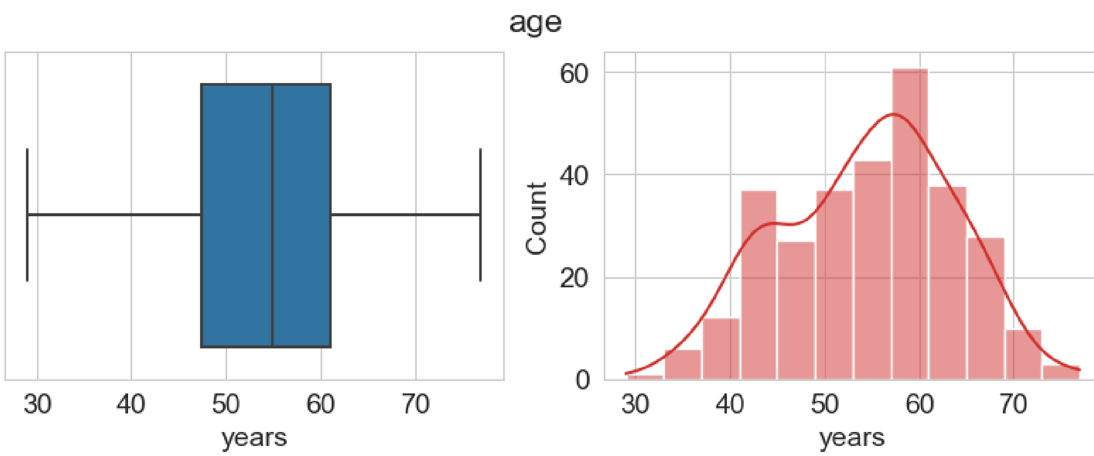
[9]:
```
age                             41
sex                              2
chest_pain_type                  4
resting_blood_pressure          49
serum_cholestoral              152
fasting_blood_sugar              2
resting_electrocard_results      3
maximum_heartrate               91
exercise_induced_angina          2
oldpeak                         40
slope_peak_exercise_segment      3
no_major_vessels_col             5
thal                             4
output                           2
dtype: int64
```

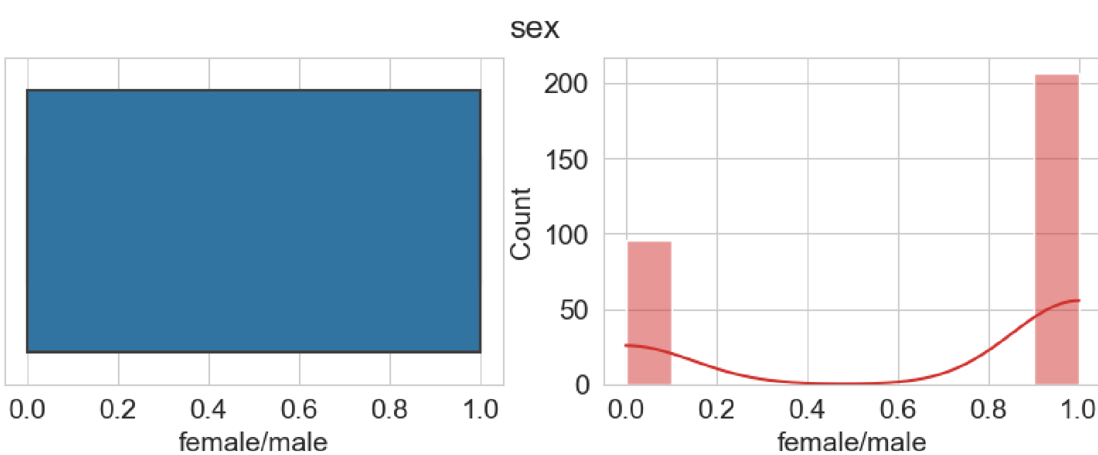
[10]:
```
# The two classes are well balanced
fig, ax = plt.subplots(figsize=(5,3))
```

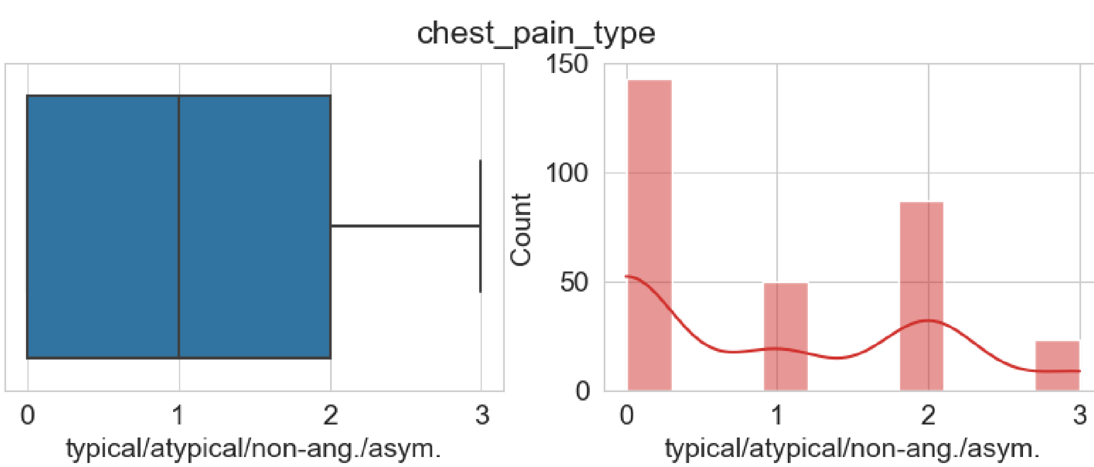
```
plt.title('Heart Attack')
ax = sns.countplot(x=df.output)
```

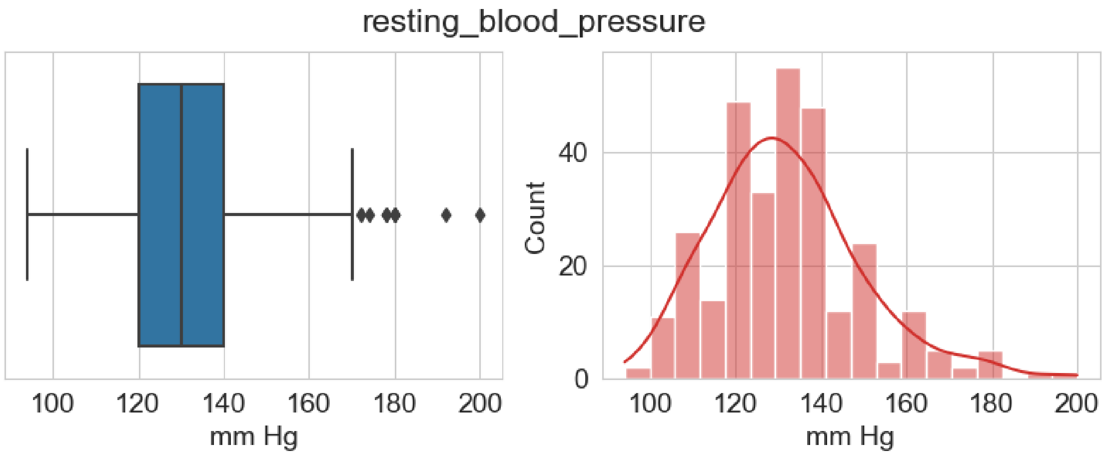


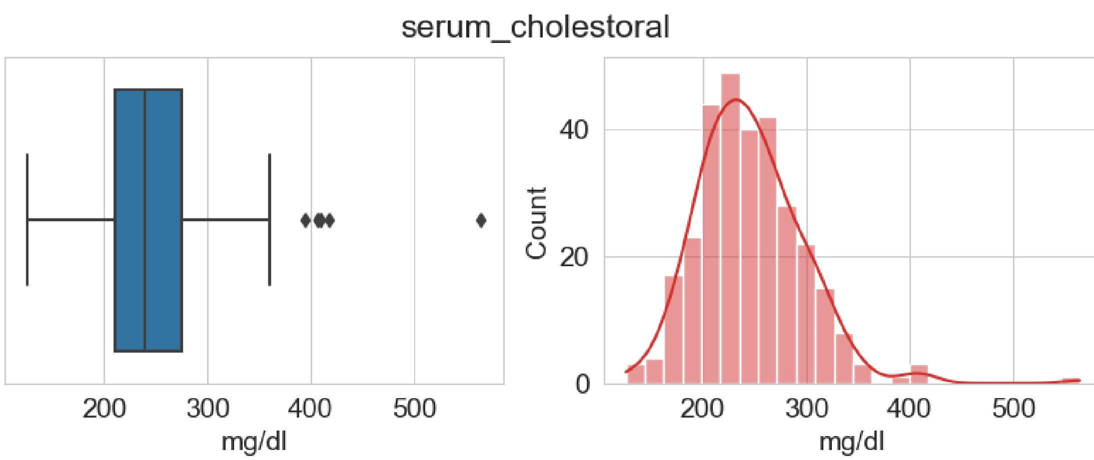

```
[11]: # Analysis of the distributions
num_features = list(df.columns[df.dtypes!=object])
num_features.remove('output')
def plot_num(feature, units):
    fig = plt.figure(figsize=(10,3))
    axes = fig.add_subplot(121)
    #,axes=plt.subplots(1,2)
    sns.boxplot(data=df, x=feature, ax=axes)
    plt.xlabel(units)
    axes = fig.add_subplot(122)
    sns.histplot(data=df, x=feature, ax=axes, color='#D0312D', kde=True)
    plt.xlabel(units)
    fig.set_size_inches(10, 3)
    plt.suptitle(feature)  # Adds a title to the entire figure
    plt.show()

units = ['years','female/male','typical/atypical/non-ang./asym.','mm Hg','mg/
 ↪dl','>120 mg/dl','normal/abnormal/hypertrophy','bps','yes/no','','up/flat/
 ↪down','#','normal/fixed/defect']
for idx, column in enumerate(num_features):
    plot_num(column,units[idx])
```

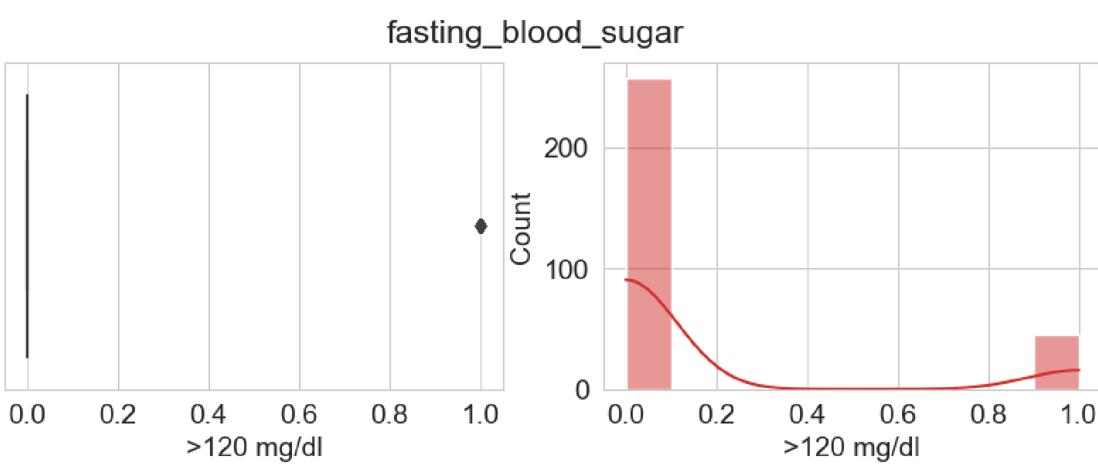

age
30
40
50
60
70
years
Count
0
20
40
60
years

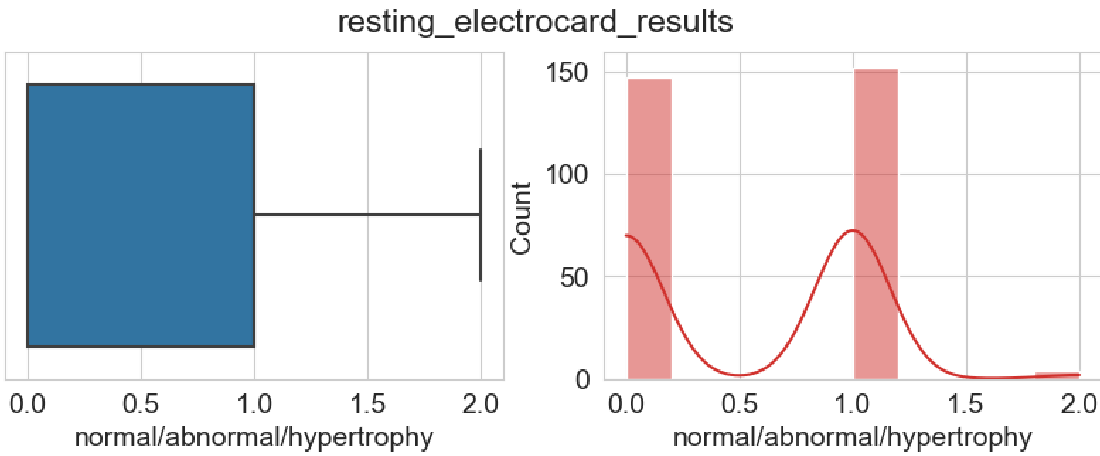

sex
0.0
0.2
0.4
0.6
0.8
1.0
female/male
Count
0
50
100
150
200
female/male

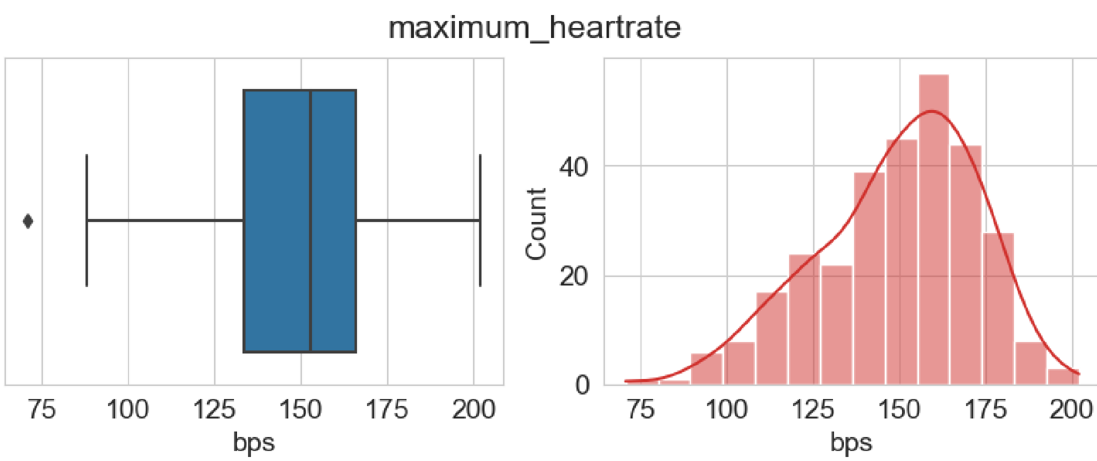

chest_pain_type
0
1
2
3
typical/atypical/non-ang./asym.
Count
0
50
100
150
typical/atypical/non-ang./asym.

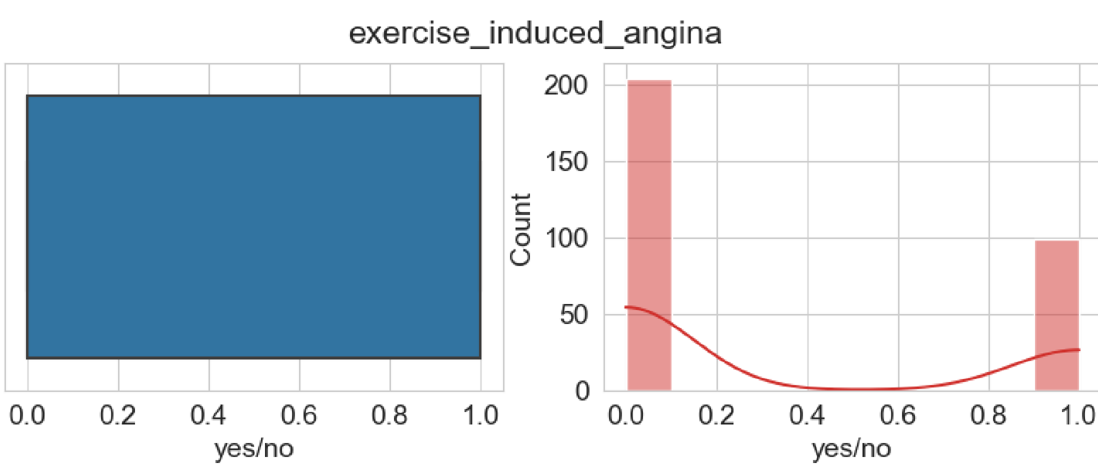

resting_blood_pressure
100 120 140 160 180 200
mm Hg
Count
0 20 40
100 120 140 160 180 200
mm Hg

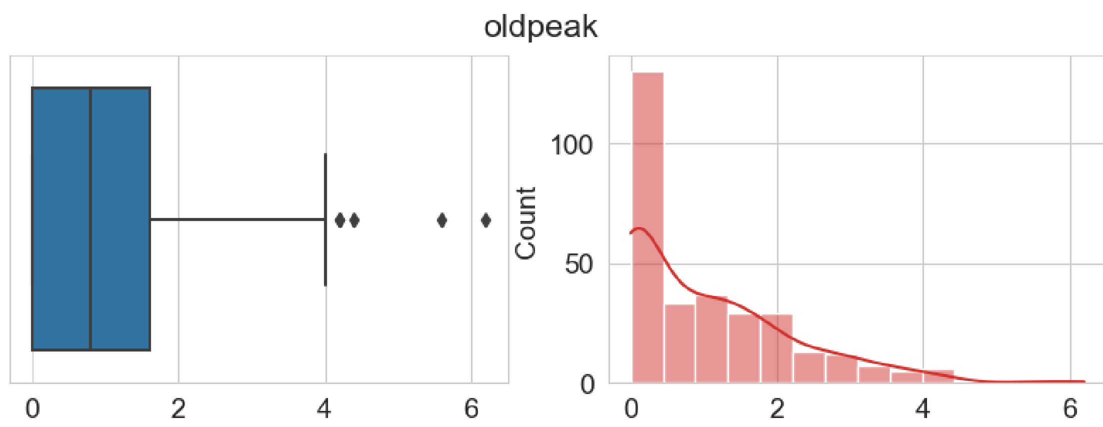

serum_cholestoral
200 300 400 500
mg/dl
Count
0 20 40
200 300 400 500
mg/dl

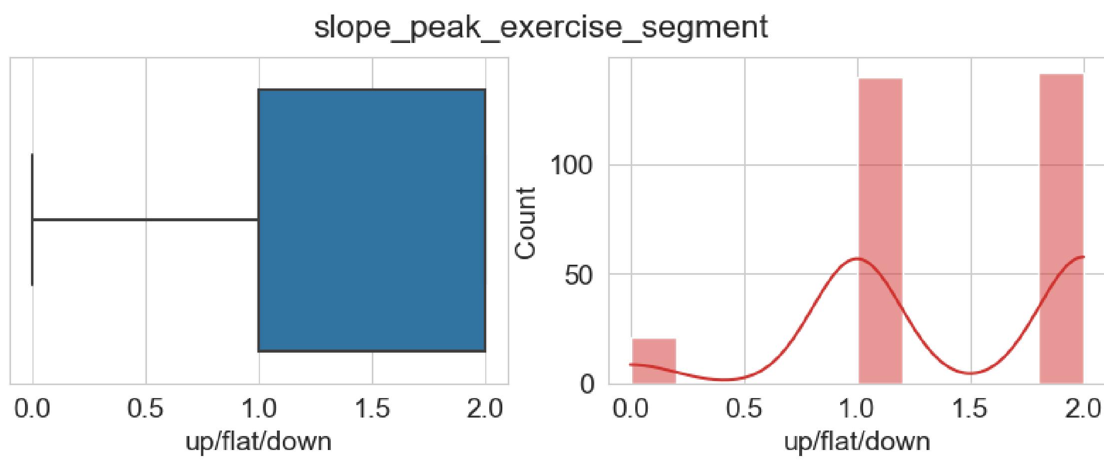

fasting_blood_sugar
0.0 0.2 0.4 0.6 0.8 1.0
>120 mg/dl
Count
0 100 200
0.0 0.2 0.4 0.6 0.8 1.0
>120 mg/dl

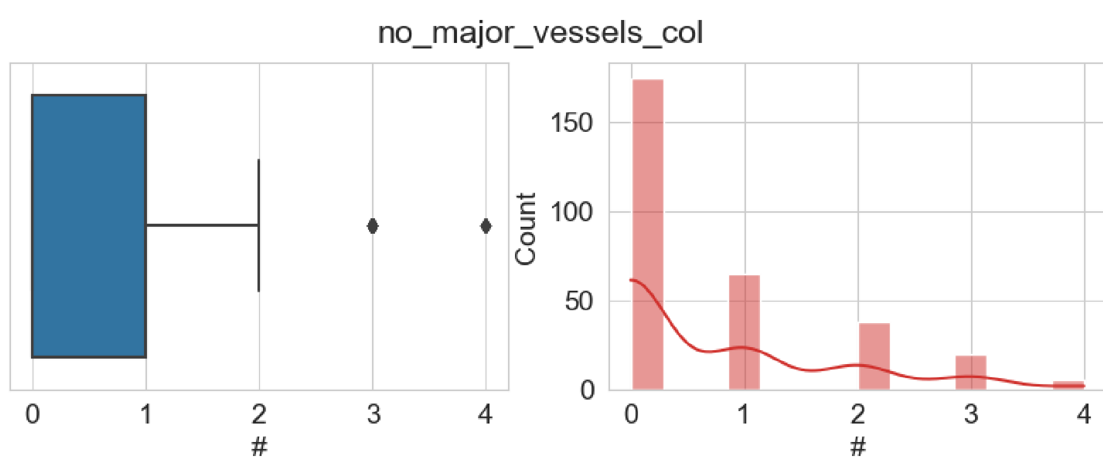

resting_electrocard_results
0.0
0.5
1.0
1.5
2.0
normal/abnormal/hypertrophy
Count
0
50
100
150
0.0
0.5
1.0
1.5
2.0
normal/abnormal/hypertrophy

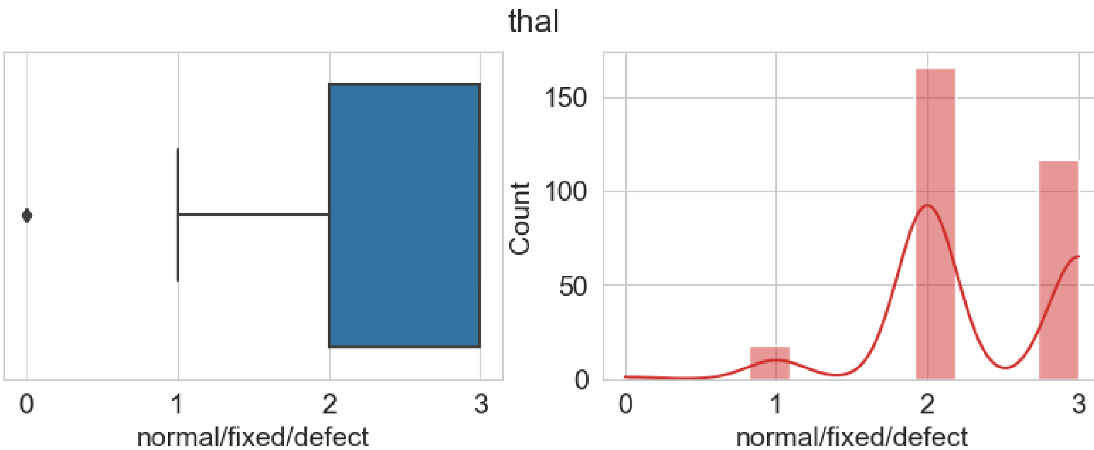

maximum_heartrate
75
100
125
150
175
200
bps
Count
0
20
40
75
100
125
150
175
200
bps


exercise_induced_angina
0.0
0.2
0.4
0.6
0.8
1.0
yes/no
Count
0
50
100
150
200
0.0
0.2
0.4
0.6
0.8
1.0
yes/no


oldpeak
Count
0
50
100
0
2
4
6


slope_peak_exercise_segment
Count
0
50
100
0.0
0.5
1.0
1.5
2.0
up/flat/down

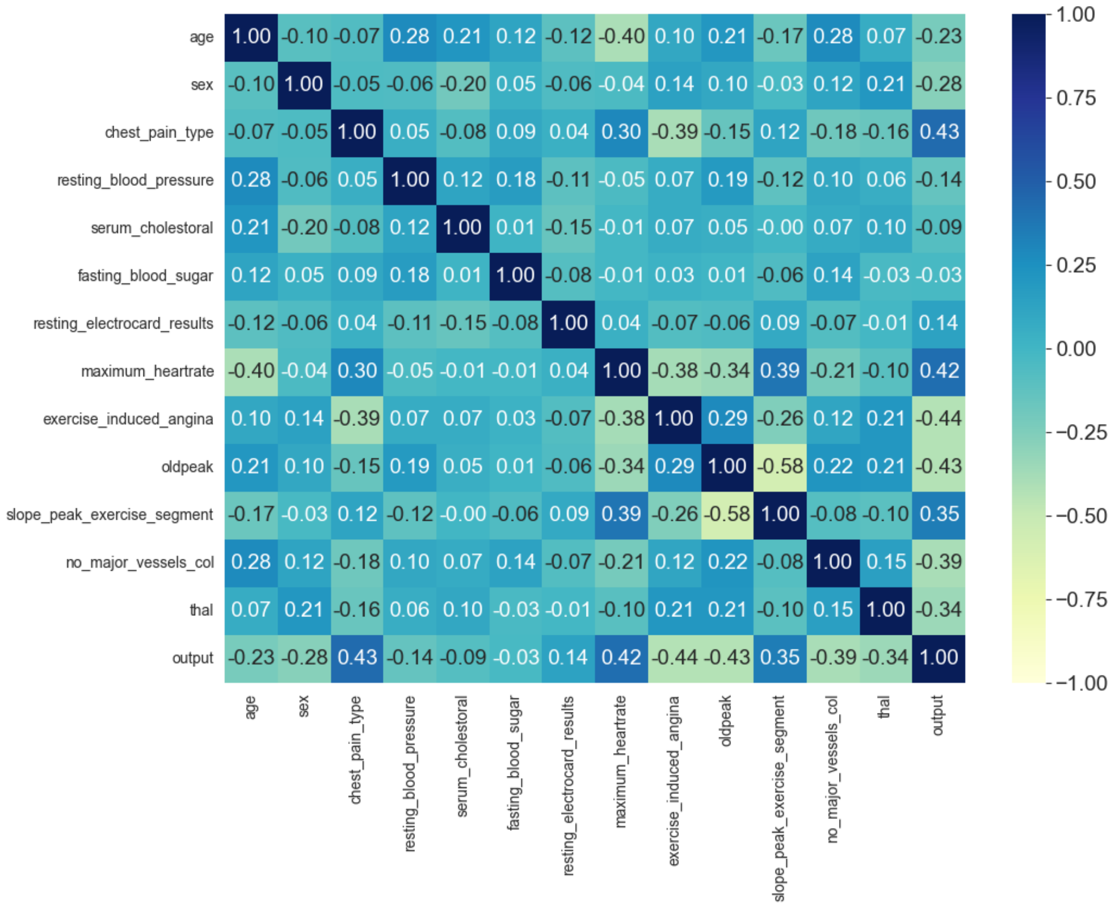

no_major_vessels_col
Count
0
50
100
150
0
1
2
3
4
#



According to these plots, some features such as "resting_blood_pressure" and "serum_cholestoral" present outliers. However, these high values might indicate risk of heart attack, so it is better to keep them.

As for the feature called "thal", the description indicates three possible values, but there are four. The one with category "0" is given by two samples only. Perhaps it is not correct. For safety, let's keep this feature unaltered.

[12]:
```
# Plot correlation matrix
def plot_correlation(df, method='pearson', figsize=(10,10)):
    '''
    This function plots the correlation of the features in a dataset.
    '''
    correlations = df.corr(method=method)
    fig = plt.figure(figsize=figsize)
    ax = fig.add_subplot()
    sns.heatmap(correlations , vmax=1, vmin=-1, annot=True, cmap="YlGnBu",␣
 ↪fmt='.2f', ax=ax)
    ax.tick_params(axis='x', labelsize=10)  # Set x-axis label size
    ax.tick_params(axis='y', labelsize=10)  # Set y-axis label size
    plt.show()

    return fig, ax
fig, ax = plot_correlation(df, figsize=(11,8))
```



The correlation matrix shows that some features present moderate correlation with the target feature.

8 Feature Engineering

[13]:
```
# Convert age into categorical
bins = [0, 40, 50, 60, 70, 80]
labels = ['29-40','40-50','50-60','60-70','70-80']
age_cat = pd.CategoricalDtype(categories=labels, ordered=True)
df['cat_age'] = pd.cut(df['age'], bins=bins, labels=labels).astype(age_cat)
```

[14]:
```
# Binary features
binary_features = ['sex', 'fasting_blood_sugar', 'exercise_induced_angina']

# Categorical features
categorical_features = ['cat_age', 'chest_pain_type',␣
↪'resting_electrocard_results', 'slope_peak_exercise_segment', 'thal']
```

```
# Numerical features
numerical_features = ['resting_blood_pressure', 'serum_cholestoral',␣
↪'maximum_heartrate', 'oldpeak', 'no_major_vessels_col']
```

```
[15]: # Convert categorical features into 'category'
for feature in categorical_features:
    df[feature] = df[feature].astype('category')

# Convert numerical and binary features into 'int32'
for feature in [numerical_features, binary_features]:
    df[feature] = df[feature].astype(int)
```

9 Train-Test Split

```
[16]: X = df.drop('output', axis=1)
y = df['output']

# Train-test-split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,␣
↪random_state=RSEED, stratify=y)

print(f"X_train: {X_train.shape[0]} samples - {X_train.shape[1]} features ")
print(f"y_train: {y_train.shape[0]} samples")
print(f"X_test: {X_test.shape[0]} samples - {X_test.shape[1]} features ")
print(f"y_test: {y_test.shape[0]} samples")
```

```
X_train: 242 samples - 14 features
y_train: 242 samples
X_test: 61 samples - 14 features
y_test: 61 samples
```

10 Dimensionality Reduction

In this particular problem consisting of predicting heart disease, reducing the number of features in the dataset may result in an improvement of the performance scores. The method called **SelectKBest** can be used to select only the most important features.

This code can be used to analyze the importance of the features. The **chi2** function can be used for categorical and binary features, and **f_classif** for numerical features.

```
select_example = SelectKBest(score_func=chi2, k='all')
select_example.fit(X_train[binary_features], y_train)
sorted(select_example.pvalues_)
```

11 Logistic Regression

[17]:
```
# Pipeline
pipe_numerical = Pipeline([
    ('scaler', StandardScaler()),
    ('kbest', SelectKBest(score_func=f_classif, k=3))
])

pipe_categorical = Pipeline([
    ('onehot', OneHotEncoder(handle_unknown='ignore', drop='first',␣
 ↪sparse_output=False)),
    ('kbest', SelectKBest(score_func=chi2, k=2))
])

pipe_binary = Pipeline([
    ('kbest', SelectKBest(score_func=chi2, k=2))
])

preprocessing = ColumnTransformer(transformers=[
    ('numerical', pipe_numerical, numerical_features),
    ('categorical', pipe_categorical, categorical_features),
    ('binary', pipe_binary, binary_features),
])

pipe_lr = Pipeline([
    ('preprocessing', preprocessing),
    ('LR', LogisticRegression(max_iter=10000))]
)
```

[18]:
```
param_lr = {'LR__penalty':('l1','l2'),
            'LR__C': [0.001, 0.01, 0.1, 1, 10, 100, 1000],
            'LR__solver': ['liblinear', 'saga']
           }

# Train, cross-validate, predict, and score
model_lr, _ = train_crossval_predict_score(pipe_lr, param_lr, X_train, y_train,␣
 ↪X_test, y_test, cv=3, scoring='f1', cross_val='full', matrix=False)
```

```
Best params: {'LR__C': 0.1, 'LR__penalty': 'l2', 'LR__solver': 'saga'}
----------------------------------------
Accuracy on training set: 0.83
Accuracy on test set: 0.85
----------------------------------------
Recall on training set: 0.89
Recall on test set: 0.94
----------------------------------------
Precision on training set: 0.82
Precision on test set: 0.82
```

```
----------------------------------------
fbeta_score on training set: 0.86
fbeta_score on test set: 0.87
----------------------------------------
roc_auc_score on trainig set:  0.9
roc_auc_score on test set:  0.92
----------------------------------------
```

12 SVM

[19]:
```
# Pipeline
pipe_numerical = Pipeline([
    ('scaler', StandardScaler()),
    ('kbest', SelectKBest(score_func=f_classif, k=3))
])

pipe_categorical = Pipeline([
    ('onehot', OneHotEncoder(handle_unknown='ignore', drop='first',␣
 ↪sparse_output=False)),
    ('kbest', SelectKBest(score_func=chi2, k=2))
])

pipe_binary = Pipeline([
    ('kbest', SelectKBest(score_func=chi2, k=2))
])

preprocessing = ColumnTransformer(transformers=[
    ('numerical', pipe_numerical, numerical_features),
    ('categorical', pipe_categorical, categorical_features),
    ('binary', pipe_binary, binary_features),
])

pipe_svm = Pipeline([
    ('preprocessing', preprocessing),
    ('SVM', SVC(probability=True, random_state=RSEED))
])
```

[20]:
```
param_svm = {'SVM__kernel':['linear', 'poly', 'rbf', 'sigmoid'],
             'SVM__C': [0.001, 0.01, 0.1, 1, 10, 100, 1000],
             'SVM__gamma': ['scale', 'auto']
            }

# Train, cross-validate, predict, and score
model_svm, _ = train_crossval_predict_score(pipe_svm, param_svm, X_train,␣
 ↪y_train, X_test, y_test, cv=3, scoring='f1', cross_val='full', matrix=False)
```

```
Best params: {'SVM__C': 1, 'SVM__gamma': 'auto', 'SVM__kernel': 'rbf'}
```

```
----------------------------------------
Accuracy on training set: 0.86
Accuracy on test set: 0.85
----------------------------------------
Recall on training set: 0.9
Recall on test set: 0.97
----------------------------------------
Precision on training set: 0.85
Precision on test set: 0.8
----------------------------------------
fbeta_score on training set: 0.88
fbeta_score on test set: 0.88
----------------------------------------
roc_auc_score on trainig set:  0.92
roc_auc_score on test set:  0.94
----------------------------------------
```

13 Random Forest

[21]:

```
# Pipeline
pipe_numerical = Pipeline([
    ('scaler', StandardScaler()),
    ('kbest', SelectKBest(score_func=f_classif, k=3))
])

pipe_categorical = Pipeline([
    ('onehot', OneHotEncoder(handle_unknown='ignore', drop='first',␣
 ↪sparse_output=False)),
    ('kbest', SelectKBest(score_func=chi2, k=5))
])

pipe_binary = Pipeline([
    ('kbest', SelectKBest(score_func=chi2, k=2))
])

preprocessing = ColumnTransformer(transformers=[
    ('numerical', pipe_numerical, numerical_features),
    ('categorical', pipe_categorical, categorical_features),
    ('binary', pipe_binary, binary_features),
])

pipe_rf = Pipeline([
    ('preprocessing', preprocessing),
    ('RF', RandomForestClassifier(random_state=RSEED, max_features = 'sqrt',␣
 ↪n_jobs=-1, verbose = 0))
])
```

[22]:
```python
param_rf = {
    'RF__n_estimators': [5, 10, 20, 50, 70, 100],
    'RF__criterion' : ['gini', 'entropy'],
    'RF__max_depth': [1, 5, 7, 10],
    'RF__min_samples_split': [2, 5, 10, 20, 30]
}

# Train, cross-validate, predict, and score
model_rf, _ = train_crossval_predict_score(pipe_rf, param_rf, X_train, y_train,␣
 ↪X_test, y_test, cv=3, scoring='f1', cross_val='full', matrix=False)
```

```
Best params: {'RF__criterion': 'entropy', 'RF__max_depth': 5,
'RF__min_samples_split': 5, 'RF__n_estimators': 10}
----------------------------------------
Accuracy on training set: 0.86
Accuracy on test set: 0.79
----------------------------------------
Recall on training set: 0.89
Recall on test set: 0.91
----------------------------------------
Precision on training set: 0.86
Precision on test set: 0.75
----------------------------------------
fbeta_score on training set: 0.87
fbeta_score on test set: 0.82
----------------------------------------
roc_auc_score on trainig set:  0.95
roc_auc_score on test set:  0.91
----------------------------------------
```

14 Soft Voting

[23]:
```python
# The group of models include: LR, SVM and RF
model_sf = VotingClassifier(estimators = [('lr', model_lr), ('svm', model_svm),␣
 ↪('rf', model_rf)], weights=[1,1,1], voting = 'soft')
model_sf.fit(X_train,y_train)
predict_and_print_scores(model_sf, X_train, y_train, X_test, y_test,␣
 ↪matrix=False)
```

```
Accuracy on training set: 0.86
Accuracy on test set: 0.84
----------------------------------------
Recall on training set: 0.89
Recall on test set: 0.97
----------------------------------------
Precision on training set: 0.86
Precision on test set: 0.78
```

```
----------------------------------------
fbeta_score on training set: 0.87
fbeta_score on test set: 0.86
----------------------------------------
roc_auc_score on trainig set:  0.94
roc_auc_score on test set:  0.94
----------------------------------------
```

15 Stacking

[24]:
```python
# In this architecture, a logistic-regression meta model is used to make the␣
↪final prediction from the output of the LR, SVM, and RF models
estimators = [('lr', model_lr), ('svm', model_svm), ('rf', model_rf)]
stacking_sk = StackingClassifier(estimators=estimators,␣
↪final_estimator=LogisticRegression(max_iter=10000), n_jobs=-1)

# Construct a pipeline with StackingClassifier
pipe_sk = Pipeline([
    ('stacking_sk', stacking_sk)
])

# Define hyperparameters only for LogisticRegression()
param_sk = {
    'stacking_sk__final_estimator__C': [0.001, 0.01, 0.1, 1, 10, 100, 1000],
    'stacking_sk__final_estimator__penalty': ['l1', 'l2'],
    'stacking_sk__final_estimator__solver': ['liblinear', 'saga']
}

model_sk, _ = train_crossval_predict_score(pipe_sk, param_sk, X_train, y_train,␣
↪X_test, y_test, cv=3, scoring='f1', cross_val='full', matrix=False)
```

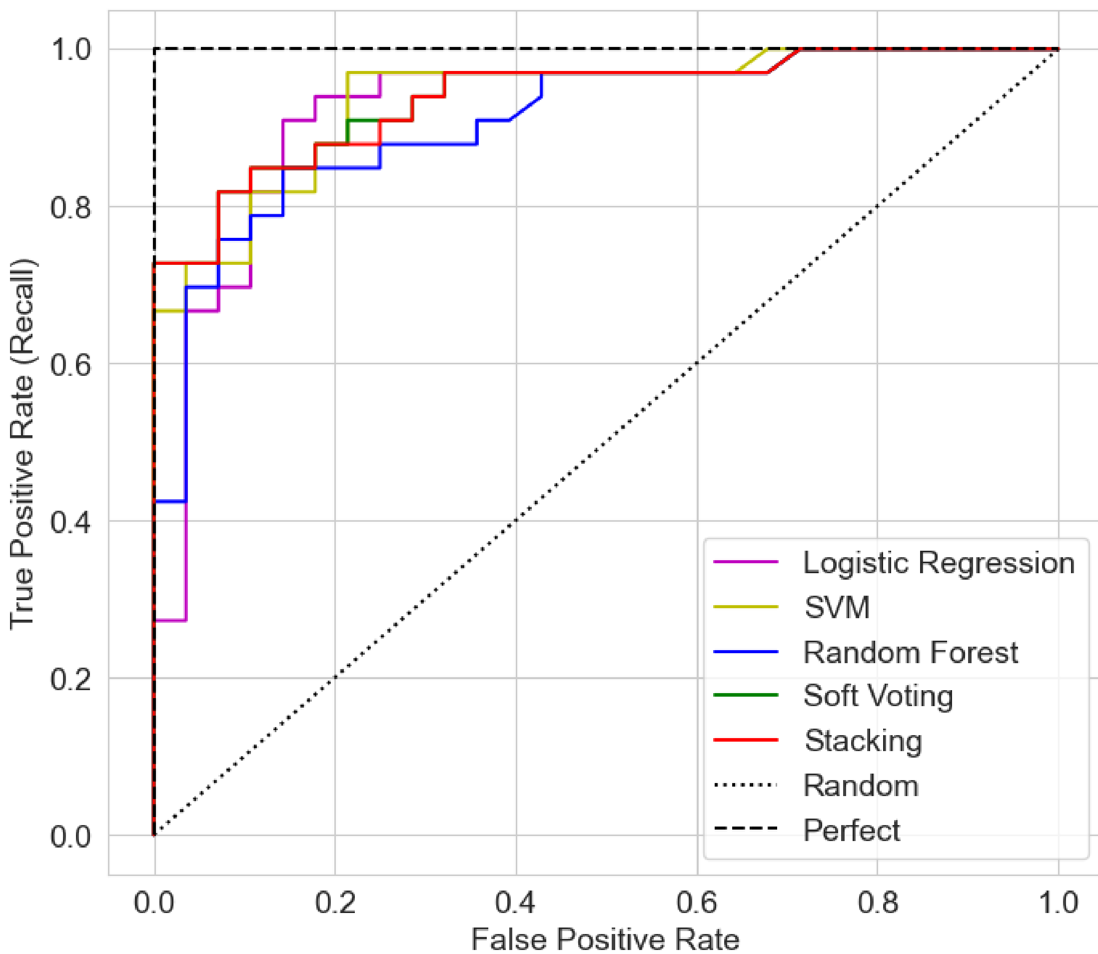
```
Best params: {'stacking_sk__final_estimator__C': 0.1,
'stacking_sk__final_estimator__penalty': 'l2',
'stacking_sk__final_estimator__solver': 'saga'}
----------------------------------------
Accuracy on training set: 0.86
Accuracy on test set: 0.82
----------------------------------------
Recall on training set: 0.91
Recall on test set: 0.97
----------------------------------------
Precision on training set: 0.85
Precision on test set: 0.76
----------------------------------------
fbeta_score on training set: 0.88
fbeta_score on test set: 0.85
----------------------------------------
```

```
roc_auc_score on trainig set:  0.94
roc_auc_score on test set:  0.94
----------------------------------------
```

16 Model Evaluation

16.1 ROC Curves

[25]:
```
# Create a dictionary with the trained models
models = {'Logistic Regression' : [model_lr, 'm-'],
          'SVM' : [model_svm, 'y-'],
          'Random Forest' : [model_rf, 'b-'],
          'Soft Voting' : [model_sf, 'g-'],
          'Stacking' : [model_sk, 'r']}
fig, ax = plot_roc_curves(models, X_test, y_test, figsize=(8,7))
```



The ROC-curve plot indicates that **Soft Voting** and **Stacking** cover a higher area than the other methods. However, it is shown that the two architectures perform worse than Logistic Regression and SVM for high true positive rates. It is also observed that Random Forest performs worse than the other ensemble learning approaches.

16.2 ROC AUC Scores

[26]:
```
# Find the model with the highest ROC AUC score
best_score = 0
for key, model in models.items():
    if key == 'logistic regression':
        score = roc_auc_score(y_test, model[0].predict_proba(X_test)[:,1])
    else:
        score = roc_auc_score(y_test, model[0].predict_proba(X_test)[:,1])
    if score > best_score:
        best_score = score
        best_model = key

print(f"Model with the best ROC_AUC score: **{best_model}**")
print(f"- ROC AUC score: {round(best_score, 2)}")
```

```
Model with the best ROC_AUC score: **Soft Voting**
- ROC AUC score: 0.94
```

The **Soft Voting** ensemble method produces the highest ROC AUC score, along with **Stacking**.

16.3 F1 Scores

[27]:
```
# Find the model with the highest F1 score for a target recall of 90%
tpr = 0.90
best_score = 0
for key, model in models.items():
    thr, _ = find_roc_threshold_tpr(model[0], X_test, y_test, tpr)
    score = f1_score(y_test, model[0].predict_proba(X_test)[:,1] >= thr)
    if score > best_score:
        best_score = score
        best_model = key
        best_thr = thr
print(f"Model with the best F1 score for a recall of {100*tpr}%:␣
 ↪**{best_model}**")
print(f"- Threshold: {round(best_thr, 2)}")
print(f"- F1 score: {round(best_score, 2)}")
```

```
Model with the best F1 score for a recall of 90.0%: **Logistic Regression**
- Threshold: 0.59
- F1 score: 0.9
```

Logistic Regression obtains the best results in therms of F1 score for a target recall of 90%.

16.4 Generalization

[28]:
```
# Find the model that achieves the lowest difference between the accuracy
↪scores on the training set and those on the test set. At the same time, the
↪best model should also produce the highest accuracy score.
lowest_diff = 1
best_score_test = 0
for key, model in models.items():
    score_train = accuracy_score(y_train, model[0].predict(X_train))
    score_test = accuracy_score(y_test, model[0].predict(X_test))
    diff = np.abs(score_train - score_test)
    if (diff <= lowest_diff) and (score_test >= best_score_test):
        lowest_diff = diff
        best_score_test = score_test
        best_model = key

print(f"Best generalizing model: **{best_model}**")
```

```
Best generalizing model: **SVM**
```

The **SVM** model is the one that best generalizes.

16.5 Confusion Matrix for a 90% Recall

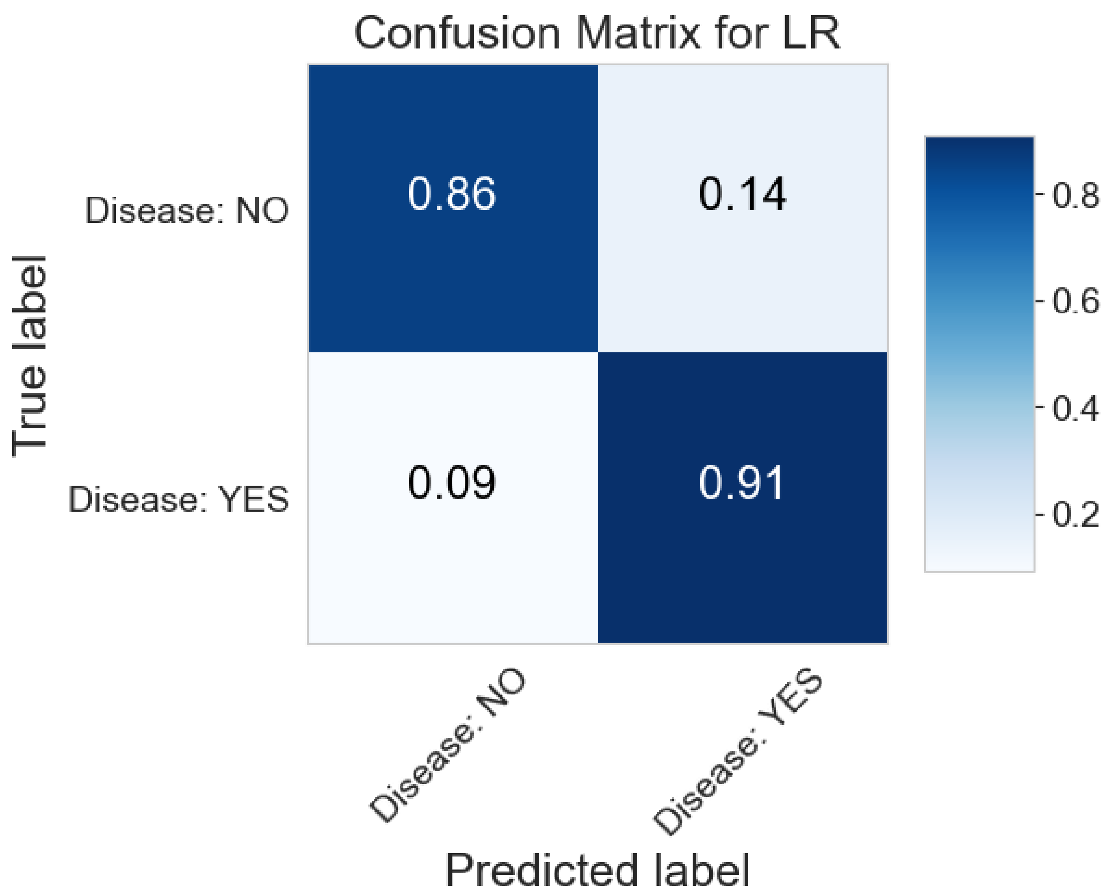
[29]:
```
# Find the false positive rate corresponding to a recall of 90% using Logistic
↪Regression and Soft Voting.
tpr = 0.90
thr_lr, fpr_lr = find_roc_threshold_tpr(model_lr, X_test, y_test, tpr)
print("Logistic Regression:")
print(f"- Threshold for a recall of {100*tpr}%: {round(thr_lr, 2)}")
print(f"- False positive rate: {round(fpr_lr, 2)}")
thr_sf, fpr_sf = find_roc_threshold_tpr(model_sf, X_test, y_test, tpr)
print("Soft Voting:")
print(f"- Threshold for a recall of {100*tpr}%: {round(thr_sf, 2)}")
print(f"- False positive rate: {round(fpr_sf, 2)}")
```

```
Logistic Regression:
- Threshold for a recall of 90.0%: 0.59
- False positive rate: 0.14
Soft Voting:
- Threshold for a recall of 90.0%: 0.59
- False positive rate: 0.21
```

Logistic Regression achieves the lowest false positive rate.

[30]:
```
# Plot confusion matrix on the test set for Logistic Regression
y_test_pred = model_lr.predict_proba(X_test)[:,1] >= thr_lr
cm = confusion_matrix(y_test, y_test_pred)
```

```
plot_confusion_matrix(cm, ['Disease: NO', 'Disease: YES'], normalize=True,␣
↪title='Confusion Matrix for LR', cmap=plt.cm.Blues, figsize=(6,6))
```



The confusion matrix shows a true positive rate of 91% (with only 9% of false negative rate) and a false positive rate of 18%, when evaluating the **Logistic Regression** model.

17 Conclusions

In this notebook, we have analyzed the potential of some ensemble architectures to enhance the prediction performance for the heart-attack database. **Soft Voting Stacking achieves the best results in terms of ROC AUC**.

The non-ensemble methods, such as SVM and Logistic Regression, perform slightly better than the ensemble approaches at high values of recall. For a target recall of 90%, **Logistic Regression obtains the best F1 score** and **SVM is the machine-learning model that best generalizes**.

According to the confusion matrix, when using **Logistic Regression**, the achieved true positive and false positive rates are, respectively, **91% and 18%**.