xgboost

September 5, 2021

1 Synopsis

This predictive modeling project aims to build a machine learning model to predict the presence or absence of cardiovascular disease based on 13 physiological features. The data comes from the Heart Disease dataset (https://archive.ics.uci.edu/ml/datasets/Heart+Disease) from the UC Irvine Machine Learning Repository.

2 Setup

Import all libraries and methods required for the project.

```
[1]: import numpy as np
     import pandas as pd
     from pandas.plotting import scatter_matrix
     import matplotlib.pyplot as plt
     from scipy.stats import shapiro
     import missingno as msno
     from sklearn.preprocessing import StandardScaler
     from sklearn.preprocessing import OneHotEncoder
     from sklearn.impute import SimpleImputer
     from sklearn.pipeline import Pipeline
     from sklearn.pipeline import FeatureUnion
     from sklearn.compose import ColumnTransformer
     from sklearn.feature_selection import SelectKBest
     from sklearn.decomposition import PCA
     from sklearn.model_selection import GridSearchCV
     from xgboost import XGBClassifier
     from pickle import dump
```

3 Load the data

Load the data into a Pandas data frame.

4 Describe the data

Setup the display system to print all decimal numbers upto the third decimal place.

```
[3]: pd.set_option("precision", 3)
```

Look at the head and tail of the data.

```
[4]: df.head()
[4]: age sex cp trestbps chol fbs restecg thalach exang oldpeak \
```

```
0
   63.0
         1.0
              1.0
                       145.0
                               233.0
                                      1.0
                                                2.0
                                                        150.0
                                                                 0.0
                                                                           2.3
   67.0
         1.0
              4.0
                       160.0
                                      0.0
                                                        108.0
                                                                 1.0
                                                                           1.5
1
                               286.0
                                                2.0
2 67.0
        1.0 4.0
                       120.0
                               229.0
                                                2.0
                                                        129.0
                                                                 1.0
                                                                           2.6
                                      0.0
3
   37.0
        1.0
              3.0
                       130.0
                               250.0
                                      0.0
                                                0.0
                                                        187.0
                                                                 0.0
                                                                           3.5
4 41.0 0.0
              2.0
                                                2.0
                                                        172.0
                       130.0
                               204.0
                                      0.0
                                                                 0.0
                                                                           1.4
```

```
slope
            ca
                 thal
                        num
     3.0
0
           0.0
                  6.0
                          0
1
     2.0
           3.0
                  3.0
                          2
2
     2.0
           2.0
                  7.0
                          1
3
     3.0
           0.0
                  3.0
                          0
4
     1.0 0.0
                  3.0
                          0
```

```
[5]: df.tail()
```

```
[5]:
                            trestbps
                                        chol
                                              fbs
                                                    restecg
                                                             thalach
                                                                       exang
                                                                               oldpeak \
           age
                 sex
                       ср
     298
          45.0
                 1.0
                      1.0
                               110.0
                                       264.0
                                              0.0
                                                        0.0
                                                                132.0
                                                                          0.0
                                                                                   1.2
     299
          68.0
                1.0
                      4.0
                               144.0
                                       193.0
                                              1.0
                                                        0.0
                                                                141.0
                                                                          0.0
                                                                                   3.4
          57.0
                               130.0
                                       131.0
                                                        0.0
                                                                          1.0
                                                                                   1.2
     300
                1.0
                      4.0
                                              0.0
                                                                115.0
     301
          57.0
                0.0
                      2.0
                               130.0
                                       236.0
                                                        2.0
                                                                174.0
                                                                          0.0
                                              0.0
                                                                                   0.0
     302
          38.0
                1.0
                      3.0
                               138.0
                                       175.0 0.0
                                                        0.0
                                                                173.0
                                                                          0.0
                                                                                   0.0
```

```
slope
                  thal
                         num
              ca
298
       2.0
             0.0
                   7.0
                           1
299
       2.0
             2.0
                   7.0
                           2
300
       2.0 1.0
                   7.0
                           3
301
       2.0
            1.0
                   3.0
                           1
302
       1.0 NaN
                   3.0
                           0
```

Look at the dimensions of the data.

[6]: df.shape

[6]: (303, 14)

The dataset appears to have 303 rows and 14 columns.

Look at the data types of each variable in the data.

[7]: df.dtypes

[7]: age float64 sex float64 float64 ср trestbps float64 float64 chol fbs float64 restecg float64 thalach float64 exang float64 oldpeak float64 slope float64 float64 ca float64 thal int64 num dtype: object

Obtain descriptive statistics for the data.

[8]: df.describe()

[8]:		age	sex	ср	trestbps	chol	fbs	restecg	\
	count	303.000	303.000	303.000	303.00	303.000	303.000	303.000	
	mean	54.439	0.680	3.158	131.69	246.693	0.149	0.990	
	std	9.039	0.467	0.960	17.60	51.777	0.356	0.995	
	min	29.000	0.000	1.000	94.00	126.000	0.000	0.000	
	25%	48.000	0.000	3.000	120.00	211.000	0.000	0.000	
	50%	56.000	1.000	3.000	130.00	241.000	0.000	1.000	
	75%	61.000	1.000	4.000	140.00	275.000	0.000	2.000	
	max	77.000	1.000	4.000	200.00	564.000	1.000	2.000	
		thalach	exang	oldpeak	slope	ca	thal	num	
	count	303.000	303.000	303.000	303.000	299.000	301.000	303.000	
	mean	149.607	0.327	1.040	1.601	0.672	4.734	0.937	
	std	22.875	0.470	1.161	0.616	0.937	1.940	1.229	
	min	71.000	0.000	0.000	1.000	0.000	3.000	0.000	
	25%	133.500	0.000	0.000	1.000	0.000	3.000	0.000	
	50%	153.000	0.000	0.800	2.000	0.000	3.000	0.000	
	75%	166.000	1.000	1.600	2.000	1.000	7.000	2.000	

max 202.000 1.000 6.200 3.000 3.000 7.000 4.000

```
Obtain the distribution of instances across different class labels.
 [9]: df["num"].value_counts()
 [9]: 0
            164
             55
      1
      2
             36
      3
             35
      4
             13
      Name: num, dtype: int64
      Obtain the correlations between the variables in the data.
[10]: df.corr(method = "pearson")
[10]:
                                         trestbps
                                                              fbs
                                                                    restecg
                                                                              thalach \
                    age
                            sex
                                     ср
                                                      chol
                  1.000 -0.098
                                 0.104
                                             0.285
                                                   0.209
                                                            0.119
                                                                       0.149
                                                                                -0.394
      age
                        1.000
                                 0.010
                                                            0.048
      sex
                -0.098
                                           -0.064 - 0.200
                                                                       0.022
                                                                                -0.049
                  0.104 0.010
                                 1.000
                                           -0.036
                                                    0.072 - 0.040
                                                                      0.068
                                                                               -0.334
      ср
```

0.092 0.204 0.162 0.127 0.223 age 0.363 sex 0.146 0.102 0.038 0.093 0.381 0.224 0.384 0.202 0.152 0.233 0.265 0.407 ср 0.065 0.189 0.117 0.099 0.134 0.158 trestbps chol 0.061 0.047 - 0.0040.119 0.014 0.071 0.145 fbs 0.026 0.006 0.060 0.071 0.059 0.085 0.114 0.134 0.128 0.025 0.184 restecg -0.343 -0.386 -0.264 -0.280 -0.415 thalach -0.3780.146 exang 1.000 0.288 0.258 0.330 0.397 oldpeak 0.288 1.000 0.578 0.296 0.341 0.504 slope 0.258 0.578 1.000 0.110 0.287 0.378 0.146 0.296 0.110 1.000 0.256 0.519 ca 0.330 0.256 0.341 0.287 1.000 0.510 thal 0.504 0.378 0.519 0.510 1.000 num 0.397

slope

oldpeak

exang

thal

num

ca

Obtain the skew of each variable in the data.

```
[11]: df.skew()
[11]: age
                  -0.209
                  -0.775
      sex
      ср
                  -0.842
      trestbps
                   0.706
      chol
                   1.136
      fbs
                   1.987
      restecg
                   0.020
      thalach
                  -0.537
      exang
                   0.743
      oldpeak
                   1.270
      slope
                   0.508
      ca
                   1.189
      thal
                   0.244
                   1.058
      num
      dtype: float64
```

Use the Shapiro-Wilk test to check if the variables in the data are Gaussian.

```
[12]:
                                             cp trestbps
                                                              chol
                                                                         fbs \
                       age
                                  sex
                                                1.8e-06 5.91e-09 5.43e-30
      p_values
                   0.00607
                            3.08e-26
                                      1.99e-19
      is_gaussian
                     False
                               False
                                         False
                                                   False
                                                             False
                                                                       False
                                                  oldpeak
                                                                           thal \
                   restecg
                             thalach
                                          exang
                                                              slope
                                                                       ca
                   1.2e-24
                            6.99e-05 3.85e-26
                                                8.18e-17
                                                           2.57e-21
                                                                        1
                                                                               1
      p_values
      is_gaussian
                               False
                                         False
                                                    False
                                                              False True
                                                                           True
                     False
                        num
                   5.59e-21
     p_values
```

is_gaussian False

The output indicates that only "ca" and "thal" are Gaussian at a 0.05 significance level. Keeping this in mind, I pick the XGBoost algorithm for modeling the problem, since this algorithm doesn't assume that its features are Gaussian.

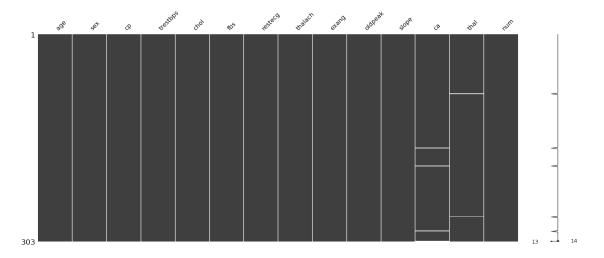
5 Visualize the data

5.1 Univariate plots

Make a missing value plot to diagnose the presence of missing values in the data.

[13]: msno.matrix(df)

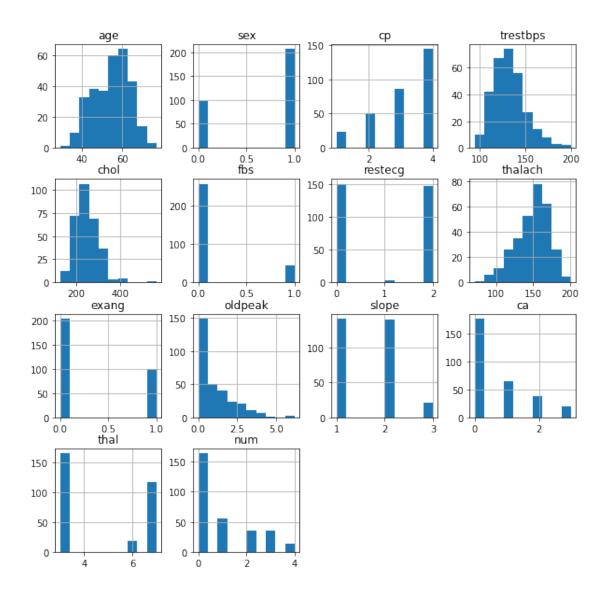
[13]: <AxesSubplot:>



The plot's output indicates that "ca" and "thal" have missing values. Hence, imputation will have to be carried out for these two variables during preprocessing.

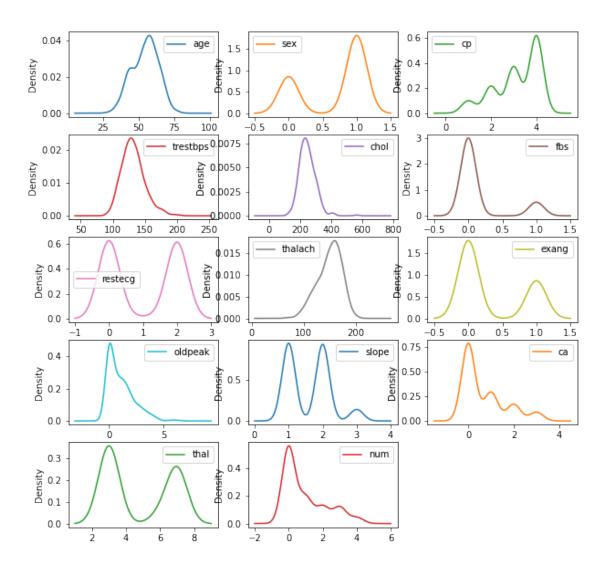
Make a histogram for each variable.

[14]: df.hist(figsize = [10, 10]) plt.show()

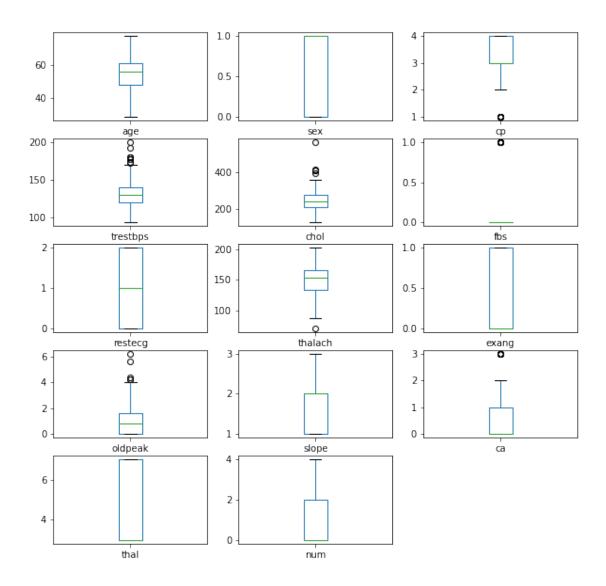


These histograms provide extremely valuable insights regarding which variables are numeric and which are categorical.

Make a density plot for each variable.



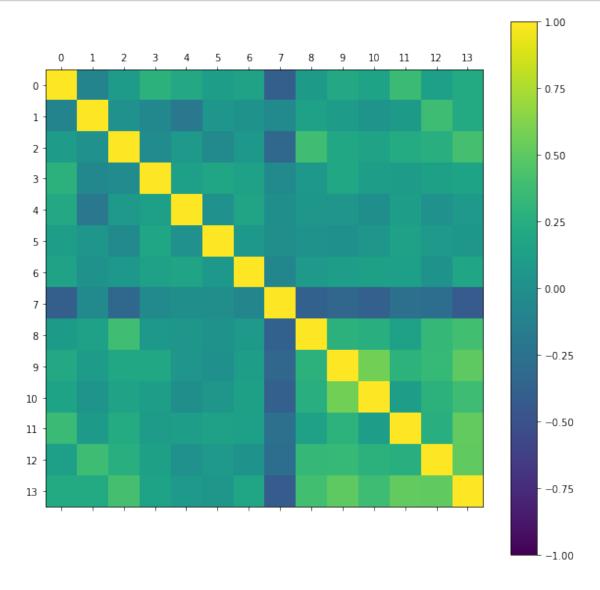
Make a boxplot for each variable.



5.2 Multivariate plots

Make a correlation matrix plot to visualize the correlation between the variables in the data.

ax.set_yticks(ticks)
plt.show()



The absense of any yellow or purple squares in the off-diagonal zones indicates that there is no pair of features which exhibits an extremely high correlation. This is favorable to the good performance of my model.

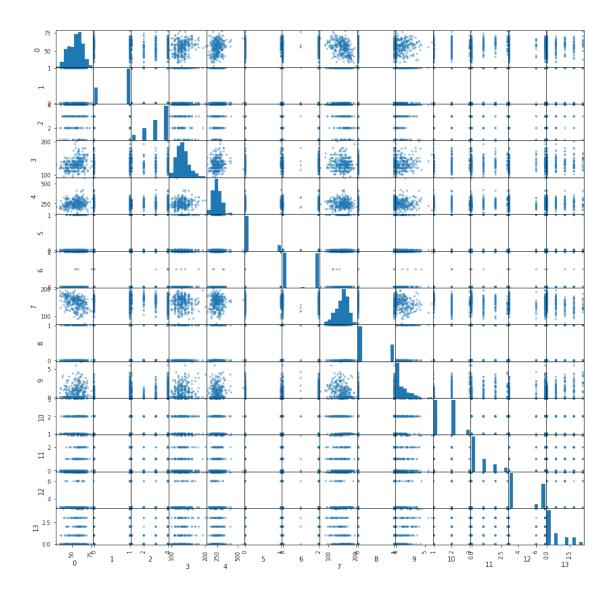
The numbered ticks along each axis in the above plot correspond to columns in the data frame as below.

[18]: pd.Series(df.columns)

[18]: 0 age 1 sex

```
2
             ср
3
      trestbps
4
           chol
5
            fbs
6
       restecg
7
       thalach
8
         exang
9
       oldpeak
10
         slope
11
12
           thal
            num
dtype: object
```

Make a scatter plot matrix for the data frame.



6 Data partitioning

Isolate the features and the target variable.

```
[22]: y
[22]: 0
              0
              2
      2
      3
      4
      298
              1
      299
              2
      300
              3
      301
              1
      302
      Name: num, Length: 303, dtype: int64
```

7 Preprocessing

According to the dataset documentation, "Experiments with the Cleveland database have concentrated on simply attempting to distinguish presence (values 1, 2, 3, 4) from absence (value 0)." Observe the current unique values in the target variable.

In its current state, the target variable has 5 unique values. I shall pool together the values 1, 2, 3 and 4 into the single value 1, to denote the presence of heart disease. I shall leave the 0 values the way they are, to denote the absence of heart disease.

```
[24]: y = y.map({0: 0,
1: 1,
2: 1,
3: 1,
4: 1})
```

```
[25]: y.value_counts()
```

```
[25]: 0 164
1 139
Name: num, dtype: int64
```

I have now converted the machine learning problem to a binary classification problem, as the dataset

documentation intended.

Refer to the dataset documentation as well as the histograms created above to ascertain which features are numeric and which are categorical.

```
[26]: categorical_vars = ["sex", "cp", "fbs", "restecg", "exang", "slope", "ca", 

→"thal"]

numeric_vars = [column for column in X.columns if (column not in 

→categorical_vars)]
```

"ca" and "thal", the two variables with missing values, are both categorical variables. Hence, imputation needs to be carried out only while preprocessing categorical variables.

For numeric variables, scale the data to a mean of 0 and a standard deviation of 1.

```
[27]: numeric_transformer = StandardScaler()
```

For categorical variables, impute missing values using most-frequent imputation and encode variables using one-hot encoding.

Merge the numeric and categorical transformers into a single preprocessor.

8 Feature selection

Extract the 10 best features from the feature list, along with the first 3 principal components. Obtain a feature union of these to make up the final feature list.

9 Tune the model parameters

I'll be training an XGBoost classifier model. Obtain the default parameters for the pipeline.

```
[31]: default_model = XGBClassifier(use_label_encoder = False)
      default_pipeline = Pipeline(steps = [
          ("preprocessor", preprocessor),
          ("feature_selector", feature_selector),
          ("model", default_model)
      ])
[32]: default_pipeline.get_params()
[32]: {'memory': None,
       'steps': [('preprocessor',
         ColumnTransformer(transformers=[('numeric', StandardScaler(),
                                           ['age', 'trestbps', 'chol', 'thalach',
                                            'oldpeak']),
                                          ('categorical',
                                          Pipeline(steps=[('imputer',
      SimpleImputer(strategy='most_frequent')),
                                                           ('one_hot',
      OneHotEncoder(handle_unknown='ignore',
      sparse=False))]),
                                           ['sex', 'cp', 'fbs', 'restecg', 'exang',
                                            'slope', 'ca', 'thal']))),
        ('feature_selector',
         FeatureUnion(transformer_list=[('select_best', SelectKBest()),
                                         ('pca', PCA(n_components=3))])),
        ('model',
         XGBClassifier(base_score=None, booster=None, colsample_bylevel=None,
                       colsample_bynode=None, colsample_bytree=None, gamma=None,
                       gpu_id=None, importance_type='gain',
      interaction_constraints=None,
                       learning_rate=None, max_delta_step=None, max_depth=None,
                       min_child_weight=None, missing=nan, monotone_constraints=None,
                       n_estimators=100, n_jobs=None, num_parallel_tree=None,
                       random_state=None, reg_alpha=None, reg_lambda=None,
                       scale_pos_weight=None, subsample=None, tree_method=None,
                       use_label_encoder=False, validate_parameters=None,
                       verbosity=None))],
       'verbose': False,
       'preprocessor': ColumnTransformer(transformers=[('numeric', StandardScaler(),
                                         ['age', 'trestbps', 'chol', 'thalach',
                                          'oldpeak']),
                                       ('categorical',
                                        Pipeline(steps=[('imputer',
      SimpleImputer(strategy='most_frequent')),
                                                         ('one_hot',
      OneHotEncoder(handle_unknown='ignore',
      sparse=False))]),
```

```
['sex', 'cp', 'fbs', 'restecg', 'exang',
                                   'slope', 'ca', 'thal'])]),
 'feature_selector': FeatureUnion(transformer_list=[('select_best',
SelectKBest()),
                                ('pca', PCA(n_components=3))]),
 'model': XGBClassifier(base_score=None, booster=None, colsample_bylevel=None,
               colsample_bynode=None, colsample_bytree=None, gamma=None,
               gpu_id=None, importance_type='gain',
interaction_constraints=None,
               learning rate=None, max delta step=None, max depth=None,
               min child weight=None, missing=nan, monotone constraints=None,
               n_estimators=100, n_jobs=None, num_parallel_tree=None,
               random_state=None, reg_alpha=None, reg_lambda=None,
               scale_pos_weight=None, subsample=None, tree_method=None,
               use_label_encoder=False, validate_parameters=None,
               verbosity=None),
 'preprocessor__n_jobs': None,
 'preprocessor_remainder': 'drop',
 'preprocessor_sparse_threshold': 0.3,
 'preprocessor_transformer_weights': None,
 'preprocessor_transformers': [('numeric',
  StandardScaler(),
   ['age', 'trestbps', 'chol', 'thalach', 'oldpeak']),
  ('categorical',
  Pipeline(steps=[('imputer', SimpleImputer(strategy='most_frequent')),
                   ('one hot'.
                    OneHotEncoder(handle_unknown='ignore', sparse=False))]),
   ['sex', 'cp', 'fbs', 'restecg', 'exang', 'slope', 'ca', 'thal'])],
 'preprocessor__verbose': False,
 'preprocessor_numeric': StandardScaler(),
 'preprocessor_categorical': Pipeline(steps=[('imputer',
SimpleImputer(strategy='most_frequent')),
                 ('one_hot',
                  OneHotEncoder(handle_unknown='ignore', sparse=False))]),
 'preprocessor_numeric_copy': True,
 'preprocessor__numeric__with_mean': True,
 'preprocessor_numeric_with_std': True,
 'preprocessor__categorical__memory': None,
 'preprocessor categorical steps': [('imputer',
  SimpleImputer(strategy='most_frequent')),
  ('one hot', OneHotEncoder(handle unknown='ignore', sparse=False))],
 'preprocessor__categorical__verbose': False,
 'preprocessor__categorical__imputer': SimpleImputer(strategy='most_frequent'),
 'preprocessor__categorical__one_hot': OneHotEncoder(handle_unknown='ignore',
sparse=False),
 'preprocessor_categorical_imputer_add_indicator': False,
 'preprocessor_categorical_imputer_copy': True,
```

```
'preprocessor_categorical_imputer_fill_value': None,
 'preprocessor_categorical_imputer_missing_values': nan,
 'preprocessor_categorical_imputer_strategy': 'most_frequent',
 'preprocessor_categorical_imputer_verbose': 0,
 'preprocessor_categorical_one_hot_categories': 'auto',
 'preprocessor_categorical_one_hot_drop': None,
 'preprocessor categorical one hot dtype': numpy.float64,
 'preprocessor_categorical_one_hot_handle_unknown': 'ignore',
 'preprocessor categorical one hot sparse': False,
 'feature selector n jobs': None,
 'feature selector transformer list': [('select best', SelectKBest()),
 ('pca', PCA(n_components=3))],
 'feature_selector__transformer_weights': None,
 'feature_selector__verbose': False,
 'feature_selector__select_best': SelectKBest(),
 'feature_selector__pca': PCA(n_components=3),
 'feature_selector__select_best__k': 10,
 'feature_selector_select_best_score_func': <function
sklearn.feature_selection._univariate_selection.f_classif(X, y)>,
 'feature_selector__pca__copy': True,
 'feature_selector__pca__iterated_power': 'auto',
 'feature_selector__pca__n_components': 3,
 'feature_selector__pca__random_state': None,
 'feature selector pca svd solver': 'auto',
 'feature_selector__pca__tol': 0.0,
 'feature_selector__pca__whiten': False,
 'model__objective': 'binary:logistic',
 'model_use_label_encoder': False,
 'model__base_score': None,
 'model__booster': None,
 'model__colsample_bylevel': None,
 'model__colsample_bynode': None,
 'model colsample bytree': None,
 'model__gamma': None,
 'model__gpu_id': None,
 'model__importance_type': 'gain',
 'model interaction constraints': None,
 'model__learning_rate': None,
 'model max delta step': None,
 'model max depth': None,
 'model min child weight': None,
 'model missing': nan,
 'model monotone constraints': None,
 'model__n_estimators': 100,
 'model__n_jobs': None,
 'model__num_parallel_tree': None,
 'model__random_state': None,
```

```
'model__reg_alpha': None,
'model__reg_lambda': None,
'model__scale_pos_weight': None,
'model__subsample': None,
'model__tree_method': None,
'model__validate_parameters': None,
'model__verbosity': None}
```

Make a grid of candidate parameters.

Perform grid search over the parameter grid.

```
[35]: grid_search.fit(X, y)
```

Fitting 5 folds for each of 240 candidates, totalling 1200 fits

```
[Parallel(n jobs=2)]: Using backend LokyBackend with 2 concurrent workers.
[Parallel(n jobs=2)]: Done 28 tasks
                                          | elapsed:
                                                       28.1s
[Parallel(n jobs=2)]: Done 124 tasks
                                          | elapsed: 2.0min
[Parallel(n_jobs=2)]: Done 284 tasks
                                          | elapsed: 4.4min
[Parallel(n_jobs=2)]: Done 508 tasks
                                          | elapsed: 7.5min
[Parallel(n_jobs=2)]: Done 796 tasks
                                          | elapsed: 11.5min
[Parallel(n_jobs=2)]: Done 1148 tasks
                                           | elapsed: 16.5min
[Parallel(n_jobs=2)]: Done 1200 out of 1200 | elapsed: 17.2min finished
[03:25:30] WARNING: /Users/travis/build/dmlc/xgboost/src/learner.cc:1095:
Starting in XGBoost 1.3.0, the default evaluation metric used with the objective
'binary:logistic' was changed from 'error' to 'logloss'. Explicitly set
eval_metric if you'd like to restore the old behavior.
```

['age',

```
'trestbps',
      'chol',
      'thalach',
      'oldpeak']),
      ('categorical',
      Pipeline(steps=[('imputer',
                SimpleImputer(strategy='most_frequent')),
               ('one_hot',
                OneHotEncoder(handle unknown='ignore',
                              sparse=False))]),
                                                                                ['sex',
                                                                                  'cp',
                                                                                  'fbs',
      'restecg',
      'exang...
                                                             tree_method=None,
                                                             use_label_encoder=False,
                                                             validate_parameters=None,
                                                             verbosity=None))]),
                   n_jobs=2,
                   param_grid={'model__colsample_bytree': [0.4, 0.6, 0.8, 1],
                                'model__learning_rate': [0.00266666666, 0.00533333333,
                                                         0.008, 0.01066666666,
                                                         0.01333333333],
                               'model__max_depth': [4, 6, 8, 10],
                               'model n estimators': [750],
                               'model_subsample': [0.5, 0.75, 1]},
                   scoring='accuracy', verbose=3)
[36]: best params = grid search.best params
      print("The best parameters obtained from the grid search are:")
      print()
      print(best_params)
     The best parameters obtained from the grid search are:
     {'model_colsample_bytree': 0.4, 'model_learning_rate': 0.00266666666,
     'model max_depth': 4, 'model n_estimators': 750, 'model subsample': 0.5}
[37]: best_accuracy = grid_search.best_score_
      print(f"The accuracy score obtained for the best parameters is {best_accuracy}")
```

The accuracy score obtained for the best parameters is 0.8249180327868852 Store the best pipeline as an estimator object.

```
[38]: best_pipeline = grid_search.best_estimator_
```

10 Save the model

Save the model to disk so that it may be conveniently loaded later, as and when it is required to make predictions on heart disease data.

```
[39]: filename = "xgboost-model.sav" dump(best_pipeline, open(filename, "wb"))
```