Data Science III with python (Class notes)

STAT 303-3

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Preface

These are class notes for the course STAT303-3. This is not the course text-book. You are required to read the relevant sections of the book as mentioned on the course website.

The course notes are currently being written, and will continue to being developed as the course progresses (just like the class notes last quarter). Please report any typos / mistakes / inconsistencies / issues with the class notes / class presentations in your comments here. Thank you!

Part I

Sklearn; Bias & Variance; KNN

1 Introduction to scikit-learn

In this chapter, we'll learn some functions from the library `sklearn` that will be useful in:

1. Splitting the data into `train` and `test`
2. Scaling data
3. Fitting a model
4. Computing model performance metrics
5. Tuning model hyperparameters* to optimize the desired performance metric

**In machine learning, a model hyperparameter is a parameter that cannot be learned from training data and must be set before training the model. Hyperparameters control aspects of the model's behavior and can greatly impact its performance. For example, the regularization parameter λ, in linear regression is a hyperparameter. You need to specify it before fitting the model. On the other hand, the beta coefficients in linear regression are parameters, as you learn them while training the model, and don't need to specify their values beforehand.*

We'll use a classification problem to illustrate the functions. However, similar functions can be used for regression problems, i.e., prediction problems with a continuous response.

```
# Importing necessary libraries
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
sns.set(font_scale=1.35)
```

Let us import the `sklearn` modules useful in developing statistical models.

```
# sklearn has 100s of models - grouped in sublibraries, such as linear_model
from sklearn.linear_model import LogisticRegression, LinearRegression

# sklearn has many tools for cleaning/processing data, also grouped in sublibraries
# splitting one dataset into train and test, computing cross validation score, cross validate
from sklearn.model_selection import train_test_split, cross_val_predict, cross_val_score
```

```
#sklearn module for scaling data
from sklearn.preprocessing import StandardScaler

#sklearn modules for computing the performance metrics
from sklearn.metrics import accuracy_score, mean_absolute_error, mean_squared_error, r2_score
roc_curve, auc, precision_score, recall_score, confusion_matrix
```

```
#Reading data
data = pd.read_csv('./Datasets/diabetes.csv')
```

Scikit-learn doesn't support the formula-like syntax of specifying the response and the predictors as in the `statsmodels` library. We need to create separate objects for predictors and response, which should be *array-like*. A Pandas DataFrame / Series or a Numpy array are *array-like* objects.

Let us reference our predictors as object `X`, and the response as object `y`.

```
# Separating the predictors and response - THIS IS HOW ALL SKLEARN OBJECTS ACCEPT DATA (diffe
y = data.Outcome
X = data.drop("Outcome", axis = 1)
```

1.1 Splitting data into `train` and `test`

Let us create train and test datasets for developing a model to predict if a person has diabetes.

```
# Creating training and test data
    # 80-20 split, which is usual - 70-30 split is also fine, 90-10 is fine if the dataset is
    # random_state to set a random seed for the splitting - reproducible results
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.2, random_state = 45)
```

Let us find the proportion of classes (*'having diabetes'* ($y = 1$) *or 'not having diabetes'* ($y = 0$)) in the complete dataset.

```
#Proportion of 0s and 1s in the complete data
y.value_counts()/y.shape
```

```
0    0.651042
1    0.348958
Name: Outcome, dtype: float64
```

Let us find the proportion of classes (*'having diabetes'* $(y = 1)$ *or 'not having diabetes'* $(y = 0)$) in the train dataset.

```
#Proportion of 0s and 1s in train data
y_train.value_counts()/y_train.shape
```

```
0    0.644951
1    0.355049
Name: Outcome, dtype: float64
```

```
#Proportion of 0s and 1s in test data
y_test.value_counts()/y_test.shape
```

```
0    0.675325
1    0.324675
Name: Outcome, dtype: float64
```

We observe that the proportion of 0s and 1s in the `train` and `test` dataset are slightly different from that in the complete `data`. In order for these datasets to be more representative of the population, they should have a proportion of 0s and 1s similar to that in the complete dataset. This is especially critical in case of imbalanced datasets, where one class is represented by a significantly smaller number of instances than the other(s).

When training a classification model on an imbalanced dataset, the model might not learn enough about the minority class, which can lead to poor generalization performance on new data. This happens because the model is biased towards the majority class, and it might even predict all instances as belonging to the majority class.

1.1.1 Stratified splitting

We will use the argument `stratify` to obtain a proportion of 0s and 1s in the `train` and `test` datasets that is similar to the proportion in the complete 'data.

```
#Stratified train-test split
X_train_stratified, X_test_stratified, y_train_stratified,\
y_test_stratified = train_test_split(X, y, test_size = 0.2, random_state = 45, stratify=y)
```

```
#Proportion of 0s and 1s in train data with stratified split
y_train_stratified.value_counts()/y_train.shape
```

```
0    0.651466
1    0.348534
Name: Outcome, dtype: float64
```

```
#Proportion of 0s and 1s in test data with stratified split
y_test_stratified.value_counts()/y_test.shape
```

```
0    0.649351
1    0.350649
Name: Outcome, dtype: float64
```

The proportion of the classes in the stratified split mimics the proportion in the complete dataset more closely.

By using stratified splitting, we ensure that both the `train` and `test` data sets have the same proportion of instances from each class, which means that the model will see enough instances from the minority class during training. This, in turn, helps the model learn to distinguish between the classes better, leading to better performance on new data.

Thus, stratified splitting helps to ensure that the model sees enough instances from each class during training, which can improve the model's ability to generalize to new data, particularly in cases where one class is underrepresented in the dataset.

Let us develop a logistic regression model for predicting if a person has diabetes.

1.2 Scaling data

In certain models, it may be important to scale data for various reasons. In a logistic regression model, scaling can help with model convergence. Scikit-learn uses a method known as gradient-descent *(not in scope of the syllabus of this course)* to obtain a solution. In case the predictors have different orders of magnitude, the algorithm may fail to converge. In such cases, it is useful to standardize the predictors so that all of them are at the same scale.

```
# With linear/logistic regression in scikit-learn, especially when the predictors have diffe
# of magn., scaling is necessary. This is to enable the training algo. which we did not cove
scaler = StandardScaler().fit(X_train)
X_train_scaled = scaler.transform(X_train)
X_test_scaled = scaler.transform(X_test) # Do NOT refit the scaler with the test data, just
```

1.3 Fitting a model

Let us fit a logistic regression model for predicting if a person has diabetes. Let us try fitting a model with the un-scaled data.

```
# Create a model object - not trained yet
logreg = LogisticRegression()

# Train the model
logreg.fit(X_train, y_train)
```

```
C:\Users\akl0407\AppData\Roaming\Python\Python38\site-packages\sklearn\linear_model\_logistic
STOP: TOTAL NO. of ITERATIONS REACHED LIMIT.

Increase the number of iterations (max_iter) or scale the data as shown in:
    https://scikit-learn.org/stable/modules/preprocessing.html
Please also refer to the documentation for alternative solver options:
    https://scikit-learn.org/stable/modules/linear_model.html#logistic-regression
  n_iter_i = _check_optimize_result(
```

```
LogisticRegression()
```

Note that the model with the un-scaled predictors fails to converge. Check out the data `X_train` to see that this may be probably due to the predictors have different orders of magnitude. For example, the predictor `DiabetesPedigreeFunction` has values in [0.078, 2.42], while the predictor `Insulin` has values in [0, 800].

Let us fit the model to the scaled data.

```
# Create a model - not trained yet
logreg = LogisticRegression()

# Train the model
logreg.fit(X_train_scaled, y_train)
```

```
LogisticRegression()
```

The model converges to a solution with the scaled data!

The coefficients of the model can be returned with the `coef_` attribute of the `LogisticRegression()` object. However, the output is not as well formatted as in the case of the `statsmodels` library since `sklearn` is developed primarily for the purpose of prediction, and not inference.

```
# Use coef_ to return the coefficients - only log reg inference you can do with sklearn
print(logreg.coef_)
```

```
[[ 0.32572891  1.20110566 -0.32046591  0.06849882 -0.21727131  0.72619528
   0.40088897  0.29698818]]
```

1.4 Computing performance metrics

1.4.1 Accuracy

Let us test the model prediction accuracy on the test data. We'll demonstrate two different functions that can be used to compute model accuracy - `accuracy_score()`, and `score()`.

The `accuracy_score()` function from the `metrics` module of the `sklearn` library is general, and can be used for any classification model. We'll use it along with the `predict()` method of the `LogisticRegression()` object, which returns the predicted class based on a threshold probability of 0.5.

```
# Get the predicted classes first
y_pred = logreg.predict(X_test_scaled)

# Use the predicted and true classes for accuracy
print(accuracy_score(y_pred, y_test)*100)
```

```
73.37662337662337
```

The `score()` method of the `LogisticRegression()` object can be used to compute the accuracy only for a logistic regression model. Note that for a `LinearRegression()` object, the `score()` method will return the model R-squared.

```
# Use .score with test predictors and response to get the accuracy
# Implements the same thing under the hood
print(logreg.score(X_test_scaled, y_test)*100)
```

```
73.37662337662337
```

1.4.2 ROC-AUC

The `roc_curve()` and `auc()` functions from the `metrics` module of the `sklearn` library can be used to compute the ROC-AUC, or the area under the ROC curve. Note that for computing ROC-AUC, we need the predicted probability, instead of the predicted class. Thus, we'll use the `predict_proba()` method of the `LogisticRegression()` object, which returns the predicted probability for the observation to belong to each of the classes, instead of using the `predict()` method, which returns the predicted class based on threshold probability of 0.5.

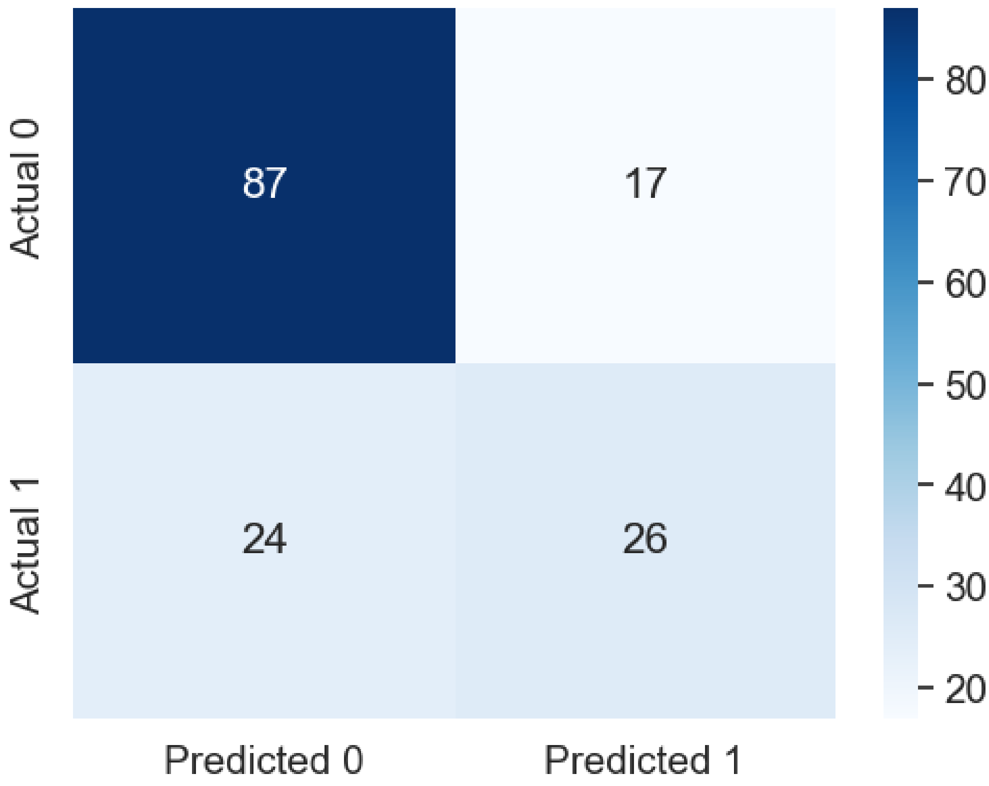
```
#Computing the predicted probability for the observation to belong to the positive class (y=
#The 2nd column in the output of predict_proba() consists of the probability of the observati
#belong to the positive class (y=1)
y_pred_prob = logreg.predict_proba(X_test_scaled)[:,1]

#Using the predicted probability computed above to find ROC-AUC
fpr, tpr, auc_thresholds = roc_curve(y_test, y_pred_prob)
print(auc(fpr, tpr))# AUC of ROC
```

```
0.7923076923076922
```

1.4.3 Confusion matrix & precision-recall

The `confusion_matrix()`, `precision_score()`, and `recall_score()` functions from the `metrics` module of the `sklearn` library can be used to compute the confusion matrix, precision, and recall respectively.

```
#Confusion matrix
cm = pd.DataFrame(confusion_matrix(y_test, y_pred), columns=['Predicted 0', 'Predicted 1'],
            index = ['Actual 0', 'Actual 1'])
sns.heatmap(cm, annot=True, cmap='Blues', fmt='g');
```




```
print("Precision: ", precision_score(y_test, y_pred))
print("Recall: ", recall_score(y_test, y_pred))
```

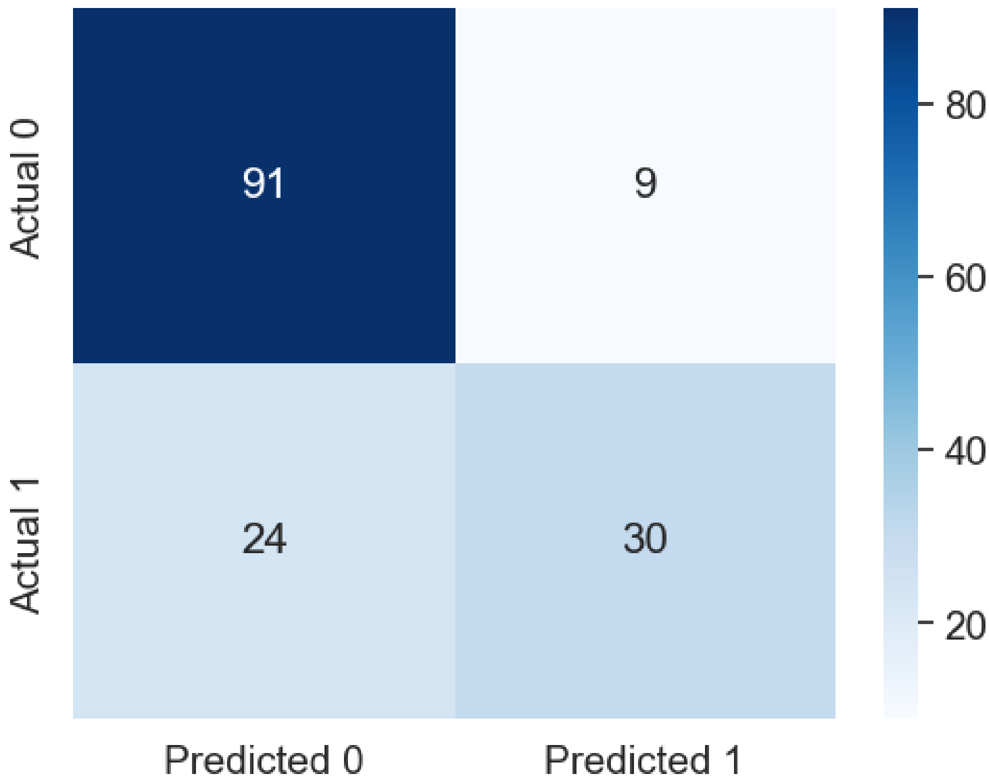
```
Precision:  0.6046511627906976
Recall:  0.52
```

Let us compute the performance metrics if we develop the model using stratified splitting.

```
# Developing the model with stratified splitting

#Scaling data
scaler = StandardScaler().fit(X_train_stratified)
X_train_stratified_scaled = scaler.transform(X_train_stratified)
X_test_stratified_scaled = scaler.transform(X_test_stratified)

# Training the model
logreg.fit(X_train_stratified_scaled, y_train_stratified)
```

```
#Computing the accuracy
y_pred_stratified = logreg.predict(X_test_stratified_scaled)
print("Accuracy: ",accuracy_score(y_pred_stratified, y_test_stratified)*100)

#Computing the ROC-AUC
y_pred_stratified_prob = logreg.predict_proba(X_test_stratified_scaled)[:,1]
fpr, tpr, auc_thresholds = roc_curve(y_test_stratified, y_pred_stratified_prob)
print("ROC-AUC: ",auc(fpr, tpr))# AUC of ROC

#Computing the precision and recall
print("Precision: ", precision_score(y_test_stratified, y_pred_stratified))
print("Recall: ", recall_score(y_test_stratified, y_pred_stratified))

#Confusion matrix
cm = pd.DataFrame(confusion_matrix(y_test_stratified, y_pred_stratified), columns=['Predicte
            index = ['Actual 0', 'Actual 1'])
sns.heatmap(cm, annot=True, cmap='Blues', fmt='g');
```

```
Accuracy:  78.57142857142857
ROC-AUC:  0.8505555555555556
Precision:  0.7692307692307693
Recall:  0.5555555555555556
```



The model with the stratified train-test split has a better performance as compared to the other model on all the performance metrics!

1.5 Tuning the model hyperparameters

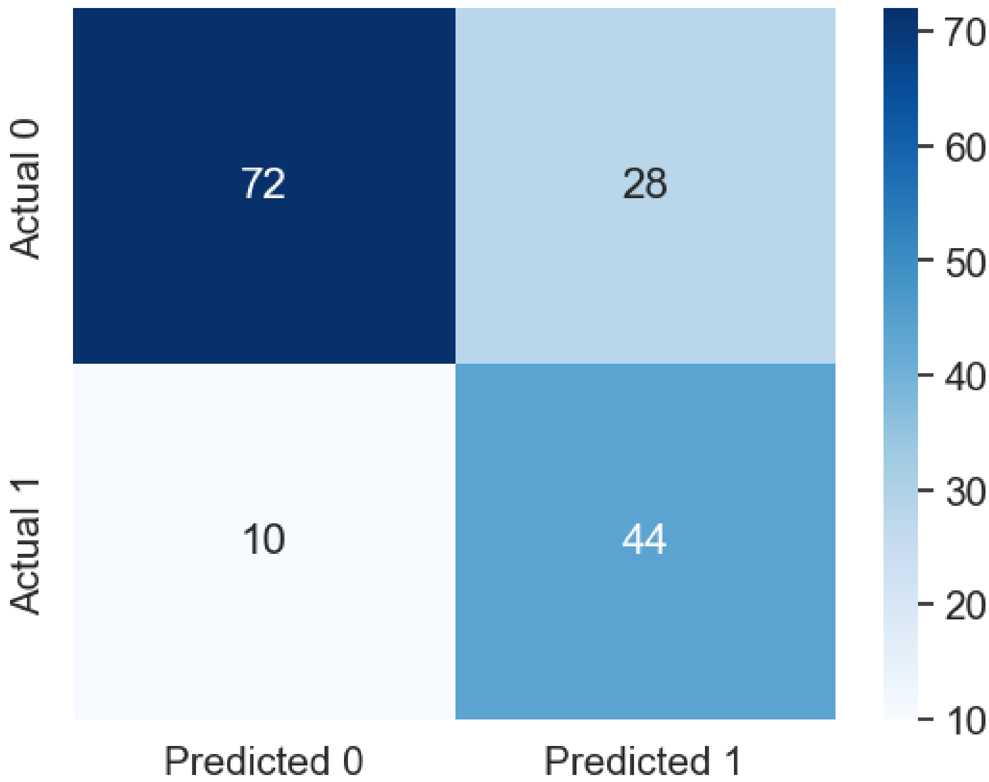
A hyperparameter (among others) that can be trained in a logistic regression model is the regularization parameter.

We may also wish to tune the decision threshold probability. Note that the decision threshold probability is not considered a hyperparameter of the model. Hyperparameters are model parameters that are set prior to training and cannot be directly adjusted by the model during training. Examples of hyperparameters in a logistic regression model include the regularization parameter, and the type of shrinkage penalty - lasso / ridge. These hyperparameters are typically optimized through a separate tuning process, such as cross-validation or grid search, before training the final model.

The performance metrics can be computed using a desired value of the threshold probability. Let us compute the performance metrics for a desired threshold probability of 0.3.

```python
# Performance metrics computation for a desired threshold probability of 0.3
desired_threshold = 0.3

# Classifying observations in the positive class (y = 1) if the predicted probability is grea
# than the desired decision threshold probability
y_pred_desired_threshold = y_pred_stratified_prob > desired_threshold
y_pred_desired_threshold = y_pred_desired_threshold.astype(int)

#Computing the accuracy
print("Accuracy: ",accuracy_score(y_pred_desired_threshold, y_test_stratified)*100)

#Computing the ROC-AUC
fpr, tpr, auc_thresholds = roc_curve(y_test_stratified, y_pred_stratified_prob)
print("ROC-AUC: ",auc(fpr, tpr))# AUC of ROC

#Computing the precision and recall
print("Precision: ", precision_score(y_test_stratified, y_pred_desired_threshold))
print("Recall: ", recall_score(y_test_stratified, y_pred_desired_threshold))

#Confusion matrix
cm = pd.DataFrame(confusion_matrix(y_test_stratified, y_pred_desired_threshold),
                  columns=['Predicted 0', 'Predicted 1'], index = ['Actual 0', 'Actual 1'])
sns.heatmap(cm, annot=True, cmap='Blues', fmt='g');
```

```
Accuracy:  75.32467532467533
ROC-AUC:  0.8505555555555556
Precision:  0.6111111111111112
Recall:  0.8148148148148148
```



1.5.1 Tuning decision threshold probability

Suppose we wish to find the optimal decision threshold probability to maximize accuracy. Note that we cannot use the test dataset to optimize model hyperparameters, as that may lead to overfitting on the test data. We'll use K-fold cross validation on train data to find the optimal decision threshold probability.

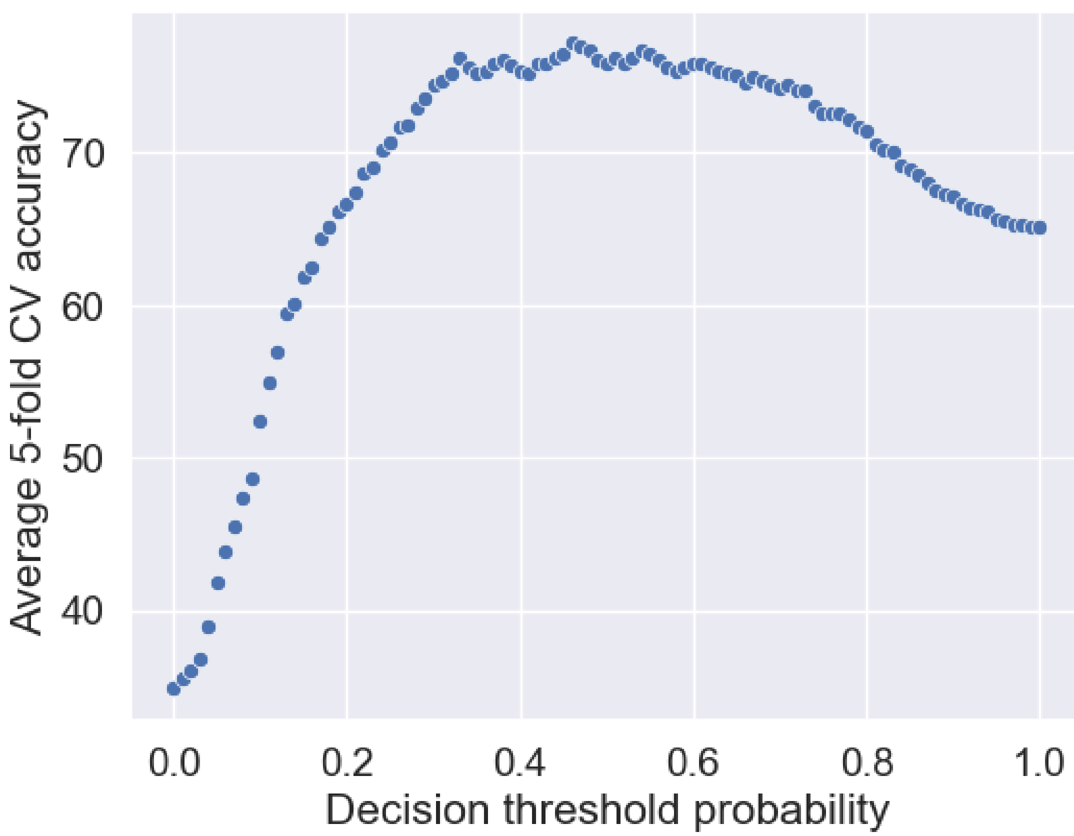
We'll use the `cross_val_predict()` function from the `model_selection` module of `sklearn` to compute the K-fold cross validated predicted probabilities. Note that this function simplifies the task of manually creating the K-folds, training the model K-times, and computing the predicted probabilities on each of the K-folds. Thereafter, the predicted probabilities will be used to find the optimal threshold probability that maximizes the classification accuracy.

```
hyperparam_vals = np.arange(0,1.01,0.01)
accuracy_iter = []

predicted_probability = cross_val_predict(LogisticRegression(), X_train_stratified_scaled,
                                          y_train_stratified, cv = 5, method = 'predict_
```

```
for threshold_prob in hyperparam_vals:
    predicted_class = predicted_probability[:,1] > threshold_prob
    predicted_class = predicted_class.astype(int)

    #Computing the accuracy
    accuracy = accuracy_score(predicted_class, y_train_stratified)*100
    accuracy_iter.append(accuracy)
```

Let us visualize the accuracy with change in decision threshold probability.

```
# Accuracy vs decision threshold probability
sns.scatterplot(x = hyperparam_vals, y = accuracy_iter)
plt.xlabel('Decision threshold probability')
plt.ylabel('Average 5-fold CV accuracy');
```



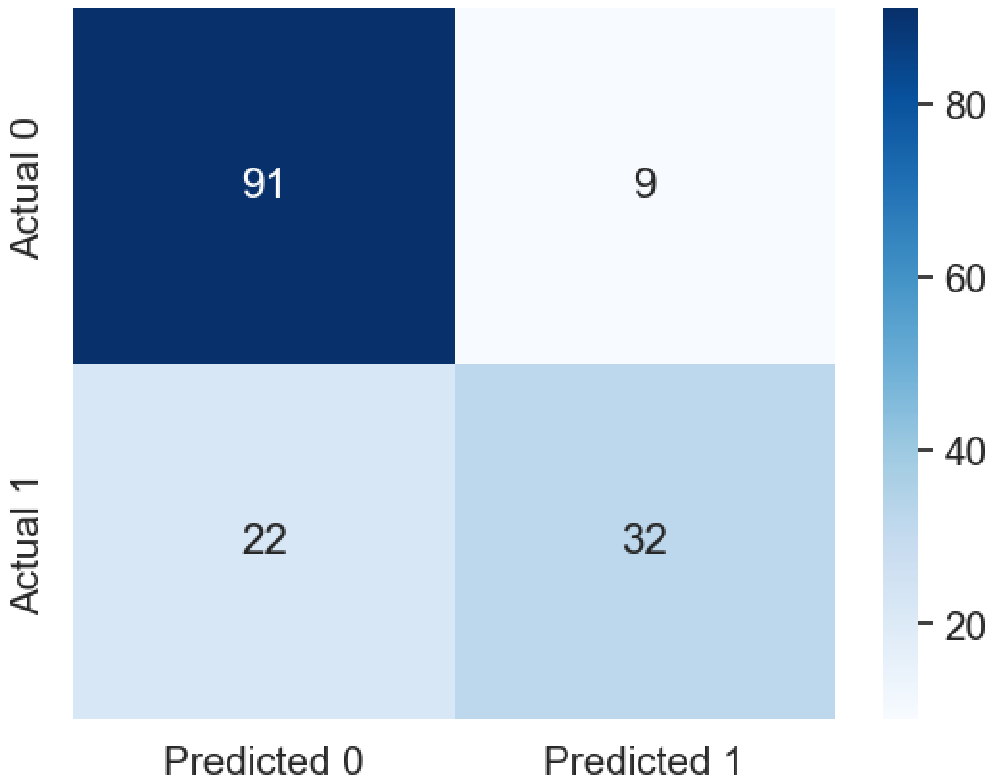
The optimal decision threshold probability is the one that maximizes the K-fold cross validation accuracy.

```
# Optimal decision threshold probability
hyperparam_vals[accuracy_iter.index(max(accuracy_iter))]
```

```
0.46
```

```
# Performance metrics computation for the optimum decision threshold probability
desired_threshold = 0.46

# Classifying observations in the positive class (y = 1) if the predicted probability is grea
# than the desired decision threshold probability
y_pred_desired_threshold = y_pred_stratified_prob > desired_threshold
y_pred_desired_threshold = y_pred_desired_threshold.astype(int)

#Computing the accuracy
print("Accuracy: ",accuracy_score(y_pred_desired_threshold, y_test_stratified)*100)

#Computing the ROC-AUC
fpr, tpr, auc_thresholds = roc_curve(y_test_stratified, y_pred_stratified_prob)
print("ROC-AUC: ",auc(fpr, tpr))# AUC of ROC

#Computing the precision and recall
print("Precision: ", precision_score(y_test_stratified, y_pred_desired_threshold))
print("Recall: ", recall_score(y_test_stratified, y_pred_desired_threshold))

#Confusion matrix
cm = pd.DataFrame(confusion_matrix(y_test_stratified, y_pred_desired_threshold),
                  columns=['Predicted 0', 'Predicted 1'], index = ['Actual 0', 'Actual 1'])
sns.heatmap(cm, annot=True, cmap='Blues', fmt='g');
```

```
Accuracy:  79.87012987012987
ROC-AUC:  0.8505555555555556
Precision:  0.7804878048780488
Recall:  0.5925925925925926
```



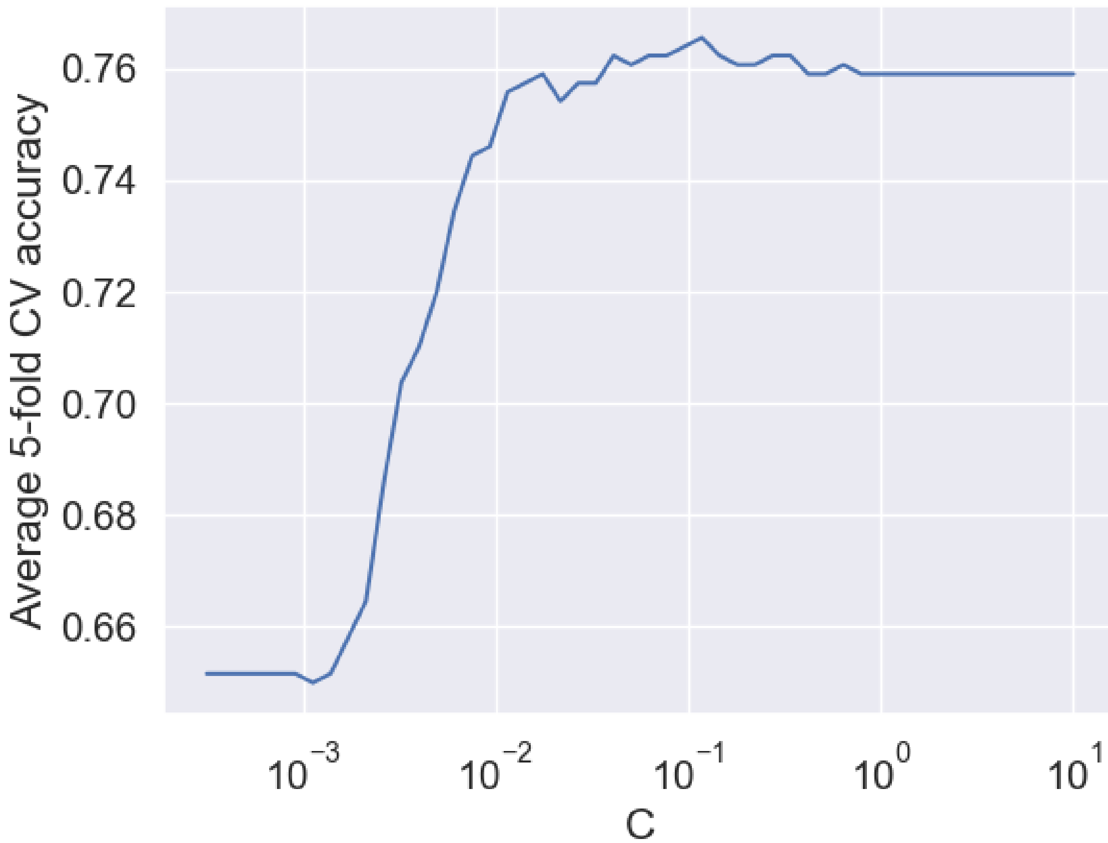
Model performance on test data has improved with the optimal decision threshold probability.

1.5.2 Tuning the regularization parameter

The `LogisticRegression()` method has a default *L2* regularization penalty, which means ridge regression.`C` is $1/\lambda$, where λ is the hyperparameter that is multiplied with the ridge penalty. `C` is 1 by default.

```
accuracy_iter = []
hyperparam_vals = 10**np.linspace(-3.5, 1)

for c_val in hyperparam_vals: # For each possible C value in your grid
    logreg_model = LogisticRegression(C=c_val) # Create a model with the C value

    accuracy_iter.append(cross_val_score(logreg_model, X_train_stratified_scaled, y_train_st
                                      scoring='accuracy', cv=5)) # Find the cv results
```

```
plt.plot(hyperparam_vals, np.mean(np.array(accuracy_iter), axis=1))
plt.xlabel('C')
plt.ylabel('Average 5-fold CV accuracy')
plt.xscale('log')
plt.show()
```



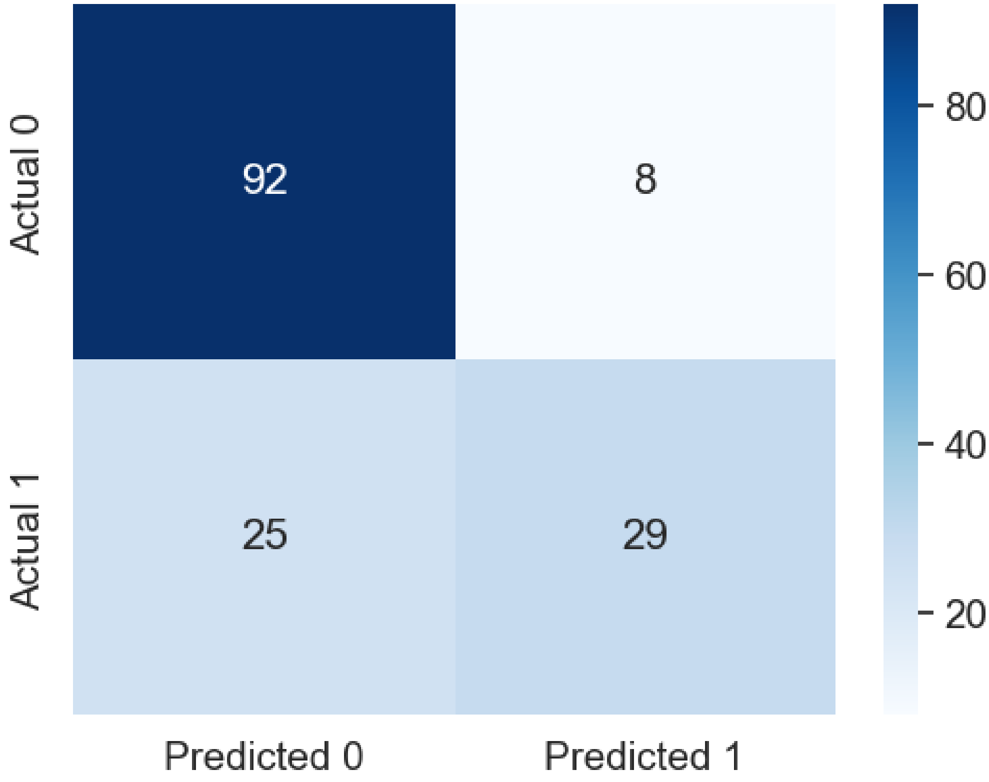

```
# Optimal value of the regularization parameter 'C'
optimal_C = hyperparam_vals[np.argmax(np.array(accuracy_iter).mean(axis=1))]
optimal_C
```

```
0.11787686347935879
```

```
# Developing the model with stratified splitting and optimal 'C'

#Scaling data
```

```
scaler = StandardScaler().fit(X_train_stratified)
X_train_stratified_scaled = scaler.transform(X_train_stratified)
X_test_stratified_scaled = scaler.transform(X_test_stratified)

# Training the model
logreg = LogisticRegression(C = optimal_C)
logreg.fit(X_train_stratified_scaled, y_train_stratified)

#Computing the accuracy
y_pred_stratified = logreg.predict(X_test_stratified_scaled)
print("Accuracy: ",accuracy_score(y_pred_stratified, y_test_stratified)*100)

#Computing the ROC-AUC
y_pred_stratified_prob = logreg.predict_proba(X_test_stratified_scaled)[:,1]
fpr, tpr, auc_thresholds = roc_curve(y_test_stratified, y_pred_stratified_prob)
print("ROC-AUC: ",auc(fpr, tpr))# AUC of ROC

#Computing the precision and recall
print("Precision: ", precision_score(y_test_stratified, y_pred_stratified))
print("Recall: ", recall_score(y_test_stratified, y_pred_stratified))

#Confusion matrix
cm = pd.DataFrame(confusion_matrix(y_test_stratified, y_pred_stratified), columns=['Predicte
            index = ['Actual 0', 'Actual 1'])
sns.heatmap(cm, annot=True, cmap='Blues', fmt='g');
```

```
Accuracy:  78.57142857142857
ROC-AUC:  0.8516666666666666
Precision:  0.7837837837837838
Recall:  0.5370370370370371
```



1.5.3 Tuning the decision threshold probability and the regularization parameter simultaneously

```
threshold_hyperparam_vals = np.arange(0,1.01,0.01)
C_hyperparam_vals = 10**np.linspace(-3.5, 1)
accuracy_iter = pd.DataFrame({'threshold':[], 'C':[], 'accuracy':[]})
iter_number = 0

for c_val in C_hyperparam_vals:
    predicted_probability = cross_val_predict(LogisticRegression(C = c_val), X_train_stratifi
                                              y_train_stratified, cv = 5, method = 'predi

    for threshold_prob in threshold_hyperparam_vals:
        predicted_class = predicted_probability[:,1] > threshold_prob
        predicted_class = predicted_class.astype(int)

        #Computing the accuracy
```

```
        accuracy = accuracy_score(predicted_class, y_train_stratified)*100
        accuracy_iter.loc[iter_number, 'threshold'] = threshold_prob
        accuracy_iter.loc[iter_number, 'C'] = c_val
        accuracy_iter.loc[iter_number, 'accuracy'] = accuracy
        iter_number = iter_number + 1
```

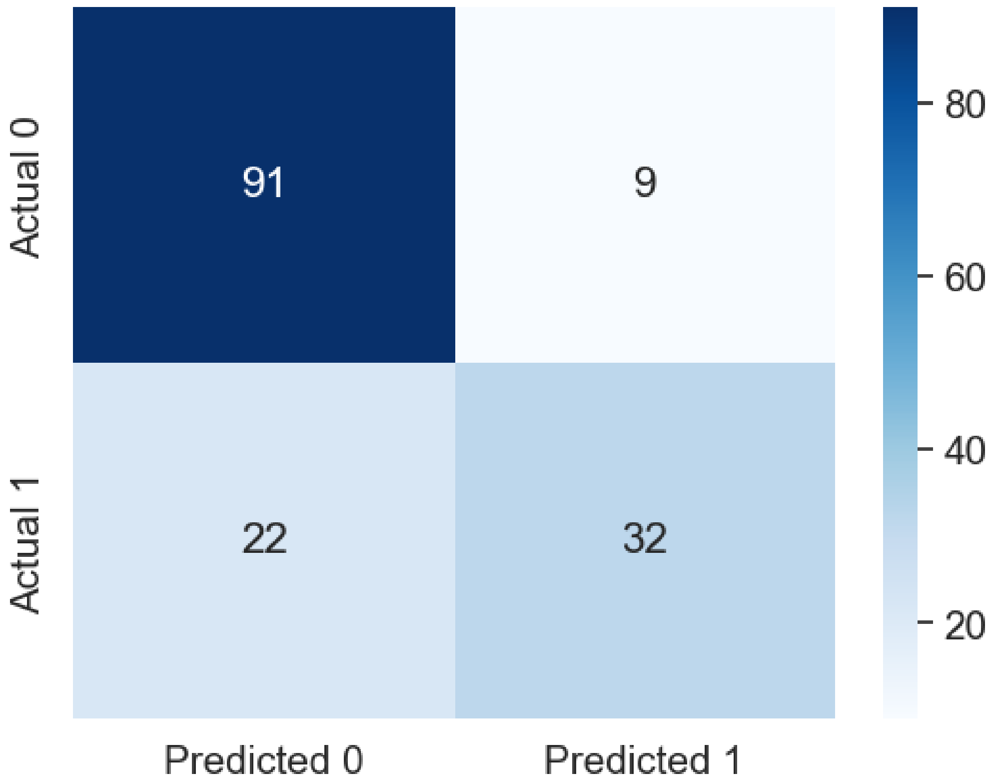
```
# Parameters for highest accuracy
optimal_C = accuracy_iter.sort_values(by = 'accuracy', ascending = False).iloc[0,:]['C']
optimal_threshold = accuracy_iter.sort_values(by = 'accuracy', ascending = False).iloc[0, :]

#Optimal decision threshold probability
print("Optimal decision threshold = ", optimal_threshold)

#Optimal C
print("Optimal C = ", optimal_C)
```

```
Optimal decision threshold =  0.46
Optimal C =  4.291934260128778
```

```
# Developing the model with stratified splitting, optimal decision threshold probability, and

#Scaling data
scaler = StandardScaler().fit(X_train_stratified)
X_train_stratified_scaled = scaler.transform(X_train_stratified)
X_test_stratified_scaled = scaler.transform(X_test_stratified)

# Training the model
logreg = LogisticRegression(C = optimal_C)
logreg.fit(X_train_stratified_scaled, y_train_stratified)

# Performance metrics computation for the optimal threshold probability
y_pred_stratified_prob = logreg.predict_proba(X_test_stratified_scaled)[:,1]

# Classifying observations in the positive class (y = 1) if the predicted probability is grea
# than the desired decision threshold probability
y_pred_desired_threshold = y_pred_stratified_prob > optimal_threshold
y_pred_desired_threshold = y_pred_desired_threshold.astype(int)

#Computing the accuracy
print("Accuracy: ",accuracy_score(y_pred_desired_threshold, y_test_stratified)*100)
```

```
#Computing the ROC-AUC
fpr, tpr, auc_thresholds = roc_curve(y_test_stratified, y_pred_stratified_prob)
print("ROC-AUC: ",auc(fpr, tpr))# AUC of ROC

#Computing the precision and recall
print("Precision: ", precision_score(y_test_stratified, y_pred_desired_threshold))
print("Recall: ", recall_score(y_test_stratified, y_pred_desired_threshold))

#Confusion matrix
cm = pd.DataFrame(confusion_matrix(y_test_stratified, y_pred_desired_threshold), columns=['Pr
            index = ['Actual 0', 'Actual 1'])
sns.heatmap(cm, annot=True, cmap='Blues', fmt='g');
```

```
Accuracy:  79.87012987012987
ROC-AUC:  0.8509259259259259
Precision:  0.7804878048780488
Recall:  0.5925925925925926
```



Later in the course, we'll see the `sklearn` function `GridSearchCV`, which is used to optimize several model hyperparameters simultaneously with K-fold cross validation, while avoiding `for` loops.

2 Bias-variance tradeoff

Read section 2.2.2 of the book before using these notes.

Note that in this course, lecture notes are not sufficient, you must read the book for better understanding. Lecture notes are just implementing the concepts of the book on a dataset, but not explaining the concepts elaborately.

In this chapter, we will show that a flexible model is likely to have high variance and low bias, while a relatively less flexible model is likely to have a high bias and low variance.

The examples considered below are motivated from the examples shown in the documentation of the bias_variance_decomp() function from the `mlxtend` library. We will first manually compute the bias and variance for understanding of the concept. Later, we will show application of the `bias_variance_decomp()` function to estimate bias and variance.

```
# Importing necessary libraries
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_squared_error
from sklearn.tree import DecisionTreeRegressor
sns.set(font_scale=1.35)
```

2.1 Simple model (Less flexible)

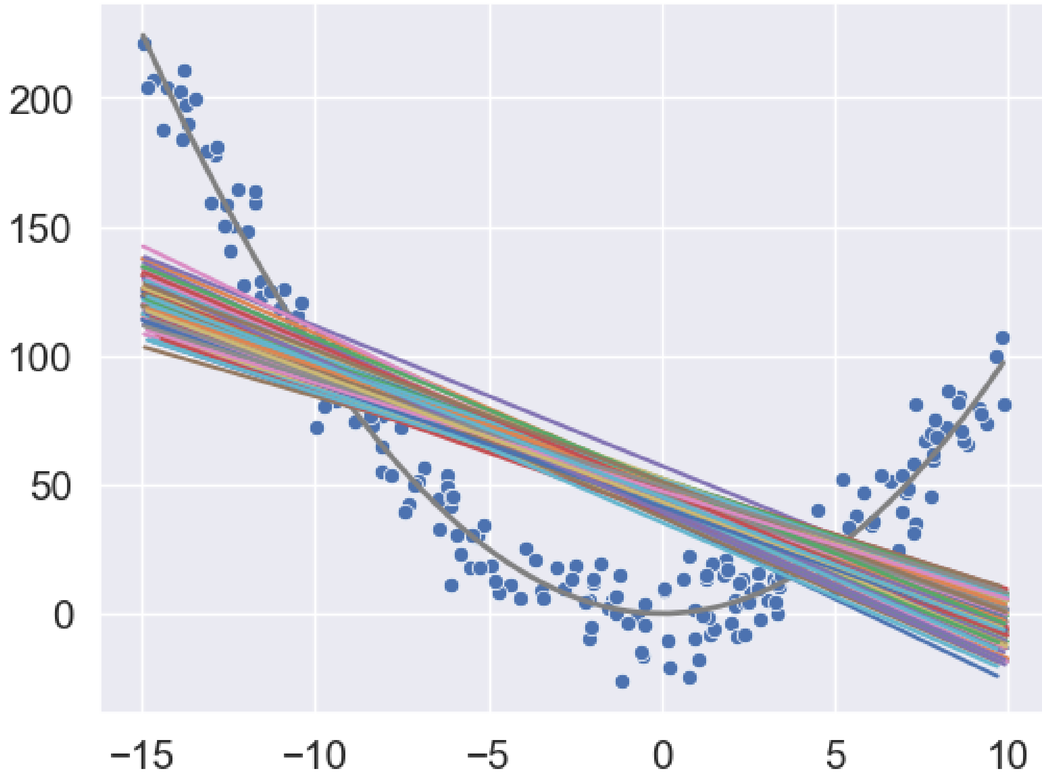
Let us consider a linear regression model as the less-flexible *(or relatively simple)* model.

We will first simulate the test dataset for which we will compute the bias and variance.

```
np.random.seed(101)

# Simulating predictor values of test data
xtest = np.random.uniform(-15, 10, 200)
```

```
# Assuming the true mean response is square of the predictor value
fxtest = xtest**2

# Simulating test response by adding noise to the true mean response
ytest = fxtest + np.random.normal(0, 10, 200)

# We will find bias and variance using a linear regression model for prediction
model = LinearRegression()
```

```
# Visualizing the data and the true mean response
sns.scatterplot(x = xtest, y = ytest)
sns.lineplot(x = xtest, y = fxtest, color = 'grey', linewidth = 2)

# Initializing objects to store predictions and mean squared error
# of 100 models developed on 100 distinct training datasets samples
pred_test = []; mse_test = []

# Iterating over each of the 100 models
for i in range(100):
    np.random.seed(i)

    # Simulating the ith training data
    x = np.random.uniform(-15, 10, 200)
    fx = x**2
    y = fx + np.random.normal(0, 10, 200)

    # Fitting the ith model on the ith training data
    model.fit(x.reshape(-1,1), y)

    # Plotting the ith model
    sns.lineplot(x = x, y = model.predict(x.reshape(-1,1)))

    # Storing the predictions of the ith model on test data
    pred_test.append(model.predict(xtest.reshape(-1,1)))

    # Storing the mean squared error of the ith model on test data
    mse_test.append(mean_squared_error(model.predict(xtest.reshape(-1,1)), ytest))
```



The above plots show that the 100 models seem to have low variance, but high bias. Note that the bias is low only around a couple of points *(x = -10 & x = 5)*.

Let us compute the average squared bias over all the test data points.

```
mean_pred = np.array(pred_test).mean(axis = 0)
sq_bias = ((mean_pred - fxtest)**2).mean()
sq_bias
```

```
2042.104126728109
```

Let us compute the average variance over all the test data points.

```
mean_var = np.array(pred_test).var(axis = 0).mean()
mean_var
```

```
28.37397844429763
```

Let us compute the mean squared error over all the test data points.

```
np.array(mse_test).mean()
```

```
2201.957555529835
```

Note that the mean squared error should be the same as the sum of squared bias, variance, and irreducible error.

The sum of squared bias, model variance, and irreducible error is:

```
sq_bias + mean_var + 100
```

```
2170.4781051724067
```

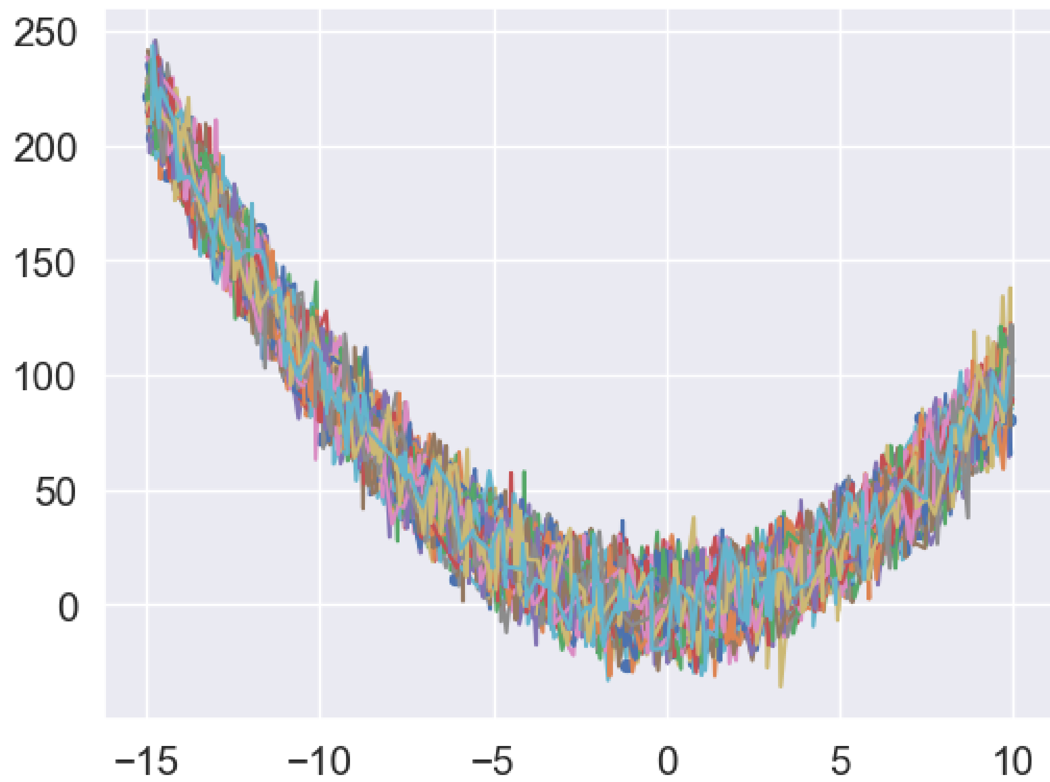
Note that this is approximately, but not exactly, the same as the mean squared error computed above as we are developing a finite number of models, and making predictions on a finite number of test data points.

2.2 Complex model (more flexible)

Let us consider a decion tree as the more flexible model.

```
np.random.seed(101)
xtest = np.random.uniform(-15, 10, 200)
fxtest = xtest**2
ytest = fxtest + np.random.normal(0, 10, 200)
model = DecisionTreeRegressor()
```

```
sns.scatterplot(x = xtest, y = ytest)
sns.lineplot(x = xtest, y = fxtest, color = 'grey', linewidth = 2)
pred_test = []; mse_test = []
for i in range(100):
    np.random.seed(i)
    x = np.random.uniform(-15, 10, 200)
    fx = x**2
    y = fx + np.random.normal(0, 10, 200)
    model.fit(x.reshape(-1,1), y)
    sns.lineplot(x = x, y = model.predict(x.reshape(-1,1)))
    pred_test.append(model.predict(xtest.reshape(-1,1)))
    mse_test.append(mean_squared_error(model.predict(xtest.reshape(-1,1)), ytest))
```



The above plots show that the 100 models seem to have high variance, but low bias.

Let us compute the average squared bias over all the test data points.

```
mean_pred = np.array(pred_test).mean(axis = 0)
sq_bias = ((mean_pred - fxtest)**2).mean()
sq_bias
```

```
1.3117561629333938
```

Let us compute the average model variance over all the test data points.

```
mean_var = np.array(pred_test).var(axis = 0).mean()
mean_var
```

```
102.5226748977198
```

Let us compute the average mean squared error over all the test data points.

```
np.array(mse_test).mean()
```

```
225.92027460924726
```

Note that the above error is approximately the same as the sum of the squared bias, model variance and the irreducible error.

Note that the relatively more flexible model has a higher variance, but lower bias as compared to the less flexible linear model. This will typically be the case, but may not be true in all scenarios. We will discuss one such scenario later.

3 KNN

Read section 4.7.6 of the book before using these notes.

Note that in this course, lecture notes are not sufficient, you must read the book for better understanding. Lecture notes are just implementing the concepts of the book on a dataset, but not explaining the concepts elaborately.

```
# Importing necessary libraries
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
sns.set(font_scale=1.35)

from sklearn.preprocessing import StandardScaler
from sklearn.neighbors import KNeighborsRegressor, KNeighborsClassifier
from sklearn.metrics import mean_squared_error
from sklearn.model_selection import cross_val_score, GridSearchCV, cross_val_predict, KFold,
```

3.1 KNN for regression

```
#Using the same datasets as used for linear regression in STAT303-2,
#so that we can compare the non-linear models with linear regression
trainf = pd.read_csv('./Datasets/Car_features_train.csv')
trainp = pd.read_csv('./Datasets/Car_prices_train.csv')
testf = pd.read_csv('./Datasets/Car_features_test.csv')
testp = pd.read_csv('./Datasets/Car_prices_test.csv')
train = pd.merge(trainf,trainp)
test = pd.merge(testf,testp)
train.head()
```

	carID	brand	model	year	transmission	mileage	fuelType	tax	mpg	engineSize	price
0	18473	bmw	6 Series	2020	Semi-Auto	11	Diesel	145	53.3282	3.0	37980
1	15064	bmw	6 Series	2019	Semi-Auto	10813	Diesel	145	53.0430	3.0	33980
2	18268	bmw	6 Series	2020	Semi-Auto	6	Diesel	145	53.4379	3.0	36850
3	18480	bmw	6 Series	2017	Semi-Auto	18895	Diesel	145	51.5140	3.0	25998
4	18492	bmw	6 Series	2015	Automatic	62953	Diesel	160	51.4903	3.0	18990

```
predictors = ['mpg', 'engineSize', 'year', 'mileage']

X_train = train[predictors]
y_train = train['price']

X_test = test[predictors]
y_test = test['price']
```

Let us scale data as we are using KNN.

3.1.1 Scaling data

```
# Scale
sc = StandardScaler()

sc.fit(X_train)
X_train_scaled = sc.transform(X_train)
X_test_scaled = sc.transform(X_test)
```

Let fit the model and compute the RMSE on test data. If the number of neighbors is not specified, the default value is taken.

3.1.2 Fitting and validating model

```
knn_model = KNeighborsRegressor()

knn_model.fit(X_train_scaled, (y_train))

y_pred = knn_model.predict(X_test_scaled)
y_pred_train = knn_model.predict(X_train_scaled)
```

```
mean_squared_error(y_test, (y_pred), squared=False)
```

```
6329.691192885354
```

```
knn_model2 = KNeighborsRegressor(n_neighbors = 5, weights='distance') # Default weights is un

knn_model2.fit(X_train_scaled, y_train)

y_pred = knn_model2.predict(X_test_scaled)

mean_squared_error(y_test, y_pred, squared=False)
```

```
6063.327598353961
```

The model seems to fit better than all the linear models in STAT303-2.

3.1.3 Hyperparameter tuning

We will use cross-validation to find the optimal value of the hyperparameter `n_neighbors`.

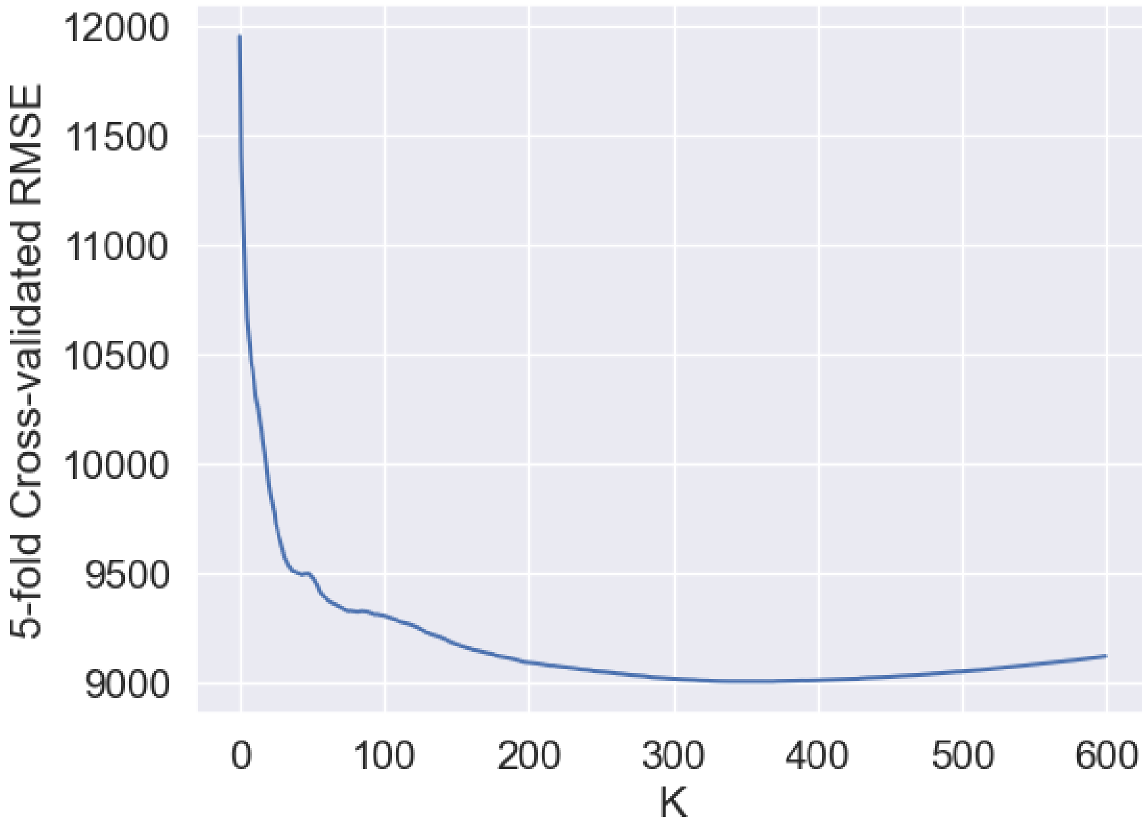
```
Ks = np.arange(1,601)

cv_scores = []

for K in Ks:
    model = KNeighborsRegressor(n_neighbors = K, weights='distance')
    score = cross_val_score(model, X_train_scaled, y_train, cv=5, scoring = 'neg_root_mean_sq
    cv_scores.append(score)
```

```
np.array(cv_scores).shape
# Each row is a K
```

```
(600, 5)
```

```
cv_scores_array = np.array(cv_scores)

avg_cv_scores = -cv_scores_array.mean(axis=1)
```

```
sns.lineplot(x = range(600), y = avg_cv_scores);
plt.xlabel('K')
plt.ylabel('5-fold Cross-validated RMSE');
```




```
avg_cv_scores.min() # Best CV score

Ks[avg_cv_scores.argmin()] # Best hyperparam value
```

```
366
```

The optimal hyperparameter value is 366. Does it seem to be too high?

```
best_model = KNeighborsRegressor(n_neighbors = Ks[avg_cv_scores.argmin()], weights='distance

best_model.fit(X_train_scaled, y_train)
```

```
y_pred = best_model.predict(X_test_scaled)

mean_squared_error(y_test, y_pred, squared=False)
```

```
7724.452068618346
```

The test error with the optimal hyperparameter value based on cross-validation is much higher than that based on the default value of the hyperparameter. Why is that?

Sometimes this may happen by chance due to the specific observations in the k folds. One option is to shuffle the dataset before splitting into folds.

The function `KFold()` can be used to shuffle the data before splitting it into folds.

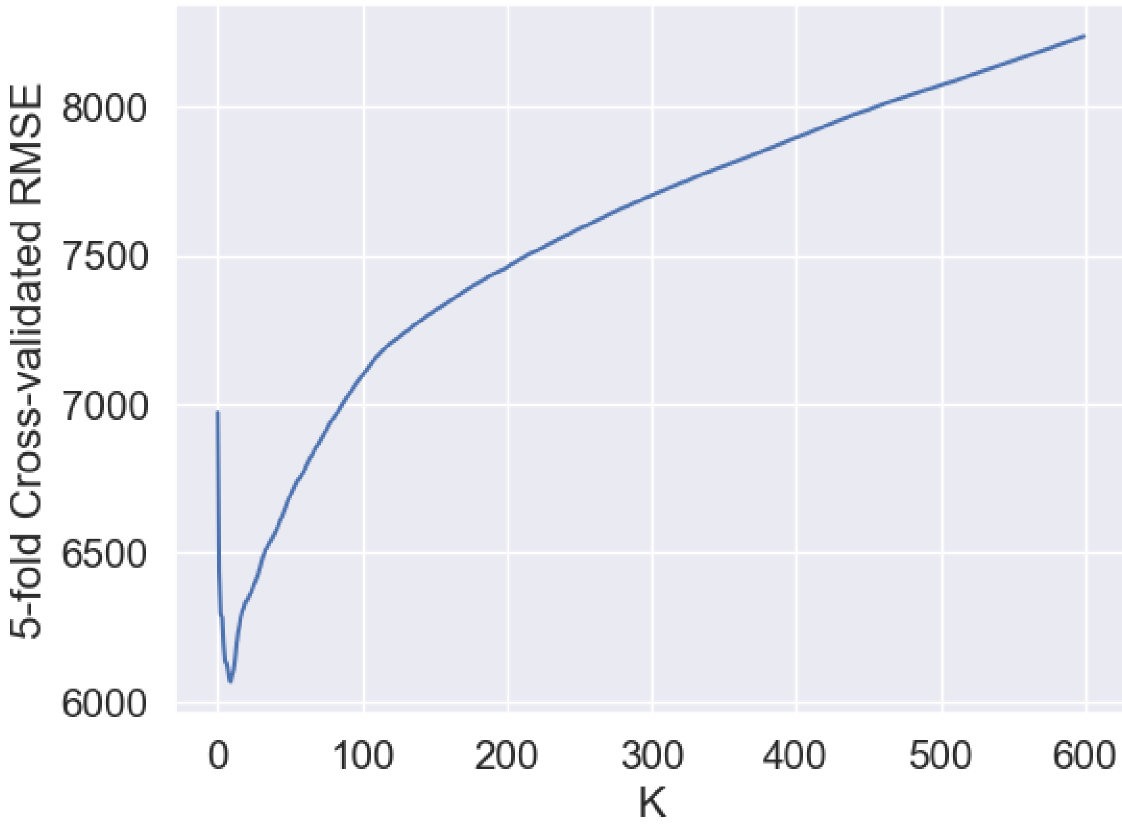
3.1.3.1 `KFold()`

```
kcv = KFold(n_splits = 5, shuffle = True, random_state = 1)
```

Now, let us again try to find the opimal K for KNN, using the new folds, based on shuffled data.

```
Ks = np.arange(1,601)

cv_scores = []

for K in Ks:
    model = KNeighborsRegressor(n_neighbors = K, weights='distance')
    score = cross_val_score(model, X_train_scaled, y_train, cv = kcv, scoring = 'neg_root_mea
    cv_scores.append(score)
```

```
cv_scores_array = np.array(cv_scores)
avg_cv_scores = -cv_scores_array.mean(axis=1)
sns.lineplot(x = range(600), y = avg_cv_scores);
plt.xlabel('K')
plt.ylabel('5-fold Cross-validated RMSE');
```



The optimal K is:

```
Ks[avg_cv_scores.argmin()]
```

```
10
```

RMSE on test data with this optimal value of K is:

```
knn_model2 = KNeighborsRegressor(n_neighbors = 10, weights='distance') # Default weights is u
knn_model2.fit(X_train_scaled, y_train)
y_pred = knn_model2.predict(X_test_scaled)
mean_squared_error(y_test, y_pred, squared=False)
```

```
6043.889393238132
```

In order to avoid these errors due the specific observations in the k folds, it will be better to repeat the k-fold cross-validation multiple times, where the data is shuffled after each k-fold cross-validation, so that the cross-validation takes place on new folds for each repetition.

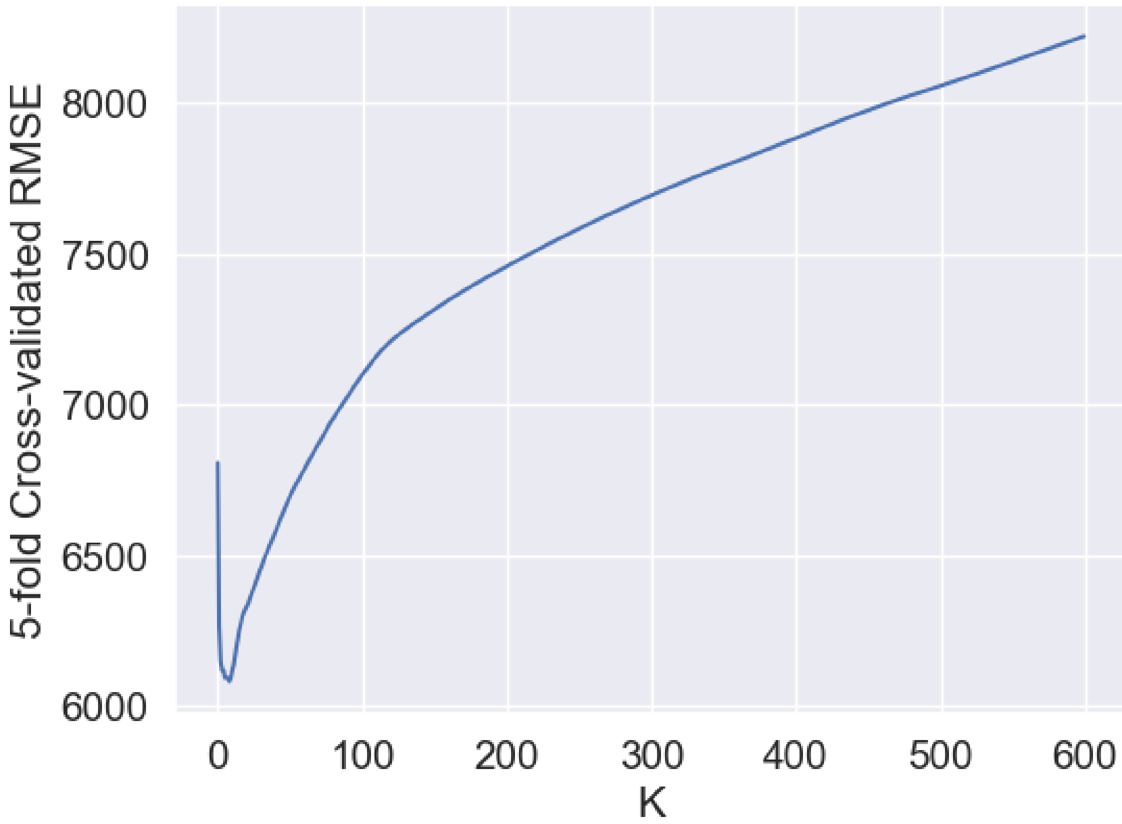
The function `RepeatedKFold()` repeats k-fold cross validation multiple times *(10 times by default)*. Let us use it to have a more robust optimal value of the number of neighbors K.

3.1.3.2 `RepeatedKFold()`

```
kcv = RepeatedKFold(n_splits = 5, random_state = 1)
```

```
Ks = np.arange(1,601)

cv_scores = []

for K in Ks:
    model = KNeighborsRegressor(n_neighbors = K, weights='distance')
    score = cross_val_score(model, X_train_scaled, y_train, cv = kcv, scoring = 'neg_root_mea
    cv_scores.append(score)
```

```
cv_scores_array = np.array(cv_scores)
avg_cv_scores = -cv_scores_array.mean(axis=1)
sns.lineplot(x = range(600), y = avg_cv_scores);
plt.xlabel('K')
plt.ylabel('5-fold Cross-validated RMSE');
```



The optimal K is:

```
Ks[avg_cv_scores.argmin()]
```

```
9
```

RMSE on test data with this optimal value of K is:

```
knn_model2 = KNeighborsRegressor(n_neighbors = 9, weights='distance') # Default weights is ur
knn_model2.fit(X_train_scaled, y_train)
y_pred = knn_model2.predict(X_test_scaled)
mean_squared_error(y_test, y_pred, squared=False)
```

```
6051.157910333279
```

3.1.4 KNN hyperparameters

The model hyperparameters can be obtained using the `get_params()` method. Note that there are other hyperparameters to tune in addition to number of neighbors. However, the number of neighbours may be the most influential hyperparameter in most cases.

```
best_model.get_params()
```

```
{'algorithm': 'auto',
 'leaf_size': 30,
 'metric': 'minkowski',
 'metric_params': None,
 'n_jobs': None,
 'n_neighbors': 366,
 'p': 2,
 'weights': 'distance'}
```

The distances and the indices of the nearest K observations to each test observation can be obtained using the `kneighbors()` method.

```
best_model.kneighbors(X_test_scaled, return_distance=True)

# Each row is a test obs
# The cols are the indices of the K Nearest Neighbors (in the training data) to the test obs
```

```
(array([[1.92799060e-02, 1.31899013e-01, 1.89662146e-01, ...,
         8.38960707e-01, 8.39293053e-01, 8.39947823e-01],
        [7.07215830e-02, 1.99916181e-01, 2.85592939e-01, ...,
         1.15445056e+00, 1.15450848e+00, 1.15512897e+00],
        [1.32608205e-03, 1.43558347e-02, 1.80622215e-02, ...,
         5.16758453e-01, 5.17378567e-01, 5.17852312e-01],
        ...,
        [1.29209535e-02, 1.59187173e-02, 3.67038947e-02, ...,
         8.48811744e-01, 8.51235616e-01, 8.55044146e-01],
        [1.84971803e-02, 1.67471541e-01, 1.69374312e-01, ...,
         7.76743422e-01, 7.76943691e-01, 7.77760930e-01],
        [4.63762129e-01, 5.88639393e-01, 7.54718535e-01, ...,
         3.16994824e+00, 3.17126663e+00, 3.17294300e+00]]),
 array([[1639, 1647, 4119, ..., 3175, 2818, 4638],
        [ 367, 1655, 1638, ..., 2010, 3600,  268],
        [ 393, 4679, 3176, ..., 4663,  357,  293],
```

```
...,
[3116, 3736, 3108, ..., 3841, 2668, 2666],
[4864, 3540, 4852, ..., 3596, 3605, 4271],
[ 435,  729, 4897, ..., 4112, 2401, 2460]], dtype=int64))
```

3.2 KNN for classification

KNN model for classification can developed and tuned in a similar manner using the sklearn function `KNeighborsClassifier()`

- For classification, KNeighborsClassifier
- Exact same inputs
  - One detail: Not common to use even numbers for K in classification because of majority voting
  - Ks = np.arange(1,41,2) –> To get the odd numbers

4 Hyperparameter tuning

In this chapter we'll introduce several functions that help with tuning hyperparameters of a machine learning model.

```
import numpy as np
import pandas as pd
from sklearn.model_selection import train_test_split, cross_val_score, cross_val_predict, \
cross_validate, GridSearchCV, RandomizedSearchCV, KFold, StratifiedKFold, RepeatedKFold, Repe
from sklearn.neighbors import KNeighborsClassifier, KNeighborsRegressor
from sklearn.preprocessing import StandardScaler
from sklearn.metrics import accuracy_score, recall_score, mean_squared_error
from scipy.stats import uniform
from skopt import BayesSearchCV
from skopt.space import Real, Categorical, Integer
import seaborn as sns
from skopt.plots import plot_objective, plot_histogram, plot_convergence
import matplotlib.pyplot as plt
import warnings
from IPython import display
```

Let us read and pre-process data first. Then we'll be ready to tune the model hyperparameters. We'll use KNN as the model. Note that KNN has multiple hyperparameters to tune, such as number of neighbors, distance metric, weights of neighbours, etc.

```
#Using the same datasets as used for linear regression in STAT303-2,
#so that we can compare the non-linear models with linear regression
trainf = pd.read_csv('./Datasets/Car_features_train.csv')
trainp = pd.read_csv('./Datasets/Car_prices_train.csv')
testf = pd.read_csv('./Datasets/Car_features_test.csv')
testp = pd.read_csv('./Datasets/Car_prices_test.csv')
train = pd.merge(trainf,trainp)
test = pd.merge(testf,testp)
train.head()
```

	carID	brand	model	year	transmission	mileage	fuelType	tax	mpg	engineSize	price
0	18473	bmw	6 Series	2020	Semi-Auto	11	Diesel	145	53.3282	3.0	37980
1	15064	bmw	6 Series	2019	Semi-Auto	10813	Diesel	145	53.0430	3.0	33980
2	18268	bmw	6 Series	2020	Semi-Auto	6	Diesel	145	53.4379	3.0	36850
3	18480	bmw	6 Series	2017	Semi-Auto	18895	Diesel	145	51.5140	3.0	25998
4	18492	bmw	6 Series	2015	Automatic	62953	Diesel	160	51.4903	3.0	18990

```
predictors = ['mpg', 'engineSize', 'year', 'mileage']
X_train = train[predictors]
y_train = train['price']
X_test = test[predictors]
y_test = test['price']

# Scale
sc = StandardScaler()

sc.fit(X_train)
X_train_scaled = sc.transform(X_train)
X_test_scaled = sc.transform(X_test)
```

4.1 GridSearchCV

The function is used to compute the cross-validated score *(MSE, RMSE, accuracy, etc.)* over a grid of hyperparameter values. This helps avoid nested `for()` loops if multiple hyperparameter values need to be tuned.

```
# GridSearchCV works in three steps:

# 1) Create the model
model = KNeighborsRegressor() # No inputs defined inside the model

# 2) Create a hyperparameter grid (as a dict)
    # the keys should be EXACTLY the same as the names of the model inputs
    # the values should be an array or list of hyperparam values you want to try out

# 30 K values x 2 weight settings x 3 metric settings = 180 different combinations in this g
grid = {'n_neighbors': np.arange(5, 151, 5), 'weights':['uniform', 'distance'],
        'metric': ['manhattan', 'euclidean', 'chebyshev']}
# 3) Create the Kfold object (Using RepeatedKFold will be more robust, but more expensive, us
# have the budget)
```

```
kfold = KFold(n_splits = 5, shuffle = True, random_state = 1)

# 4) Create the CV object
# Look at the documentation to see the order in which the objects must be specified within tl
gcv = GridSearchCV(model, grid, cv = kfold, scoring = 'neg_root_mean_squared_error', n_jobs =

# Fit the models, and cross-validate
gcv.fit(X_train_scaled, y_train)
```

```
Fitting 5 folds for each of 180 candidates, totalling 900 fits
```

```
GridSearchCV(cv=KFold(n_splits=5, random_state=1, shuffle=True),
             estimator=KNeighborsRegressor(), n_jobs=-1,
             param_grid={'metric': ['manhattan', 'euclidean', 'chebyshev'],
                         'n_neighbors': array([  5,  10,  15,  20,  25,  30,  35,  40,  45,
        70,  75,  80,  85,  90,  95, 100, 105, 110, 115, 120, 125, 130,
       135, 140, 145, 150]),
                         'weights': ['uniform', 'distance']},
             scoring='neg_root_mean_squared_error', verbose=10)
```

The optimal estimator based on cross-validation is:

```
gcv.best_estimator_
```

```
KNeighborsRegressor(metric='manhattan', n_neighbors=10, weights='distance')
```

The optimal hyperparameter values *(based on those considered in the grid search)* are:

```
gcv.best_params_
```

```
{'metric': 'manhattan', 'n_neighbors': 10, 'weights': 'distance'}
```

The cross-validated root mean squared error for the optimal hyperparameter values is:

```
-gcv.best_score_
```

```
5740.928686723918
```

The RMSE on test data for the optimal hyperparameter values is:

```
y_pred = gcv.predict(X_test_scaled)
mean_squared_error(y_test, y_pred, squared=False)
```

```
5747.466851437544
```

Note that the error is further reduced as compared to the case when we tuned only one hyperparameter in the previous chatper. We must tune all the hyperparameters that can effect prediction accuracy, in order to get the most accurate model.

The results for each cross-validation are stored in the `cv_results_` attribute.

```
pd.DataFrame(gcv.cv_results_).head()
```

	mean_fit_time	std_fit_time	mean_score_time	std_score_time	param_metric	param_n_neighb
0	0.011169	0.005060	0.011768	0.001716	manhattan	5
1	0.009175	0.001934	0.009973	0.000631	manhattan	5
2	0.008976	0.001092	0.012168	0.001323	manhattan	10
3	0.007979	0.000001	0.011970	0.000892	manhattan	10
4	0.006781	0.000748	0.012367	0.001017	manhattan	15

These results can be useful to see if other hyperparameter values are almost equally good.

For example, the next two best optimal values of the hyperparameter correspond to neighbors being 15 and 5 respectively. As the test error has a high variance, the best hyperparameter values need not necessarily be actually optimal.

```
pd.DataFrame(gcv.cv_results_).sort_values(by = 'rank_test_score').head()
```

	mean_fit_time	std_fit_time	mean_score_time	std_score_time	param_metric	param_n_neighb
3	0.007979	0.000001	0.011970	0.000892	manhattan	10
5	0.009374	0.004829	0.013564	0.001850	manhattan	15
1	0.009175	0.001934	0.009973	0.000631	manhattan	5
7	0.007977	0.001092	0.017553	0.002054	manhattan	20
9	0.007777	0.000748	0.019349	0.003374	manhattan	25

Let us compute the RMSE on test data based on the 2nd and 3rd best hyperparameter values.

```
model = KNeighborsRegressor(n_neighbors=15, metric='manhattan', weights='distance').fit(X_tra
mean_squared_error(model.predict(X_test_scaled), y_test, squared = False)
```

```
5800.418957612656
```

```
model = KNeighborsRegressor(n_neighbors=5, metric='manhattan', weights='distance').fit(X_tra
mean_squared_error(model.predict(X_test_scaled), y_test, squared = False)
```

```
5722.4859230146685
```

We can see that the RMSE corresponding to the 3rd best hyperparameter value is the least. Due to variance in test errors, it may be a good idea to consider the set of top few best hyperparameter values, instead of just considering the best one.

4.2 RandomizedSearchCV()

In case of many possible values of hyperparameters, it may be comptaionally very expensive to use `GridSearchCV()`. In such cases, `RandomizedSearchCV()` can be used to compute the cross-validated score on a randomly selected subset of hyperparameter values from the specified grid. The number of values can be fixed by the user, as per the available budget.

```
# RandomizedSearchCV works in three steps:

# 1) Create the model
model = KNeighborsRegressor() # No inputs defined inside the model

# 2) Create a hyperparameter grid (as a dict)
    # the keys should be EXACTLY the same as the names of the model inputs
    # the values should be an array or list of hyperparam values, or distribution of hyperpa


grid = {'n_neighbors': range(1, 500), 'weights':['uniform', 'distance'],
        'metric': ['minkowski'], 'p': uniform(loc=1, scale=10)} #We can specify a distributi
                                                                #for continuous hyperparamet

# 3) Create the Kfold object (Using RepeatedKFold will be more robust, but more expensive, u
# have the budget)
kfold = KFold(n_splits = 5, shuffle = True, random_state = 1)
```

```
# 4) Create the CV object
# Look at the documentation to see the order in which the objects must be specified within th
gcv = RandomizedSearchCV(model, param_distributions = grid, cv = kfold, n_iter = 180, random_
                          scoring = 'neg_root_mean_squared_error', n_jobs = -1, verbose = 10)

# Fit the models, and cross-validate
gcv.fit(X_train_scaled, y_train)
```

```
Fitting 5 folds for each of 180 candidates, totalling 900 fits
```

```
RandomizedSearchCV(cv=KFold(n_splits=5, random_state=1, shuffle=True),
                   estimator=KNeighborsRegressor(), n_iter=180, n_jobs=-1,
                   param_distributions={'metric': ['minkowski'],
                                        'n_neighbors': range(1, 500),
                                        'p': <scipy.stats._distn_infrastructure.rv_continuous
                                        'weights': ['uniform', 'distance']},
                   random_state=10, scoring='neg_root_mean_squared_error',
                   verbose=10)
```

```
gcv.best_params_
```

```
{'metric': 'minkowski',
 'n_neighbors': 3,
 'p': 1.252639454318171,
 'weights': 'uniform'}
```

```
gcv.best_score_
```

```
-6239.171627183809
```

```
y_pred = gcv.predict(X_test_scaled)
mean_squared_error(y_test, y_pred, squared=False)
```

```
6176.533397589911
```

Note that in this example, `RandomizedSearchCV()` helps search for optimal values of the hyperparameter p over a continuous domain space. In this dataset, $p = 1$ seems to be the optimal value. However, if the optimal value was somewhere in the middle of a larger continuous domain space *(instead of the boundary of the domain space)*, and there were several other hyperparameters, some of which were not influencing the response *(effect sparsity)*, `RandomizedSearchCV()` is likely to be more effective in estimating the optimal value of the continuous hyperparameter.

The advantages of `RandomizedSearchCV()` over `GridSearchCV()` are:

1. `RandomizedSearchCV()` fixes the computational cost in case of large number of hyperparameters / large number of levels of individual hyperparameters. If there are n hyper parameters, each with 3 levels, the number of all possible hyperparameter values will be 3^n. The computational cost increase exponentially with increase in number of hyperparameters.

2. In case of a hyperparameter having continuous values, the distribution of the hyperparameter can be specified in `RandomizedSearchCV()`.

3. In case of effect sparsity of hyperparameters, i.e., if only a few hyperparameters significantly effect prediction accuracy, `RandomizedSearchCV()` is likely to consider more unique values of the influential hyperparameters as compared to `GridSearchCV()`, and is thus likely to provide more optimal hyperparameter values as compared to `GridSearchCV()`. The figure below shows effect sparsity where there are 2 hyperparameters, but only one of them is associated with the cross-validated score, Here, it is more likely that the optimal cross-validated score will be obtained by `RandomizedSearchCV()`, as it is evaluating the model on 9 unique values of the relevant hyperparameter, instead of just 3.

```
<IPython.core.display.Image object>
```

4.3 `BayesSearchCV()`

Unlike the grid search and random search, which treat hyperparameter sets independently, the Bayesian optimization is an informed search method, meaning that it learns from previous iterations. The number of trials in this approach is determined by the user.

- The function begins by computing the cross-validated score by randomly selecting a few hyperparameter values from the specified disttribution of hyperparameter values.
- Based on the data of hyperparameter values tested *(predictors)*, and the cross-validated score *(the response)*, a Gaussian process model is developed to estimate the cross-validated score & the uncertainty in the estimate in the entire space of the hyperparameter values

- A criterion that "explores" uncertain regions of the space of hyperparameter values *(where it is difficult to predict cross-validated score)*, and "exploits" promising regions of the space are of hyperparameter values *(where the cross-validated score is predicted to minimize)* is used to suggest the next hyperparameter value that will potentially minimize the cross-validated score
- Cross-validated score is computed at the suggested hyperparameter value, the Gaussian process model is updated, and the previous step is repeated, until a certain number of iterations specified by the user.

To summarize, instead of blindly testing the model for the specified hyperparameter values *(as in `GridSearchCV()`)*, or randomly testing the model on certain hyperparameter values *(as in `RandomizedSearchCV()`)*, `BayesSearchCV()` smartly tests the model for those hyperparameter values that are likely to reduce the cross-validated score. The algorithm becomes "smarter" as it "learns" more with increasing iterations.

Here is a nice blog, if you wish to understand more about the Bayesian optimization procedure.

```
# BayesSearchCV works in three steps:

# 1) Create the model
model = KNeighborsRegressor(metric = 'minkowski') # No inputs defined inside the model

# 2) Create a hyperparameter grid (as a dict)
# the keys should be EXACTLY the same as the names of the model inputs
# the values should be the distribution of hyperparameter values. Lists and NumPy arrays can
# also be used

grid = {'n_neighbors': Integer(1, 500), 'weights': Categorical(['uniform', 'distance']),
       'p': Real(1, 10, prior = 'uniform')}

# 3) Create the Kfold object (Using RepeatedKFold will be more robust, but more expensive,
# use it if you have the budget)
kfold = KFold(n_splits = 5, shuffle = True, random_state = 1)

# 4) Create the CV object
# Look at the documentation to see the order in which the objects must be specified within
# the function
gcv = BayesSearchCV(model, search_spaces = grid, cv = kfold, n_iter = 180, random_state = 10
                         scoring = 'neg_root_mean_squared_error', n_jobs = -1)

# Fit the models, and cross-validate
```

```
# Sometimes the Gaussian process model predicting the cross-validated score suggests a
# "promising point" (i.e., set of hyperparameter values) for cross-validation that it has
# already suggested earlier. In such  a case a warning is raised, and the objective
# function (i.e., the cross-validation score) is computed at a randomly selected point
# (as in RandomizedSearchCV()). This feature helps the algorithm explore other regions of
# the hyperparameter space, rather than only searching in the promising regions. Thus, it
# balances exploration (of the hyperparameter space) with exploitation (of the promising
# regions of the hyperparameter space)

warnings.filterwarnings("ignore")
gcv.fit(X_train_scaled, y_train)
warnings.resetwarnings()
```

The optimal hyperparameter values *(based on Bayesian search)* on the provided distribution of hyperparameter values are:

```
gcv.best_params_
```

```
OrderedDict([('n_neighbors', 9),
             ('p', 1.0008321732366932),
             ('weights', 'distance')])
```

The cross-validated root mean squared error for the optimal hyperparameter values is:

```
-gcv.best_score_
```

```
5756.172382596493
```

The RMSE on test data for the optimal hyperparameter values is:

```
y_pred = gcv.predict(X_test_scaled)
mean_squared_error(y_test, y_pred, squared=False)
```

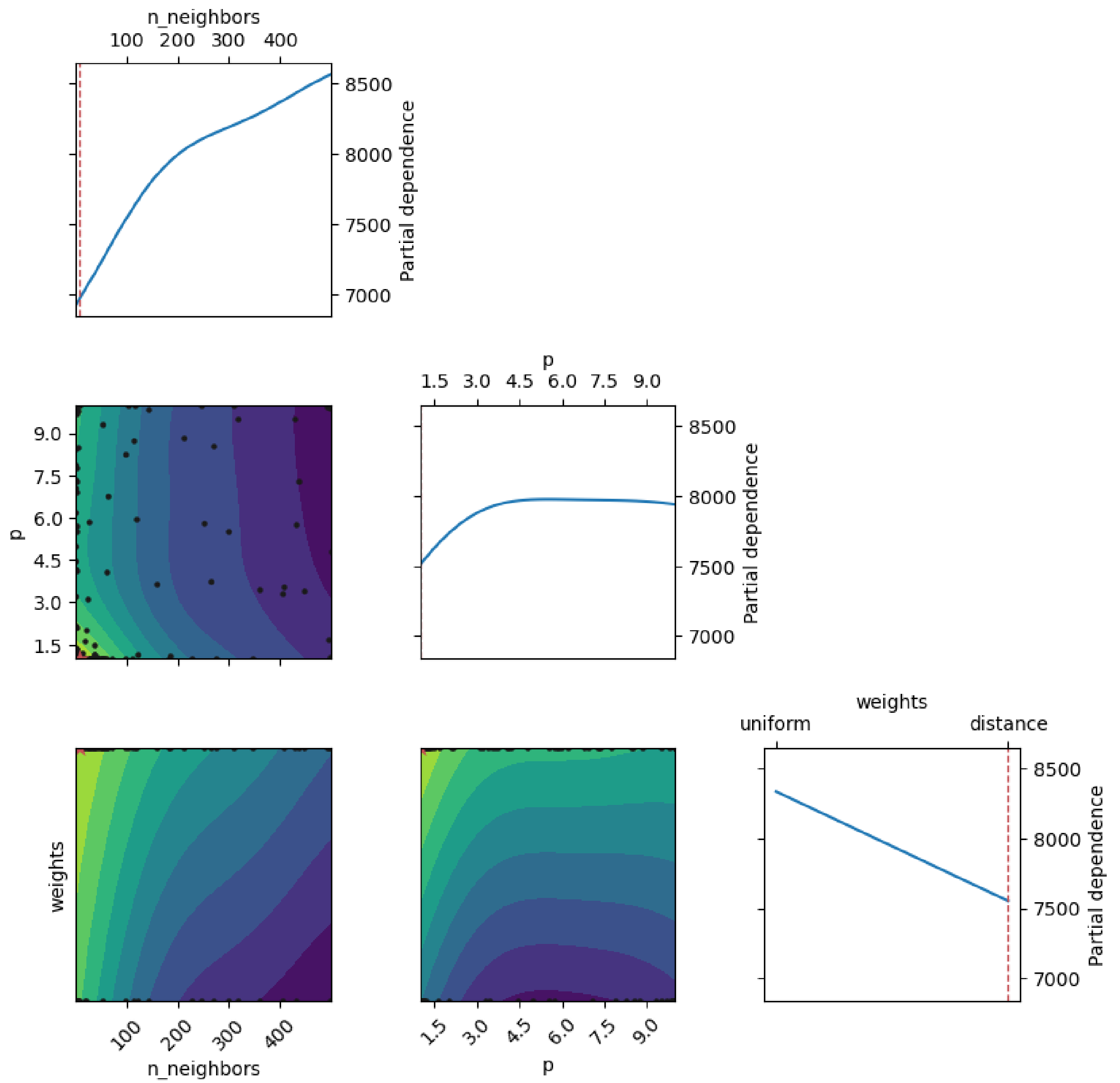
```
5740.432278861367
```

4.3.1 Diagonosis of cross-validated score optimization

Below are the partial dependence plots of the objective function *(i.e., the cross-validated score)*. The cross-validated score predictions are based on the most recently updated model *(i.e., the updated Gaussian Process model at the end of* ***n_iter*** *iterations specified by the user)* that predicts the cross-validated score.

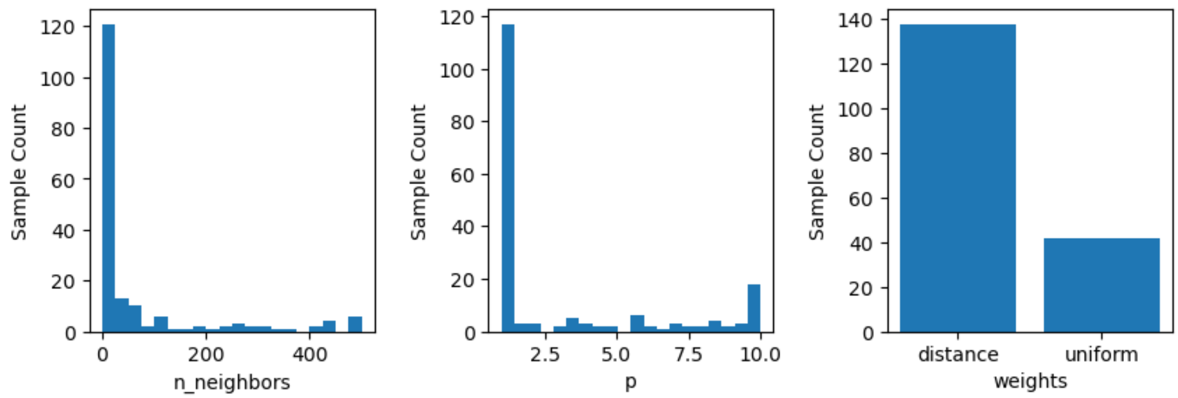
Check the plot_objective() documentation to interpret the plots.

```
plot_objective(gcv.optimizer_results_[0],
                   dimensions=["n_neighbors", "p", "weights"], size = 3)
plt.show();
```



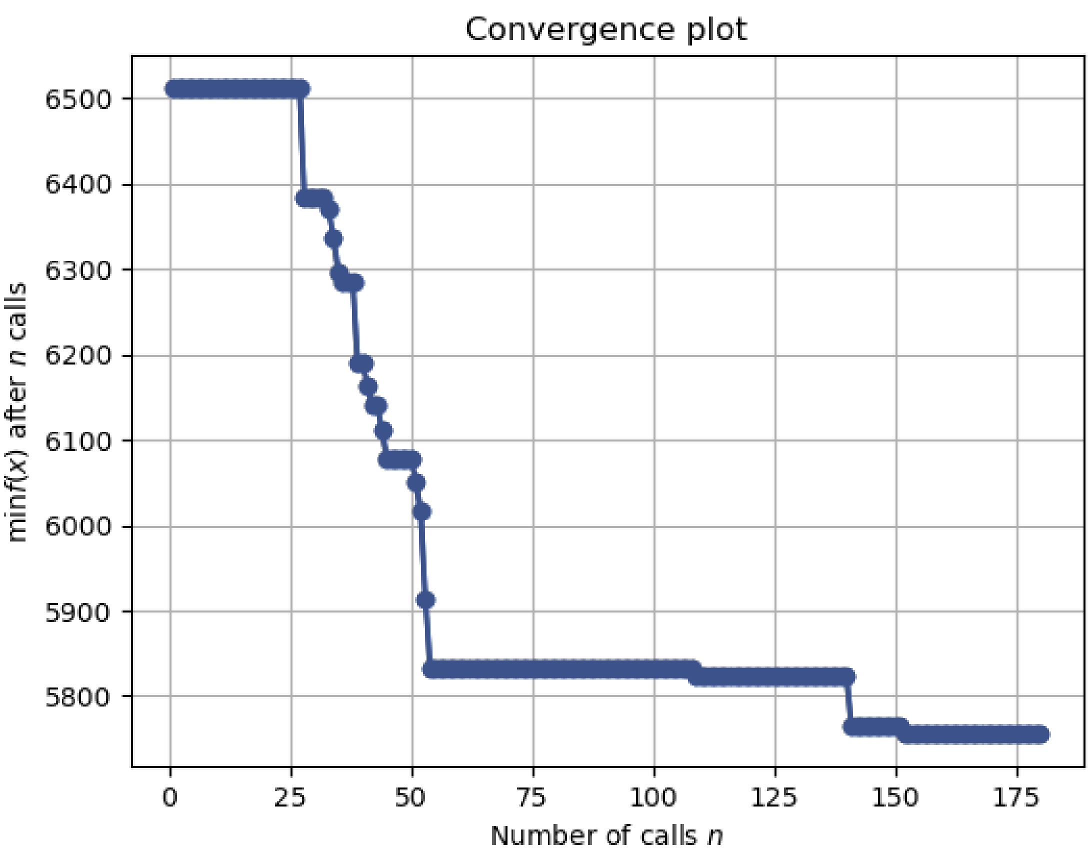
The frequence of individual hyperparameter values considered can also be visualized as below.

```
fig, ax = plt.subplots(1, 3, figsize = (10, 3))
plt.subplots_adjust(wspace=0.4)
plot_histogram(gcv.optimizer_results_[0], 0, ax = ax[0])
plot_histogram(gcv.optimizer_results_[0], 1, ax = ax[1])
plot_histogram(gcv.optimizer_results_[0], 2, ax = ax[2])
plt.show()
```



Below is the plot showing the minimum cross-validated score computed obtained until 'n' hyperparameter values are considered for cross-validation.

```
plot_convergence(gcv.optimizer_results_)
plt.show()
```



Note that the cross-validated error is close to the optmial value in the 53rd iteration itself.

The cross-validated error at the 53rd iteration is:

```
gcv.optimizer_results_[0]['func_vals'][53]
```

```
5831.87280274334
```

The hyperparameter values at the 53rd iterations are:

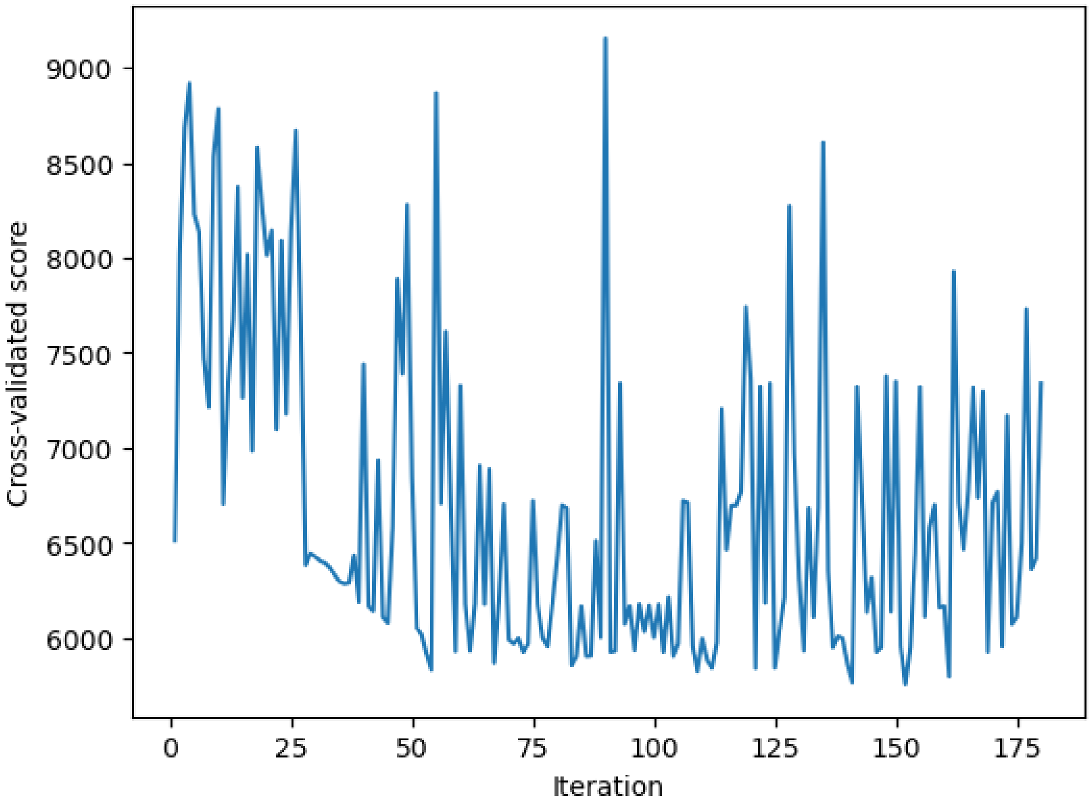
```
gcv.optimizer_results_[0]['x_iters'][53]
```

```
[15, 1.0, 'distance']
```

Note that this is the 2nd most optimal hyperparameter value based on `GridSearchCV()`.

Below is the plot showing the cross-validated score computed at each of the 180 hyperparameter values considered for cross-validation. The plot shows that the algorithm seems to explore new regions of the domain space, instead of just exploting the promising ones. There is a balance between exploration and exploitation for finding the optimal hyperparameter values that minimize the objective function *(i.e., the function that models the cross-validated score)*.

```
sns.lineplot(x = range(1, 181), y = gcv.optimizer_results_[0]['func_vals'])
plt.xlabel('Iteration')
plt.ylabel('Cross-validated score')
plt.show();
```



The advantages of `BayesSearchCV()` over `GridSearchCV()` and `RandomizedSearchCV()` are:

1. The Bayesian Optimization approach gives the benefit that we can give a much larger range of possible values, since over time we identify and exploit the most promising regions and discard the not so promising ones. Plain grid-search would burn computational resources to explore all regions of the domain space with the same granularity, even the not promising ones. Since we search much more effectively in Bayesian search, we can search over a larger domain space.

2. BayesSearch CV may help us identify the optimal hyperparameter value in fewer iterations if the Gaussian process model estimating the cross-validated score is relatively accurate. However, this is not certain. Grid and random search are completely uninformed by past evaluations, and as a result, often spend a significant amount of time evaluating "bad" hyperparameters.

3. BayesSearch CV is more reliable in cases of a large search space, where random selection may miss sampling values from optimal regions of the search space.

The disadvantages of `BayesSearchCV()` over `GridSearchCV()` and `RandomizedSearchCV()` are:

1. `BayesSearchCV()` has a cost of learning from past data, i.e., updating the model that predicts the cross-validated score after every iteration of evaluating the cross-validated score on a new hyperparameter value. This cost will continue to increase as more and more data is collected. There is no such cost in `GridSearchCV()` and `RandomizedSearchCV()` as there is no learning. This implies that each iteration of `BayesSearchCV()` will take a longer time than each iteration of `GridSearchCV()` / `RandomizedSearchCV()`. Thus, even if `BayesSearchCV()` finds the optimal hyperparameter value in fewer iterations, it may take more time than `GridSearchCV()` / `RandomizedSearchCV()` for the same.
2. The success of `BayesSearchCV()` depends on the predictions and associated uncertainty estimated by the Gaussian process (GP) model that predicts the cross-validated score. The GP model, although works well in general, may not be suitable for certain datasets, or may take a relatively large number of iterations to learn for certain datasets.

4.3.2 Live monitoring of cross-validated score

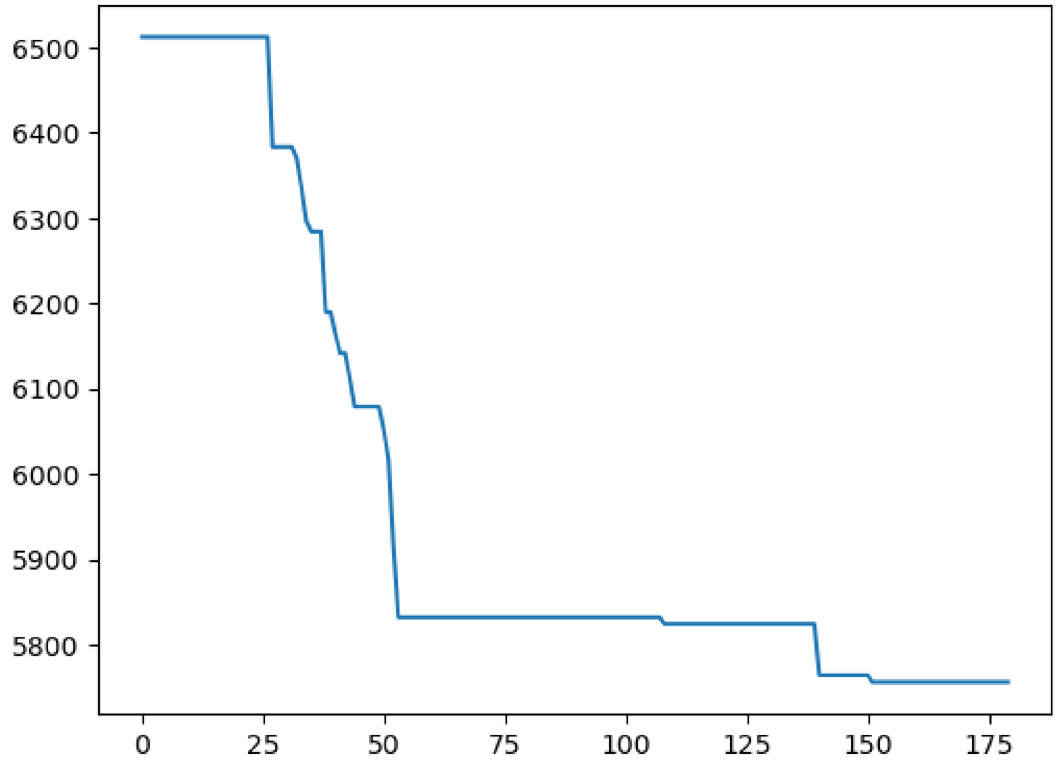
Note that it will be useful monitor the cross-validated score while the Bayesian Search CV code is running, and stop the code as soon as the desired accuracy is reached, or the optimal cross-validated score doesn't seem to improve. The `fit()` method of the `BayesSeaerchCV()` object has a `callback` argument that can be used as follows:

```
model = KNeighborsRegressor(metric = 'minkowski') # No inputs defined inside the model
grid = {'n_neighbors': Integer(1, 500), 'weights': Categorical(['uniform', 'distance']),
       'p': Real(1, 10, prior = 'uniform')}

kfold = KFold(n_splits = 5, shuffle = True, random_state = 1)
gcv = BayesSearchCV(model, search_spaces = grid, cv = kfold, n_iter = 180, random_state = 10
                         scoring = 'neg_root_mean_squared_error', n_jobs = -1)
```

```
paras = list(gcv.search_spaces.keys())
paras.sort()

def monitor(optim_result):
    cv_values = pd.Series(optim_result['func_vals']).cummin()
    display.clear_output(wait = True)
    min_ind = pd.Series(optim_result['func_vals']).argmin()
    print(paras, "=", optim_result['x_iters'][min_ind], pd.Series(optim_result['func_vals'])
    sns.lineplot(cv_values)
    plt.show()
```

```
gcv.fit(X_train_scaled, y_train, callback = monitor)
```

```
['n_neighbors', 'p', 'weights'] = [9, 1.0008321732366932, 'distance'] 5756.172382596493
```




```
BayesSearchCV(cv=KFold(n_splits=5, random_state=1, shuffle=True),
              estimator=KNeighborsRegressor(), n_iter=180, n_jobs=-1,
              random_state=10, scoring='neg_root_mean_squared_error',
              search_spaces={'n_neighbors': Integer(low=1, high=500, prior='uniform', transf
                             'p': Real(low=1, high=10, prior='uniform', transform='normalize
                             'weights': Categorical(categories=('uniform', 'distance'), prio
```

4.4 cross_validate()

We have used `cross_val_score()` and `cross_val_predict()` so far.

When can we use one over the other?

The function `cross_validate()` is similar to `cross_val_score()` except that it has the option to return multiple cross-validated metrics, instead of a single one.

Consider the heart disease classification problem, where the response is `target` *(whether the person has a heart disease or not).*

```
data = pd.read_csv('Datasets/heart_disease_classification.csv')
data.head()
```

	age	sex	cp	trestbps	chol	fbs	restecg	thalach	exang	oldpeak	slope	ca	thal	target
0	63	1	3	145	233	1	0	150	0	2.3	0	0	1	1
1	37	1	2	130	250	0	1	187	0	3.5	0	0	2	1
2	41	0	1	130	204	0	0	172	0	1.4	2	0	2	1
3	56	1	1	120	236	0	1	178	0	0.8	2	0	2	1
4	57	0	0	120	354	0	1	163	1	0.6	2	0	2	1

Let us pre-process the data.

```
# First, separate the response and the predictors
y = data['target']
X = data.drop('target', axis=1)
```

```
# Separate the data (X,y) into training and test

# Inputs:
    # data
    # train-test ratio
    # random_state for reproducible code

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=20, st

# stratify=y makes sure the class 0 to class 1 ratio in the training and test sets are kept
```

```
model = KNeighborsClassifier()
sc = StandardScaler()
sc.fit(X_train)
X_train_scaled = sc.transform(X_train)
X_test_scaled = sc.transform(X_test)
```

Suppose we want to take recall above a certain threshold with the highest precision possible. `cross_validate()` computes the cross-validated score for multiple metrics - rest is the same as `cross_val_score()`.

```
Ks = np.arange(10,200,10)

scores = []

for K in Ks:
    model = KNeighborsClassifier(n_neighbors=K) # Keeping distance uniform
    scores.append(cross_validate(model, X_train_scaled, y_train, cv=5, scoring = ['accuracy'
```

```
scores

# The output is now a list of dicts - easy to convert to a df

df_scores = pd.DataFrame(scores) # We need to handle test_recall and test_precision cols

df_scores['CV_recall'] = df_scores['test_recall'].apply(np.mean)
df_scores['CV_precision'] = df_scores['test_precision'].apply(np.mean)
df_scores['CV_accuracy'] = df_scores['test_accuracy'].apply(np.mean)

df_scores.index = Ks # We can set K values as indices for convenience


#df_scores
# What happens as K increases?
    # Recall increases (not monotonically)
    # Precision decreases (not monotonically)
# Why?
    # Check the class distribution in the data - more obs with class 1
    # As K gets higher, the majority class overrules (visualized in the slides)
    # More 1s means less FNs - higher recall
    # More 1s means more FPs - lower precision
# Would this be the case for any dataset?
    # NO!! Depends on what the majority class is!
```

Suppose we wish to have the maximum possible precision for at least 95% recall.

The optimal 'K' will be:

```
df_scores.loc[df_scores['CV_recall'] > 0.95, 'CV_precision'].idxmax()
```

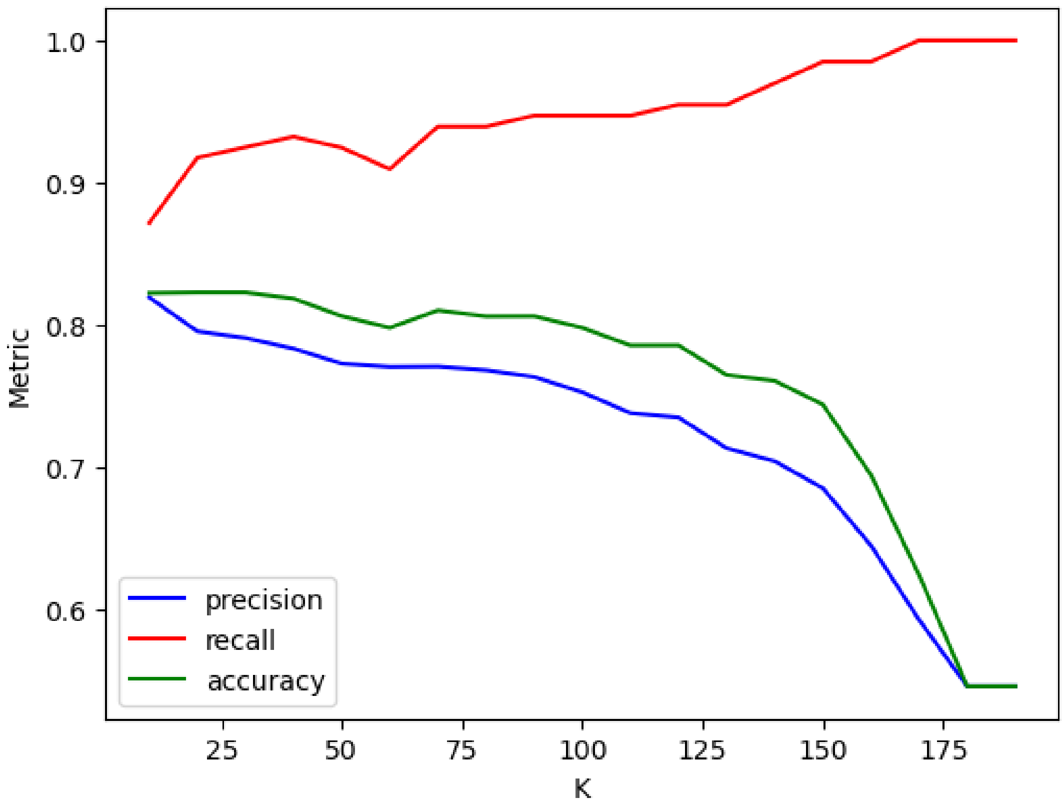
```
120
```

The cross-validated precision, recall and accuracy for the optimal 'K' are:

```
df_scores.loc[120, ['CV_recall', 'CV_precision', 'CV_accuracy']]
```

```
CV_recall       0.954701
CV_precision    0.734607
CV_accuracy     0.785374
Name: 120, dtype: object
```

```
sns.lineplot(x = df_scores.index, y = df_scores.CV_precision, color = 'blue', label = 'preci
sns.lineplot(x = df_scores.index, y = df_scores.CV_recall, color = 'red', label = 'recall')
sns.lineplot(x = df_scores.index, y = df_scores.CV_accuracy, color = 'green', label = 'accura
plt.ylabel('Metric')
plt.xlabel('K')
plt.show()
```



Part II

Tree based models

5 Regression trees

Read section 8.1.1 of the book before using these notes.

Note that in this course, lecture notes are not sufficient, you must read the book for better understanding. Lecture notes are just implementing the concepts of the book on a dataset, but not explaining the concepts elaborately.

```
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.metrics import mean_squared_error, r2_score
from sklearn.model_selection import cross_val_score, train_test_split, KFold, RepeatedKFold,
GridSearchCV, ParameterGrid, RandomizedSearchCV
from sklearn.tree import DecisionTreeRegressor
from skopt import BayesSearchCV
from skopt.space import Integer, Categorical, Real
from IPython import display

#Libraries for visualizing trees
from sklearn.tree import export_graphviz, export_text
from six import StringIO
from IPython.display import Image
import pydotplus
import time as tm
```

```
#Using the same datasets as used for linear regression in STAT303-2,
#so that we can compare the non-linear models with linear regression
trainf = pd.read_csv('./Datasets/Car_features_train.csv')
trainp = pd.read_csv('./Datasets/Car_prices_train.csv')
testf = pd.read_csv('./Datasets/Car_features_test.csv')
testp = pd.read_csv('./Datasets/Car_prices_test.csv')
train = pd.merge(trainf,trainp)
test = pd.merge(testf,testp)
train.head()
```

	carID	brand	model	year	transmission	mileage	fuelType	tax	mpg	engineSize	price
0	18473	bmw	6 Series	2020	Semi-Auto	11	Diesel	145	53.3282	3.0	37980
1	15064	bmw	6 Series	2019	Semi-Auto	10813	Diesel	145	53.0430	3.0	33980
2	18268	bmw	6 Series	2020	Semi-Auto	6	Diesel	145	53.4379	3.0	36850
3	18480	bmw	6 Series	2017	Semi-Auto	18895	Diesel	145	51.5140	3.0	25998
4	18492	bmw	6 Series	2015	Automatic	62953	Diesel	160	51.4903	3.0	18990

5.1 Building a regression tree

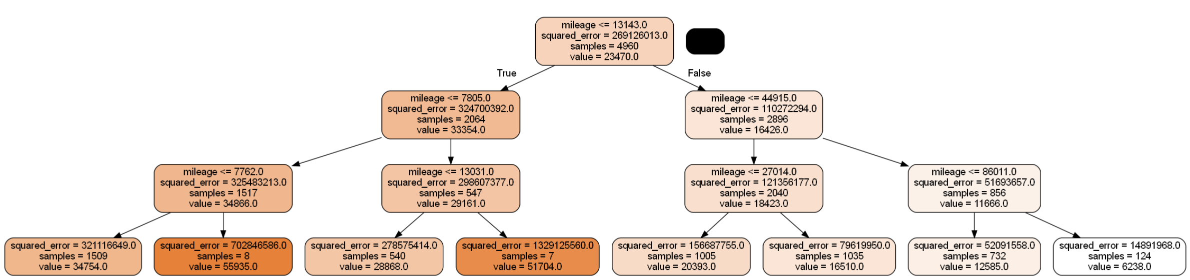
Develop a regression tree to predict car price based on mileage

```
X = train['mileage']
y = train['price']
```

```
#Defining the object to build a regression tree
model = DecisionTreeRegressor(random_state=1, max_depth=3)

#Fitting the regression tree to the data
model.fit(X.values.reshape(-1,1), y)
```

```
DecisionTreeRegressor(max_depth=3, random_state=1)
```

```
#Visualizing the regression tree
dot_data = StringIO()
export_graphviz(model, out_file=dot_data,
                filled=True, rounded=True,
                feature_names =['mileage'],precision=0)
graph = pydotplus.graph_from_dot_data(dot_data.getvalue())
graph.write_png('car_price_tree.png')
Image(graph.create_png())
```

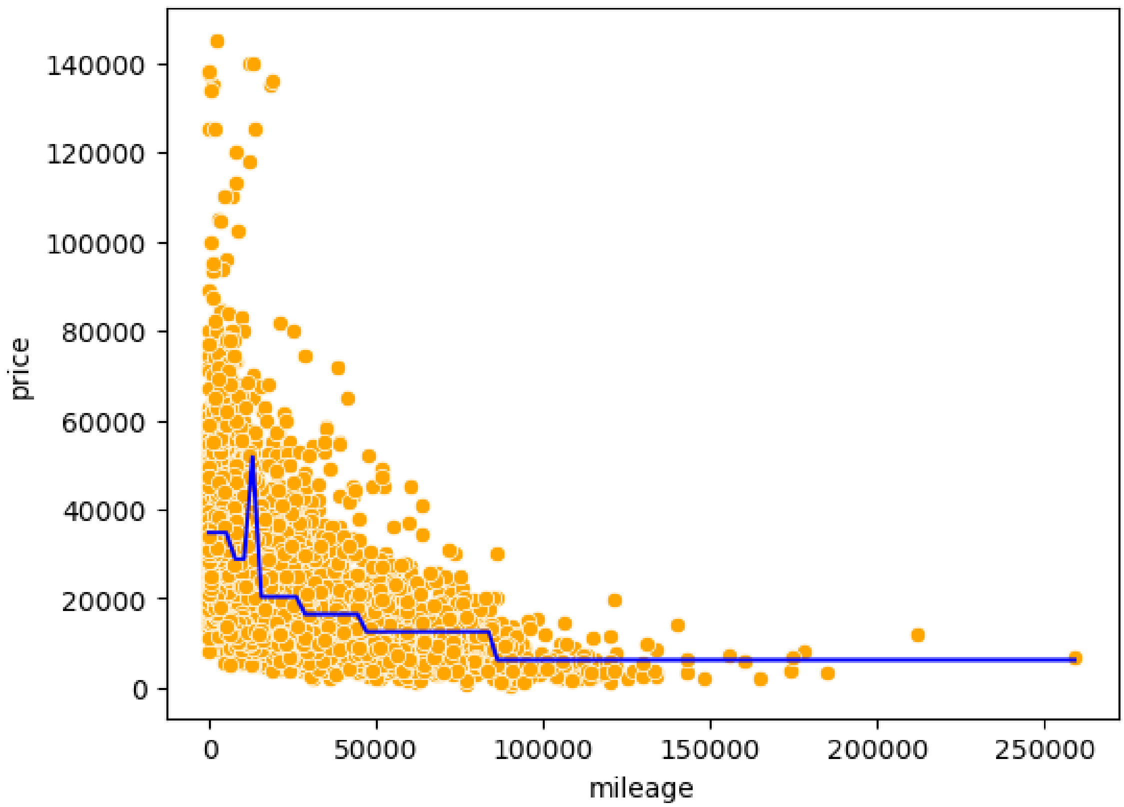


```
#prediction on test data
pred=model.predict(test[['mileage']].values)
```

```
#RMSE on test data
np.sqrt(mean_squared_error(test.price, pred))
```

```
13764.798425410803
```

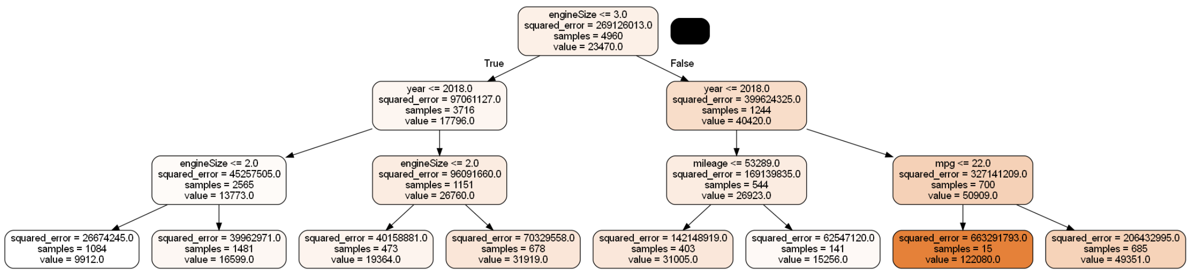
```
#Visualizing the model fit
Xtest = np.linspace(min(X), max(X), 100)
pred_test = model.predict(Xtest.reshape(-1,1))
sns.scatterplot(x = 'mileage', y = 'price', data = train, color = 'orange')
sns.lineplot(x = Xtest, y = pred_test, color = 'blue');
```



All cars falling within the same terminal node have the same predicted price, which is seen as flat line segments in the above model curve.

Develop a regression tree to predict car price based on `mileage`, `mpg`, `engineSize` and `year`

```python
X = train[['mileage','mpg','year','engineSize']]
model = DecisionTreeRegressor(random_state=1, max_depth=3)
model.fit(X, y)
dot_data = StringIO()
export_graphviz(model, out_file=dot_data,
                filled=True, rounded=True,
                feature_names =['mileage','mpg','year','engineSize'],precision=0)
graph = pydotplus.graph_from_dot_data(dot_data.getvalue())
graph.write_png('car_price_tree.png')
Image(graph.create_png())
```



The model can also be visualized in the text format as below.

```python
print(export_text(model))
```

```
|--- feature_3 <= 2.75
|   |--- feature_2 <= 2018.50
|   |   |--- feature_3 <= 1.75
|   |   |   |--- value: [9912.24]
|   |   |--- feature_3 >  1.75
|   |   |   |--- value: [16599.03]
|   |--- feature_2 >  2018.50
|   |   |--- feature_3 <= 1.90
|   |   |   |--- value: [19363.81]
|   |   |--- feature_3 >  1.90
|   |   |   |--- value: [31919.42]
|--- feature_3 >  2.75
|   |--- feature_2 <= 2017.50
|   |   |--- feature_0 <= 53289.00
|   |   |   |--- value: [31004.63]
|   |   |--- feature_0 >  53289.00
|   |   |   |--- value: [15255.91]
|   |--- feature_2 >  2017.50
```

```
|   |   |--- feature_1 <= 21.79
|   |   |   |--- value: [122080.00]
|   |   |--- feature_1 >  21.79
|   |   |   |--- value: [49350.79]
```

5.2 Optimizing parameters to improve the regression tree

Let us find the optimal depth of the tree and the number of terminal nodes (leaves) by cross validation.

5.2.1 Range of hyperparameter values

First, we'll find the minimum and maximum possible values of the depth and leaves, and then find the optimal value in that range.

```
model = DecisionTreeRegressor(random_state=1)
model.fit(X, y)

print("Maximum tree depth =", model.get_depth())

print("Maximum leaves =", model.get_n_leaves())
```

```
Maximum tree depth = 29
Maximum leaves = 4845
```

5.2.2 Cross validation: Coarse grid

We'll use the `sklearn` function `GridSearchCV` to find the optimal hyperparameter values over a grid of possible values. By default, `GridSearchCV` returns the optimal hyperparameter values based on the coefficient of determination R^2. However, the `scoring` argument of the function can be used to find the optimal parameters based on several different criteria as mentioned in the scoring-parameter documentation.

```
#Finding cross-validation error for trees
parameters = {'max_depth':range(2,30, 3),'max_leaf_nodes':range(2,4900, 100)}
cv = KFold(n_splits = 5,shuffle=True,random_state=1)
model = GridSearchCV(DecisionTreeRegressor(random_state=1), parameters, n_jobs=-1,verbose=1,c
model.fit(X, y)
print (model.best_score_, model.best_params_)
```

```
Fitting 5 folds for each of 490 candidates, totalling 2450 fits
0.8433100904754441 {'max_depth': 11, 'max_leaf_nodes': 302}
```

Let us find the optimal hyperparameters based on root mean squared error (RMSE), instead of R^2. Let us compute R^2 as well during cross validation, as we can compute multiple performance metrics using the `scoring` argument. However, when computing multiple performance metrics, we will need to specify the performance metric used to find the optimal hyperparameters with the `refit` argument.

```
#Finding cross-validation error for trees
parameters = {'max_depth':range(2,30, 3),'max_leaf_nodes':range(2,4900, 100)}
cv = KFold(n_splits = 5,shuffle=True,random_state=1)
model = GridSearchCV(DecisionTreeRegressor(random_state=1), parameters, n_jobs=-1,verbose=1,c
                    scoring=['neg_root_mean_squared_error', 'r2'], refit = 'neg_root_mean_squ
model.fit(X, y)
print (model.best_score_, model.best_params_)
```

```
Fitting 5 folds for each of 490 candidates, totalling 2450 fits
-6475.329183576911 {'max_depth': 11, 'max_leaf_nodes': 302}
```

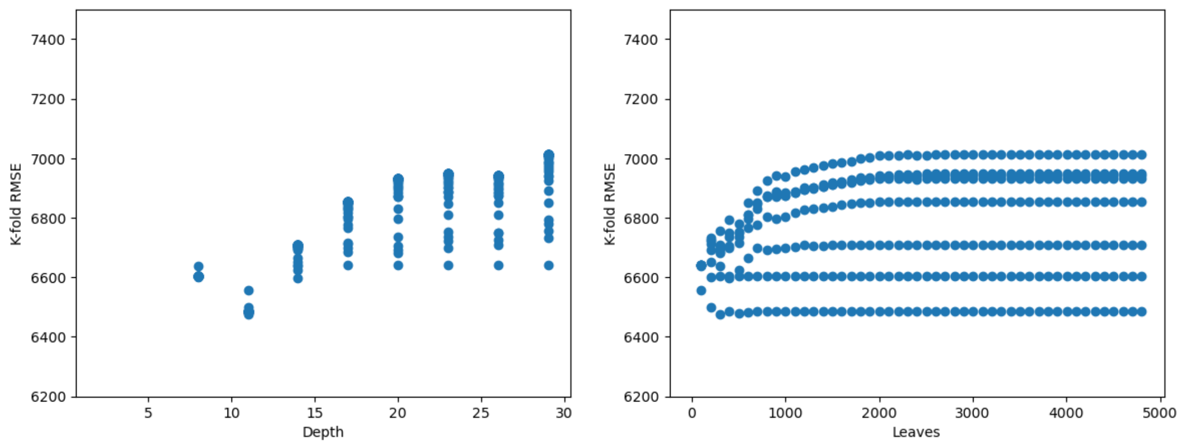
Note that as the `GridSearchCV` function maximizes the performance metric to find the optimal hyperparameters, we are maximizing the negative root mean squared error (`neg_root_mean_squared_error`), and the function returns the optimal negative mean squared error.

Let us visualize the mean squared error based on the hyperparameter values. We'll use the cross validation results stored in the `cv_results_` attribute of the `GridSearchCV` `fit()` object.

```
#Detailed results of k-fold cross validation
cv_results = pd.DataFrame(model.cv_results_)
cv_results.head()
```

	mean_fit_time	std_fit_time	mean_score_time	std_score_time	param_max_depth	param_max
0	0.010178	7.531409e-04	0.003791	0.000415	2	2
1	0.009574	1.758238e-03	0.003782	0.000396	2	102
2	0.009774	7.458305e-04	0.003590	0.000488	2	202
3	0.009568	4.953541e-04	0.003391	0.000489	2	302
4	0.008976	6.843901e-07	0.003192	0.000399	2	402

```
fig, axes = plt.subplots(1,2,figsize=(14,5))
plt.subplots_adjust(wspace=0.2)
axes[0].plot(cv_results.param_max_depth, (-cv_results.mean_test_neg_root_mean_squared_error)
axes[0].set_ylim([6200, 7500])
axes[0].set_xlabel('Depth')
axes[0].set_ylabel('K-fold RMSE')
axes[1].plot(cv_results.param_max_leaf_nodes, (-cv_results.mean_test_neg_root_mean_squared_e
axes[1].set_ylim([6200, 7500])
axes[1].set_xlabel('Leaves')
axes[1].set_ylabel('K-fold RMSE');
```



We observe that for a depth of around 8-14, and number of leaves within 1000, we get the lowest K-fold RMSE. So, we should do a finer search in that region to obtain more precise hyperparameter values.

5.2.3 Cross validation: Finer grid

```
#Finding cross-validation error for trees
start_time = tm.time()
parameters = {'max_depth':range(8,15),'max_leaf_nodes':range(2,1000)}
cv = KFold(n_splits = 5,shuffle=True,random_state=1)
model = GridSearchCV(DecisionTreeRegressor(random_state=1), parameters, n_jobs=-1,verbose=1,c
                    scoring = 'neg_root_mean_squared_error')
model.fit(X, y)
print (model.best_score_, model.best_params_)
print("Time taken =", round((tm.time() - start_time)/60), "minutes")
```

```
Fitting 5 folds for each of 6986 candidates, totalling 34930 fits
-6414.468922119372 {'max_depth': 10, 'max_leaf_nodes': 262}
Time taken = 2 minutes
```

From the above cross-validation, the optimal hyperparameter values are `max_depth = 10` and `max_leaf_nodes = 262`. Note that the cross-validation score with finer grid is only slightly lower than the course grid. However, depending on the dataset, the finer grid may lead to more benefit.

```
#Developing the tree based on optimal hyperparameters found by cross-validation
model = DecisionTreeRegressor(random_state=1, max_depth=10,max_leaf_nodes=262)
model.fit(X, y)
```

```
DecisionTreeRegressor(max_depth=10, max_leaf_nodes=262, random_state=1)
```

```
#RMSE on test data
Xtest = test[['mileage','mpg','year','engineSize']]
np.sqrt(mean_squared_error(test.price, model.predict(Xtest)))
```

```
6921.0404660552895
```

The RMSE for the decision tree is lower than that of linear regression models with these four predictors. This may be probably due to car price having a highly non-linear association with the predictors.

Note that we may also use `RandomizedSearchCV()` or `BayesSearchCV()` to optimze the hyperparameters.

Predictor importance: The importance of a predictor is computed as the (normalized) total reduction of the criterion (SSE in case of regression trees) brought by that predictor.

Warning: impurity-based feature importances can be misleading for high cardinality features (many unique values) *Source: https://scikit-learn.org/stable/modules/generated/sklearn.tree.DecisionTreeRegres*

Why?

Because high cardinality predictors will tend to overfit. When the predictors have high cardinality, it means they form little groups *(in the leaf nodes)* and then the model "learns" the individuals, instead of "learning" the general trend. The higher the cardinality of the predictor, the more prone is the model to overfitting.

```
model.feature_importances_
```

```
array([0.04490344, 0.15882336, 0.29739951, 0.49887369])
```

Engine size is the most important predictor, followed by *year*, which is followed by *mpg*, and *mileage* is the least important predictor.

5.3 Cost complexity pruning

While optimizing parameters above, we optimized them within a range that we thought was reasonable. While doing so, we restricted ourselves to considering only a subset of the unpruned tree. Thus, we could have missed out on finding the optimal tree (or the best model).

With cost complexity pruning, we first develop an unpruned tree without any restrictions. Then, using cross validation, we find the optimal value of the tuning parameter α. All the non-terminal nodes for which α_{eff} is smaller that the optimal α will be pruned. You will need to check out the link below to understand this better.

Check out a detailed explanation of how cost complexity pruning is implemented in sklearn at: https://scikit-learn.org/stable/modules/tree.html#minimal-cost-complexity-pruning

Here are some informative visualizations that will help you understand what is happening in cost complexity pruning: https://scikit-learn.org/stable/auto_examples/tree/plot_cost_complexity_pruning.html#sphx-glr-auto-examples-tree-plot-cost-complexity-pruning-py

```
model = DecisionTreeRegressor(random_state = 1)#model without any restrictions
path= model.cost_complexity_pruning_path(X,y)# Compute the pruning path during Minimal Cost-C
```

```
alphas=path['ccp_alphas']
```

```
len(alphas)
```

```
4126
```

```
start_time = tm.time()
cv = KFold(n_splits = 5,shuffle=True,random_state=1)
tree = GridSearchCV(DecisionTreeRegressor(random_state=1), param_grid = {'ccp_alpha':alphas}
                     scoring = 'neg_mean_squared_error',n_jobs=-1,verbose=1,cv=cv)
tree.fit(X, y)
print (tree.best_score_, tree.best_params_)
print("Time taken =",round((tm.time()-start_time)/60), "minutes")
```

```
Fitting 5 folds for each of 4126 candidates, totalling 20630 fits
-44150619.209031895 {'ccp_alpha': 143722.94076639024}
Time taken = 2 minutes
```

The code took 2 minutes to run on a dataset of about 5000 observations and 4 predictors.

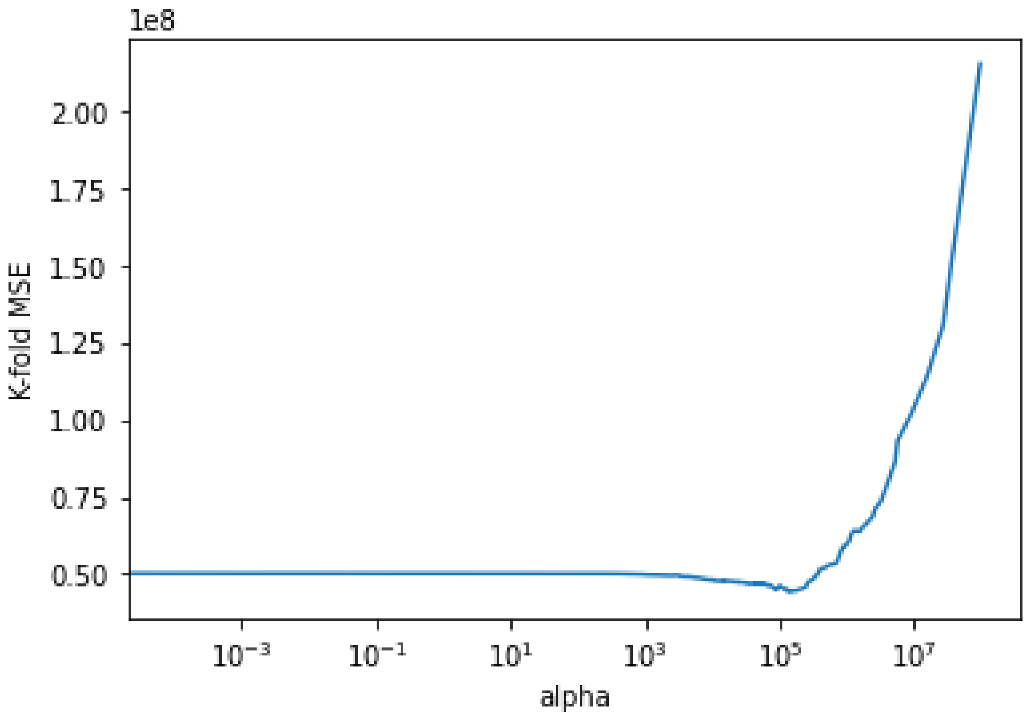
```
model = DecisionTreeRegressor(ccp_alpha=143722.94076639024,random_state=1)
model.fit(X, y)
pred = model.predict(Xtest)
np.sqrt(mean_squared_error(test.price, pred))
```

```
7306.592294294368
```

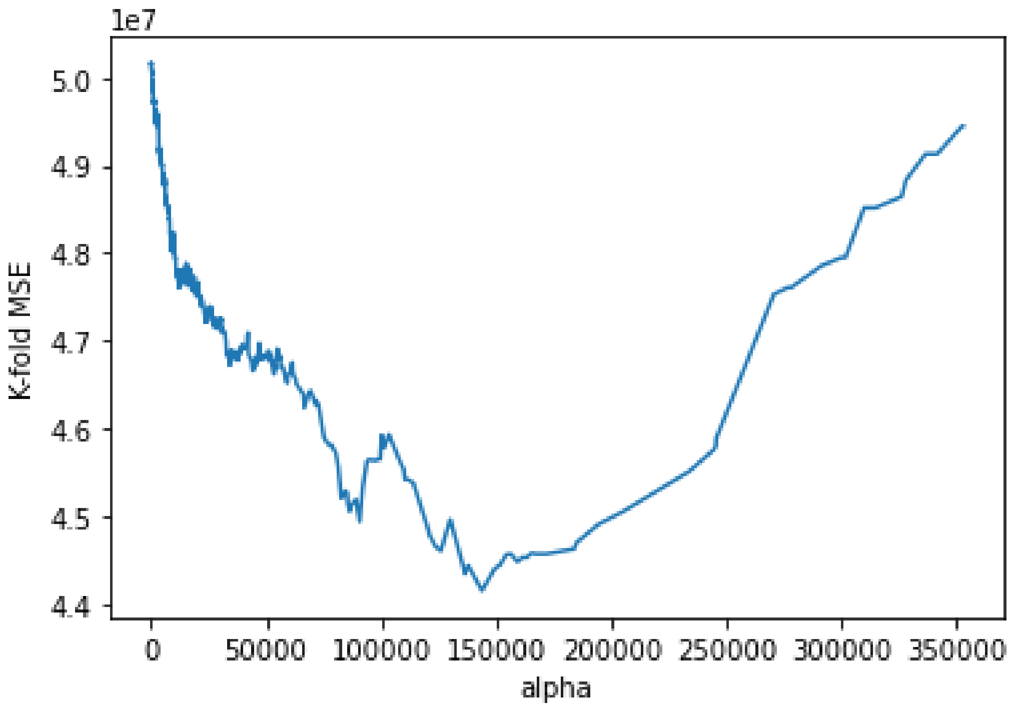
The RMSE for the decision tree with cost complexity pruning is lower than that of linear regression models and spline regression models (including MARS), with these four predictors. However, it is higher than the one obtained with tuning tree parameters using grid search (shown previously). Cost complexity pruning considers a completely unpruned tree unlike the 'grid search' method of searching over a grid of hyperparameters such as `max_depth` and `max_leaf_nodes`, and thus may seem to be more comprehensive than the 'grid search' approach. However, both the approaches may consider trees that are not considered by the other approach, and thus either one may provide a more accurate model. Depending on the grid of parameters chosen for cross validation, the grid search method may be more or less comprehensive than cost complexity pruning.

```
gridcv_results = pd.DataFrame(tree.cv_results_)
cv_error = -gridcv_results['mean_test_score']
```

```
#Visualizing the 5-fold cross validation error vs alpha
plt.plot(alphas,cv_error)
plt.xscale('log')
plt.xlabel('alpha')
plt.ylabel('K-fold MSE');
```




```
#Zooming in the above visualization to see the alpha where the 5-fold cross validation error
plt.plot(alphas[0:4093],cv_error[0:4093])
plt.xlabel('alpha')
plt.ylabel('K-fold MSE');
```



5.3.1 Depth vs alpha; Node counts vs alpha

```
stime = time.time()
trees=[]
for i in alphas:
    tree = DecisionTreeRegressor(ccp_alpha=i,random_state=1)
    tree.fit(X, train['price'])
    trees.append(tree)
print(time.time()-stime)
```

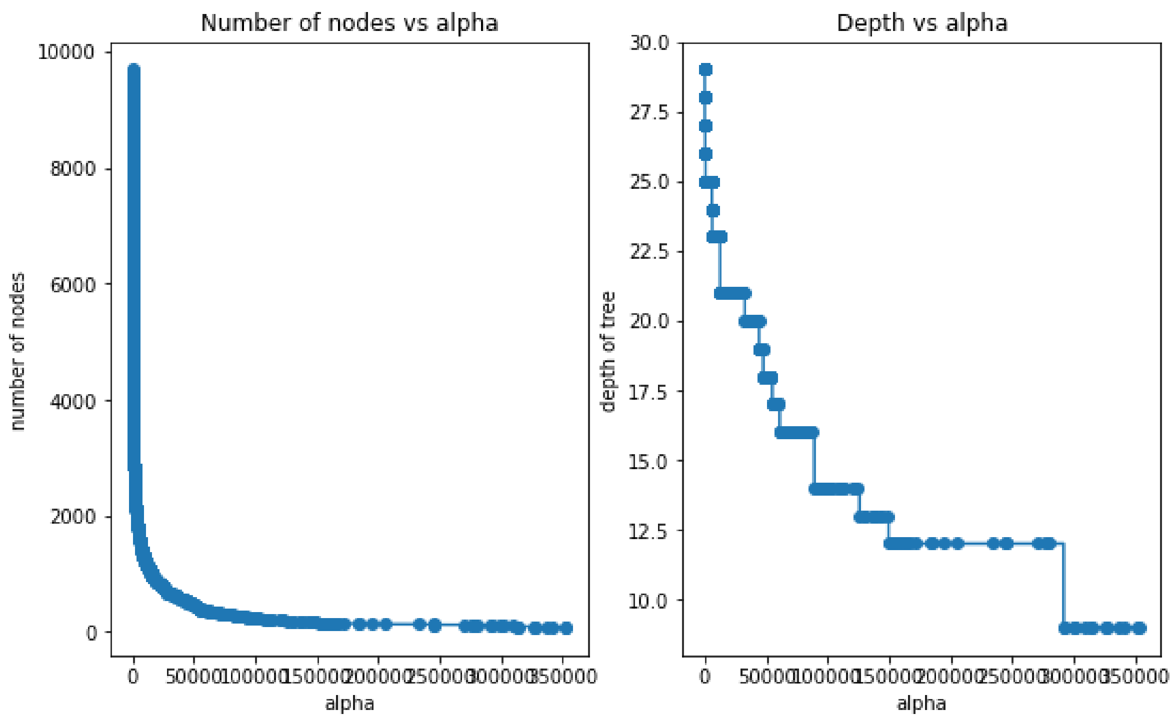
```
268.10325384140015
```

This code takes 4.5 minutes to run

```
node_counts = [clf.tree_.node_count for clf in trees]
depth = [clf.tree_.max_depth for clf in trees]
```

```
fig, ax = plt.subplots(1, 2,figsize=(10,6))
ax[0].plot(alphas[0:4093], node_counts[0:4093], marker="o", drawstyle="steps-post")#Plotting
ax[0].set_xlabel("alpha")
ax[0].set_ylabel("number of nodes")
ax[0].set_title("Number of nodes vs alpha")
ax[1].plot(alphas[0:4093], depth[0:4093], marker="o", drawstyle="steps-post")#Plotting the zo
ax[1].set_xlabel("alpha")
ax[1].set_ylabel("depth of tree")
ax[1].set_title("Depth vs alpha")
#fig.tight_layout()
```

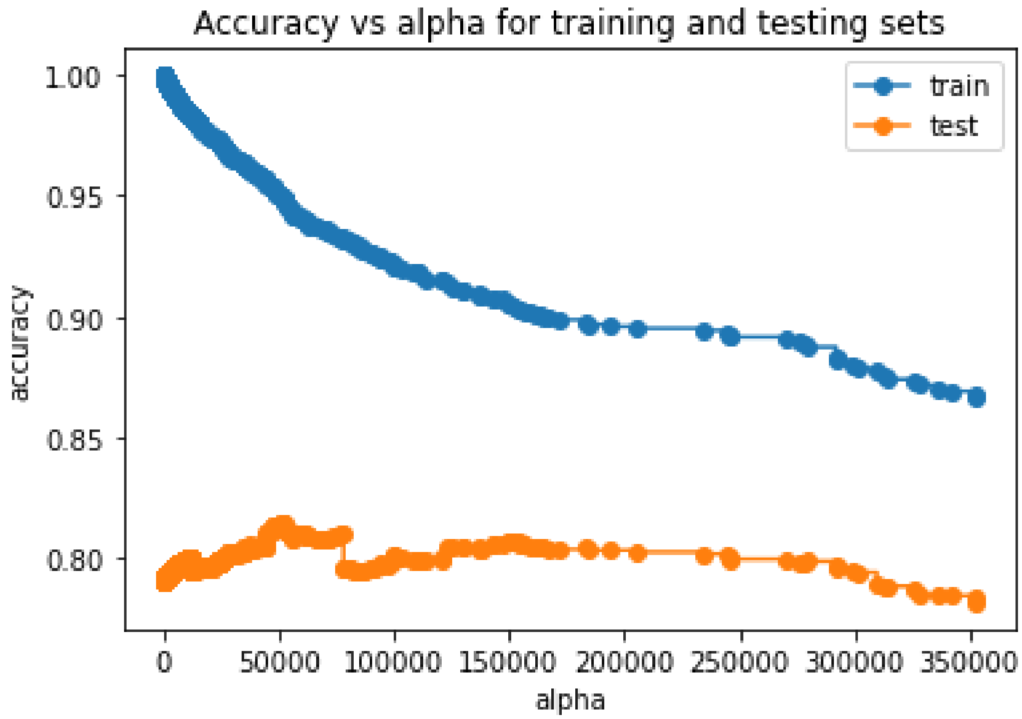
```
Text(0.5, 1.0, 'Depth vs alpha')
```



5.3.2 Train and test accuracies (R-squared) vs alpha

```
train_scores = [clf.score(X, y) for clf in trees]
test_scores = [clf.score(Xtest, test.price) for clf in trees]
```

```
fig, ax = plt.subplots()
ax.set_xlabel("alpha")
ax.set_ylabel("accuracy")
ax.set_title("Accuracy vs alpha for training and testing sets")
ax.plot(alphas[0:4093], train_scores[0:4093], marker="o", label="train", drawstyle="steps-pos
ax.plot(alphas[0:4093], test_scores[0:4093], marker="o", label="test", drawstyle="steps-post"
ax.legend()
plt.show()
```



6 Classification trees

Read section 8.1.2 of the book before using these notes.

Note that in this course, lecture notes are not sufficient, you must read the book for better understanding. Lecture notes are just implementing the concepts of the book on a dataset, but not explaining the concepts elaborately.

```
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.metrics import mean_squared_error
from sklearn.model_selection import cross_val_score,train_test_split, cross_val_predict
from sklearn.metrics import roc_curve, precision_recall_curve, auc, make_scorer, recall_score
from sklearn.model_selection import StratifiedKFold, KFold
from sklearn.tree import DecisionTreeClassifier
from sklearn.model_selection import GridSearchCV

#Libraries for visualizing trees
from sklearn.tree import export_graphviz
from six import StringIO
from IPython.display import Image
import pydotplus

import time as time
```

```
train = pd.read_csv('./Datasets/diabetes_train.csv')
test = pd.read_csv('./Datasets/diabetes_test.csv')
```

```
test.head()
```

	Pregnancies	Glucose	BloodPressure	SkinThickness	Insulin	BMI	DiabetesPedigreeFunction	Age
0	6	148	72	35	0	33.6	0.627	50
1	2	197	70	45	543	30.5	0.158	53

	Pregnancies	Glucose	BloodPressure	SkinThickness	Insulin	BMI	DiabetesPedigreeFunction	Age
2	1	115	70	30	96	34.6	0.529	32
3	8	99	84	0	0	35.4	0.388	50
4	7	147	76	0	0	39.4	0.257	43

6.1 Building a classification tree

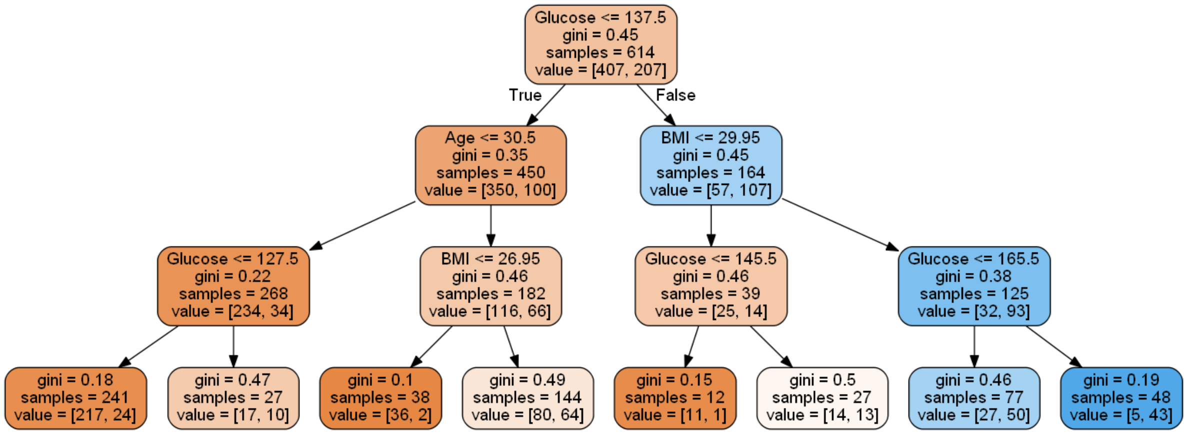
Develop a classification tree to predict if a person has diabetes.

```
X = train.drop(columns = 'Outcome')
Xtest = test.drop(columns = 'Outcome')
y = train['Outcome']
ytest = test['Outcome']
```

```
#Defining the object to build a classification tree
model = DecisionTreeClassifier(random_state=1, max_depth=3)

#Fitting the regression tree to the data
model.fit(X, y)
```

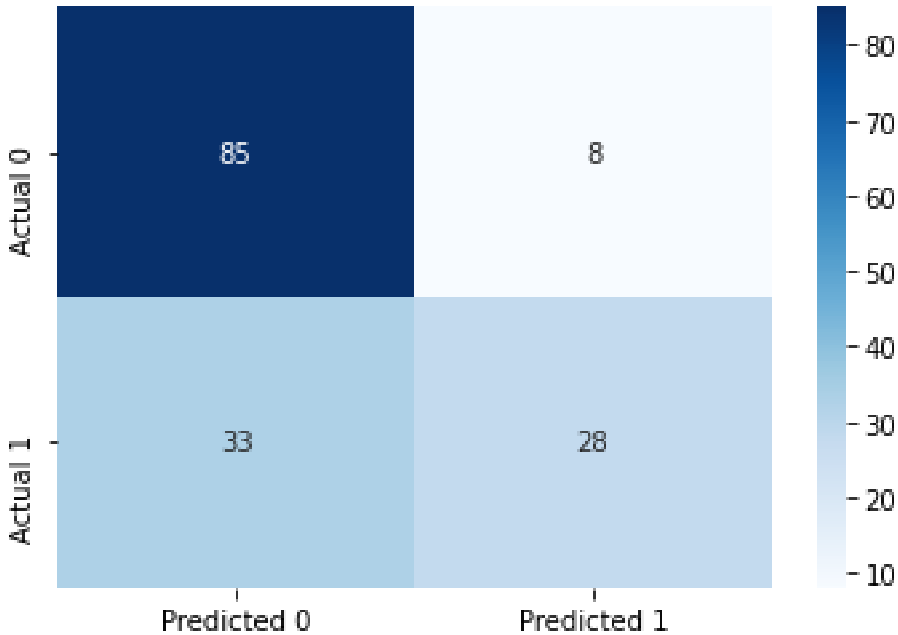
```
DecisionTreeClassifier(max_depth=3, random_state=1)
```

```
#Visualizing the regression tree
dot_data = StringIO()
export_graphviz(model, out_file=dot_data,
                filled=True, rounded=True,
                feature_names =X.columns,precision=2)
graph = pydotplus.graph_from_dot_data(dot_data.getvalue())
#graph.write_png('car_price_tree.png')
Image(graph.create_png())
```




```
# Performance metrics computation

#Computing the accuracy
y_pred = model.predict(Xtest)
print("Accuracy: ",accuracy_score(y_pred, ytest)*100)

#Computing the ROC-AUC
y_pred_prob = model.predict_proba(Xtest)[:,1]
fpr, tpr, auc_thresholds = roc_curve(ytest, y_pred_prob)
print("ROC-AUC: ",auc(fpr, tpr))# AUC of ROC

#Computing the precision and recall
print("Precision: ", precision_score(ytest, y_pred))
print("Recall: ", recall_score(ytest, y_pred))

#Confusion matrix
cm = pd.DataFrame(confusion_matrix(ytest, y_pred), columns=['Predicted 0', 'Predicted 1'],
            index = ['Actual 0', 'Actual 1'])
sns.heatmap(cm, annot=True, cmap='Blues', fmt='g');
```

```
Accuracy:  73.37662337662337
ROC-AUC:  0.8349197955226512
Precision:  0.7777777777777778
Recall:  0.45901639344262296
```



6.2 Optimizing hyperparameters to optimize performance

In case of diabetes, it is important to reduce FNR (False negative rate) or maximize recall. This is because if a person has diabetes, the consequences of predicting that they don't have diabetes can be much worse than the other way round.

Let us find the optimal depth of the tree and the number of terminal nods (leaves) that minimizes the FNR or maximizes recall.

Find the maximum values of depth and number of leaves.

```
#Defining the object to build a regression tree
model = DecisionTreeClassifier(random_state=1)

#Fitting the regression tree to the data
model.fit(X, y)
```

```
DecisionTreeClassifier(random_state=1)
```

```
# Maximum number of leaves
model.get_n_leaves()
```

```
118
```

```python
# Maximum depth
model.get_depth()
```

```
14
```

```python
#Defining parameters and the range of values over which to optimize
param_grid = {
    'max_depth': range(2,14),
    'max_leaf_nodes': range(2,118),
    'max_features': range(1, 9)
}
```

```python
#Grid search to optimize parameter values

start_time = time.time()
skf = StratifiedKFold(n_splits=5)#The folds are made by preserving the percentage of samples

#Minimizing FNR is equivalent to maximizing recall
grid_search = GridSearchCV(DecisionTreeClassifier(random_state=1), param_grid, scoring=['pre
                           refit="recall", cv=skf, n_jobs=-1, verbose = True)
grid_search.fit(X, y)

# make the predictions
y_pred = grid_search.predict(Xtest)

print('Train accuracy : %.3f'%grid_search.best_estimator_.score(X, y))
print('Test accuracy : %.3f'%grid_search.best_estimator_.score(Xtest, ytest))
print('Best recall Through Grid Search : %.3f'%grid_search.best_score_)

print('Best params for recall')
print(grid_search.best_params_)

print("Time taken =", round((time.time() - start_time)), "seconds")
```

```
Fitting 5 folds for each of 11136 candidates, totalling 55680 fits
Train accuracy : 0.785
Test accuracy : 0.675
Best recall Through Grid Search : 0.658
Best params for recall
{'max_depth': 4, 'max_features': 2, 'max_leaf_nodes': 8}
Time taken = 70 seconds
```

6.3 Optimizing the decision threshold probability

Note that decision threshold probability is not tuned with `GridSearchCV` because `GridSearchCV` is a technique used for hyperparameter tuning in machine learning models, and the decision threshold probability is not a hyperparameter of the model.

The decision threshold is set to 0.5 by default during hyperparameter tuning with `GridSearchCV`.

`GridSearchCV` is used to tune hyperparameters that control the internal settings of a machine learning model, such as learning rate, regularization strength, and maximum tree depth, among others. These hyperparameters affect the model's internal behavior and performance. On the other hand, the decision threshold is an external parameter that is used to interpret the model's output and make predictions based on the predicted probabilities.

To tune the decision threshold, one typically needs to manually adjust it after the model has been trained and evaluated using a specific set of hyperparameter values. This can be done using methods, which involve evaluating the model's performance at different decision threshold values and selecting the one that best meets the desired trade-off between false positives and false negatives based on the specific problem requirements.

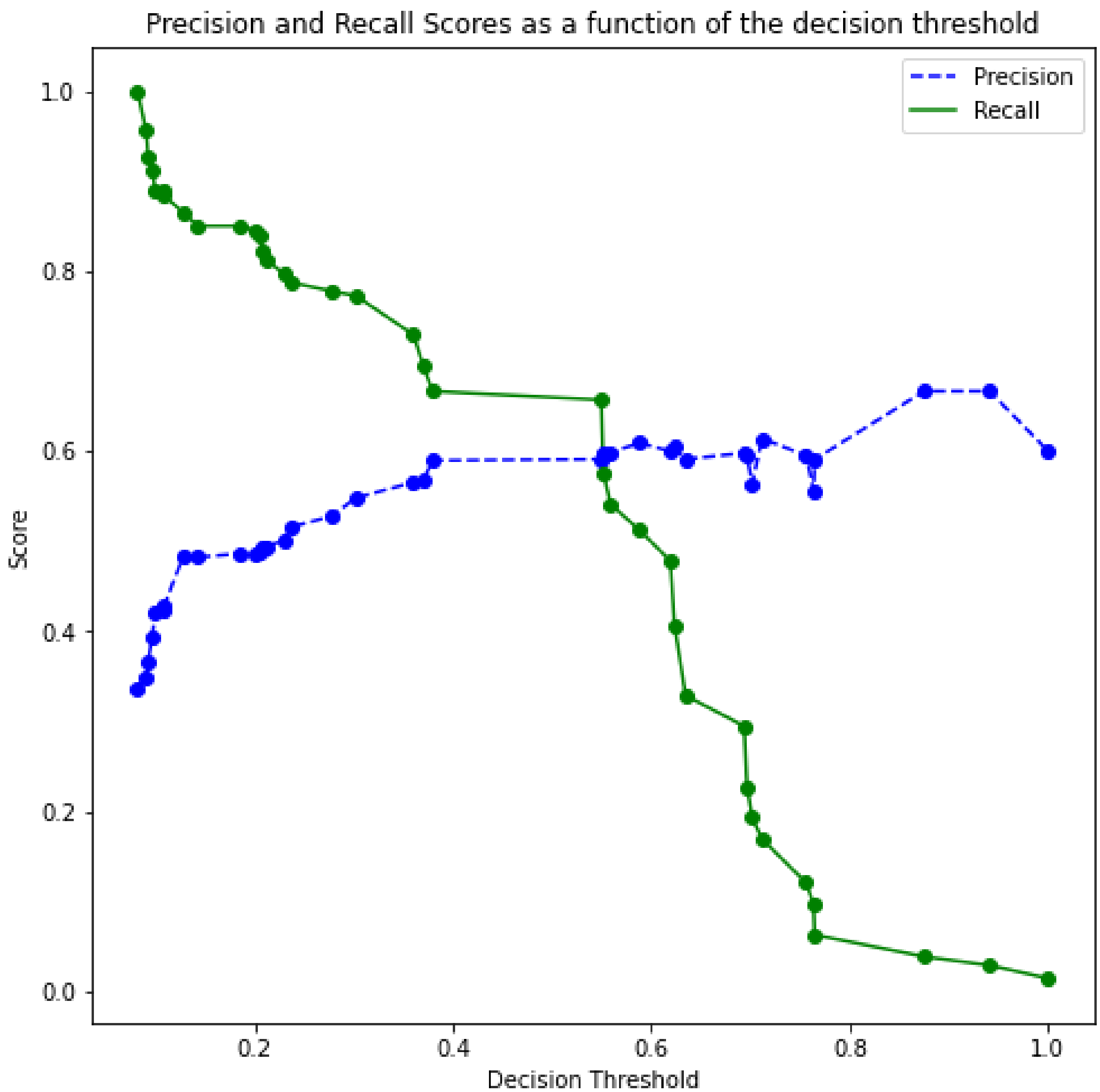
As the recall will always be 100% for a decision threshold probability of zero, we'll find a decision threshold probability that balances recall with another performance metric such as precision, false positive rate, accuracy, etc. Below are a couple of examples that show we can balance recall with (1) precision or (2) false positive rate.

6.3.1 Balancing recall with precision

We can find a threshold probability that balances recall with precision.

```
model = DecisionTreeClassifier(random_state=1, max_depth = 4, max_leaf_nodes=8, max_features=

# Note that we are using the cross-validated predicted probabilities, instead of directly usi
# predicted probabilities on train data, as the model may be overfitting on the train data, a
# may lead to misleading results
cross_val_ypred = cross_val_predict(DecisionTreeClassifier(random_state=1, max_depth = 4,
                                                        max_leaf_nodes=8, max_features=2), X
                                              y, cv = 5, method = 'predict_proba')

p, r, thresholds = precision_recall_curve(y, cross_val_ypred[:,1])
def plot_precision_recall_vs_threshold(precisions, recalls, thresholds):
    plt.figure(figsize=(8, 8))
    plt.title("Precision and Recall Scores as a function of the decision threshold")
```

```
    plt.plot(thresholds, precisions[:-1], "b--", label="Precision")
    plt.plot(thresholds, recalls[:-1], "g-", label="Recall")
    plt.plot(thresholds, precisions[:-1], "o", color = 'blue')
    plt.plot(thresholds, recalls[:-1], "o", color = 'green')
    plt.ylabel("Score")
    plt.xlabel("Decision Threshold")
    plt.legend(loc='best')
    plt.legend()
plot_precision_recall_vs_threshold(p, r, thresholds)
```




```
# Thresholds with precision and recall
np.concatenate([thresholds.reshape(-1,1), p[:-1].reshape(-1,1), r[:-1].reshape(-1,1)], axis
```

```
array([[0.08196721, 0.33713355, 1.        ],
       [0.09045226, 0.34982332, 0.95652174],
       [0.09248555, 0.36641221, 0.92753623],
       [0.0964467 , 0.39293139, 0.91304348],
       [0.1       , 0.42105263, 0.88888889],
```

```
       [0.10810811, 0.42298851, 0.88888889],
       [0.10869565, 0.42857143, 0.88405797],
       [0.12820513, 0.48378378, 0.8647343 ],
       [0.14285714, 0.48219178, 0.85024155],
       [0.18518519, 0.48618785, 0.85024155],
       [0.2       , 0.48611111, 0.84541063],
       [0.20512821, 0.48876404, 0.84057971],
       [0.20833333, 0.49418605, 0.82125604],
       [0.21276596, 0.49411765, 0.8115942 ],
       [0.22916667, 0.50151976, 0.79710145],
       [0.23684211, 0.51582278, 0.78743961],
       [0.27777778, 0.52786885, 0.77777778],
       [0.3015873 , 0.54794521, 0.77294686],
       [0.36      , 0.56554307, 0.7294686 ],
       [0.3697479 , 0.56692913, 0.69565217],
       [0.37931034, 0.58974359, 0.66666667],
       [0.54954955, 0.59130435, 0.65700483],
       [0.55172414, 0.59798995, 0.57487923],
       [0.55882353, 0.59893048, 0.5410628 ],
       [0.58823529, 0.6091954 , 0.51207729],
       [0.61904762, 0.6       , 0.47826087],
       [0.62337662, 0.60431655, 0.4057971 ],
       [0.63461538, 0.59130435, 0.32850242],
       [0.69354839, 0.59803922, 0.29468599],
       [0.69642857, 0.59493671, 0.22705314],
       [0.70149254, 0.56338028, 0.19323671],
       [0.71153846, 0.61403509, 0.16908213],
       [0.75609756, 0.5952381 , 0.12077295],
       [0.76363636, 0.55555556, 0.09661836],
       [0.76470588, 0.59090909, 0.06280193],
       [0.875     , 0.66666667, 0.03864734],
       [0.94117647, 0.66666667, 0.02898551],
       [1.        , 0.6       , 0.01449275]])
```

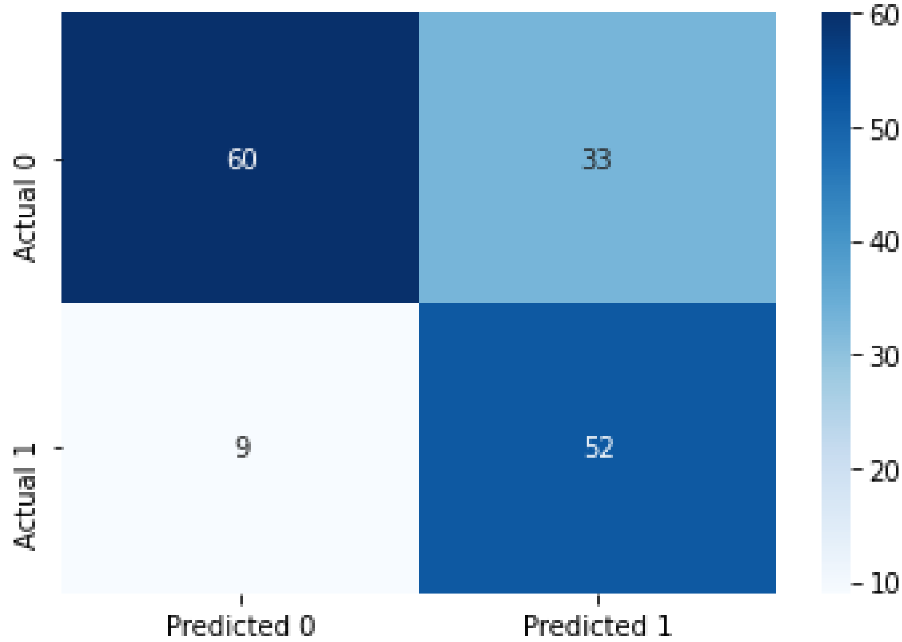
Suppose, we wish to have at least 80% recall, with the highest possible precision. Then, based on the precision-recall curve *(or the table above)*, we should have a decision threshold probability of 0.21.

Let's assess the model's performance on test data with a threshold probability of 0.21.

```
# Performance metrics computation for the optimum decision threshold probability
desired_threshold = 0.21
```

```
y_pred_prob = model.predict_proba(Xtest)[:,1]

# Classifying observations in the positive class (y = 1) if the predicted probability is grea
# than the desired decision threshold probability
y_pred = y_pred_prob > desired_threshold
y_pred = y_pred.astype(int)

#Computing the accuracy
print("Accuracy: ",accuracy_score(y_pred, ytest)*100)

#Computing the ROC-AUC
fpr, tpr, auc_thresholds = roc_curve(ytest, y_pred_prob)
print("ROC-AUC: ",auc(fpr, tpr))# AUC of ROC

#Computing the precision and recall
print("Precision: ", precision_score(ytest, y_pred))
print("Recall: ", recall_score(ytest, y_pred))

#Confusion matrix
cm = pd.DataFrame(confusion_matrix(ytest, y_pred),
                  columns=['Predicted 0', 'Predicted 1'], index = ['Actual 0', 'Actual 1'])
sns.heatmap(cm, annot=True, cmap='Blues', fmt='g');
```

```
Accuracy:  72.72727272727273
ROC-AUC:  0.7544509078089194
Precision:  0.611764705882353
Recall:  0.8524590163934426
```



6.3.2 Balancing recall with false positive rate

Suppose we wish to balance recall with false positive rate. We can optimize the model to maximize ROC-AUC, and then choose a point on the ROC-curve that balances recall with the false positive rate.

```
# Defining parameters and the range of values over which to optimize
param_grid = {
    'max_depth': range(2,14),
    'max_leaf_nodes': range(2,118),
    'max_features': range(1, 9)
}
```

```
#Grid search to optimize parameter values

start_time = time.time()
skf = StratifiedKFold(n_splits=5)#The folds are made by preserving the percentage of samples

#Minimizing FNR is equivalent to maximizing recall
grid_search = GridSearchCV(DecisionTreeClassifier(random_state=1), param_grid, scoring=['pre
                            'roc_auc'], refit="roc_auc", cv=skf, n_jobs=-1, verbose = True)
grid_search.fit(X, y)
```

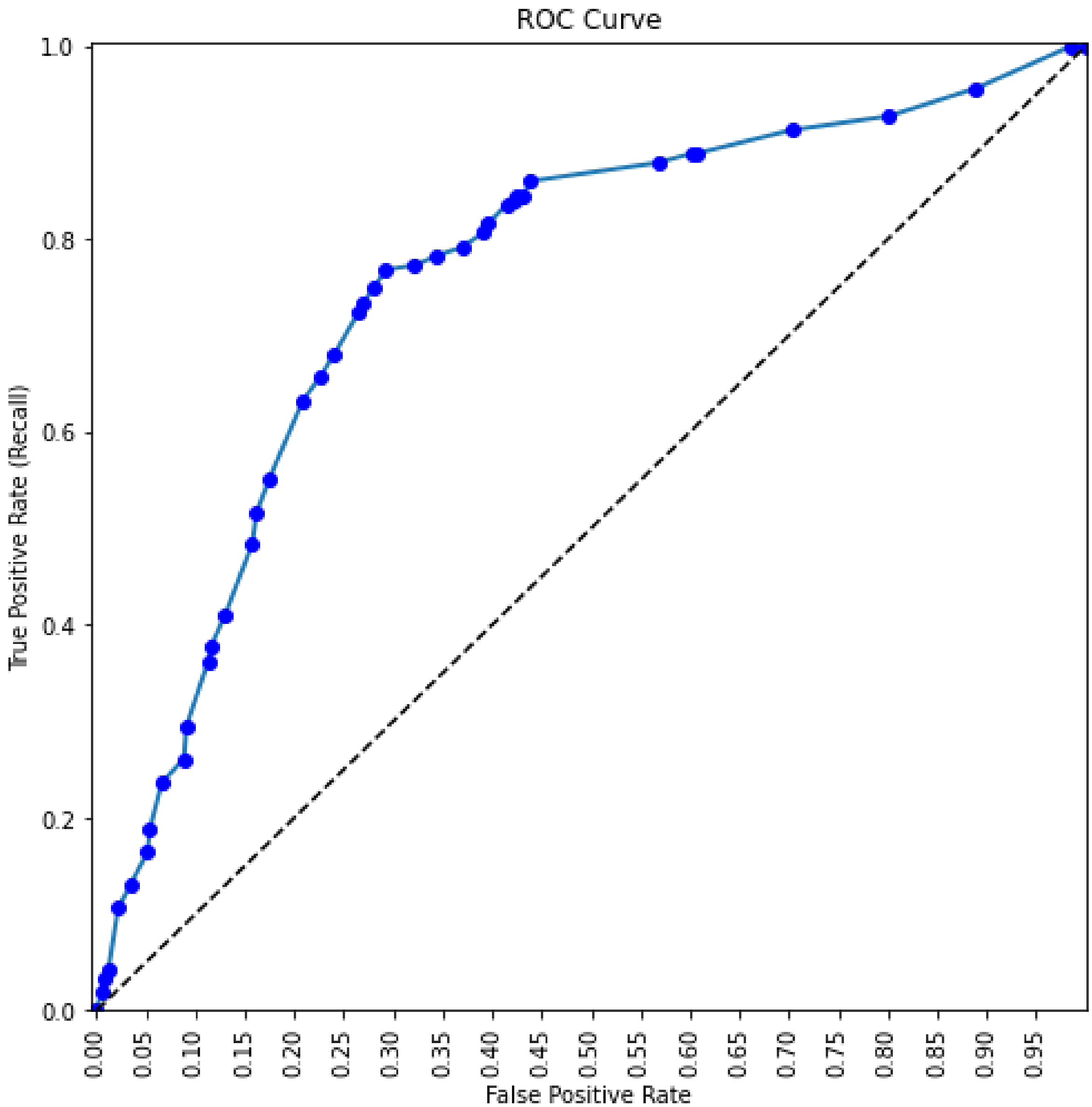
```
# make the predictions
y_pred = grid_search.predict(Xtest)

print('Best params for recall')
print(grid_search.best_params_)

print("Time taken =", round((time.time() - start_time)), "seconds")
```

```
Fitting 5 folds for each of 11136 candidates, totalling 55680 fits
Best params for recall
{'max_depth': 6, 'max_features': 2, 'max_leaf_nodes': 9}
Time taken = 72 seconds
```

```
model = DecisionTreeClassifier(random_state=1, max_depth = 6, max_leaf_nodes=9, max_features=
```

```
cross_val_ypred = cross_val_predict(DecisionTreeClassifier(random_state=1, max_depth = 6,
                                                           max_leaf_nodes=9, max_features=2)
                                              y, cv = 5, method = 'predict_proba')

fpr, tpr, auc_thresholds = roc_curve(y, cross_val_ypred[:,1])
print(auc(fpr, tpr))# AUC of ROC
def plot_roc_curve(fpr, tpr, label=None):
    plt.figure(figsize=(8,8))
    plt.title('ROC Curve')
    plt.plot(fpr, tpr, linewidth=2, label=label)
    plt.plot(fpr, tpr, 'o', color = 'blue')
    plt.plot([0, 1], [0, 1], 'k--')
    plt.axis([-0.005, 1, 0, 1.005])
    plt.xticks(np.arange(0,1, 0.05), rotation=90)
    plt.xlabel("False Positive Rate")
    plt.ylabel("True Positive Rate (Recall)")

fpr, tpr, auc_thresholds = roc_curve(y, cross_val_ypred[:,1])
plot_roc_curve(fpr, tpr)
```

```
0.7605075431162388
```




```
# Thresholds with TPR and FPR
all_thresholds = np.concatenate([auc_thresholds.reshape(-1,1), tpr.reshape(-1,1), fpr.reshape
recall_more_than_80 = all_thresholds[all_thresholds[:,1]>0.8,:]
# As the values in 'recall_more_than_80' are arranged in increasing order of recall and decre
# the first value will provide the maximum threshold probability for the recall to be more th
# We wish to find the maximum threshold probability to obtain the minimum possible FPR
recall_more_than_80[0]
```

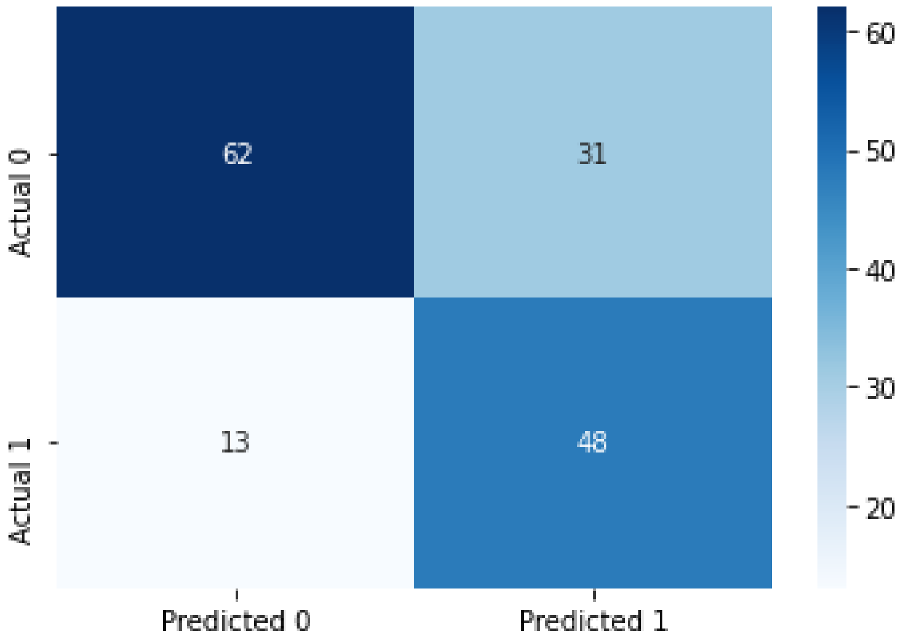
```
array([0.21276596, 0.80676329, 0.39066339])
```

Suppose, we wish to have at least 80% recall, with the lowest possible precision. Then, based on the ROC-AUC curve, we should have a decision threshold probability of 0.21.

Let's assess the model's performance on test data with a threshold probability of 0.21.

```
# Performance metrics computation for the optimum decision threshold probability
desired_threshold = 0.21

y_pred_prob = model.predict_proba(Xtest)[:,1]

# Classifying observations in the positive class (y = 1) if the predicted probability is grea
# than the desired decision threshold probability
y_pred = y_pred_prob > desired_threshold
y_pred = y_pred.astype(int)

#Computing the accuracy
print("Accuracy: ",accuracy_score(y_pred, ytest)*100)

#Computing the ROC-AUC
fpr, tpr, auc_thresholds = roc_curve(ytest, y_pred_prob)
print("ROC-AUC: ",auc(fpr, tpr))# AUC of ROC

#Computing the precision and recall
print("Precision: ", precision_score(ytest, y_pred))
print("Recall: ", recall_score(ytest, y_pred))

#Confusion matrix
cm = pd.DataFrame(confusion_matrix(ytest, y_pred),
                  columns=['Predicted 0', 'Predicted 1'], index = ['Actual 0', 'Actual 1'])
sns.heatmap(cm, annot=True, cmap='Blues', fmt='g');
```

```
Accuracy:  71.42857142857143
ROC-AUC:  0.7618543980257358
Precision:  0.6075949367088608
Recall:  0.7868852459016393
```



6.4 Cost complexity pruning

Just as we did cost complexity pruning in a regression tree, we can do it to optimize the model for a classification tree.

```
model = DecisionTreeClassifier(random_state = 1)#model without any restrictions
path= model.cost_complexity_pruning_path(X,y)# Compute the pruning path during Minimal Cost-C
```

```
alphas=path['ccp_alphas']
len(alphas)
```

```
58
```

```
#Grid search to optimize parameter values

skf = StratifiedKFold(n_splits=5)
grid_search = GridSearchCV(DecisionTreeClassifier(random_state = 1), param_grid = {'ccp_alpha
                                                   scoring=['precision','recall','accuracy'],
                                                   refit="recall", cv=skf, n_jobs=-1, verbose
grid_search.fit(X, y)
```

```python
# make the predictions
y_pred = grid_search.predict(Xtest)

print('Best params for recall')
print(grid_search.best_params_)
```

```
Fitting 5 folds for each of 58 candidates, totalling 290 fits
Best params for recall
{'ccp_alpha': 0.010561291712538737}
```

```python
# Model with the optimal value of 'ccp_alpha'
model = DecisionTreeClassifier(ccp_alpha=0.01435396,random_state=1)
model.fit(X, y)
```

```
DecisionTreeClassifier(ccp_alpha=0.01435396, random_state=1)
```

Now we can tune the decision threshold probability to balance recall with another performance metrics as shown earlier in Section 4.3.

7 Bagging

Read section 8.2.1 of the book before using these notes.

Note that in this course, lecture notes are not sufficient, you must read the book for better understanding. Lecture notes are just implementing the concepts of the book on a dataset, but not explaining the concepts elaborately.

```
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.model_selection import cross_val_score,train_test_split, KFold, GridSearchCV, Pa
RandomizedSearchCV
from sklearn.tree import DecisionTreeRegressor,DecisionTreeClassifier
from sklearn.ensemble import BaggingRegressor,BaggingClassifier
from sklearn.linear_model import LinearRegression, LogisticRegression
from sklearn.neighbors import KNeighborsRegressor
from sklearn.metrics import roc_curve, precision_recall_curve, auc, make_scorer, recall_score
accuracy_score, precision_score, confusion_matrix, mean_squared_error, r2_score, mean_squared
from skopt import BayesSearchCV
from skopt.space import Real, Integer, Categorical
from skopt.plots import plot_convergence, plot_histogram, plot_objective
from IPython import display
import itertools as it
from sklearn.preprocessing import StandardScaler

#Libraries for visualizing trees
from sklearn.tree import export_graphviz, export_text
from six import StringIO
from IPython.display import Image
import pydotplus
import time as time
import warnings
```

```
#Using the same datasets as in linear regression in STAT303-2,
#so that we can compare the non-linear models with linear regression
```

```
trainf = pd.read_csv('./Datasets/Car_features_train.csv')
trainp = pd.read_csv('./Datasets/Car_prices_train.csv')
testf = pd.read_csv('./Datasets/Car_features_test.csv')
testp = pd.read_csv('./Datasets/Car_prices_test.csv')
train = pd.merge(trainf,trainp)
test = pd.merge(testf,testp)
train.head()
```

	carID	brand	model	year	transmission	mileage	fuelType	tax	mpg	engineSize	price
0	18473	bmw	6 Series	2020	Semi-Auto	11	Diesel	145	53.3282	3.0	37980
1	15064	bmw	6 Series	2019	Semi-Auto	10813	Diesel	145	53.0430	3.0	33980
2	18268	bmw	6 Series	2020	Semi-Auto	6	Diesel	145	53.4379	3.0	36850
3	18480	bmw	6 Series	2017	Semi-Auto	18895	Diesel	145	51.5140	3.0	25998
4	18492	bmw	6 Series	2015	Automatic	62953	Diesel	160	51.4903	3.0	18990

```
X = train[['mileage','mpg','year','engineSize']]
Xtest = test[['mileage','mpg','year','engineSize']]
y = train['price']
ytest = test['price']
```

7.1 Bagging regression trees

Bag regression trees to develop a model to predict car price using the predictors `mileage`,`mpg`,`year`,and `engineSize`.

```
#Bagging the results of 10 decision trees to predict car price
model = BaggingRegressor(estimator=DecisionTreeRegressor(), n_estimators=10, random_state=1,
                        n_jobs=-1).fit(X, y)
```

```
np.sqrt(mean_squared_error(test.price, model.predict(Xtest)))
```

```
5752.0779571060875
```

The RMSE has reduced a lot by averaging the predictions of 10 trees. The RMSE for a single tree model with optimized parameters was around 7000.

7.1.1 Model accuracy vs number of trees

How does the model accuracy vary with the number of trees?

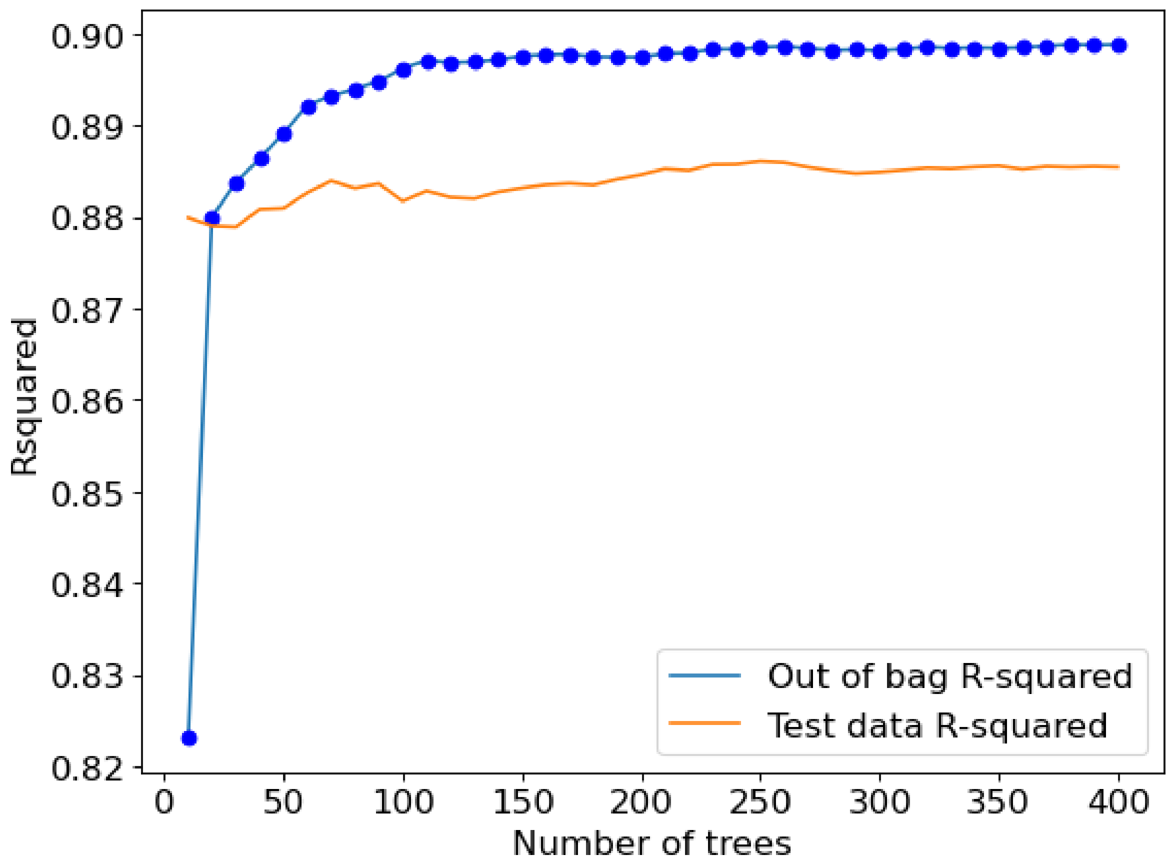
As we increase the number of trees, it will tend to reduce the variance of individual trees leading to a more accurate prediction.

```
#Finding model accuracy vs number of trees
warnings.filterwarnings("ignore")
oob_rsquared={};test_rsquared={};oob_rmse={};test_rmse = {}
for i in np.linspace(10,400,40,dtype=int):
    model = BaggingRegressor(estimator=DecisionTreeRegressor(), n_estimators=i, random_state=
                    n_jobs=-1,oob_score=True).fit(X, y)
    oob_rsquared[i]=model.oob_score_  #Returns the out-of_bag R-squared of the model
    test_rsquared[i]=model.score(Xtest,ytest) #Returns the test R-squared of the model
    oob_rmse[i]=np.sqrt(mean_squared_error(model.oob_prediction_,y))
    test_rmse[i]=np.sqrt(mean_squared_error(model.predict(Xtest),ytest))
warnings.resetwarnings()

# The hidden warning is: "Some inputs do not have OOB scores. This probably means too few
# estimators were used to compute any reliable oob estimates." This warning will appear
# in case of small number of estimators. In such a case, some observations may be use
# by all the estimators, and their OOB score can't be computed
```

As we are bagging only 10 trees in the first iteration, some of the observations are selected in every bootstrapped sample, and thus they don't have an out-of-bag error, which is producing the warning. For every observation to have an out-of-bag error, the number of trees must be sufficiently large.

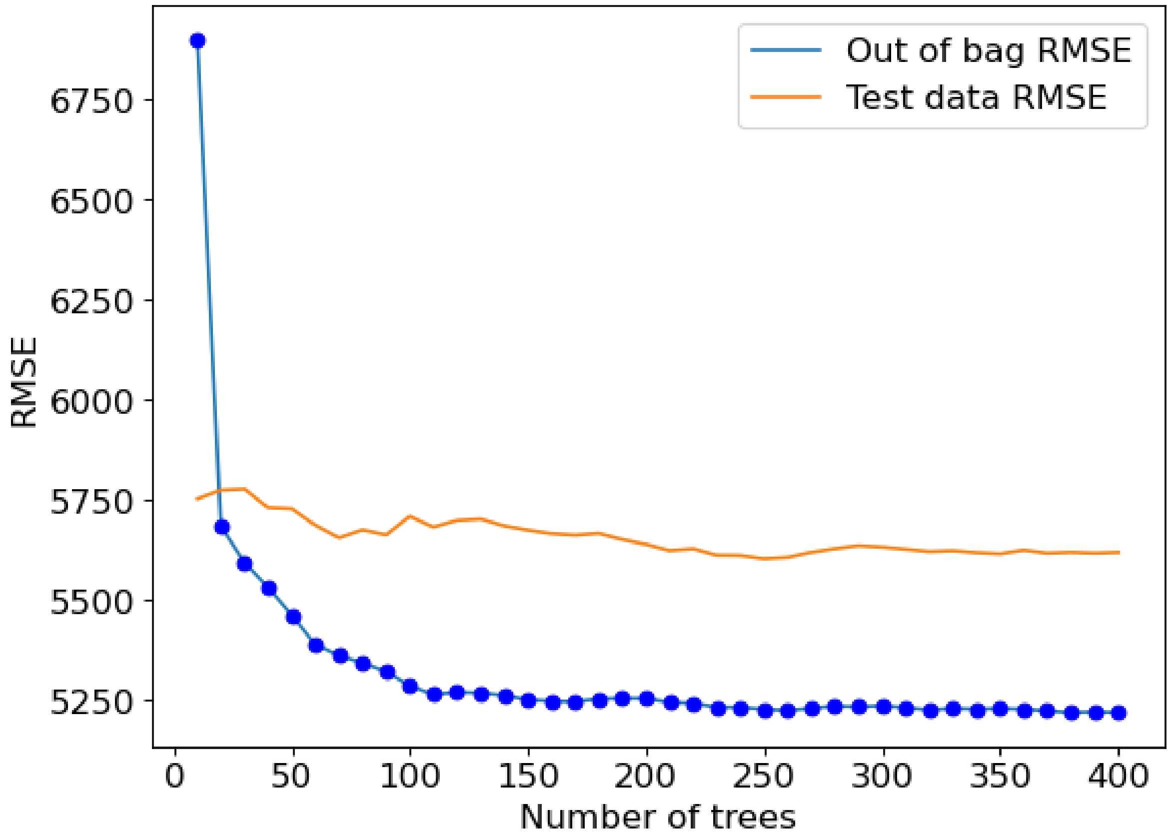
Let us visualize the out-of-bag (OOB) R-squared and R-squared on test data vs the number of trees.

```
plt.rcParams.update({'font.size': 15})
plt.figure(figsize=(8, 6), dpi=80)
plt.plot(oob_rsquared.keys(),oob_rsquared.values(),label = 'Out of bag R-squared')
plt.plot(oob_rsquared.keys(),oob_rsquared.values(),'o',color = 'blue')
plt.plot(test_rsquared.keys(),test_rsquared.values(), label = 'Test data R-squared')
plt.xlabel('Number of trees')
plt.ylabel('Rsquared')
plt.legend();
```



The out-of-bag R-squared initially increases, and then stabilizes after a certain number of trees (around 150 in this case). Note that increasing the number of trees further will not lead to overfitting. However, increasing the number of trees will increase the computations. Thus, we don't need to develop more trees once the R-squared stabilizes.

```
#Visualizing out-of-bag RMSE and test data RMSE
plt.rcParams.update({'font.size': 15})
plt.figure(figsize=(8, 6), dpi=80)
plt.plot(oob_rmse.keys(),oob_rmse.values(),label = 'Out of bag RMSE')
plt.plot(oob_rmse.keys(),oob_rmse.values(),'o',color = 'blue')
plt.plot(test_rmse.keys(),test_rmse.values(), label = 'Test data RMSE')
plt.xlabel('Number of trees')
plt.ylabel('RMSE')
plt.legend()
```



A similar trend can be seen by plotting out-of-bag RMSE and test RMSE. Note that RMSE is proportional to R-squared. We only need to visualize one of RMSE or R-squared to find the optimal number of trees.

```
#Bagging with 150 trees
model = BaggingRegressor(base_estimator=DecisionTreeRegressor(), n_estimators=150, random_sta
                         oob_score=True,n_jobs=-1).fit(X, y)
```

```
#OOB R-squared
model.oob_score_
```

```
0.897561533100511
```

```
#RMSE on test data
pred = model.predict(Xtest)
np.sqrt(mean_squared_error(test.price, pred))
```

```
5673.756466489405
```

7.1.2 Optimizing bagging hyperparameters using grid search

More parameters of a bagged regression tree model can be optimized using the typical approach of k-fold cross validation over a grid of parameter values.

Note that we don't need to tune the number of trees in bagging as we know that the higher the number of trees, the lower will be the expected MSE. So, we will tune all the hyperparameters for a fixed number of trees. Once we have obtained the optimal hyperparameter values, we'll keep increasing the number of trees until the gains are neglible.

```
n_samples = train.shape[0]
n_features = train.shape[1]

params = {'base_estimator': [DecisionTreeRegressor(random_state = 1),LinearRegression()],#Com
          'n_estimators': [100],
          'max_samples': [0.5,1.0],
          'max_features': [0.5,1.0],
          'bootstrap': [True, False],
          'bootstrap_features': [True, False]}

cv = KFold(n_splits=5,shuffle=True,random_state=1)
bagging_regressor_grid = GridSearchCV(BaggingRegressor(random_state=1, n_jobs=-1),
                                      param_grid =params, cv=cv, n_jobs=-1, verbose=1)
bagging_regressor_grid.fit(X, y)

print('Train R^2 Score : %.3f'%bagging_regressor_grid.best_estimator_.score(X, y))
print('Test R^2 Score : %.3f'%bagging_regressor_grid.best_estimator_.score(Xtest, ytest))
print('Best R^2 Score Through Grid Search : %.3f'%bagging_regressor_grid.best_score_)
print('Best Parameters : ',bagging_regressor_grid.best_params_)
```

```
Fitting 5 folds for each of 32 candidates, totalling 160 fits
Train R^2 Score : 0.986
Test R^2 Score : 0.882
Best R^2 Score Through Grid Search : 0.892
Best Parameters :  {'base_estimator': DecisionTreeRegressor(random_state=1), 'bootstrap': Tru
```

You may use the object `bagging_regressor_grid` to directly make the prediction.

```
np.sqrt(mean_squared_error(test.price, bagging_regressor_grid.predict(Xtest)))
```

```
5708.308794847089
```

Note that once the model has been tuned and the optimal hyperparameters identified, we can keep increasing the number of trees until it ceases to benefit.

```
#Model with optimal hyperparameters and increased number of trees
model = BaggingRegressor(base_estimator=DecisionTreeRegressor(), n_estimators=500, random_sta
                        oob_score=True,n_jobs=-1,bootstrap_features=False,bootstrap=True,
                        max_features=1.0,max_samples=1.0).fit(X, y)
```

```
#RMSE on test data
np.sqrt(mean_squared_error(test.price, model.predict(Xtest)))
```

```
5624.685464926517
```

7.2 Bagging for classification

Bag classification tree models to predict if a person has diabetes.

```
train = pd.read_csv('./Datasets/diabetes_train.csv')
test = pd.read_csv('./Datasets/diabetes_test.csv')
```

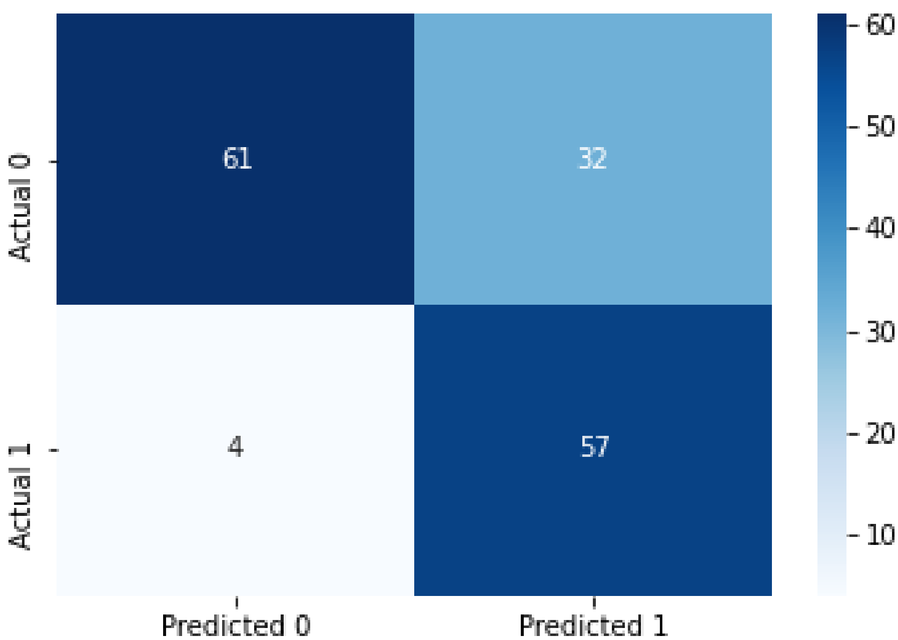
```
X = train.drop(columns = 'Outcome')
Xtest = test.drop(columns = 'Outcome')
y = train['Outcome']
ytest = test['Outcome']
```

```
#Bagging the results of 10 decision trees to predict car price
model = BaggingClassifier(base_estimator=DecisionTreeClassifier(), n_estimators=150, random_s
                        n_jobs=-1).fit(X, y)
```

```
# Performance metrics computation for the optimum decision threshold probability
desired_threshold = 0.23

y_pred_prob = model.predict_proba(Xtest)[:,1]

# Classifying observations in the positive class (y = 1) if the predicted probability is grea
# than the desired decision threshold probability
y_pred = y_pred_prob > desired_threshold
y_pred = y_pred.astype(int)
```

```
#Computing the accuracy
print("Accuracy: ",accuracy_score(y_pred, ytest)*100)

#Computing the ROC-AUC
fpr, tpr, auc_thresholds = roc_curve(ytest, y_pred_prob)
print("ROC-AUC: ",auc(fpr, tpr))# AUC of ROC

#Computing the precision and recall
print("Precision: ", precision_score(ytest, y_pred))
print("Recall: ", recall_score(ytest, y_pred))

#Confusion matrix
cm = pd.DataFrame(confusion_matrix(ytest, y_pred),
                  columns=['Predicted 0', 'Predicted 1'], index = ['Actual 0', 'Actual 1'])
sns.heatmap(cm, annot=True, cmap='Blues', fmt='g');
```

```
Accuracy:  76.62337662337663
ROC-AUC:  0.8766084963863917
Precision:  0.6404494382022472
Recall:  0.9344262295081968
```



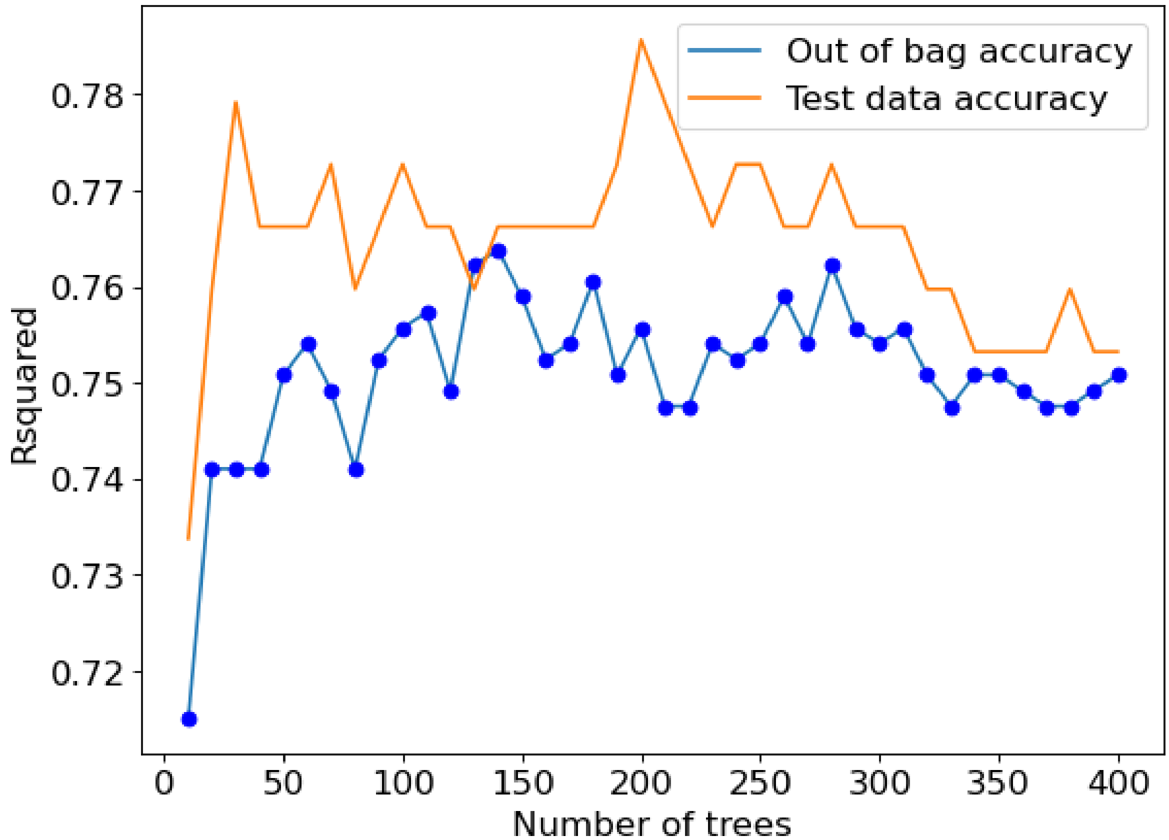
As a result of bagging, we obtain a model (with a threshold probabiltiy cutoff of 0.23) that has a better performance on test data in terms of almost all the metrics - accuracy, precision (comparable performance), recall, and ROC-AUC, as compared the single tree classification model (with a threshold probability cutoff of 0.23). Note that we have not yet tuned the model using `GridSearchCv` here, which is shown towards the end of this chapter.

7.2.1 Model accuracy vs number of trees

```
#Finding model accuracy vs number of trees
oob_accuracy={};test_accuracy={};oob_rmse={};test_rmse = {}
for i in np.linspace(10,400,40,dtype=int):
    model = BaggingClassifier(base_estimator=DecisionTreeClassifier(), n_estimators=i, randon
                        n_jobs=-1,oob_score=True).fit(X, y)
    oob_accuracy[i]=model.oob_score_  #Returns the out-of_bag R-squared of the model
    test_accuracy[i]=model.score(Xtest,ytest) #Returns the test R-squared of the model
```

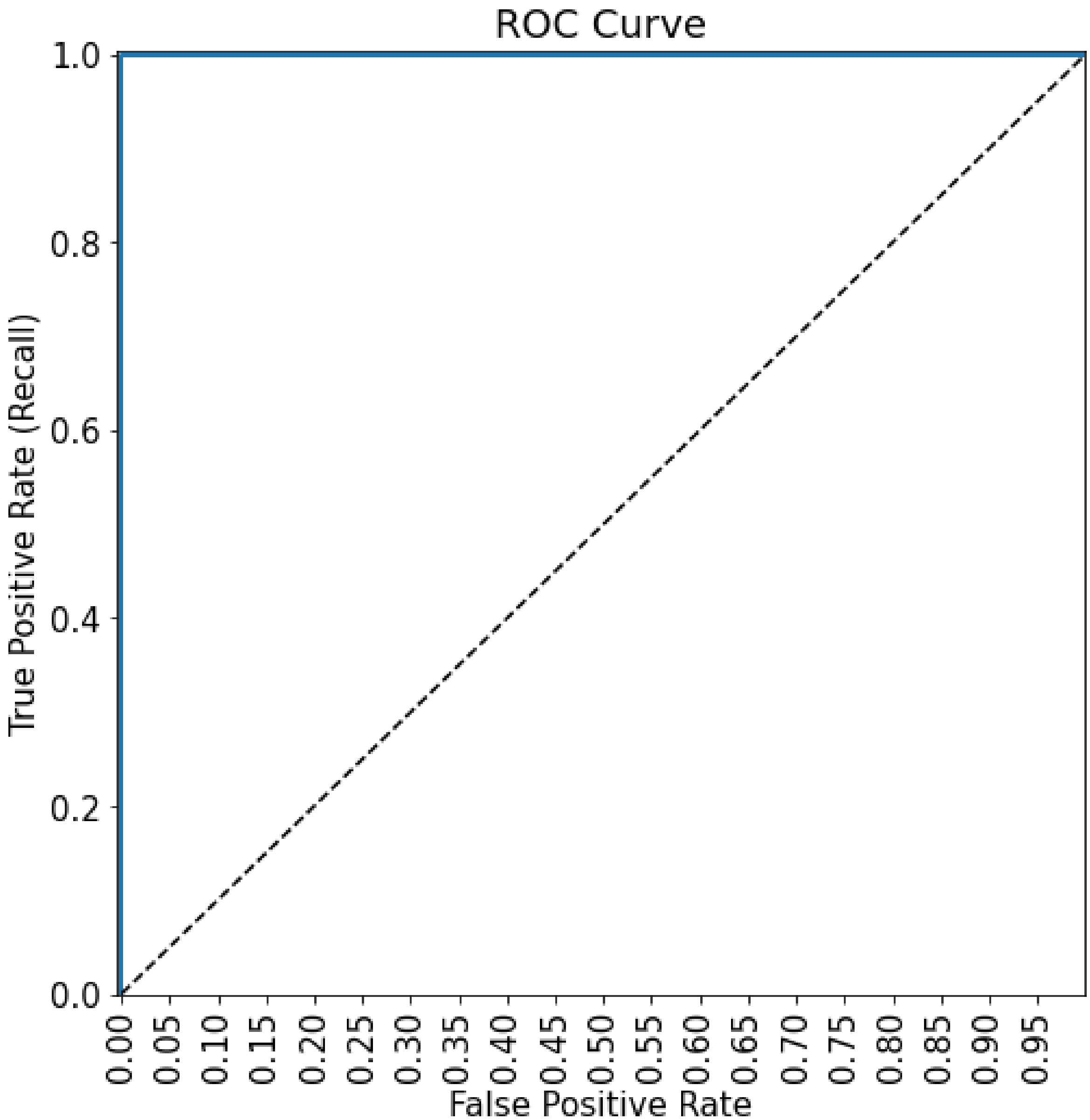
```
C:\Users\akl0407\Anaconda3\lib\site-packages\sklearn\ensemble\_bagging.py:640: UserWarning: S
  warn("Some inputs do not have OOB scores. "
C:\Users\akl0407\Anaconda3\lib\site-packages\sklearn\ensemble\_bagging.py:644: RuntimeWarning
  oob_decision_function = (predictions /
```

```
plt.rcParams.update({'font.size': 15})
plt.figure(figsize=(8, 6), dpi=80)
plt.plot(oob_accuracy.keys(),oob_accuracy.values(),label = 'Out of bag accuracy')
plt.plot(oob_accuracy.keys(),oob_accuracy.values(),'o',color = 'blue')
plt.plot(test_accuracy.keys(),test_accuracy.values(), label = 'Test data accuracy')
plt.xlabel('Number of trees')
plt.ylabel('Rsquared')
plt.legend()
```




```
#ROC curve on training data
ypred = model.predict_proba(X)[:, 1]
fpr, tpr, auc_thresholds = roc_curve(y, ypred)
print(auc(fpr, tpr))# AUC of ROC
def plot_roc_curve(fpr, tpr, label=None):

    plt.figure(figsize=(8,8))
    plt.title('ROC Curve')
    plt.plot(fpr, tpr, linewidth=2, label=label)
    plt.plot([0, 1], [0, 1], 'k--')
    plt.axis([-0.005, 1, 0, 1.005])
    plt.xticks(np.arange(0,1, 0.05), rotation=90)
    plt.xlabel("False Positive Rate")
    plt.ylabel("True Positive Rate (Recall)")

fpr, tpr, auc_thresholds = roc_curve(y, ypred)
plot_roc_curve(fpr, tpr)
```

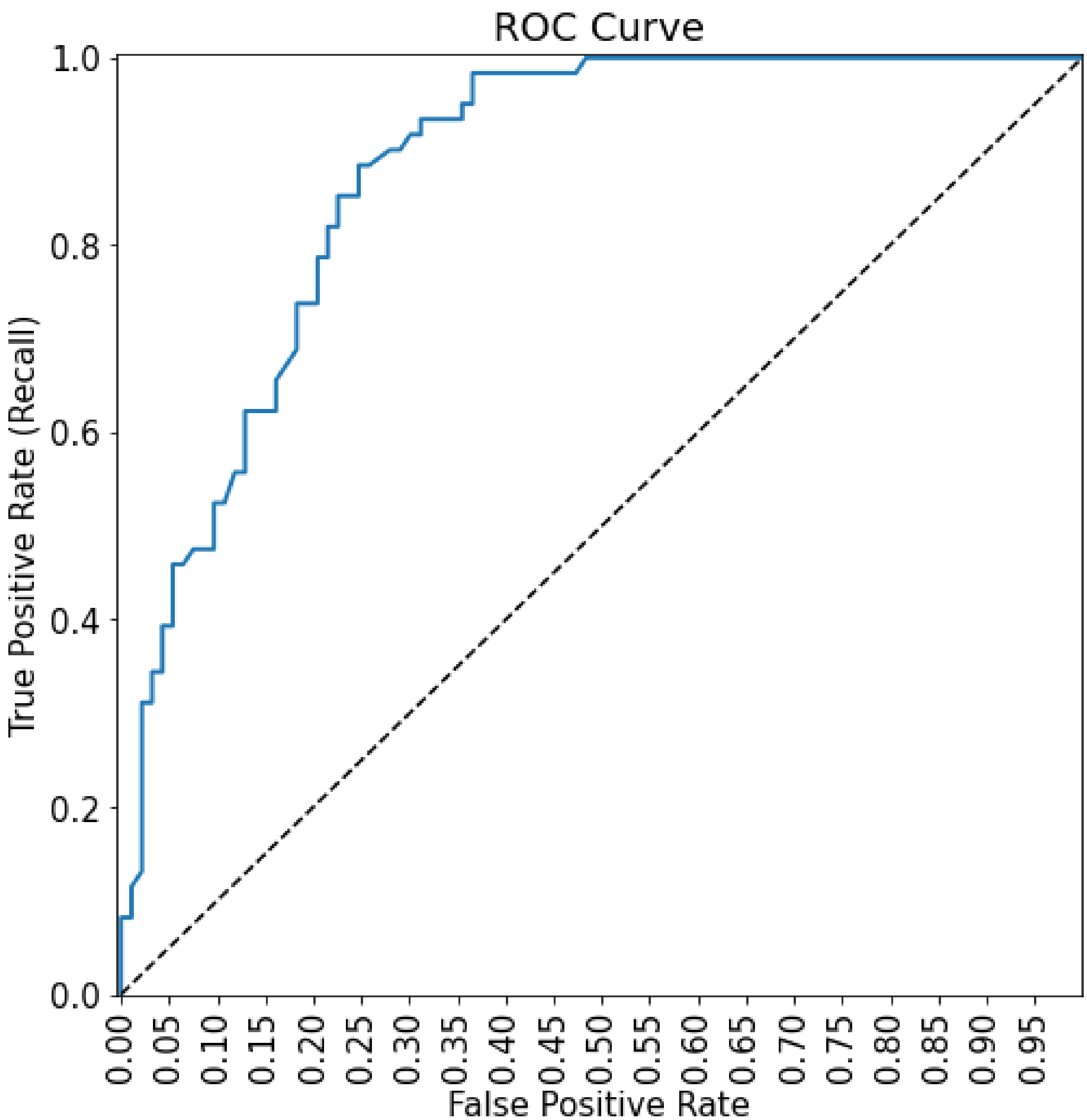
```
1.0
```



Note that there is perfect separation in train data as ROC-AUC = 1. This shows that the model is probably overfitting. However, this also shows that, despite the reduced variance *(as compared to a single tree)*, the bagged tree model is flexibly enough to perfectly separate the classes.

```
#ROC curve on test data
ypred = model.predict_proba(Xtest)[:, 1]
fpr, tpr, auc_thresholds = roc_curve(ytest, ypred)
print("ROC-AUC = ",auc(fpr, tpr))# AUC of ROC
def plot_roc_curve(fpr, tpr, label=None):

    plt.figure(figsize=(8,8))
    plt.title('ROC Curve')
    plt.plot(fpr, tpr, linewidth=2, label=label)
    plt.plot([0, 1], [0, 1], 'k--')
    plt.axis([-0.005, 1, 0, 1.005])
    plt.xticks(np.arange(0,1, 0.05), rotation=90)
    plt.xlabel("False Positive Rate")
    plt.ylabel("True Positive Rate (Recall)")

fpr, tpr, auc_thresholds = roc_curve(ytest, ypred)
plot_roc_curve(fpr, tpr)
```

```
ROC-AUC =  0.8781949585757096
```



7.2.2 Optimizing bagging hyperparameters using grid search

More parameters of a bagged classification tree model can be optimized using the typical approach of k-fold cross validation over a grid of parameter values.

```
n_samples = train.shape[0]
n_features = train.shape[1]

params = {'base_estimator': [DecisionTreeClassifier(random_state = 1),LogisticRegression()],
          'n_estimators': [150,200,250],
          'max_samples': [0.5,1.0],
          'max_features': [0.5,1.0],
          'bootstrap': [True, False],
          'bootstrap_features': [True, False]}

cv = KFold(n_splits=5,shuffle=True,random_state=1)
bagging_classifier_grid = GridSearchCV(BaggingClassifier(random_state=1, n_jobs=-1),
                                      param_grid =params, cv=cv, n_jobs=-1, verbose=1,
                                      scoring = ['precision', 'recall'], refit='recall')
bagging_classifier_grid.fit(X, y)

print('Train accuracy : %.3f'%bagging_classifier_grid.best_estimator_.score(X, y))
print('Test accuracy : %.3f'%bagging_classifier_grid.best_estimator_.score(Xtest, ytest))
print('Best accuracy Through Grid Search : %.3f'%bagging_classifier_grid.best_score_)
print('Best Parameters : ',bagging_classifier_grid.best_params_)
```

```
Fitting 5 folds for each of 96 candidates, totalling 480 fits
Train accuracy : 1.000
Test accuracy : 0.786
Best accuracy Through Grid Search : 0.573
Best Parameters :  {'base_estimator': DecisionTreeClassifier(random_state=1), 'bootstrap': T
```

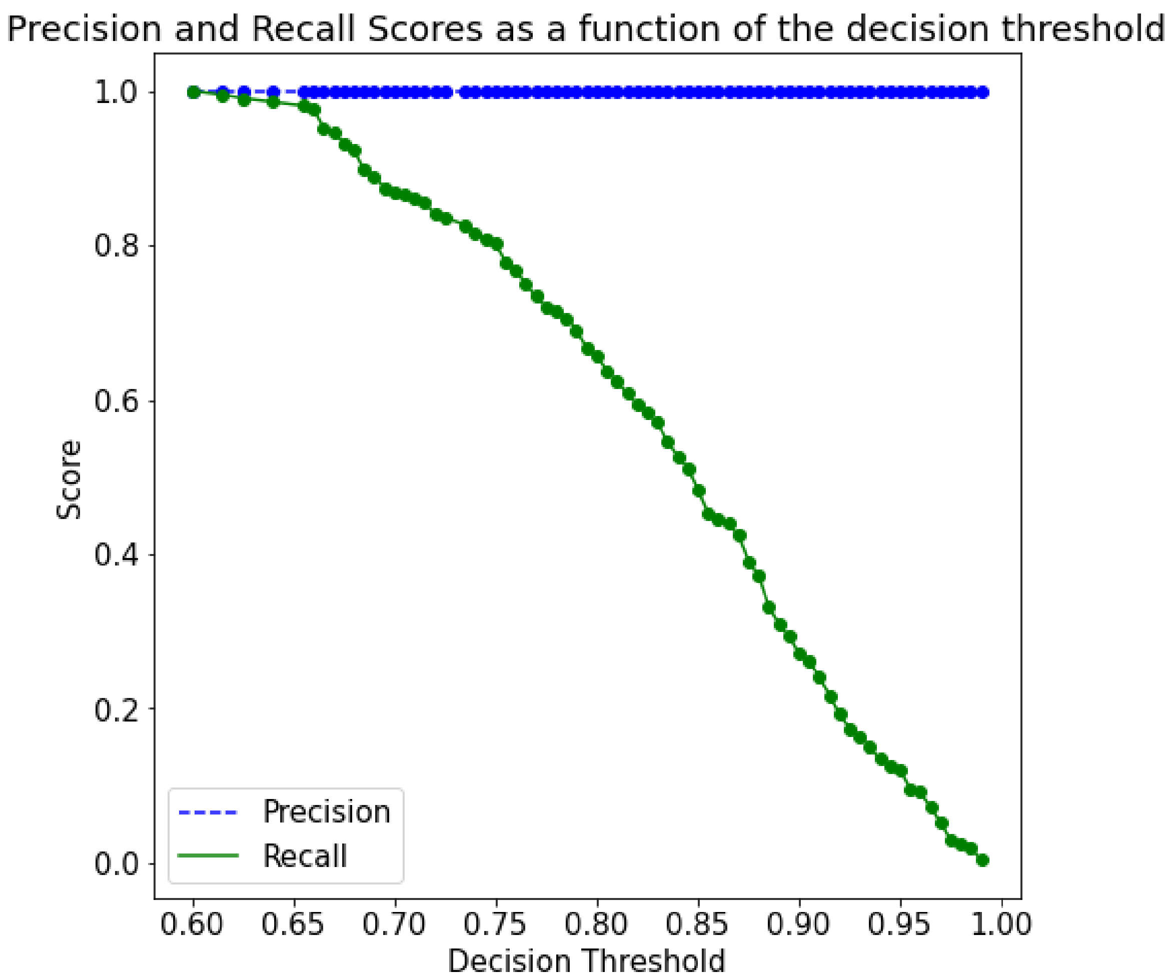
7.2.3 Tuning the decision threshold probability

We'll find a decision threshold probability that balances recall with precision.

```
model = BaggingClassifier(base_estimator=DecisionTreeClassifier(random_state=1), n_estimator
                          random_state=1,max_features=1.0, oob_score=True,
                        max_samples=1.0,n_jobs=-1,bootstrap=True,bootstrap_features=False).fi
```

As the model is overfitting on the train data, it will not be a good idea to tune the decision threshold probability based on the precision-recall curve on train data, as shown in the figure below.

```python
ypred = model.predict_proba(X)[:,1]
p, r, thresholds = precision_recall_curve(y, ypred)
def plot_precision_recall_vs_threshold(precisions, recalls, thresholds):
    plt.figure(figsize=(8, 8))
    plt.title("Precision and Recall Scores as a function of the decision threshold")
    plt.plot(thresholds, precisions[:-1], "b--", label="Precision")
    plt.plot(thresholds, recalls[:-1], "g-", label="Recall")
    plt.plot(thresholds, precisions[:-1], "o", color = 'blue')
    plt.plot(thresholds, recalls[:-1], "o", color = 'green')
    plt.ylabel("Score")
    plt.xlabel("Decision Threshold")
    plt.legend(loc='best')
    plt.legend()
plot_precision_recall_vs_threshold(p, r, thresholds)
```



Instead, we should make the precision-recall curve using the out-of-bag predictions, as shown below. The method `oob_decision_function_` provides the predicted probability.

```
ypred = model.oob_decision_function_[:,1]
p, r, thresholds = precision_recall_curve(y, ypred)
def plot_precision_recall_vs_threshold(precisions, recalls, thresholds):
    plt.figure(figsize=(8, 8))
    plt.title("Precision and Recall Scores as a function of the decision threshold")
    plt.plot(thresholds, precisions[:-1], "b--", label="Precision")
    plt.plot(thresholds, recalls[:-1], "g-", label="Recall")
    plt.plot(thresholds, precisions[:-1], "o", color = 'blue')
    plt.plot(thresholds, recalls[:-1], "o", color = 'green')
    plt.ylabel("Score")
    plt.xlabel("Decision Threshold")
```

```
    plt.legend(loc='best')
    plt.legend()
plot_precision_recall_vs_threshold(p, r, thresholds)
```

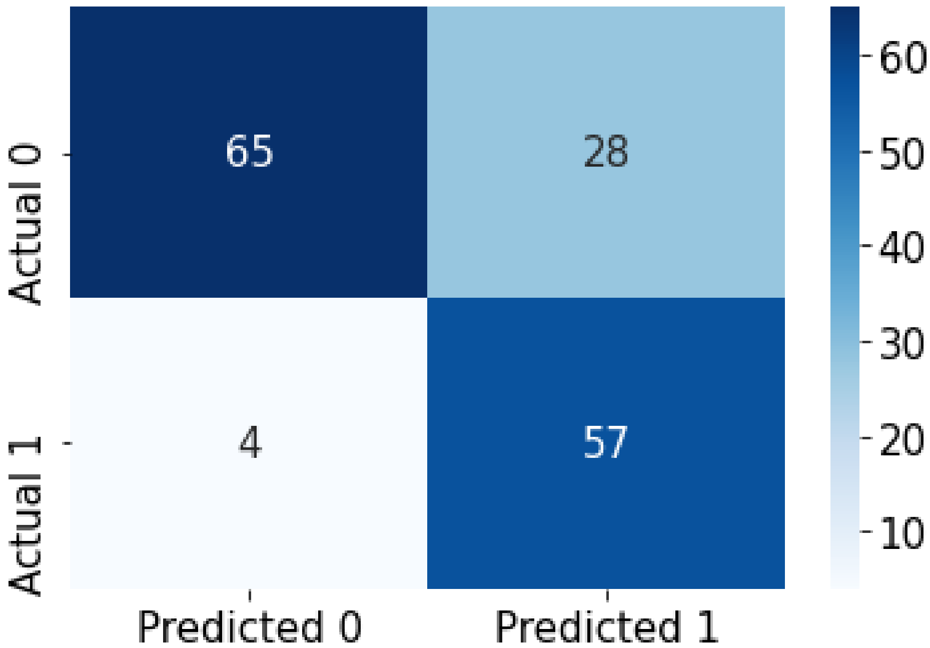

```
# Thresholds with precision and recall
all_thresholds = np.concatenate([thresholds.reshape(-1,1), p[:-1].reshape(-1,1), r[:-1].resha
recall_more_than_80 = all_thresholds[all_thresholds[:,2]>0.8,:]
# As the values in 'recall_more_than_80' are arranged in decreasing order of recall and incre
# the last value will provide the maximum threshold probability for the recall to be more tha
# We wish to find the maximum threshold probability to obtain the maximum possible precision
recall_more_than_80[recall_more_than_80.shape[0]-1]
```

```
array([0.2804878 , 0.53205128, 0.80193237])
```

Suppose, we wish to have at least 80% recall, with the highest possible precision. Then, based on the precision-recall curve, we should have a decision threshold probability of 0.28.

```
# Performance metrics computation for the optimum decision threshold probability
desired_threshold = 0.28

y_pred_prob = model.predict_proba(Xtest)[:,1]

# Classifying observations in the positive class (y = 1) if the predicted probability is grea
# than the desired decision threshold probability
y_pred = y_pred_prob > desired_threshold
y_pred = y_pred.astype(int)

#Computing the accuracy
print("Accuracy: ",accuracy_score(y_pred, ytest)*100)

#Computing the ROC-AUC
fpr, tpr, auc_thresholds = roc_curve(ytest, y_pred_prob)
print("ROC-AUC: ",auc(fpr, tpr))# AUC of ROC

#Computing the precision and recall
print("Precision: ", precision_score(ytest, y_pred))
print("Recall: ", recall_score(ytest, y_pred))

#Confusion matrix
cm = pd.DataFrame(confusion_matrix(ytest, y_pred),
                  columns=['Predicted 0', 'Predicted 1'], index = ['Actual 0', 'Actual 1'])
sns.heatmap(cm, annot=True, cmap='Blues', fmt='g');
```

```
Accuracy:  79.22077922077922
ROC-AUC:  0.8802221047065044
Precision:  0.6705882352941176
Recall:  0.9344262295081968
```



Note that this model has a better performance than the untuned bagged model earlier, and the single tree classification model, as expected.

8 Bagging (addendum)

This notebook provides examples to:

1. Compare tuning bagging hyperparameters with OOB validation and k-fold cross-validation.
2. Compare bagging tuned models with untuned models.

```
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.model_selection import cross_val_score,train_test_split, KFold, GridSearchCV, Pa
RandomizedSearchCV, RepeatedKFold
from sklearn.tree import DecisionTreeRegressor,DecisionTreeClassifier
from sklearn.ensemble import BaggingRegressor,BaggingClassifier
from sklearn.linear_model import LinearRegression, LogisticRegression
from sklearn.neighbors import KNeighborsRegressor
from sklearn.metrics import roc_curve, precision_recall_curve, auc, make_scorer, recall_score
accuracy_score, precision_score, confusion_matrix, mean_squared_error, r2_score, mean_squared
from skopt import BayesSearchCV
from skopt.space import Real, Integer, Categorical
from skopt.plots import plot_convergence, plot_histogram, plot_objective
from IPython import display
import itertools as it

#Libraries for visualizing trees
from sklearn.tree import export_graphviz, export_text
from six import StringIO
from IPython.display import Image
import pydotplus
import time as time
import warnings
```

```
#Using the same datasets as in linear regression in STAT303-2,
#so that we can compare the non-linear models with linear regression
trainf = pd.read_csv('./Datasets/Car_features_train.csv')
trainp = pd.read_csv('./Datasets/Car_prices_train.csv')
testf = pd.read_csv('./Datasets/Car_features_test.csv')
testp = pd.read_csv('./Datasets/Car_prices_test.csv')
train = pd.merge(trainf,trainp)
test = pd.merge(testf,testp)
train.head()
```

	carID	brand	model	year	transmission	mileage	fuelType	tax	mpg	engineSize	price
0	18473	bmw	6 Series	2020	Semi-Auto	11	Diesel	145	53.3282	3.0	37980
1	15064	bmw	6 Series	2019	Semi-Auto	10813	Diesel	145	53.0430	3.0	33980
2	18268	bmw	6 Series	2020	Semi-Auto	6	Diesel	145	53.4379	3.0	36850
3	18480	bmw	6 Series	2017	Semi-Auto	18895	Diesel	145	51.5140	3.0	25998
4	18492	bmw	6 Series	2015	Automatic	62953	Diesel	160	51.4903	3.0	18990

```
X = train[['mileage','mpg','year','engineSize']]
Xtest = test[['mileage','mpg','year','engineSize']]
y = train['price']
ytest = test['price']
```

1. Tree without tuning
2. Tree performance improves with tuning
3. Bagging tuned tree
4. Bagging untuned tree - better, how?
5. Tuning bagged model - OOB
6. Tuning bagged model - BayesSearchCV
7. warm start
8. Bagging KNN - no need to tune number of neighbors

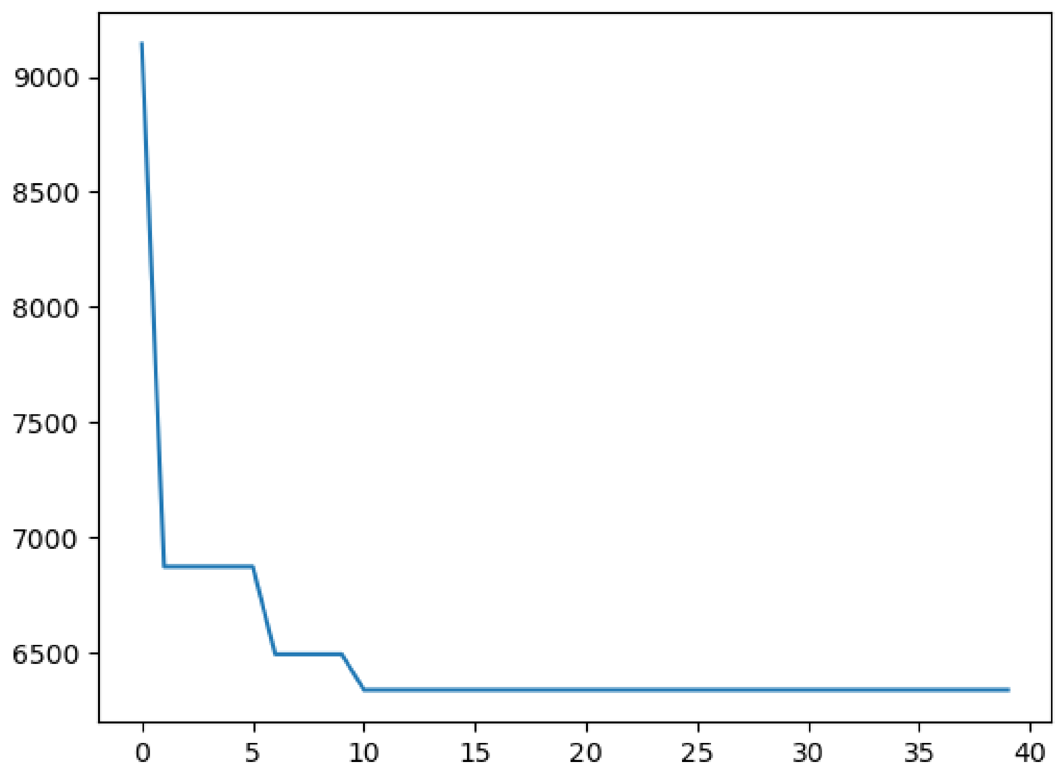
8.1 Tree without tuning

```
model = DecisionTreeRegressor()
cv = KFold(n_splits=5, shuffle=True, random_state=1)
-np.mean(cross_val_score(model, X, y, scoring='neg_root_mean_squared_error', cv = cv))
```

```
7056.960817154941
```

```
param_grid = {'max_depth': Integer(2, 30)}
gcv = BayesSearchCV(model, search_spaces = param_grid, cv = cv, n_iter = 40, random_state = 
                         scoring = 'neg_root_mean_squared_error', n_jobs = -1)
paras = list(gcv.search_spaces.keys())
paras.sort()

def monitor(optim_result):
    cv_values = pd.Series(optim_result['func_vals']).cummin()
    display.clear_output(wait = True)
    min_ind = pd.Series(optim_result['func_vals']).argmin()
    print(paras, "=", optim_result['x_iters'][min_ind], pd.Series(optim_result['func_vals'])
    sns.lineplot(cv_values)
    plt.show()
gcv.fit(X, y, callback = monitor)
```

```
['max_depth'] = [10] 6341.1481858990355
```




```
BayesSearchCV(cv=KFold(n_splits=5, random_state=1, shuffle=True),
```

```
estimator=DecisionTreeRegressor(), n_iter=40, n_jobs=-1,
random_state=10, scoring='neg_root_mean_squared_error',
search_spaces={'max_depth': Integer(low=2, high=30, prior='uniform', transform=
```

8.2 Performance of tree improves with tuning

```
model = DecisionTreeRegressor(max_depth=10)
cv = KFold(n_splits=5, shuffle=True, random_state=1)
-np.mean(cross_val_score(model, X, y, scoring='neg_root_mean_squared_error', cv = cv))
```

```
6442.494300778735
```

8.3 Bagging tuned trees

```
model = BaggingRegressor(DecisionTreeRegressor(max_depth = 10), oob_score=True, n_estimators
mean_squared_error(model.oob_prediction_, y, squared = False)
```

```
5354.357809020438
```

8.4 Bagging untuned trees

```
model = BaggingRegressor(DecisionTreeRegressor(), oob_score=True, n_estimators = 100).fit(X,
mean_squared_error(model.oob_prediction_, y, squared = False)
```

```
5248.720845665685
```

Why is bagging tuned trees worse than bagging untuned trees?

In the tuned tree here, the reduction in variance by controlling maximum depth resulted in an increas in bias of indivudual trees. Bagging trees only reduces the variance, but not the bias of the indivudal trees. Thus, bagging high bias models will result in a high-bias model, while bagging high variance models may result in a low variance model if the models are not highly correlated.

Bagging tuned models may provide a better performance as compared to bagging untuned models if the reduction in variance of the individual models is high enough to overshadow the increase in bias, and increase in pairwise correlation of the individual models.

8.5 Tuning bagged model - OOB

```
param_grid1 = {'max_samples': [0.25, 0.5, 0.75, 1.0],
             'max_features': [2, 3, 4],
             'bootstrap_features': [True, False]}
param_grid2 = {'max_samples': [0.25, 0.5, 0.75, 1.0],
             'max_features': [1],
              'bootstrap_features': [False]}
param_list1 = list(it.product(*[values for key, values in param_grid1.items()]))
param_list2 = list(it.product(*[values for key, values in param_grid2.items()]))
param_list = param_list1 + param_list2
```

```
oob_score_pr = []
for pr in param_list:
    model = BaggingRegressor(DecisionTreeRegressor(), max_samples=pr[0], max_features=pr[1],
                            bootstrap_features=pr[2], n_jobs = -1, oob_score=True, n_estimato
    oob_score_pr.append(mean_squared_error(model.oob_prediction_, y, squared=False))
```

What is the benefit of OOB validation to tune hyperparameters in bagging?

It is much cheaper than k-fold cross-validation, as only $1/k$ of the models are trained with OOB validation as compared to k-fold cross-validation. However, the cost of training individual models is lower in k-fold cross-validation as models are trained on a smaller dataset. Typically, OOB will be faster than k-fold cross-validation. The higher the value of k, the more faster OOB validation will be as compared to k-fold cross-validation.

8.6 Tuning without k-fold cross-validation

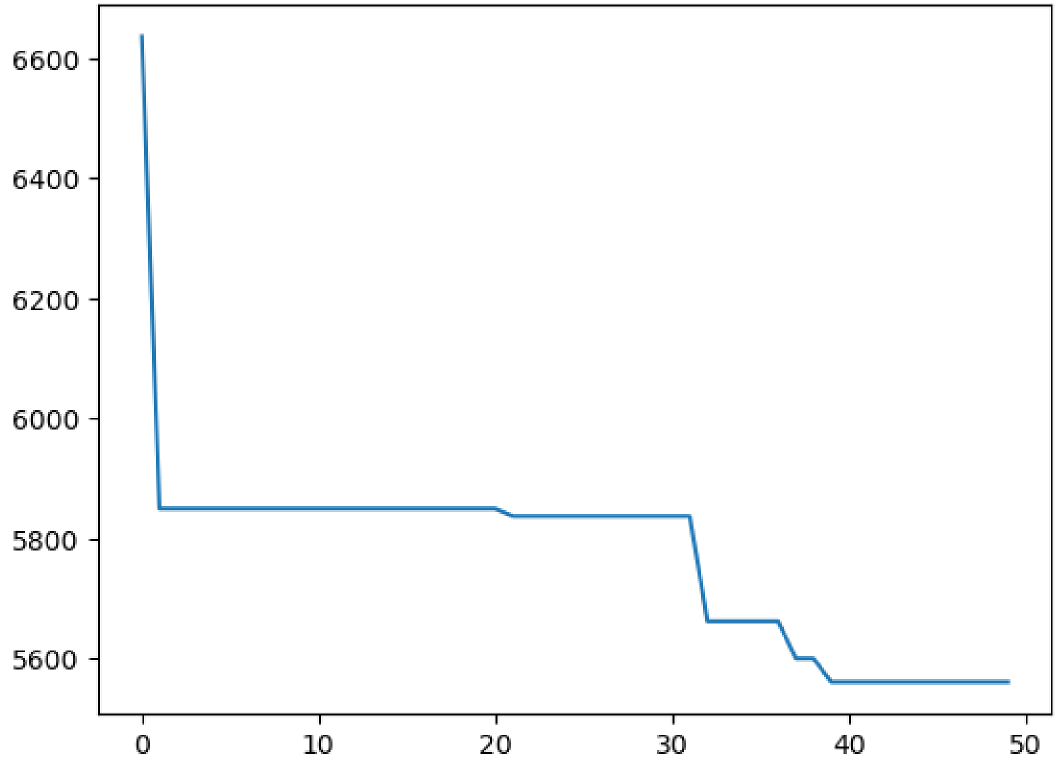
When hyperparameters can be tuned with OOB validation, what is the benefit of using k-fold cross-validation?

1. Hyperparameters cannot be tuned over continuous spaces with OOB validation.
2. OOB score is not computed if samping is done without replacement *(`bootstrap = False`)*. Thus, for tuning the `bootstrap` hyperparameter, k-fold cross-validation will need to be used.

```
def monitor(optim_result):
    cv_values = pd.Series(optim_result['func_vals']).cummin()
    display.clear_output(wait = True)
    min_ind = pd.Series(optim_result['func_vals']).argmin()
    print(paras, "=", optim_result['x_iters'][min_ind], pd.Series(optim_result['func_vals'])
    sns.lineplot(cv_values)
    plt.show()
```

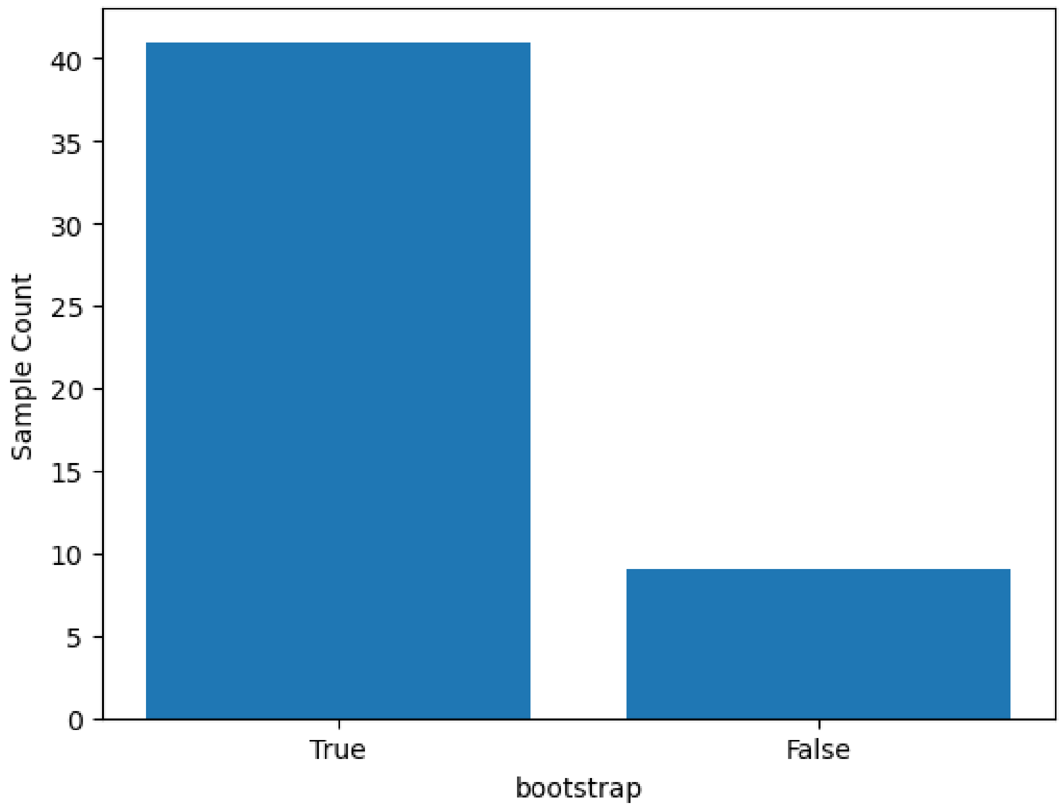
```
param_grid = {'max_samples': Real(0.2, 1.0),
             'max_features': Integer(1, 4),
             'bootstrap_features': [True, False],
              'bootstrap': [True, False]}
gcv = BayesSearchCV(BaggingRegressor(DecisionTreeRegressor(), bootstrap=False),
                    search_spaces = param_grid, cv = cv, n_jobs = -1,
                  scoring='neg_root_mean_squared_error')

paras = list(gcv.search_spaces.keys())
paras.sort()

gcv.fit(X, y, callback=monitor)
```

```
['bootstrap', 'bootstrap_features', 'max_features', 'max_samples'] = [True, False, 4, 0.8061
```

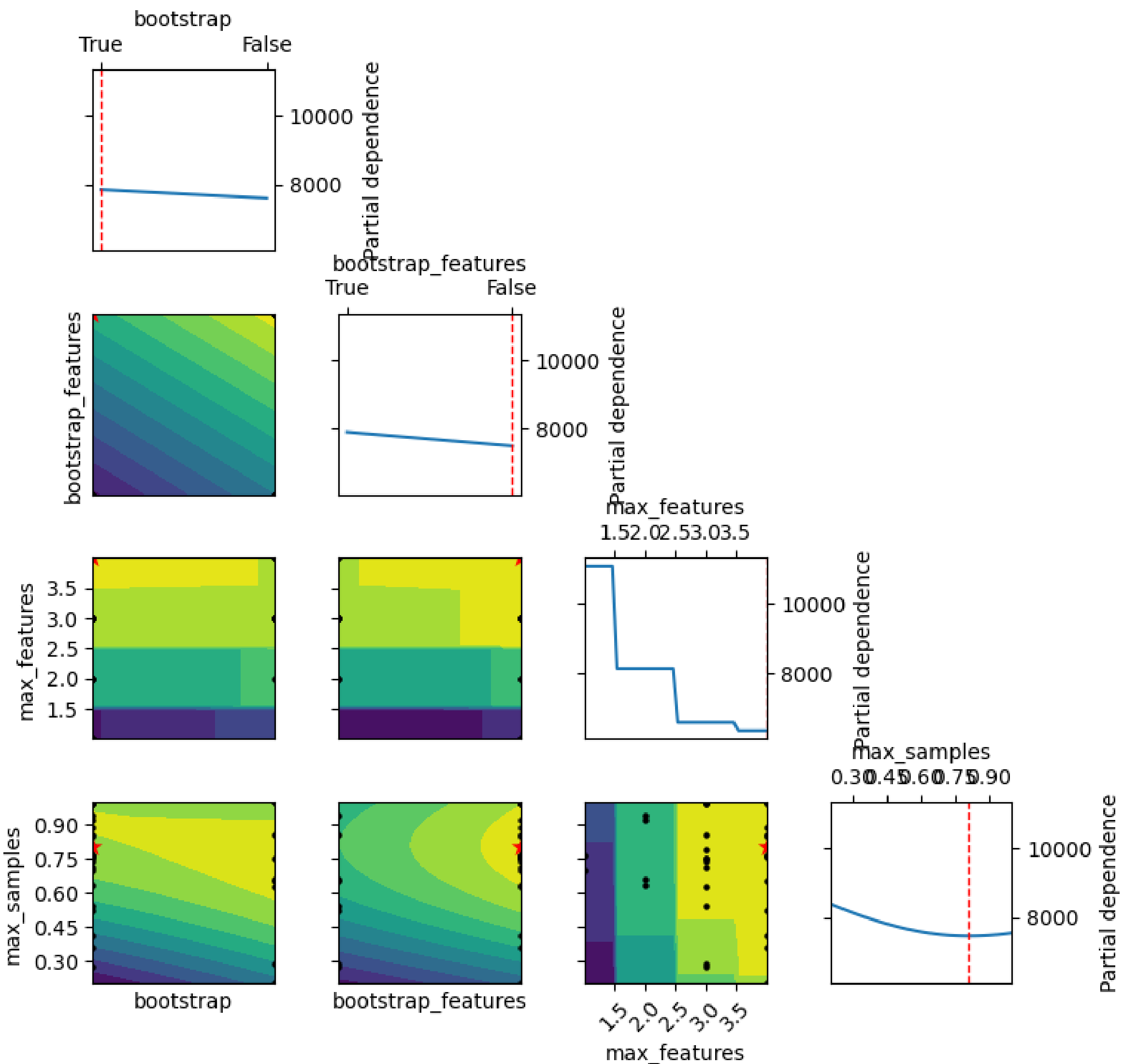



```
BayesSearchCV(cv=KFold(n_splits=5, random_state=1, shuffle=True),
              estimator=BaggingRegressor(bootstrap=False,
                                         estimator=DecisionTreeRegressor()),
              n_jobs=-1, scoring='neg_root_mean_squared_error',
              search_spaces={'bootstrap': [True, False],
                             'bootstrap_features': [True, False],
                             'max_features': Integer(low=1, high=4, prior='uniform', transfo
                             'max_samples': Real(low=0.2, high=1.0, prior='uniform', transfo
```

```
plot_histogram(gcv.optimizer_results_[0],0)
```




```
plot_objective(gcv.optimizer_results_[0])
```



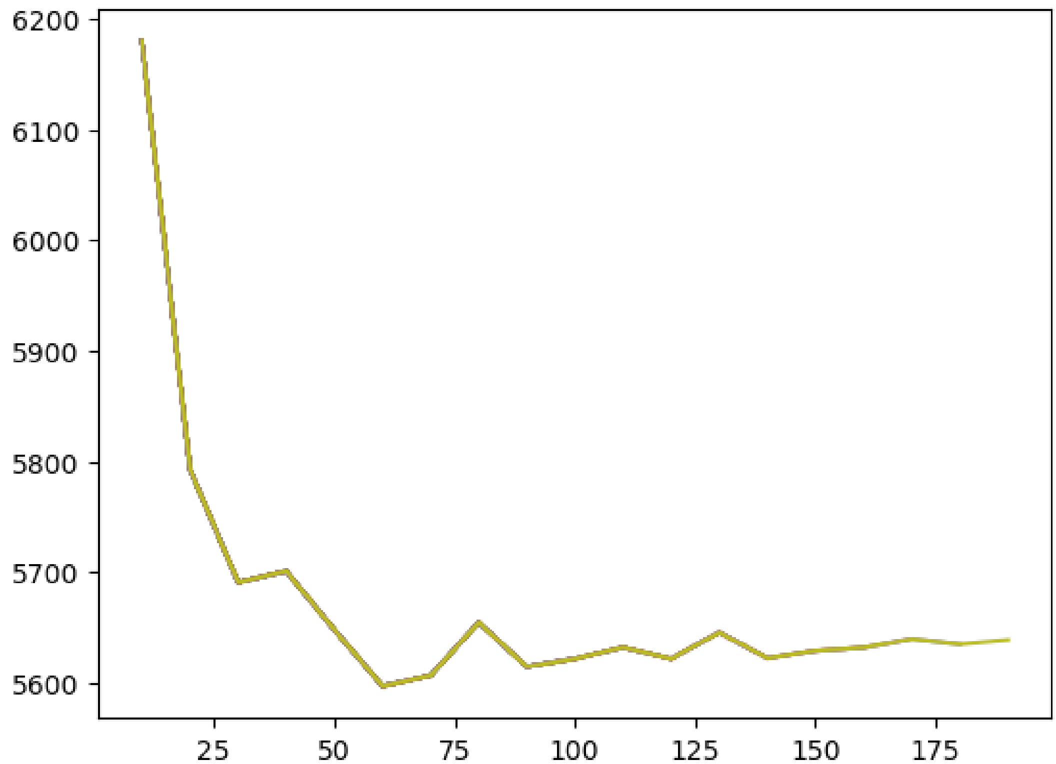
8.7 warm start

What is the purpose of warm_start?

The purpose of `warm_start` is to avoid developing trees from scratch, and incrementally add trees to monitor the validation error. However, note that OOB score is not computed with `warm_start`. Thus, a validation set approach will need to be adopted to tune number of trees.

A cheaper approach to tune number of estimators is to just use trial and error, and stop increasing once the cross-validation error / OOB error / validation set error stabilizes.

```
model = BaggingRegressor(DecisionTreeRegressor(), oob_score=False, n_estimators = 5,
                        warm_start=True).fit(X, y)
rmse = []
for i in range(10, 200, 10):
    model.n_estimators = i
    model.fit(X, y)
    rmse.append(mean_squared_error(model.predict(Xtest), ytest, squared=False))
    sns.lineplot(x = range(10, i+1, 10), y = rmse)
```



8.8 Bagging KNN

Should we bag a tuned KNN model or an untuned one?

```
from sklearn.preprocessing import StandardScaler
```

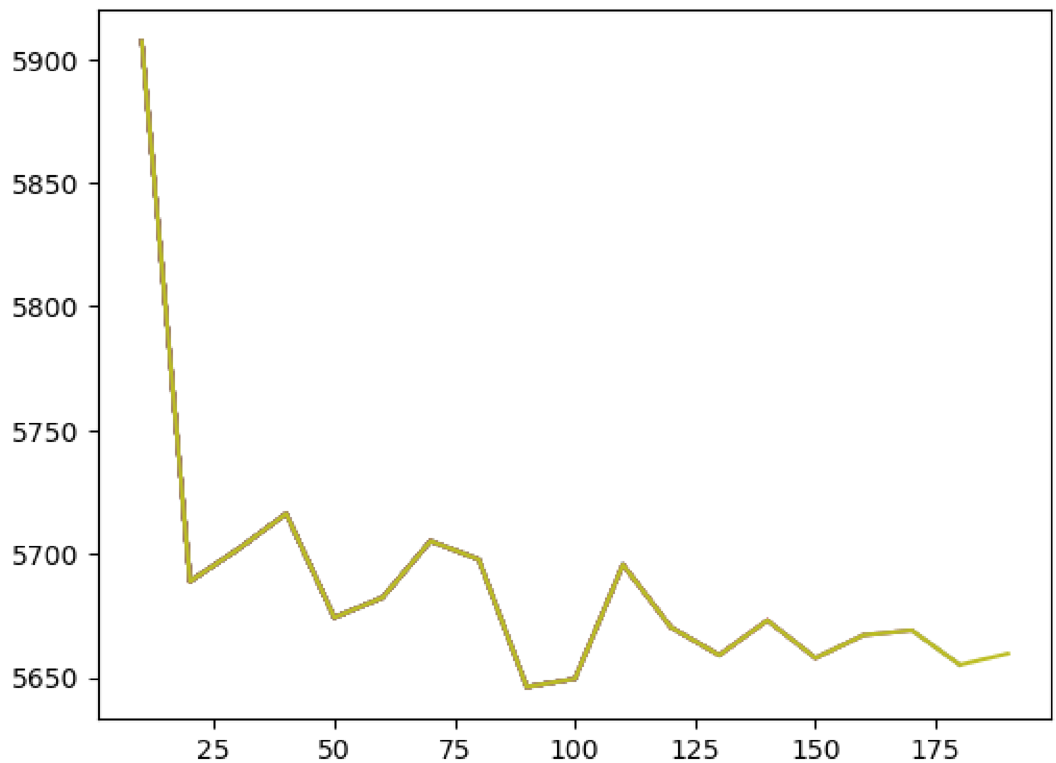
```
model = KNeighborsRegressor(n_neighbors=9) # optimal neigbors
scaler = StandardScaler()
scaler.fit(X)
X_scaled = scaler.transform(X)
-np.mean(cross_val_score((model), X_scaled, y, cv = cv,
                         scoring='neg_root_mean_squared_error', n_jobs = -1))
```

6972.997277781689

```
model = KNeighborsRegressor(n_neighbors=1)
scaler = StandardScaler()
scaler.fit(X)
X_scaled = scaler.transform(X)
-np.mean(cross_val_score(BaggingRegressor(model), X_scaled, y, cv = cv,
                         scoring='neg_root_mean_squared_error', n_jobs = -1))
```

6254.305462266355

```
model = BaggingRegressor(DecisionTreeRegressor(), n_estimators=5, warm_start=True)
model.fit(X, y)
rmse = []
for i in range(10, 200,10):
    model.n_estimators = i
    model.fit(X, y)
    rmse.append(mean_squared_error(model.predict(Xtest), ytest, squared=False))
    sns.lineplot(x = range(10, i + 1, 10), y = rmse)
```



5900
5850
5800
5750
5700
5650
25
50
75
100
125
150
175

9 Random Forest

Read section 8.2.2 of the book before using these notes.

Note that in this course, lecture notes are not sufficient, you must read the book for better understanding. Lecture notes are just implementing the concepts of the book on a dataset, but not explaining the concepts elaborately.

```
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.metrics import mean_squared_error
from sklearn.model_selection import cross_val_score,train_test_split
from sklearn.model_selection import KFold
from sklearn.tree import DecisionTreeRegressor,DecisionTreeClassifier
from sklearn.model_selection import GridSearchCV, ParameterGrid
from sklearn.ensemble import BaggingRegressor,BaggingClassifier,RandomForestRegressor,RandomF
from sklearn.linear_model import LinearRegression,LogisticRegression
from sklearn.neighbors import KNeighborsRegressor
from sklearn.metrics import roc_curve, precision_recall_curve, auc, make_scorer, recall_score
accuracy_score, precision_score, confusion_matrix, mean_squared_error, r2_score

import itertools as it

#Libraries for visualizing trees
from sklearn.tree import export_graphviz
from six import StringIO
from IPython.display import Image
import pydotplus
import time as time
import warnings
```

```
#Using the same datasets as used for linear regression in STAT303-2,
#so that we can compare the non-linear models with linear regression
trainf = pd.read_csv('./Datasets/Car_features_train.csv')
trainp = pd.read_csv('./Datasets/Car_prices_train.csv')
```

```
testf = pd.read_csv('./Datasets/Car_features_test.csv')
testp = pd.read_csv('./Datasets/Car_prices_test.csv')
train = pd.merge(trainf,trainp)
test = pd.merge(testf,testp)
train.head()
```

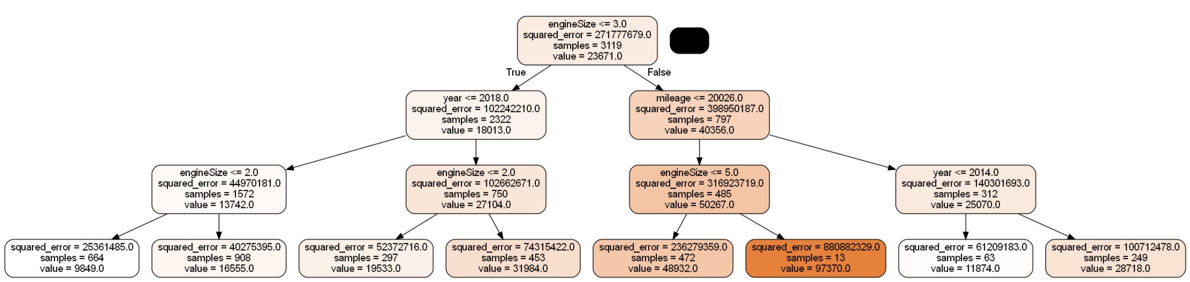
	carID	brand	model	year	transmission	mileage	fuelType	tax	mpg	engineSize	price
0	18473	bmw	6 Series	2020	Semi-Auto	11	Diesel	145	53.3282	3.0	37980
1	15064	bmw	6 Series	2019	Semi-Auto	10813	Diesel	145	53.0430	3.0	33980
2	18268	bmw	6 Series	2020	Semi-Auto	6	Diesel	145	53.4379	3.0	36850
3	18480	bmw	6 Series	2017	Semi-Auto	18895	Diesel	145	51.5140	3.0	25998
4	18492	bmw	6 Series	2015	Automatic	62953	Diesel	160	51.4903	3.0	18990

```
X = train[['mileage','mpg','year','engineSize']]
Xtest = test[['mileage','mpg','year','engineSize']]
y = train['price']
ytest = test['price']
```

Let us make a bunch of small trees with bagging, so that we can visualize and see if they are being dominated by a particular predictor or predictor(s).

```
#Bagging the results of 10 decision trees to predict car price
model = BaggingRegressor(estimator=DecisionTreeRegressor(max_depth=3), n_estimators=10, rando
                        n_jobs=-1).fit(X, y)
```

```
#Change the index of model.estimators_[index] to visualize the 10 bagged trees, one at a tim
dot_data = StringIO()
export_graphviz(model.estimators_[0], out_file=dot_data,
                filled=True, rounded=True,
                feature_names =['mileage','mpg','year','engineSize'],precision=0)
graph = pydotplus.graph_from_dot_data(dot_data.getvalue())
#graph.write_png('car_price_tree.png')
Image(graph.create_png())
```



Each of the 10 bagged trees seems to be dominated by the `engineSize` predictor, thereby making the trees highly correlated. Average of highly correlated random variables has a higher variance than the average of lesser correlated random variables. Thus, highly correlated trees will tend to have a relatively high prediction variance despite averaging their predictions.

```
#Feature importance can be found by averaging the feature importance in individual trees
feature_importances = np.mean([
    tree.feature_importances_ for tree in model.estimators_
], axis=0)
feature_importances
```

```
array([0.13058631, 0.03965966, 0.22866077, 0.60109325])
```

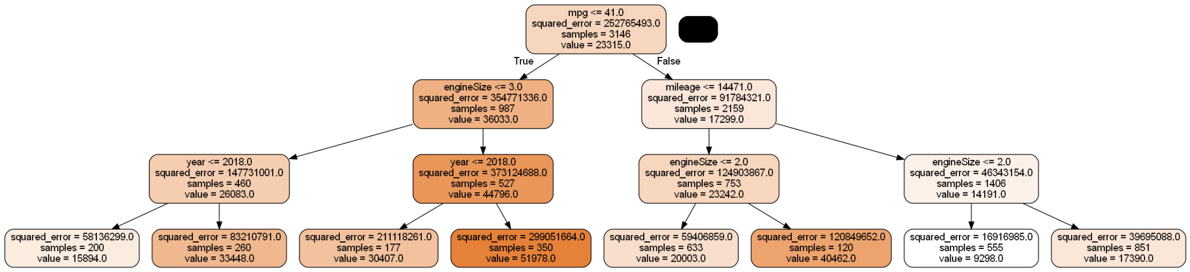
We can see that `engineSize` has the highest importance among predictors, supporting the visualization that it dominates the trees.

9.1 Random Forest for regression

Now, let us visualize small trees with the random forest algorithm to see if a predictor dominates all the trees.

```
#Averaging the results of 10 decision trees, while randomly considering sqrt(4)=2 predictors
#to split, to predict car price
model = RandomForestRegressor(n_estimators=10, random_state=1,max_features="sqrt",max_depth=3
                        n_jobs=-1).fit(X, y)
```

```
#Change the index of model.estimators_[index] to visualize the 10 random forest trees, one at
dot_data = StringIO()
export_graphviz(model.estimators_[4], out_file=dot_data,
                filled=True, rounded=True,
                feature_names =['mileage','mpg','year','engineSize'],precision=0)
graph = pydotplus.graph_from_dot_data(dot_data.getvalue())
#graph.write_png('car_price_tree.png')
Image(graph.create_png())
```



As two of the four predictors are randomly selected for splitting each node, **`engineSize`** no longer seems to dominate the trees. This will tend to reduce correlation among trees, thereby reducing the prediction variance, which in turn will tend to improve prediction accuracy.

```
#Averaging the results of 10 decision trees, while randomly considering sqrt(4)=2 predictors
#to split, to predict car price
model = RandomForestRegressor(n_estimators=10, random_state=1,max_features="sqrt",
                              n_jobs=-1).fit(X, y)
```

```
model.feature_importances_
```

```
array([0.16370584, 0.35425511, 0.18552673, 0.29651232])
```

Note that the feature importance of **`engineSize`** is reduced in random forests (as compared to bagged trees), and it no longer dominates the trees.

```
np.sqrt(mean_squared_error(test.price, model.predict(Xtest)))
```

```
5856.022395768459
```

The RMSE is similar to that obtained by bagging. We will discuss the comparison later.

9.1.1 Model accuracy vs number of trees

How does the model accuracy vary with the number of trees?

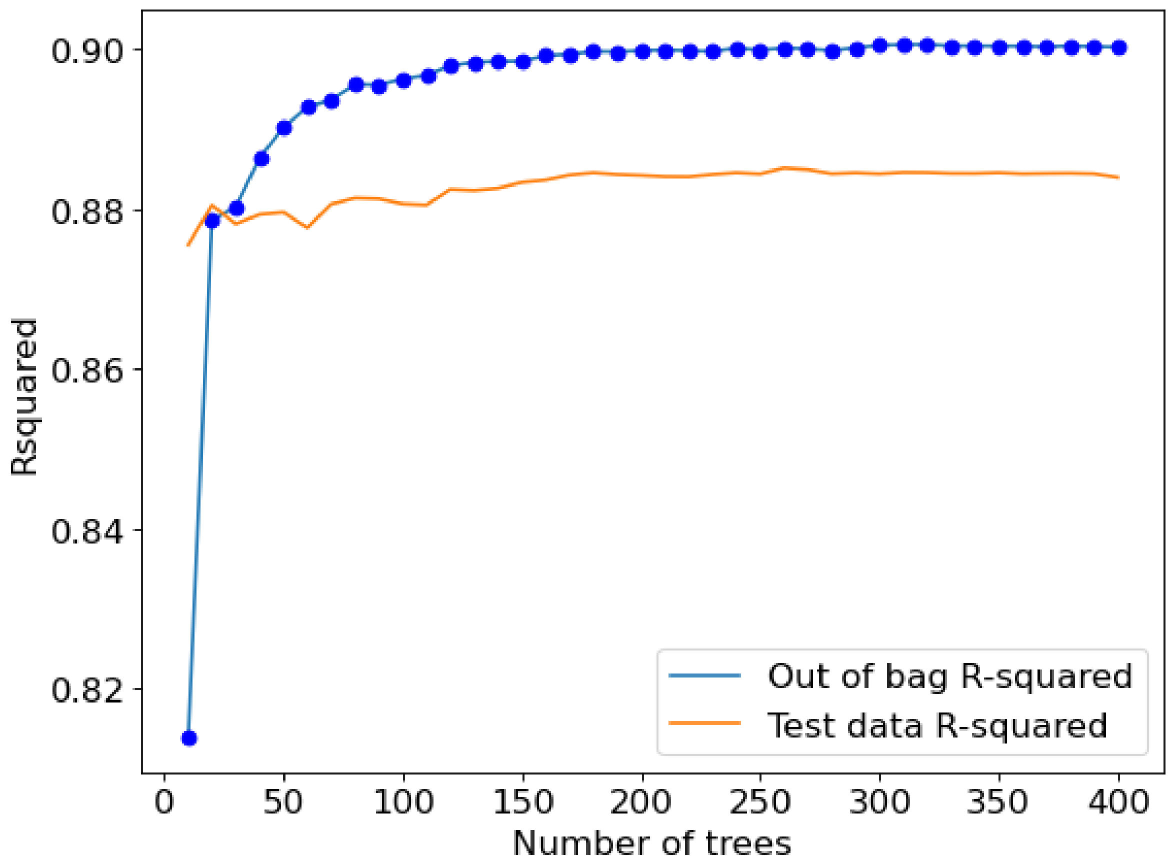
As we increase the number of trees, it will tend to reduce the variance of individual trees leading to a more accurate prediction.

```
#Finding model accuracy vs number of trees
warnings.filterwarnings("ignore")
oob_rsquared={};test_rsquared={};oob_rmse={};test_rmse = {}

for i in np.linspace(10,400,40,dtype=int):
    model = RandomForestRegressor(n_estimators=i, random_state=1,max_features="sqrt",
                        n_jobs=-1,oob_score=True).fit(X, y)
    oob_rsquared[i]=model.oob_score_  #Returns the out-of_bag R-squared of the model
    test_rsquared[i]=model.score(Xtest,ytest) #Returns the test R-squared of the model
    oob_rmse[i]=np.sqrt(mean_squared_error(model.oob_prediction_,y))
    test_rmse[i]=np.sqrt(mean_squared_error(model.predict(Xtest),ytest))

warnings.resetwarnings()

# The hidden warning is: "Some inputs do not have OOB scores. This probably means too few
# estimators were used to compute any reliable oob estimates." This warning will appear
# in case of small number of estimators. In such a case, some observations may be use
# by all the estimators, and their OOB score can't be computed
```

As we are ensemble only 10 trees in the first iteration, some of the observations are selected in every bootstrapped sample, and thus they don't have an out-of-bag error, which is producing the warning. For every observation to have an out-of-bag error, the number of trees must be sufficiently large.

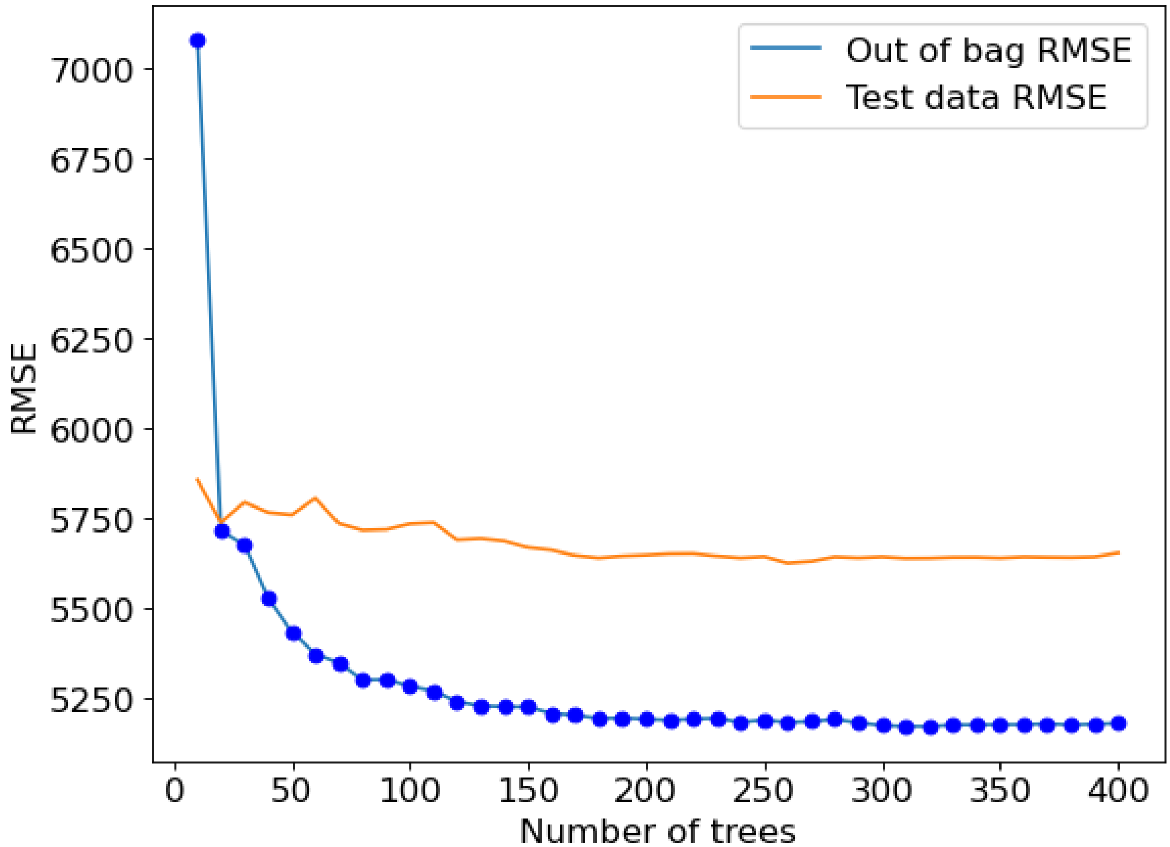
Let us visualize the out-of-bag (OOB) R-squared and R-squared on test data vs the number of trees.

```
plt.rcParams.update({'font.size': 15})
plt.figure(figsize=(8, 6), dpi=80)
plt.plot(oob_rsquared.keys(),oob_rsquared.values(),label = 'Out of bag R-squared')
plt.plot(oob_rsquared.keys(),oob_rsquared.values(),'o',color = 'blue')
plt.plot(test_rsquared.keys(),test_rsquared.values(), label = 'Test data R-squared')
plt.xlabel('Number of trees')
plt.ylabel('Rsquared')
plt.legend();
```



The out-of-bag R-squared initially increases, and then stabilizes after a certain number of trees (around 200 in this case). Note that increasing the number of trees further will not lead to overfitting. However, increasing the number of trees will increase the computations. Thus, the number of trees developed should be the number beyond which the R-squared stabilizes.

```
#Visualizing out-of-bag RMSE and test data RMSE
plt.rcParams.update({'font.size': 15})
plt.figure(figsize=(8, 6), dpi=80)
plt.plot(oob_rmse.keys(),oob_rmse.values(),label = 'Out of bag RMSE')
plt.plot(oob_rmse.keys(),oob_rmse.values(),'o',color = 'blue')
plt.plot(test_rmse.keys(),test_rmse.values(), label = 'Test data RMSE')
plt.xlabel('Number of trees')
plt.ylabel('RMSE')
plt.legend();
```



A similar trend can be seen by plotting out-of-bag RMSE and test RMSE. Note that RMSE is proportional to R-squared. You only need to visualize one of RMSE or R-squared to find the optimal number of trees.

```
#Bagging with 150 trees
model = RandomForestRegressor(n_estimators=200, random_state=1,max_features="sqrt",
                        oob_score=True,n_jobs=-1).fit(X, y)
```

```
#OOB R-squared
model.oob_score_
```

```
0.8998265006519903
```

```
#RMSE on test data
pred = model.predict(Xtest)
np.sqrt(mean_squared_error(test.price, pred))
```

```
5647.195064555622
```

9.1.2 Tuning random forest

The Random forest object has options to set parameters such as depth, leaves, minimum number of observations in a leaf etc., for individual trees. These parameters are useful to prune a decision tree model consisting of a single tree, in order to avoid overfitting due to high variance of an unpruned tree.

Pruning individual trees in random forests is not likely to add much value, since averaging a sufficient number of unpruned trees reduces the variance of the trees, which enhances prediction accuracy. Pruning individual trees is unlikely to further reduce the prediction variance.

Here is a comment from page 596 of the The Elements of Statistical Learning that supports the above statement: *Segal (2004) demonstrates small gains in performance by controlling the depths of the individual trees grown in random forests. Our experience is that using full-grown trees seldom costs much, and results in one less tuning parameter.*

Below we attempt to optimize parameters that prune individual trees. However, as expected, it does not result in a substantial increase in prediction accuracy.

Also, note that we don't need to tune the number of trees in random forest with `GridSearchCV`. As we know the prediction accuracy will keep increasing with number of trees, we can tune the other hyperparameters with a constant value for the number of trees.

```
model.estimators_[0].get_n_leaves()
```

```
3086
```

```
model.estimators_[0].get_depth()
```

```
29
```

Coarse grid search

```
#Optimizing with OOB score takes half the time as compared to cross validation.
#The number of models developed with OOB score tuning is one-fifth of the number of models d
#5-fold cross validation
start_time = time.time()

n_samples = train.shape[0]
n_features = train.shape[1]

params = {'max_depth': [5, 10, 15, 20, 25, 30],
```

```
          'max_leaf_nodes':[600, 1200, 1800, 2400, 3000],
          'max_features': [1,2,3,4]}

param_list=list(it.product(*(params[Name] for Name in params)))

oob_score = [0]*len(param_list)
i=0
for pr in param_list:
    model = RandomForestRegressor(random_state=1,oob_score=True,verbose=False,
                    n_estimators = 100, max_depth=pr[0],
                    max_leaf_nodes=pr[1], max_features=pr[2], n_jobs=-1).fit(X,y)
    oob_score[i] = mean_squared_error(model.oob_prediction_, y, squared=False)
    i=i+1

end_time = time.time()
print("time taken = ", (end_time-start_time)/60, " minutes")
print("Best params = ", param_list[np.argmin(oob_score)])
print("Optimal OOB validation RMSE = ", np.min(oob_score))
```

```
time taken =  1.230358862876892  minutes
Best params =  (15, 1800, 3)
Optimal OOB validation RMSE =  5243.408784594606
```

Finer grid search

Based on the coarse grid search, hyperparameters will be tuned in a finer grid around the optimal hyperparamter values obtained.

```
#Optimizing with OOB score takes half the time as compared to cross validation.
#The number of models developed with OOB score tuning is one-fifth of the number of models de
#5-fold cross validation
start_time = time.time()

n_samples = train.shape[0]
n_features = train.shape[1]

params = {'max_depth': [12, 15, 18],
          'max_leaf_nodes':[1600, 1800, 2000],
          'max_features': [1,2,3,4]}

param_list=list(it.product(*(params[Name] for Name in params)))
```

```
oob_score = [0]*len(param_list)
i=0
for pr in param_list:
    model = RandomForestRegressor(random_state=1,oob_score=True,verbose=False,
             n_estimators = 100, max_depth=pr[0], max_leaf_nodes=pr[1],
                    max_features=pr[2], n_jobs=-1).fit(X,y)
    oob_score[i] = mean_squared_error(model.oob_prediction_, y, squared=False)
    i=i+1

end_time = time.time()
print("time taken = ", (end_time-start_time)/60, " minutes")
print("Best params = ", param_list[np.argmin(oob_score)])
print("Optimal OOB validation RMSE = ", np.min(oob_score))
```

```
time taken =  0.4222299337387085  minutes
Best params =  (15, 1800, 3)
Best score =  5243.408784594606
```

```
#Model with optimal parameters
model = RandomForestRegressor(n_estimators = 100, random_state=1, max_leaf_nodes = 1800, max_
                        oob_score=True,n_jobs=-1, max_features=3).fit(X, y)
```

```
#RMSE on test data
np.sqrt(mean_squared_error(test.price, model.predict(Xtest)))
```

```
5671.410705964455
```

Optimizing depth and leaves of individual trees didn't improve the prediction accuracy of the model. Important parameters to optimize in random forests will be the number of trees (`n_estimators`), and number of predictors considered at each split (`max_features`). However, sometimes individual pruning of trees may be useful. This may happen when the increase in bias in individual trees *(when pruned)* is lesser than the decrease in variance of the tree. However, if the pairwise correlation coefficient ρ of the trees increases by a certain extent on pruning, pruning may again be not useful.

```
#Tuning only n_estimators and max_features produces similar results
start_time = time.time()
params = {'max_features': [1,2,3,4]}

param_list=list(it.product(*(params[Name] for Name in params)))
```

```
oob_score = [0]*len(param_list)
i=0
for pr in param_list:
    model = RandomForestRegressor(random_state=1,oob_score=True,verbose=False,
                    n_estimators = 100, max_features=pr[0], n_jobs=-1).fit(X,y)
    oob_score[i] = mean_squared_error(model.oob_prediction_, y, squared=False)
    i=i+1

end_time = time.time()
print("time taken = ", (end_time-start_time)/60, " minutes")
print("Best params = ", param_list[np.argmin(oob_score)])
print("Optimal OOB validation RMSE = ", np.min(oob_score))
```

```
time taken =  0.02856200933456421  minutes
Best params =  (3,)
Best score (R-squared) =  5252.291978670057
```

```
#Model with optimal parameters
model = RandomForestRegressor(n_estimators=100, random_state=1,
                        n_jobs=-1, max_features=3).fit(X, y)
np.sqrt(mean_squared_error(test.price, model.predict(Xtest)))
```

```
5656.561522632323
```

Considering hyperparameters involving pruning, we observe a marginal decrease in the out-of-bag RMSE. Thus, other hyperparameters *(such as `max_features` and `max_samples`)* must be prioritized for tuning over hyperparameters involving pruning.

9.2 Random forest for classification

Random forest model to predict if a person has diabetes.

```
train = pd.read_csv('./Datasets/diabetes_train.csv')
test = pd.read_csv('./Datasets/diabetes_test.csv')
```

```
X = train.drop(columns = 'Outcome')
Xtest = test.drop(columns = 'Outcome')
y = train['Outcome']
ytest = test['Outcome']
```

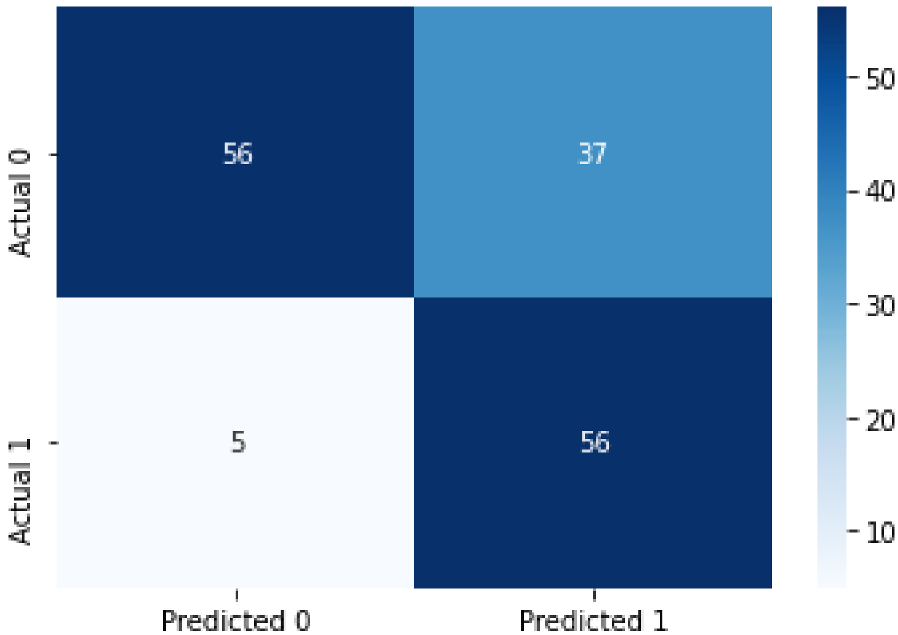
```
#Ensembling the results of 10 decision trees
model = RandomForestClassifier(n_estimators=200, random_state=1,max_features="sqrt",n_jobs=-
```

```
#Feature importance for Random forest
np.mean([tree.feature_importances_ for tree in model.estimators_],axis=0)
```

```
array([0.08380406, 0.25403736, 0.09000104, 0.07151063, 0.07733353,
       0.16976023, 0.12289303, 0.13066012])
```

```
# Performance metrics computation for the optimum decision threshold probability
desired_threshold = 0.23

y_pred_prob = model.predict_proba(Xtest)[:,1]

# Classifying observations in the positive class (y = 1) if the predicted probability is grea
# than the desired decision threshold probability
y_pred = y_pred_prob > desired_threshold
y_pred = y_pred.astype(int)

#Computing the accuracy
print("Accuracy: ",accuracy_score(y_pred, ytest)*100)

#Computing the ROC-AUC
fpr, tpr, auc_thresholds = roc_curve(ytest, y_pred_prob)
print("ROC-AUC: ",auc(fpr, tpr))# AUC of ROC

#Computing the precision and recall
print("Precision: ", precision_score(ytest, y_pred))
print("Recall: ", recall_score(ytest, y_pred))

#Confusion matrix
cm = pd.DataFrame(confusion_matrix(ytest, y_pred),
                  columns=['Predicted 0', 'Predicted 1'], index = ['Actual 0', 'Actual 1'])
sns.heatmap(cm, annot=True, cmap='Blues', fmt='g');
```

```
Accuracy:  72.72727272727273
ROC-AUC:  0.8744050766790058
Precision:  0.6021505376344086
Recall:  0.9180327868852459
```



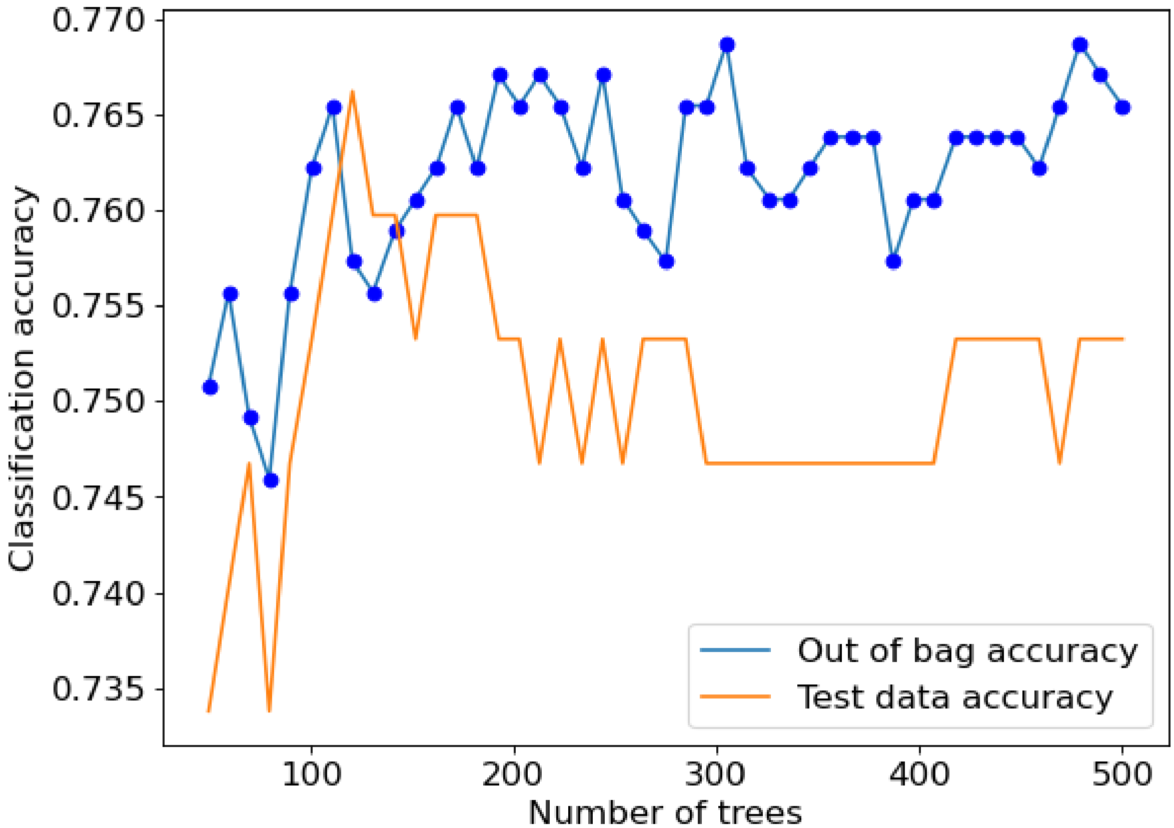
The model obtained above is similar to the one obtained by bagging. We'll discuss the comparison later.

9.2.1 Model accuracy vs number of trees

```
#Finding model accuracy vs number of trees
oob_accuracy={};test_accuracy={};oob_precision={}; test_precision = {}
for i in np.linspace(50,500,45,dtype=int):
    model = RandomForestClassifier(n_estimators=i, random_state=1,max_features="sqrt",n_jobs=
    oob_accuracy[i]=model.oob_score_  #Returns the out-of_bag R-squared of the model
    test_accuracy[i]=model.score(Xtest,ytest) #Returns the test R-squared of the model
    oob_pred = (model.oob_decision_function_[:,1]>=0.5).astype(int)
    oob_precision[i] = precision_score(y, oob_pred)
    test_pred = model.predict(Xtest)
    test_precision[i] = precision_score(ytest, test_pred)
```

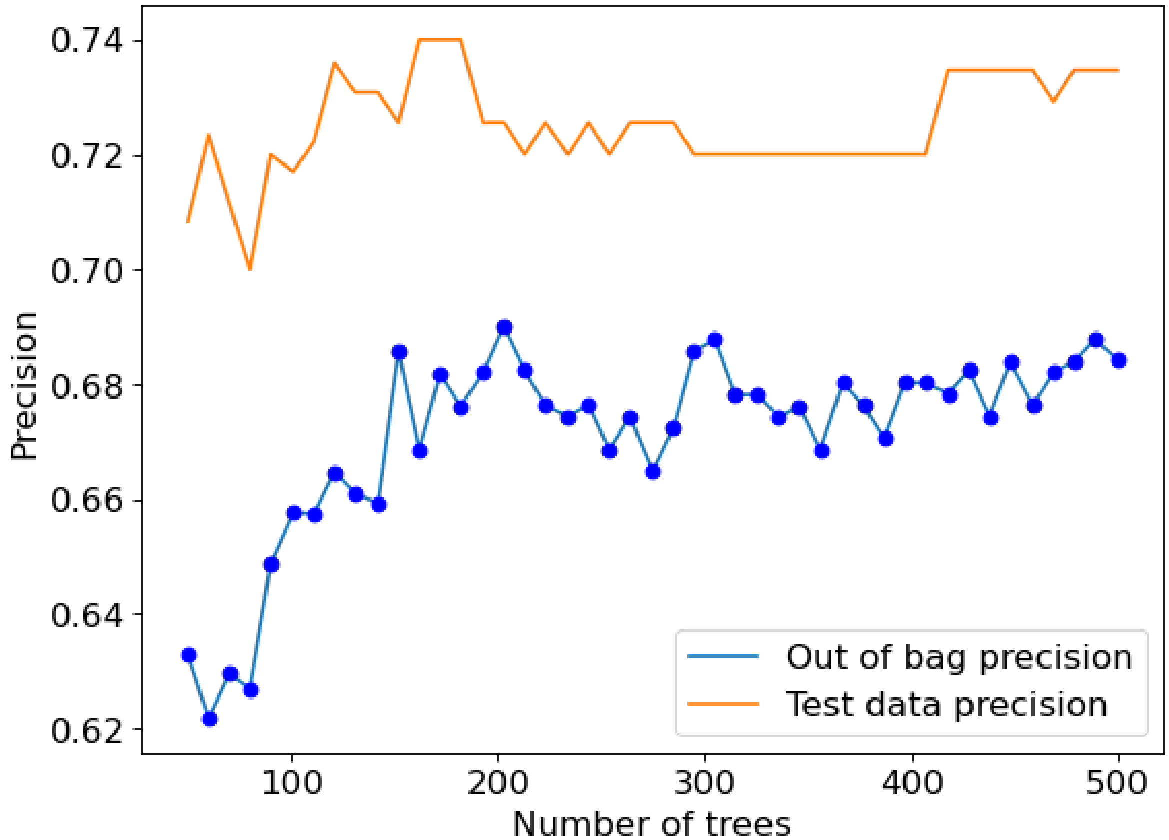
```
plt.rcParams.update({'font.size': 15})
plt.figure(figsize=(8, 6), dpi=80)
plt.plot(oob_accuracy.keys(),oob_accuracy.values(),label = 'Out of bag accuracy')
plt.plot(oob_accuracy.keys(),oob_accuracy.values(),'o',color = 'blue')
plt.plot(test_accuracy.keys(),test_accuracy.values(), label = 'Test data accuracy')
```

```
plt.xlabel('Number of trees')
plt.ylabel('Classification accuracy')
plt.legend();
```



We can also plot other metrics of interest such as out-of-bag precision vs number of trees.

```
#Precision vs number of trees
plt.rcParams.update({'font.size': 15})
plt.figure(figsize=(8, 6), dpi=80)
plt.plot(oob_precision.keys(),oob_precision.values(),label = 'Out of bag precision')
plt.plot(oob_precision.keys(),oob_precision.values(),'o',color = 'blue')
plt.plot(test_precision.keys(),test_precision.values(), label = 'Test data precision')

plt.xlabel('Number of trees')
plt.ylabel('Precision')
plt.legend();
```



9.2.2 Tuning random forest

Here we tune the number of predictors to be considered at each node for the split to maximize recall.

```
start_time = time.time()

params = {'n_estimators': [500],
          'max_features': range(1,9),
         }

param_list=list(it.product(*(params[Name] for Name in list(params.keys()))))
oob_recall = [0]*len(param_list)

i=0
for pr in param_list:
    model = RandomForestClassifier(random_state=1,oob_score=True,verbose=False,n_estimators =
```

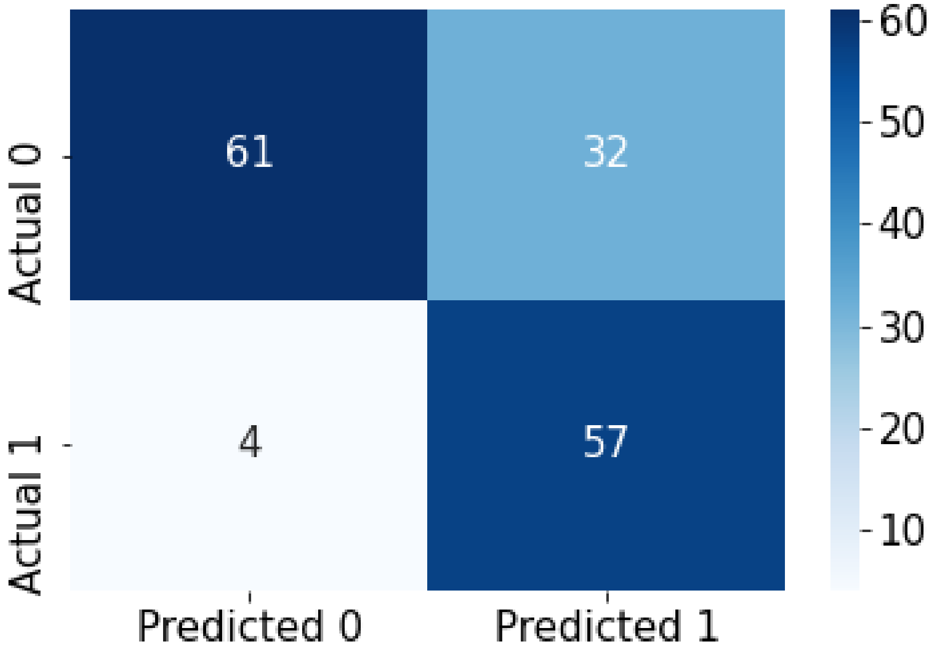
```
                                  max_features=pr[1], n_jobs=-1).fit(X,y)

    oob_pred = (model.oob_decision_function_[:,1]>=0.5).astype(int)
    oob_recall[i] = recall_score(y, oob_pred)
    i=i+1

end_time = time.time()
print("time taken = ", (end_time-start_time)/60, " minutes")
print("max recall = ", np.max(oob_recall))
print("params= ", param_list[np.argmax(oob_recall)])
```

```
time taken =  0.08032723267873128  minutes
max recall =  0.5990338164251208
params=  (500, 8)
```

```
model = RandomForestClassifier(random_state=1,n_jobs=-1,max_features=8,n_estimators=500).fit
```

```
# Performance metrics computation for the optimum decision threshold probability
desired_threshold = 0.23

y_pred_prob = model.predict_proba(Xtest)[:,1]

# Classifying observations in the positive class (y = 1) if the predicted probability is grea
# than the desired decision threshold probability
y_pred = y_pred_prob > desired_threshold
y_pred = y_pred.astype(int)

#Computing the accuracy
print("Accuracy: ",accuracy_score(y_pred, ytest)*100)

#Computing the ROC-AUC
fpr, tpr, auc_thresholds = roc_curve(ytest, y_pred_prob)
print("ROC-AUC: ",auc(fpr, tpr))# AUC of ROC

#Computing the precision and recall
print("Precision: ", precision_score(ytest, y_pred))
print("Recall: ", recall_score(ytest, y_pred))

#Confusion matrix
cm = pd.DataFrame(confusion_matrix(ytest, y_pred),
                  columns=['Predicted 0', 'Predicted 1'], index = ['Actual 0', 'Actual 1'])
sns.heatmap(cm, annot=True, cmap='Blues', fmt='g');
```

```
Accuracy:  76.62337662337663
ROC-AUC:  0.8787237793054822
Precision:  0.6404494382022472
Recall:  0.9344262295081968
```




```
model.feature_importances_
```

```
array([0.069273  , 0.31211579, 0.08492953, 0.05225877, 0.06179047,
       0.17732674, 0.12342981, 0.1188759 ])
```

9.3 Random forest vs Bagging

We saw in the above examples that the performance of random forest was similar to that of bagged trees. This may happen in some cases including but not limited to:

1. All the predictors are more or less equally important, and the bagged trees are not highly correlated.

2. One of the predictors dominates the trees, resulting in highly correlated trees. However, each of the highly correlated trees have high prediction accuracy, leading to overall high prediction accuracy of the bagged trees despite the high correlation.

When can random forests perform poorly: When the number of variables is large, but the fraction of relevant variables small, random forests are likely to perform poorly with small m (fraction of predictors considered for each split). At each split the chance can be small that the relevant variables will be selected. - *Elements of Statistical Learning, page 596*.

However, in general, random forests are expected to decorrelate and improve the bagged trees.

Let us consider a classification example.

```
data = pd.read_csv('Heart.csv')
data.dropna(inplace = True)
data.head()
```

	Age	Sex	ChestPain	RestBP	Chol	Fbs	RestECG	MaxHR	ExAng	Oldpeak	Slope	Ca
0	63	1	typical	145	233	1	2	150	0	2.3	3	0.0
1	67	1	asymptomatic	160	286	0	2	108	1	1.5	2	3.0
2	67	1	asymptomatic	120	229	0	2	129	1	2.6	2	2.0
3	37	1	nonanginal	130	250	0	0	187	0	3.5	3	0.0
4	41	0	nontypical	130	204	0	2	172	0	1.4	1	0.0

In the above dataset, we wish to predict if a person has acquired heart disease (AHD = 'Yes'), based on their symptoms.

```
#Response variable
y = pd.get_dummies(data['AHD'])['Yes']

#Creating a dataframe for predictors with dummy variables replacing the categorical variables
X = data.drop(columns = ['AHD','ChestPain','Thal'])
X = pd.concat([X,pd.get_dummies(data['ChestPain']),pd.get_dummies(data['Thal'])],axis=1)
X.head()
```

	Age	Sex	RestBP	Chol	Fbs	RestECG	MaxHR	ExAng	Oldpeak	Slope	Ca	asymptomatic
0	63	1	145	233	1	2	150	0	2.3	3	0.0	0
1	67	1	160	286	0	2	108	1	1.5	2	3.0	1
2	67	1	120	229	0	2	129	1	2.6	2	2.0	1
3	37	1	130	250	0	0	187	0	3.5	3	0.0	0

	Age	Sex	RestBP	Chol	Fbs	RestECG	MaxHR	ExAng	Oldpeak	Slope	Ca	asymptomatic
4	41	0	130	204	0	2	172	0	1.4	1	0.0	0

```
X.shape
```

```
(297, 18)
```

```
#Creating train and test datasets
Xtrain,Xtest,ytrain,ytest = train_test_split(X,y,train_size = 0.5,random_state=1)
```

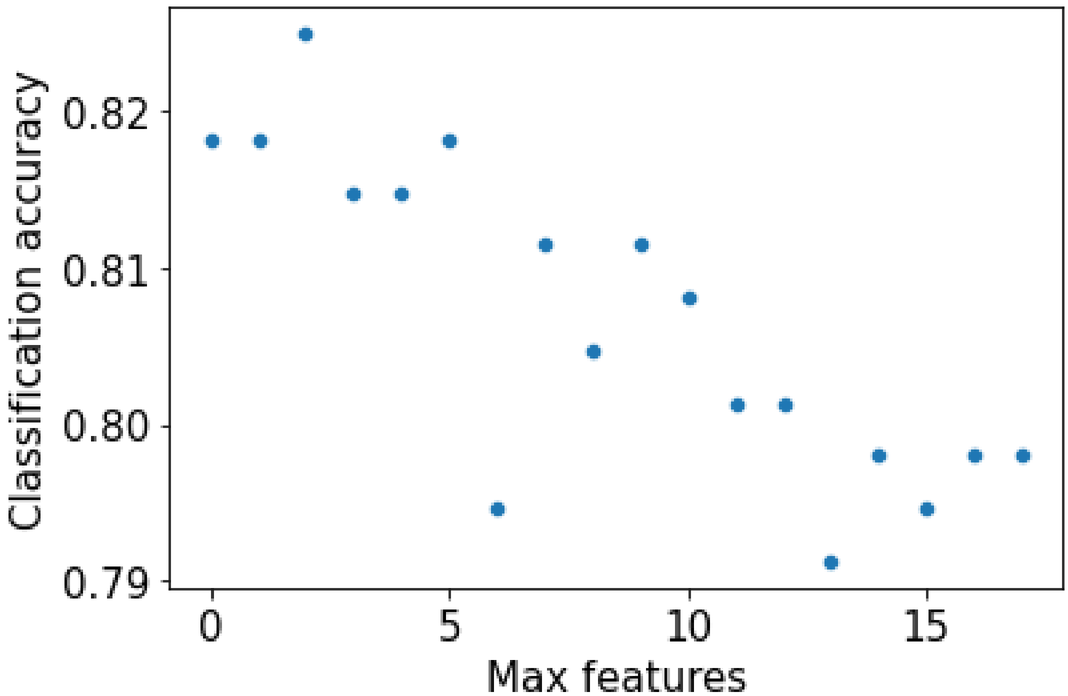
Tuning random forest

```
#Tuning the random forest parameters
start_time = time.time()

oob_score = {}

i=0
for pr in range(1,19):
    model = RandomForestClassifier(random_state=1,oob_score=True,verbose=False,n_estimators =
                                   max_features=pr, n_jobs=-1).fit(X,y)
    oob_score[i] = model.oob_score_
    i=i+1

end_time = time.time()
print("time taken = ", (end_time-start_time)/60, " minutes")
print("max accuracy = ", np.max(list(oob_score.values())))
print("Best value of max_features= ", np.argmax(list(oob_score.values()))+1)
```

```
time taken =  0.21557459433873494  minutes
max accuracy =  0.8249158249158249
Best value of max_features=  3
```

```
sns.scatterplot(x = oob_score.keys(),y = oob_score.values())
plt.xlabel('Max features')
plt.ylabel('Classification accuracy')
```

```
Text(0, 0.5, 'Classification accuracy')
```



Note that as the value of `max_features` is increasing, the accuracy is decreasing. This is probably due to the trees getting correlated as we consider more predictors for each split.

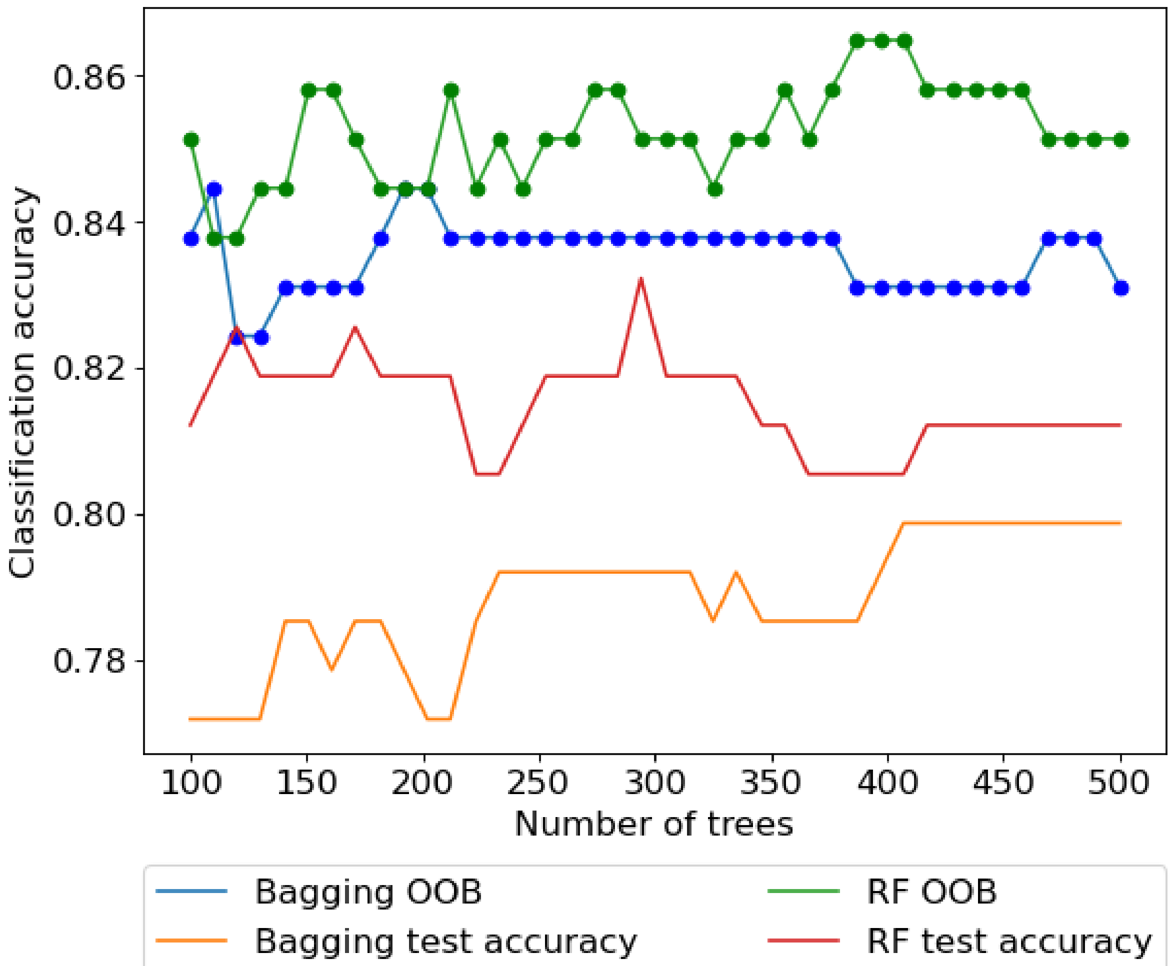
```
#Finding model accuracy vs number of trees
oob_accuracy={};test_accuracy={};
oob_accuracy2={};test_accuacy2={};

for i in np.linspace(100,500,40,dtype=int):
    #Bagging
    model = BaggingClassifier(base_estimator=DecisionTreeClassifier(), n_estimators=i, random
                        n_jobs=-1,oob_score=True).fit(Xtrain, ytrain)
    oob_accuracy[i]=model.oob_score_  #Returns the out-of-bag classification accuracy of the
    test_accuracy[i]=model.score(Xtest,ytest) #Returns the classification accuracy of the mod

    #Random forest
    model2 = RandomForestClassifier(n_estimators=i, random_state=1,max_features=3,
                        n_jobs=-1,oob_score=True).fit(Xtrain, ytrain)
    oob_accuracy2[i]=model2.oob_score_  #Returns the out-of-bag classification accuracy of th
    test_accuacy2[i]=model2.score(Xtest,ytest) #Returns the classification accuracy of the mo
```

```
#Feature importance for bagging
np.mean([tree.feature_importances_ for tree in model.estimators_],axis=0)
```

```
array([0.04381883, 0.05913479, 0.08585651, 0.07165678, 0.00302965,
       0.00903484, 0.05890448, 0.01223421, 0.072461  , 0.01337919,
       0.17495662, 0.18224651, 0.00527156, 0.00953965, 0.00396654,
       0.00163193, 0.09955286, 0.09332406])
```

Note that no predictor is too important to consider. That's why a small value of three for `max_features` is likely to decorrelate trees without compromising the quality of predictions.

```
plt.rcParams.update({'font.size': 15})
plt.figure(figsize=(8, 6), dpi=80)
plt.plot(oob_accuracy.keys(),oob_accuracy.values(),label = 'Bagging OOB')
plt.plot(oob_accuracy.keys(),oob_accuracy.values(),'o',color = 'blue')
plt.plot(test_accuracy.keys(),test_accuracy.values(), label = 'Bagging test accuracy')

plt.plot(oob_accuracy2.keys(),oob_accuracy2.values(),label = 'RF OOB')
plt.plot(oob_accuracy2.keys(),oob_accuracy2.values(),'o',color = 'green')
plt.plot(test_accuacy2.keys(),test_accuacy2.values(), label = 'RF test accuracy')

plt.xlabel('Number of trees')
plt.ylabel('Classification accuracy')
plt.legend(bbox_to_anchor=(0, -0.15, 1, 0), loc=2, ncol=2, mode="expand", borderaxespad=0)
```



In the above example we observe that random forest does improve over bagged trees in terms of classification accuracy. Unlike the previous two examples, the optimal value of `max_features` for random forests is much smaller than the total number of available predictors, thereby making the random forest model much different than the bagged tree model.

10 Adaptive Boosting

Read section 8.2.3 of the book before using these notes.

Note that in this course, lecture notes are not sufficient, you must read the book for better understanding. Lecture notes are just implementing the concepts of the book on a dataset, but not explaining the concepts elaborately.

For the exact algorithms underlying the AdaBoost algorithm, check out the papers `AdaBoostRegressor()` and `AdaBoostClassifier()`.

10.1 Hyperparameters

There are 3 important parameters to tune in AdaBoost:

1. Number of trees
2. Depth of each tree
3. Learning rate

Let us visualize the accuracy of AdaBoost when we independently tweak each of the above parameters.

```
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.metrics import mean_squared_error
from sklearn.model_selection import cross_val_score,train_test_split, KFold, cross_val_predi
from sklearn.metrics import mean_squared_error,r2_score,roc_curve,auc,precision_recall_curve
recall_score, precision_score, confusion_matrix
from sklearn.tree import DecisionTreeRegressor,DecisionTreeClassifier
from sklearn.model_selection import GridSearchCV, ParameterGrid, StratifiedKFold
from sklearn.ensemble import BaggingRegressor,BaggingClassifier,AdaBoostRegressor,AdaBoostCla
RandomForestRegressor
from sklearn.linear_model import LinearRegression,LogisticRegression
from sklearn.neighbors import KNeighborsRegressor
```

```
import itertools as it
import time as time

from skopt import BayesSearchCV
from skopt.space import Real, Categorical, Integer
from skopt.plots import plot_objective, plot_histogram, plot_convergence
import warnings
from IPython import display
```

```
#Using the same datasets as used for linear regression in STAT303-2,
#so that we can compare the non-linear models with linear regression
trainf = pd.read_csv('./Datasets/Car_features_train.csv')
trainp = pd.read_csv('./Datasets/Car_prices_train.csv')
testf = pd.read_csv('./Datasets/Car_features_test.csv')
testp = pd.read_csv('./Datasets/Car_prices_test.csv')
train = pd.merge(trainf,trainp)
test = pd.merge(testf,testp)
train.head()
```

	carID	brand	model	year	transmission	mileage	fuelType	tax	mpg	engineSize	price
0	18473	bmw	6 Series	2020	Semi-Auto	11	Diesel	145	53.3282	3.0	37980
1	15064	bmw	6 Series	2019	Semi-Auto	10813	Diesel	145	53.0430	3.0	33980
2	18268	bmw	6 Series	2020	Semi-Auto	6	Diesel	145	53.4379	3.0	36850
3	18480	bmw	6 Series	2017	Semi-Auto	18895	Diesel	145	51.5140	3.0	25998
4	18492	bmw	6 Series	2015	Automatic	62953	Diesel	160	51.4903	3.0	18990

```
X = train[['mileage','mpg','year','engineSize']]
Xtest = test[['mileage','mpg','year','engineSize']]
y = train['price']
ytest = test['price']
```

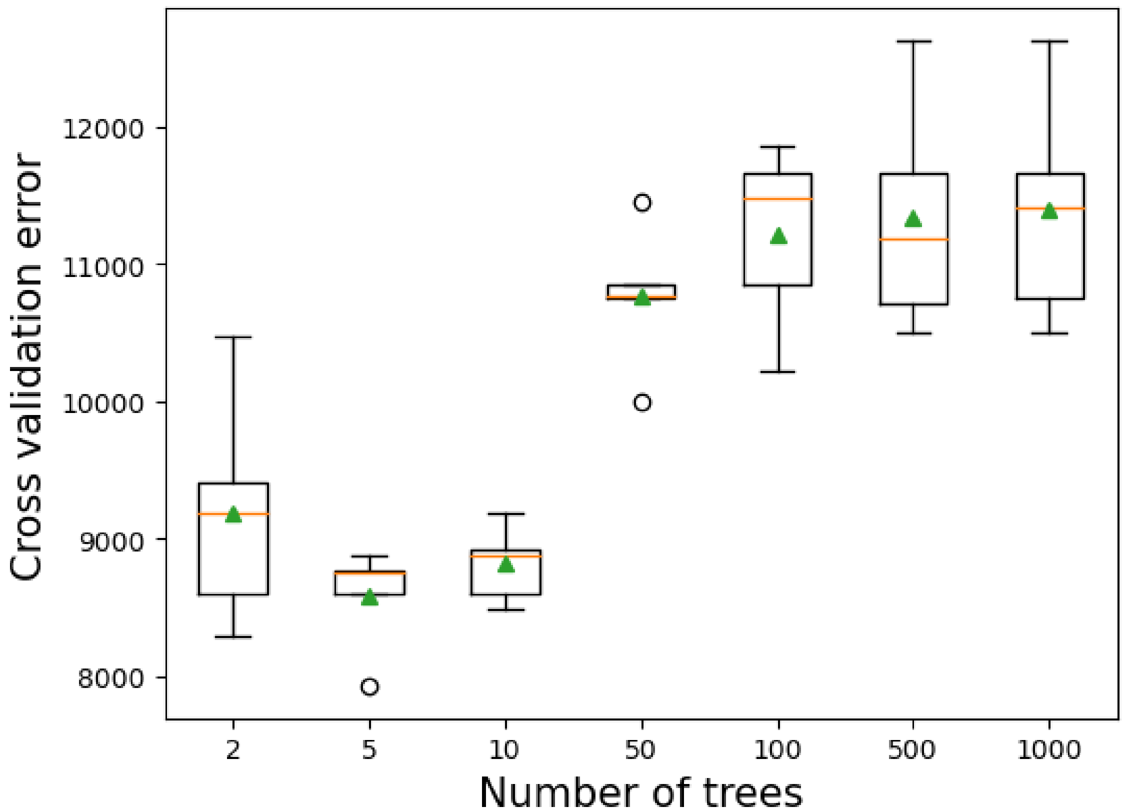
10.2 AdaBoost for regression

10.2.1 Number of trees vs cross validation error

As the number of trees increases, the prediction bias will decrease, and the prediction variance will increase. Thus, there will be an optimal number of trees that minimizes the prediction error.

```
def get_models():
    models = dict()
    # define number of trees to consider
    n_trees = [2, 5, 10, 50, 100, 500, 1000]
    for n in n_trees:
        models[str(n)] = AdaBoostRegressor(n_estimators=n,random_state=1)
    return models

# evaluate a given model using cross-validation
def evaluate_model(model, X, y):
    # define the evaluation procedure
    cv = KFold(n_splits=5, shuffle=True, random_state=1)
    # evaluate the model and collect the results
    scores = -cross_val_score(model, X, y, scoring='neg_root_mean_squared_error', cv=cv, n_jo
    return scores

# get the models to evaluate
models = get_models()
# evaluate the models and store results
results, names = list(), list()
for name, model in models.items():
    # evaluate the model
    scores = evaluate_model(model, X, y)
    # store the results
    results.append(scores)
    names.append(name)
    # summarize the performance along the way
    print('>%s %.3f (%.3f)' % (name, np.mean(scores), np.std(scores)))
# plot model performance for comparison
plt.boxplot(results, labels=names, showmeans=True)
plt.ylabel('Cross validation error',fontsize=15)
plt.xlabel('Number of trees',fontsize=15);
```

```
>2 9190.253 (757.408)
>5 8583.629 (341.406)
>10 8814.328 (248.891)
>50 10763.138 (465.677)
>100 11217.783 (602.642)
>500 11336.088 (763.288)
>1000 11390.043 (752.446)
```



10.2.2 Depth of tree vs cross validation error

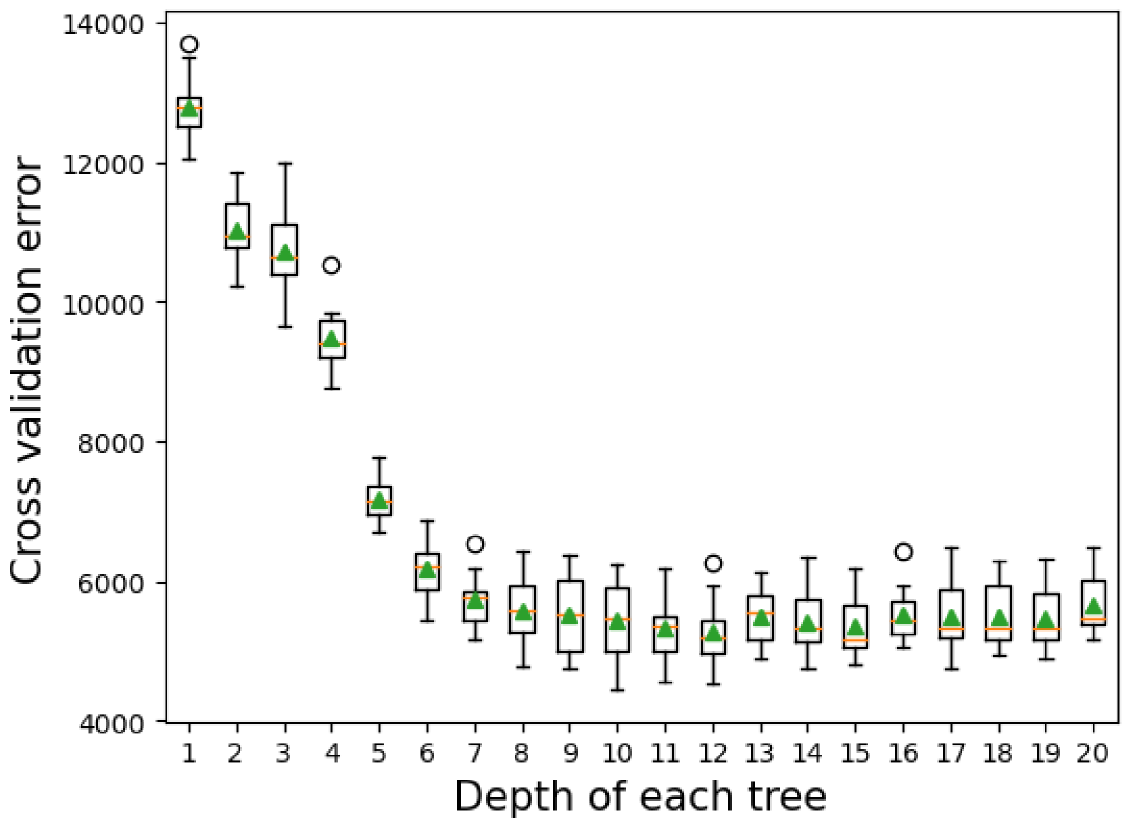
As the depth of each weak learner (decision tree) increases, the complexity of the weak learner will increase. As the complexity increases, the prediction bias will decrease, while the prediction variance will increase. Thus, there will be an optimal depth for each weak learner that minimizes the prediction error.

```
# get a list of models to evaluate
def get_models():
    models = dict()
    # explore depths from 1 to 10
    for i in range(1,21):
        # define base model
        base = DecisionTreeRegressor(max_depth=i)
        # define ensemble model
        models[str(i)] = AdaBoostRegressor(base_estimator=base,n_estimators=50)
    return models
```

```
# evaluate a given model using cross-validation
def evaluate_model(model, X, y):
    # define the evaluation procedure
    cv = KFold(n_splits=10, shuffle=True, random_state=1)
    # evaluate the model and collect the results
    scores = -cross_val_score(model, X, y, scoring='neg_root_mean_squared_error', cv=cv, n_j
    return scores

# get the models to evaluate
models = get_models()
# evaluate the models and store results
results, names = list(), list()
for name, model in models.items():
    # evaluate the model
    scores = evaluate_model(model, X, y)
    # store the results
    results.append(scores)
    names.append(name)
    # summarize the performance along the way
    print('>%s %.3f (%.3f)' % (name, np.mean(scores), np.std(scores)))
plt.boxplot(results, labels=names, showmeans=True)
plt.ylabel('Cross validation error',fontsize=15)
plt.xlabel('Depth of each tree',fontsize=15);
```

```
>1 12798.764 (490.538)
>2 11031.451 (465.520)
>3 10739.302 (636.517)
>4 9491.714 (466.764)
>5 7184.489 (324.484)
>6 6181.533 (411.394)
>7 5746.902 (407.451)
>8 5587.726 (473.619)
>9 5526.291 (541.512)
>10 5444.928 (554.170)
>11 5321.725 (455.899)
>12 5279.581 (492.785)
>13 5494.982 (393.469)
>14 5423.982 (488.564)
>15 5369.485 (441.799)
>16 5536.739 (409.166)
>17 5511.002 (517.384)
```

```
>18 5510.922 (478.285)
>19 5482.119 (465.565)
>20 5667.969 (468.964)
```



10.2.3 Learning rate vs cross validation error

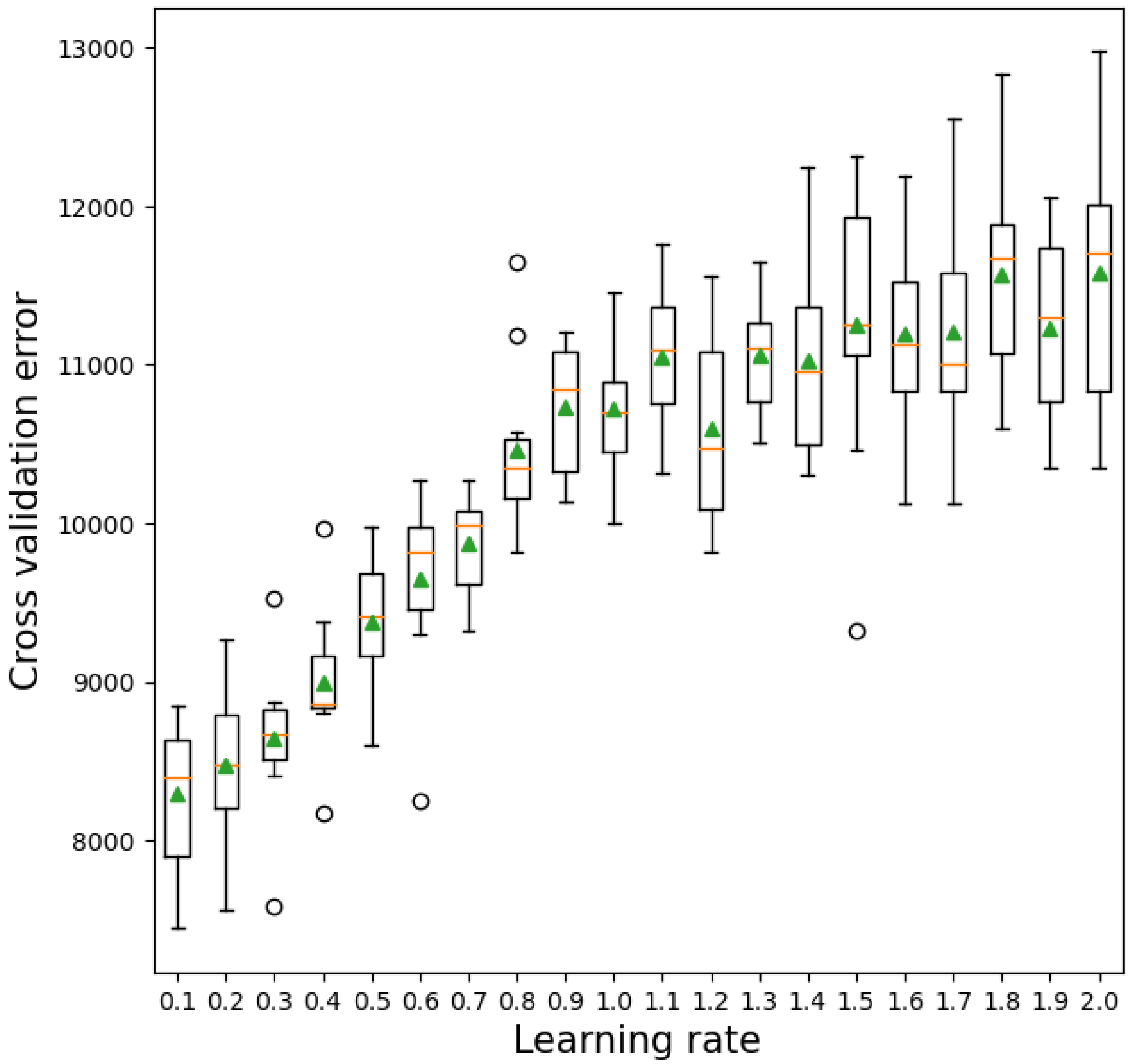
The optimal learning rate will depend on the number of trees, and vice-versa. If the learning rate is too low, it will take several trees to "learn" the response. If the learning rate is high, the response will be "learned" quickly (with fewer) trees. Learning too quickly will be prone to overfitting, while learning too slowly will be computationally expensive. Thus, there will be an optimal learning rate to minimize the prediction error.

```
def get_models():
    models = dict()
    # explore learning rates from 0.1 to 2 in 0.1 increments
    for i in np.arange(0.1, 2.1, 0.1):
        key = '%.1f' % i
```

```
        models[key] = AdaBoostRegressor(learning_rate=i)
    return models

# evaluate a given model using cross-validation
def evaluate_model(model, X, y):
    # define the evaluation procedure
    cv = KFold(n_splits=10, shuffle=True, random_state=1)
    # evaluate the model and collect the results
    scores = -cross_val_score(model, X, y, scoring='neg_root_mean_squared_error', cv=cv, n_jo
    return scores

# get the models to evaluate
models = get_models()
# evaluate the models and store results
results, names = list(), list()
for name, model in models.items():
    # evaluate the model
    scores = evaluate_model(model, X, y)
    # store the results
    results.append(scores)
    names.append(name)
    # summarize the performance along the way
    print('>%s %.1f (%.1f)' % (name, np.mean(scores), np.std(scores)))
# plot model performance for comparison
plt.figure(figsize=(7, 7))
plt.boxplot(results, labels=names, showmeans=True)
plt.ylabel('Cross validation error',fontsize=15)
plt.xlabel('Learning rate',fontsize=15);
```

```
>0.1 8291.9 (452.4)
>0.2 8475.7 (465.3)
>0.3 8648.5 (458.8)
>0.4 8995.5 (438.6)
>0.5 9376.1 (388.2)
>0.6 9655.3 (551.8)
>0.7 9877.3 (319.8)
>0.8 10466.8 (528.3)
>0.9 10728.9 (386.8)
>1.0 10720.2 (410.6)
>1.1 11043.9 (432.5)
>1.2 10602.5 (570.0)
>1.3 11058.8 (362.1)
```

```
>1.4 11022.7 (616.0)
>1.5 11252.5 (839.3)
>1.6 11195.3 (604.5)
>1.7 11206.3 (636.1)
>1.8 11569.1 (674.6)
>1.9 11232.3 (605.6)
>2.0 11581.0 (824.8)
```



10.2.4 Tuning AdaBoost for regression

As the optimal value of the parameters depend on each other, we need to optimize them simultaneously.

```
model = AdaBoostRegressor(random_state=1)
grid = dict()
grid['n_estimators'] = [10, 50, 100,200]
grid['learning_rate'] = [0.0001, 0.001, 0.01,0.1, 1.0]
grid['estimator'] = [DecisionTreeRegressor(max_depth=3), DecisionTreeRegressor(max_depth=5),
                          DecisionTreeRegressor(max_depth=10),DecisionTreeRegressor(max_dept
# define the evaluation procedure
cv = KFold(n_splits=5, shuffle=True, random_state=1)
# define the grid search procedure
grid_search = GridSearchCV(estimator=model, param_grid=grid, n_jobs=-1, cv=cv, scoring='neg_
# execute the grid search
grid_result = grid_search.fit(X, y)
# summarize the best score and configuration
print("Best: %f using %s" % (-grid_result.best_score_, grid_result.best_params_))
# summarize all scores that were evaluated
means = grid_result.cv_results_['mean_test_score']
stds = grid_result.cv_results_['std_test_score']
params = grid_result.cv_results_['params']
```

```
Best: 5346.490675 using {'estimator': DecisionTreeRegressor(max_depth=10), 'learning_rate':
```

Note that for tuning `max_depth` of the base estimator - decision tree, we specified 4 different base estimators with different depths. However, there is a more concise way to do that. We can specify the `max_depth` of the estimator by adding a double underscore "`__`" between the `estimator` and the hyperparameter that we wish to tune *(`max_depth` here)*, and then specify its potential values in the `grid` itself as shown below. However, we'll then need to add `DecisionTreeRegressor()` as the estimator within the `AdaBoostRegressor()` function.

```
model = AdaBoostRegressor(random_state=1, estimator = DecisionTreeRegressor(random_state=1))
grid = dict()
grid['n_estimators'] = [10, 50, 100,200]
grid['learning_rate'] = [0.0001, 0.001, 0.01,0.1, 1.0]
grid['estimator__max_depth'] = [3, 5, 10, 15]
# define the evaluation procedure
cv = KFold(n_splits=5, shuffle=True, random_state=1)
# define the grid search procedure
```

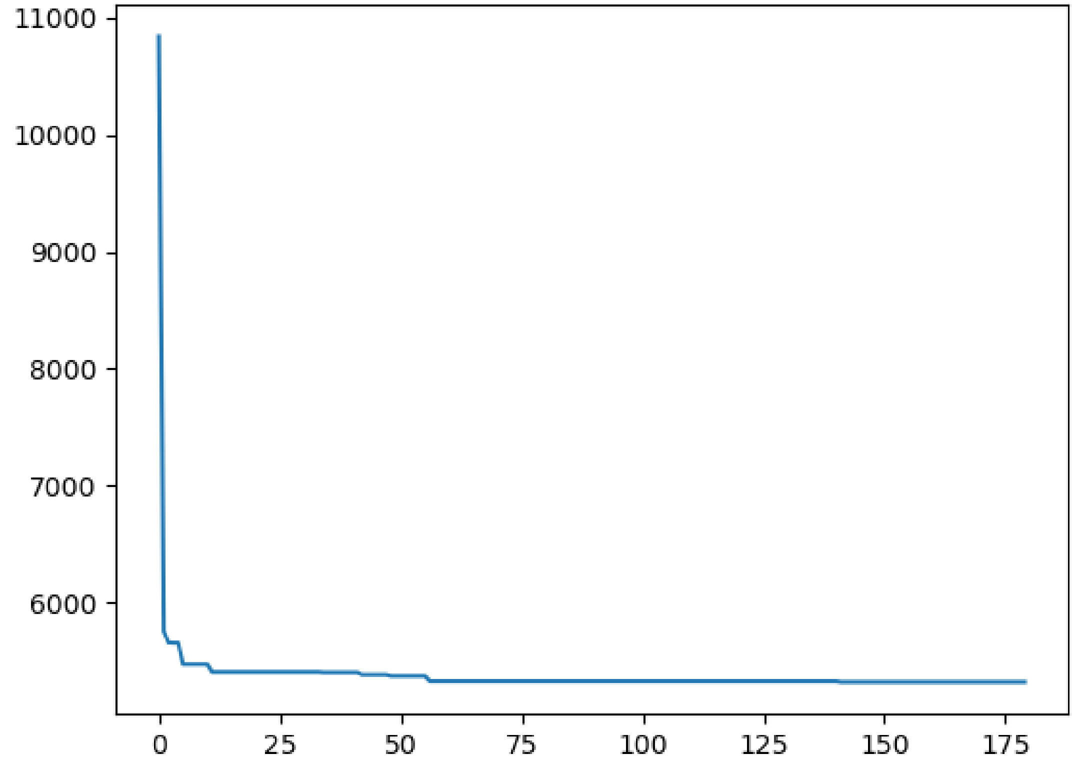
```
grid_search = GridSearchCV(estimator=model, param_grid=grid, n_jobs=-1, cv=cv, scoring='neg_
# execute the grid search
grid_result = grid_search.fit(X, y)
# summarize the best score and configuration
print("Best: %f using %s" % (-grid_result.best_score_, grid_result.best_params_))
# summarize all scores that were evaluated
means = grid_result.cv_results_['mean_test_score']
stds = grid_result.cv_results_['std_test_score']
params = grid_result.cv_results_['params']
```

```
Best: 5346.490675 using {'estimator__max_depth': 10, 'learning_rate': 1.0, 'n_estimators': 50
```

The BayesSearchCV() approach also coverges to a slightly different set of optimal hyperparameter values. However, it gives a similar cross-validated RMSE. This is possible. There may be multiple hyperparameter values that are different from each other, but similar in performance. It may be a good idea to ensemble models based on these two distinct set of hyperparameter values that give an equally accurate model.

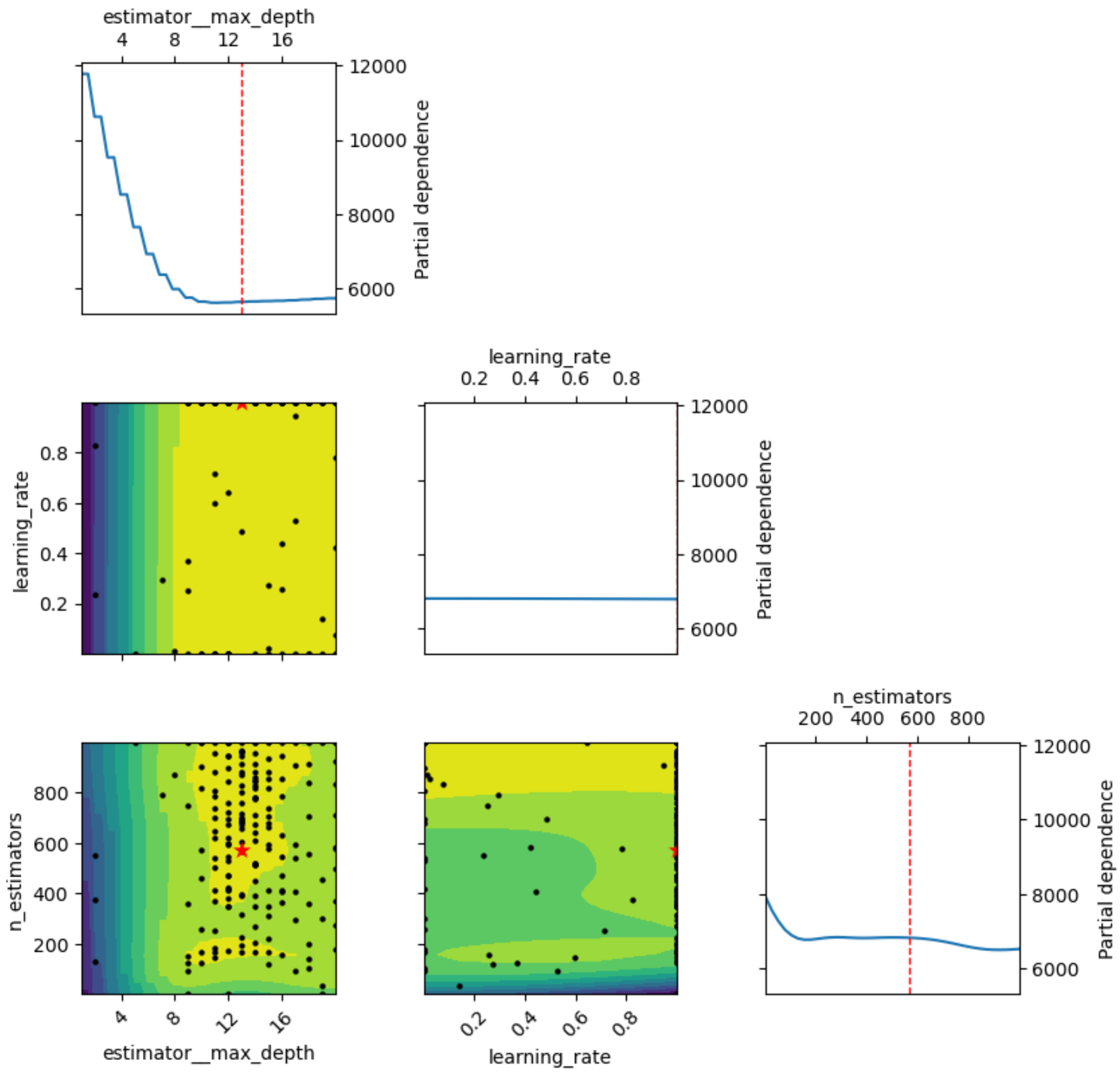
```
model = AdaBoostRegressor(estimator=DecisionTreeRegressor())
grid = dict()
grid['n_estimators'] = Integer(2, 1000)
grid['learning_rate'] = Real(0.0001, 1.0)
grid['estimator__max_depth'] = Integer(1, 20)

kfold = KFold(n_splits = 5, shuffle = True, random_state = 1)
gcv = BayesSearchCV(model, search_spaces = grid, cv = kfold, n_iter = 180, random_state = 10
                         scoring = 'neg_root_mean_squared_error', n_jobs = -1)
paras = list(gcv.search_spaces.keys())
paras.sort()

def monitor(optim_result):
    cv_values = pd.Series(optim_result['func_vals']).cummin()
    display.clear_output(wait = True)
    min_ind = pd.Series(optim_result['func_vals']).argmin()
    print(paras, "=", optim_result['x_iters'][min_ind], pd.Series(optim_result['func_vals'])
    sns.lineplot(cv_values)
    plt.show()
gcv.fit(X, y, callback = monitor)
```

```
['estimator__max_depth', 'learning_rate', 'n_estimators'] = [13, 1.0, 570] 5325.017602505734
```

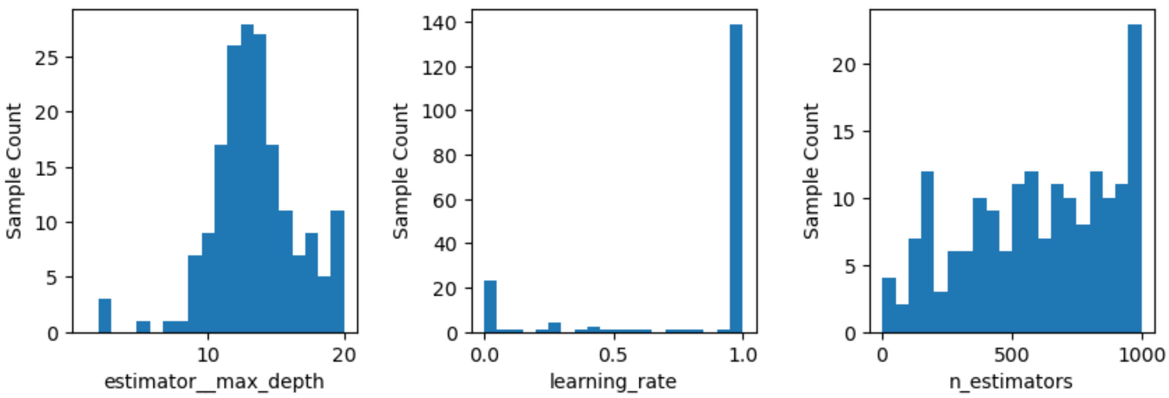



```
BayesSearchCV(cv=KFold(n_splits=5, random_state=1, shuffle=True),
              estimator=AdaBoostRegressor(estimator=DecisionTreeRegressor()),
              n_iter=180, n_jobs=-1, random_state=10,
              scoring='neg_root_mean_squared_error',
              search_spaces={'estimator__max_depth': Integer(low=1, high=20, prior='uniform'
                             'learning_rate': Real(low=0.0001, high=1.0, prior='uniform', tra
                             'n_estimators': Integer(low=2, high=1000, prior='uniform', trans
```

```
plot_objective(gcv.optimizer_results_[0],
                   dimensions=['estimator__max_depth', 'learning_rate', 'n_estimators'], size
plt.show();
```




```python
fig, ax = plt.subplots(1, 3, figsize = (10, 3))
plt.subplots_adjust(wspace=0.4)
plot_histogram(gcv.optimizer_results_[0], 0, ax = ax[0])
plot_histogram(gcv.optimizer_results_[0], 1, ax = ax[1])
plot_histogram(gcv.optimizer_results_[0], 2, ax = ax[2])
plt.show()
```




```
#Model based on the optimal hyperparameters
model = AdaBoostRegressor(estimator=DecisionTreeRegressor(max_depth=10),n_estimators=50,lear
                          random_state=1).fit(X,y)
```

```
#RMSE of the optimized model on test data
pred1=model.predict(Xtest)
print("AdaBoost model RMSE = ", np.sqrt(mean_squared_error(model.predict(Xtest),ytest)))
```

```
AdaBoost model RMSE =  5693.165811600585
```

```
#Model based on the optimal hyperparameters
model = AdaBoostRegressor(estimator=DecisionTreeRegressor(max_depth=13),n_estimators=570,lea
                          random_state=1).fit(X,y)
```

```
#RMSE of the optimized model on test data
pred2=model.predict(Xtest)
print("AdaBoost model RMSE = ", np.sqrt(mean_squared_error(model.predict(Xtest),ytest)))
```

```
AdaBoost model RMSE =  5434.852990644646
```

```
model = RandomForestRegressor(n_estimators=300, random_state=1,
                        n_jobs=-1, max_features=2).fit(X, y)
pred3 = model.predict(Xtest)
print("Random Forest model RMSE = ", np.sqrt(mean_squared_error(model.predict(Xtest),ytest))
```

```
Random Forest model RMSE =  5642.45839697972
```

```
#Ensemble modeling
pred = 0.33*pred1+0.33*pred2 + 0.34*pred3
print("Ensemble model RMSE = ", np.sqrt(mean_squared_error(pred,ytest)))
```

```
Ensemble model RMSE =  5402.832128650372
```

Combined, the random forest model and the Adaboost models do better than each of the individual models.

10.3 AdaBoost for classification

Below is the AdaBoost implementation on a classification problem. The takeaways are the same as that of the regression problem above.

```
train = pd.read_csv('./Datasets/diabetes_train.csv')
test = pd.read_csv('./Datasets/diabetes_test.csv')
```

```
X = train.drop(columns = 'Outcome')
Xtest = test.drop(columns = 'Outcome')
y = train['Outcome']
ytest = test['Outcome']
```

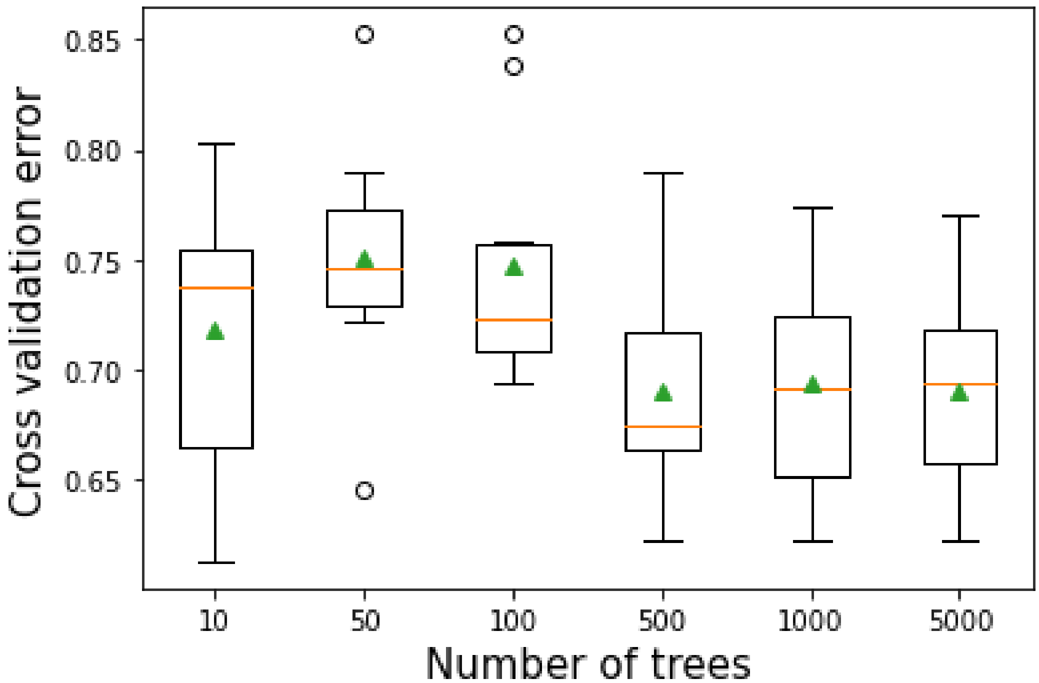
10.3.1 Number of trees vs cross validation accuracy

```
def get_models():
    models = dict()
    # define number of trees to consider
    n_trees = [10, 50, 100, 500, 1000, 5000]
    for n in n_trees:
        models[str(n)] = AdaBoostClassifier(n_estimators=n,random_state=1)
    return models

# evaluate a given model using cross-validation
def evaluate_model(model, X, y):
    # define the evaluation procedure
    cv = StratifiedKFold(n_splits=10, shuffle=True, random_state=1)
    # evaluate the model and collect the results
```

```
    scores = cross_val_score(model, X, y, scoring='accuracy', cv=cv, n_jobs=-1)
    return scores

# get the models to evaluate
models = get_models()
# evaluate the models and store results
results, names = list(), list()
for name, model in models.items():
    # evaluate the model
    scores = evaluate_model(model, X, y)
    # store the results
    results.append(scores)
    names.append(name)
    # summarize the performance along the way
    print('>%s %.3f (%.3f)' % (name, np.mean(scores), np.std(scores)))
# plot model performance for comparison
plt.boxplot(results, labels=names, showmeans=True)
plt.ylabel('Cross validation error',fontsize=15)
plt.xlabel('Number of trees',fontsize=15)
```

```
>10 0.718 (0.060)
>50 0.751 (0.051)
>100 0.748 (0.053)
>500 0.690 (0.045)
>1000 0.694 (0.048)
>5000 0.691 (0.044)
```

```
Text(0.5, 0, 'Number of trees')
```



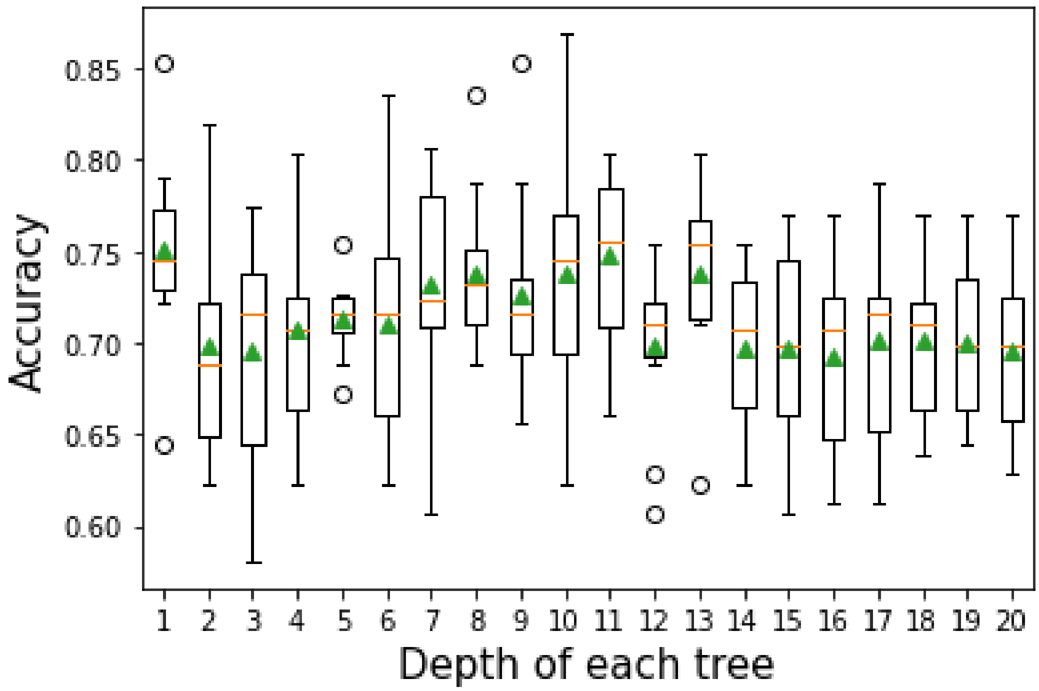
10.3.2 Depth of each tree vs cross validation accuracy

```
# get a list of models to evaluate
def get_models():
    models = dict()
    # explore depths from 1 to 10
    for i in range(1,21):
        # define base model
        base = DecisionTreeClassifier(max_depth=i)
        # define ensemble model
        models[str(i)] = AdaBoostClassifier(estimator=base)
    return models

# evaluate a given model using cross-validation
def evaluate_model(model, X, y):
    # define the evaluation procedure
    cv = StratifiedKFold(n_splits=10, shuffle=True, random_state=1)
    # evaluate the model and collect the results
    scores = cross_val_score(model, X, y, scoring='accuracy', cv=cv, n_jobs=-1)
    return scores
```

```python
# get the models to evaluate
models = get_models()
# evaluate the models and store results
results, names = list(), list()
for name, model in models.items():
    # evaluate the model
    scores = evaluate_model(model, X, y)
    # store the results
    results.append(scores)
    names.append(name)
    # summarize the performance along the way
    print('>%s %.3f (%.3f)' % (name, np.mean(scores), np.std(scores)))
plt.boxplot(results, labels=names, showmeans=True)
plt.ylabel('Accuracy',fontsize=15)
plt.xlabel('Depth of each tree',fontsize=15)
```

```
>1 0.751 (0.051)
>2 0.699 (0.063)
>3 0.696 (0.062)
>4 0.707 (0.055)
>5 0.713 (0.021)
>6 0.710 (0.061)
>7 0.733 (0.057)
>8 0.738 (0.044)
>9 0.727 (0.053)
>10 0.738 (0.065)
>11 0.748 (0.048)
>12 0.699 (0.044)
>13 0.738 (0.047)
>14 0.697 (0.041)
>15 0.697 (0.052)
>16 0.692 (0.052)
>17 0.702 (0.056)
>18 0.702 (0.045)
>19 0.700 (0.040)
>20 0.696 (0.042)
```

```
Text(0.5, 0, 'Depth of each tree')
```



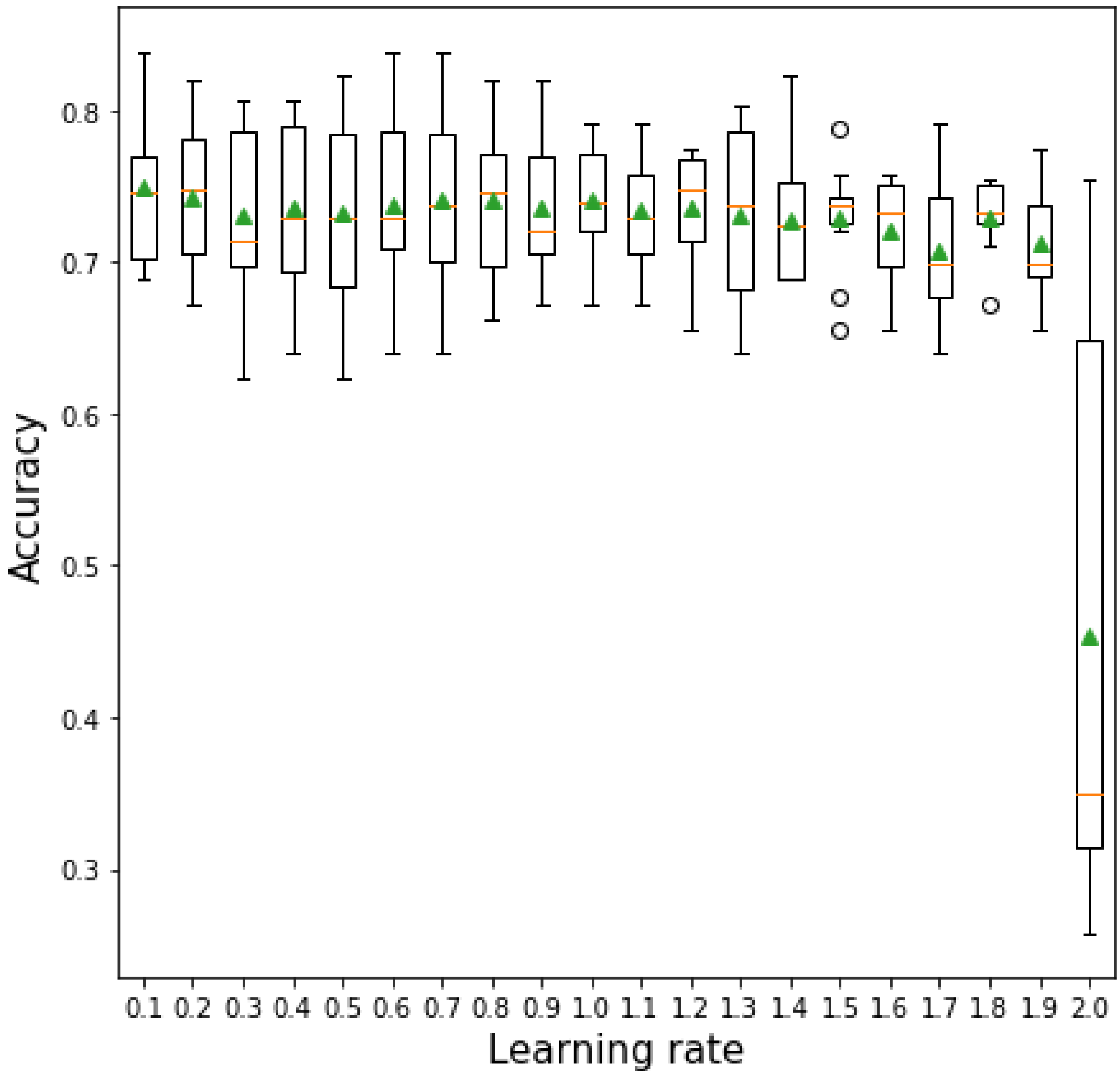
10.3.3 Learning rate vs cross validation accuracy

```
def get_models():
    models = dict()
    # explore learning rates from 0.1 to 2 in 0.1 increments
    for i in np.arange(0.1, 2.1, 0.1):
        key = '%.1f' % i
        models[key] = AdaBoostClassifier(learning_rate=i)
    return models

# evaluate a given model using cross-validation
def evaluate_model(model, X, y):
    # define the evaluation procedure
    cv = KFold(n_splits=10, shuffle=True, random_state=1)
    # evaluate the model and collect the results
    scores = cross_val_score(model, X, y, scoring='accuracy', cv=cv, n_jobs=-1)
    return scores

# get the models to evaluate
models = get_models()
```

```python
# evaluate the models and store results
results, names = list(), list()
for name, model in models.items():
    # evaluate the model
    scores = evaluate_model(model, X, y)
    # store the results
    results.append(scores)
    names.append(name)
    # summarize the performance along the way
    print('>%s %.3f (%.3f)' % (name, np.mean(scores), np.std(scores)))
# plot model performance for comparison
plt.figure(figsize=(7, 7))
plt.boxplot(results, labels=names, showmeans=True)
plt.ylabel('Accuracy',fontsize=15)
plt.xlabel('Learning rate',fontsize=15)
```

```
>0.1 0.749 (0.052)
>0.2 0.743 (0.050)
>0.3 0.731 (0.057)
>0.4 0.736 (0.053)
>0.5 0.733 (0.062)
>0.6 0.738 (0.058)
>0.7 0.741 (0.056)
>0.8 0.741 (0.049)
>0.9 0.736 (0.048)
>1.0 0.741 (0.035)
>1.1 0.734 (0.037)
>1.2 0.736 (0.038)
>1.3 0.731 (0.057)
>1.4 0.728 (0.041)
>1.5 0.730 (0.036)
>1.6 0.720 (0.038)
>1.7 0.707 (0.045)
>1.8 0.730 (0.024)
>1.9 0.712 (0.033)
>2.0 0.454 (0.191)
```

```
Text(0.5, 0, 'Learning rate')
```



10.3.4 Tuning AdaBoost Classifier hyperparameters

```
model = AdaBoostClassifier(random_state=1, estimator = DecisionTreeClassifier())
grid = dict()
grid['n_estimators'] = [10, 50, 100,200,500]
grid['learning_rate'] = [0.0001, 0.001, 0.01,0.1, 1.0]
grid['estimator__max_depth'] = [1, 2, 3, 4]
# define the evaluation procedure
```

```
cv = StratifiedKFold(n_splits=5, shuffle=True, random_state=1)
# define the grid search procedure
grid_search = GridSearchCV(estimator=model, param_grid=grid, n_jobs=-1, cv=cv,
                          verbose = True)
# execute the grid search
grid_result = grid_search.fit(X, y)
# summarize the best score and configuration
print("Best: %f using %s" % (grid_result.best_score_, grid_result.best_params_))
# summarize all scores that were evaluated
means = grid_result.cv_results_['mean_test_score']
stds = grid_result.cv_results_['std_test_score']
params = grid_result.cv_results_['params']
#for mean, stdev, param in zip(means, stds, params):
#    print("%f (%f) with: %r" % (mean, stdev, param)
```

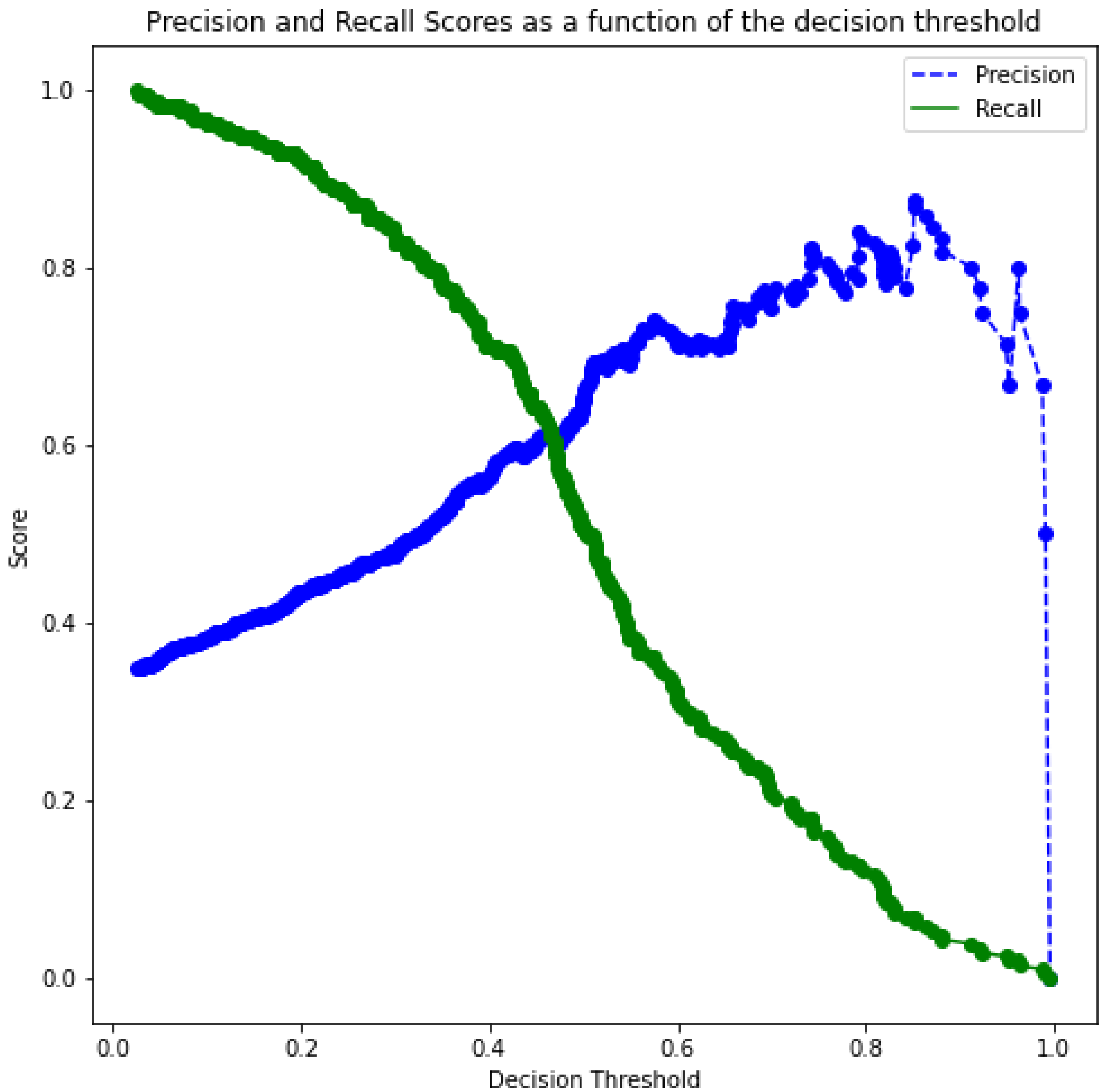
```
Fitting 5 folds for each of 100 candidates, totalling 500 fits
Best: 0.763934 using {'estimator__max_depth': 3, 'learning_rate': 0.01, 'n_estimators': 200}
```

10.3.5 Tuning the decision threshold probability

We'll find a decision threshold probability that balances recall with precision.

```
#Model based on the optimal parameters
model = AdaBoostClassifier(random_state=1, estimator = DecisionTreeClassifier(max_depth=3),le
                          n_estimators=200).fit(X,y)

# Note that we are using the cross-validated predicted probabilities, instead of directly usi
# predicted probabilities on train data, as the model may be overfitting on the train data, a
# may lead to misleading results
cross_val_ypred = cross_val_predict(AdaBoostClassifier(random_state=1,base_estimator = Decisi
                          n_estimators=200), X, y, cv = 5, method = 'predict_proba')

p, r, thresholds = precision_recall_curve(y, cross_val_ypred[:,1])
def plot_precision_recall_vs_threshold(precisions, recalls, thresholds):
    plt.figure(figsize=(8, 8))
    plt.title("Precision and Recall Scores as a function of the decision threshold")
    plt.plot(thresholds, precisions[:-1], "b--", label="Precision")
    plt.plot(thresholds, recalls[:-1], "g-", label="Recall")
    plt.plot(thresholds, precisions[:-1], "o", color = 'blue')
    plt.plot(thresholds, recalls[:-1], "o", color = 'green')
    plt.ylabel("Score")
```

```
    plt.xlabel("Decision Threshold")
    plt.legend(loc='best')
    plt.legend()
plot_precision_recall_vs_threshold(p, r, thresholds)
```




```
# Thresholds with precision and recall
all_thresholds = np.concatenate([thresholds.reshape(-1,1), p[:-1].reshape(-1,1), r[:-1].resha
recall_more_than_80 = all_thresholds[all_thresholds[:,2]>0.8,:]
```

```
# As the values in 'recall_more_than_80' are arranged in decreasing order of recall and incre
# the last value will provide the maximum threshold probability for the recall to be more tha
# We wish to find the maximum threshold probability to obtain the maximum possible precision
recall_more_than_80[recall_more_than_80.shape[0]-1]
```

```
array([0.33488762, 0.50920245, 0.80193237])
```

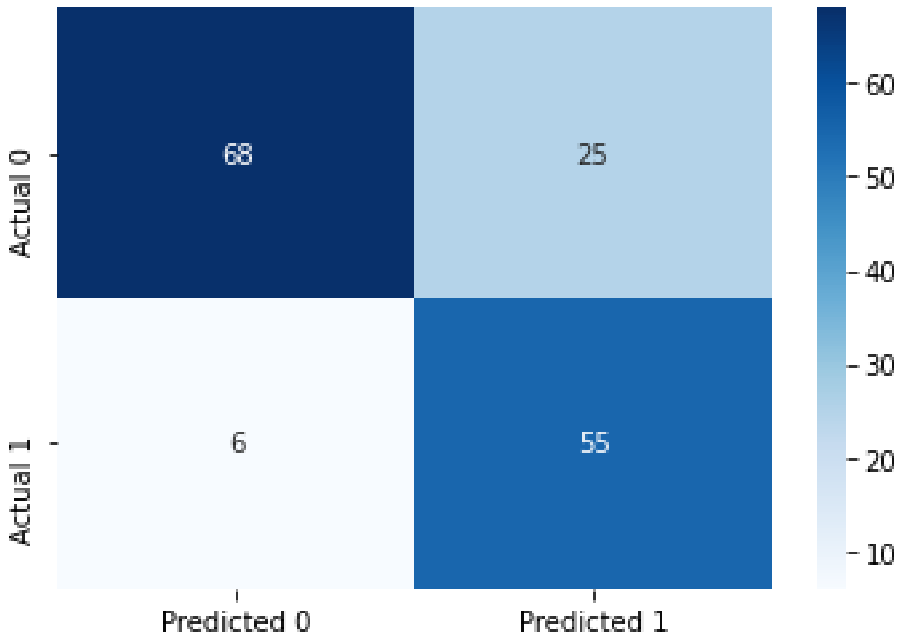
```
#Optimal decision threshold probability
thres = recall_more_than_80[recall_more_than_80.shape[0]-1][0]
thres
```

```
0.3348876199649718
```

```
# Performance metrics computation for the optimum decision threshold probability
desired_threshold = thres

y_pred_prob = model.predict_proba(Xtest)[:,1]

# Classifying observations in the positive class (y = 1) if the predicted probability is grea
# than the desired decision threshold probability
y_pred = y_pred_prob > desired_threshold
y_pred = y_pred.astype(int)

#Computing the accuracy
print("Accuracy: ",accuracy_score(y_pred, ytest)*100)

#Computing the ROC-AUC
fpr, tpr, auc_thresholds = roc_curve(ytest, y_pred_prob)
print("ROC-AUC: ",auc(fpr, tpr))# AUC of ROC

#Computing the precision and recall
print("Precision: ", precision_score(ytest, y_pred))
print("Recall: ", recall_score(ytest, y_pred))

#Confusion matrix
cm = pd.DataFrame(confusion_matrix(ytest, y_pred),
                  columns=['Predicted 0', 'Predicted 1'], index = ['Actual 0', 'Actual 1'])
sns.heatmap(cm, annot=True, cmap='Blues', fmt='g');
```

```
Accuracy:  79.87012987012987
```

```
ROC-AUC:  0.8884188260179798
Precision:  0.6875
Recall:  0.9016393442622951
```



The above model is similar to the one obtained with bagging / random forest. However, adaptive boosting may lead to better classification performance as compared to bagging / random forest.

11 Gradient Boosting

Check the gradient boosting algorithm in section 10.10.2 of the book, [Elements of Statistical Learning] before using these notes.

Note that in this course, lecture notes are not sufficient, you must read the book for better understanding. Lecture notes are just implementing the concepts of the book on a dataset, but not explaining the concepts elaborately.

11.1 Hyperparameters

There are 5 important parameters to tune in Gradient boosting:

1. Number of trees
2. Depth of each tree
3. Learning rate
4. Subsample fraction
5. Maximum features

Let us visualize the accuracy of Gradient boosting when we independently tweak each of the above parameters.

```
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.metrics import mean_squared_error
from sklearn.model_selection import cross_val_score,train_test_split, KFold, cross_val_predi
from sklearn.metrics import mean_squared_error,r2_score,roc_curve,auc,precision_recall_curve
recall_score, precision_score, confusion_matrix
from sklearn.tree import DecisionTreeRegressor,DecisionTreeClassifier
from sklearn.model_selection import GridSearchCV, ParameterGrid, StratifiedKFold
from sklearn.ensemble import GradientBoostingRegressor,GradientBoostingClassifier, BaggingReg
from sklearn.linear_model import LinearRegression,LogisticRegression
```

```
from sklearn.neighbors import KNeighborsRegressor
import itertools as it
import time as time

from skopt import BayesSearchCV
from skopt.space import Real, Categorical, Integer
from skopt.plots import plot_objective, plot_histogram, plot_convergence
import warnings
from IPython import display
```

```
#Using the same datasets as used for linear regression in STAT303-2,
#so that we can compare the non-linear models with linear regression
trainf = pd.read_csv('./Datasets/Car_features_train.csv')
trainp = pd.read_csv('./Datasets/Car_prices_train.csv')
testf = pd.read_csv('./Datasets/Car_features_test.csv')
testp = pd.read_csv('./Datasets/Car_prices_test.csv')
train = pd.merge(trainf,trainp)
test = pd.merge(testf,testp)
train.head()
```

	carID	brand	model	year	transmission	mileage	fuelType	tax	mpg	engineSize	price
0	18473	bmw	6 Series	2020	Semi-Auto	11	Diesel	145	53.3282	3.0	37980
1	15064	bmw	6 Series	2019	Semi-Auto	10813	Diesel	145	53.0430	3.0	33980
2	18268	bmw	6 Series	2020	Semi-Auto	6	Diesel	145	53.4379	3.0	36850
3	18480	bmw	6 Series	2017	Semi-Auto	18895	Diesel	145	51.5140	3.0	25998
4	18492	bmw	6 Series	2015	Automatic	62953	Diesel	160	51.4903	3.0	18990

```
X = train[['mileage','mpg','year','engineSize']]
Xtest = test[['mileage','mpg','year','engineSize']]
y = train['price']
ytest = test['price']
```

11.2 Gradient boosting for regression

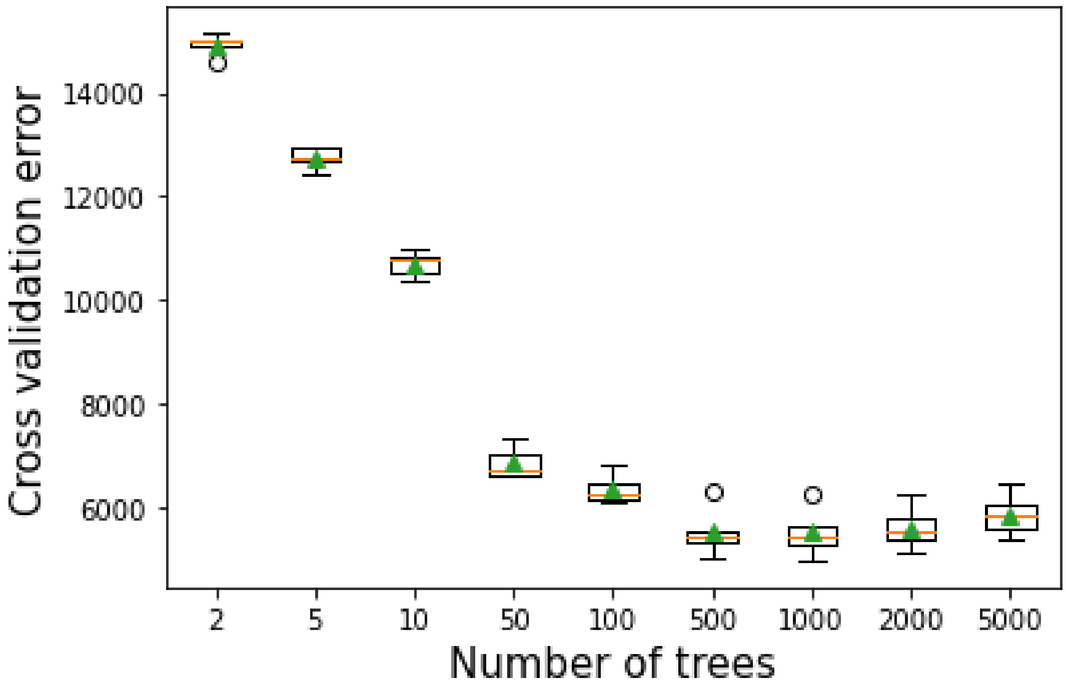
11.2.1 Number of trees vs cross validation error

As per the documentation, Gradient boosting is fairly robust *(as compared to AdaBoost)* to over-fitting (why?) so a large number usually results in better performance. Note that the number of trees still need to be tuned for optimal performance.

```
def get_models():
    models = dict()
    # define number of trees to consider
    n_trees = [2, 5, 10, 50, 100, 500, 1000, 2000, 5000]
    for n in n_trees:
        models[str(n)] = GradientBoostingRegressor(n_estimators=n,random_state=1,loss='huber
    return models

# evaluate a given model using cross-validation
def evaluate_model(model, X, y):
    # define the evaluation procedure
    cv = KFold(n_splits=5, shuffle=True, random_state=1)
    # evaluate the model and collect the results
    scores = np.sqrt(-cross_val_score(model, X, y, scoring='neg_mean_squared_error', cv=cv, n
    return scores

# get the models to evaluate
models = get_models()
# evaluate the models and store results
results, names = list(), list()
for name, model in models.items():
    # evaluate the model
    scores = evaluate_model(model, X, y)
    # store the results
    results.append(scores)
    names.append(name)
    # summarize the performance along the way
    print('>%s %.3f (%.3f)' % (name, np.mean(scores), np.std(scores)))
# plot model performance for comparison
plt.boxplot(results, labels=names, showmeans=True)
plt.ylabel('Cross validation error',fontsize=15)
plt.xlabel('Number of trees',fontsize=15)
```

```
>2 14927.566 (179.475)
>5 12743.148 (189.408)
>10 10704.199 (226.234)
>50 6869.066 (278.885)
>100 6354.656 (270.097)
>500 5515.622 (424.516)
>1000 5515.251 (427.767)
>2000 5600.041 (389.687)
>5000 5854.168 (362.223)
```

```
Text(0.5, 0, 'Number of trees')
```



11.2.2 Depth of tree vs cross validation error

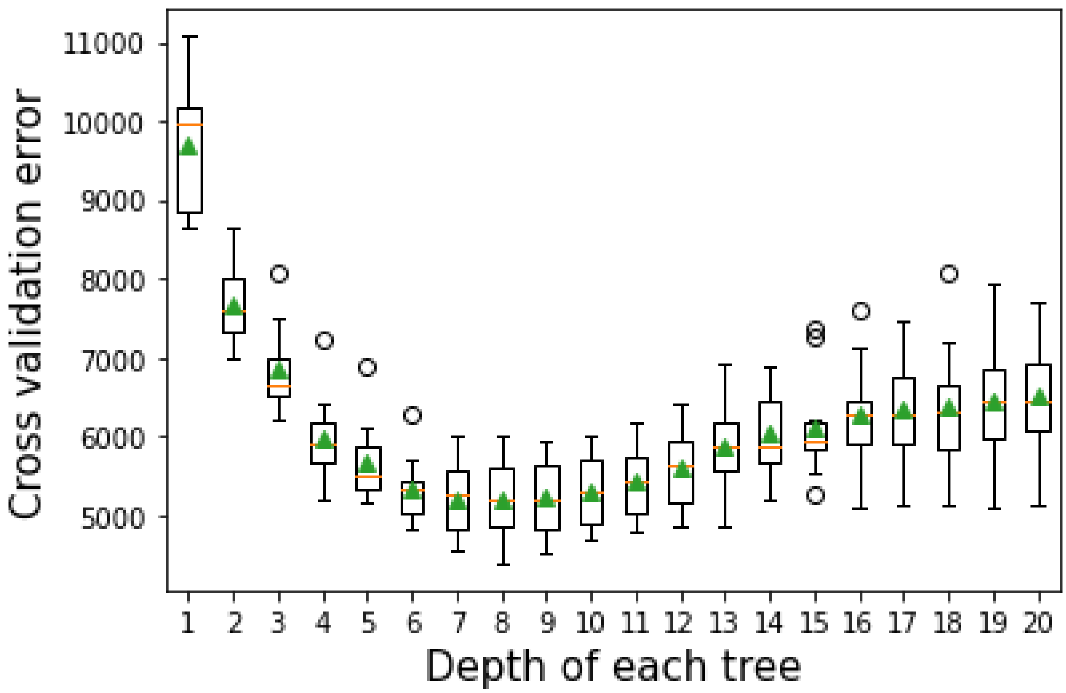
As the depth of each weak learner (decision tree) increases, the complexity of the weak learner will increase. As the complexity increases, the prediction bias will decrease, while the prediction variance will increase. Thus, there will be an optimal depth of each weak learner that minimizes the prediction error.

```
# get a list of models to evaluate
def get_models():
    models = dict()
    # explore depths from 1 to 10
    for i in range(1,21):
        # define ensemble model
        models[str(i)] = GradientBoostingRegressor(n_estimators=50,random_state=1,max_depth=
    return models

# evaluate a given model using cross-validation
def evaluate_model(model, X, y):
    # define the evaluation procedure
```

```
    cv = KFold(n_splits=10, shuffle=True, random_state=1)
    # evaluate the model and collect the results
    scores = np.sqrt(-cross_val_score(model, X, y, scoring='neg_mean_squared_error', cv=cv, n
    return scores

# get the models to evaluate
models = get_models()
# evaluate the models and store results
results, names = list(), list()
for name, model in models.items():
    # evaluate the model
    scores = evaluate_model(model, X, y)
    # store the results
    results.append(scores)
    names.append(name)
    # summarize the performance along the way
    print('>%s %.3f (%.3f)' % (name, np.mean(scores), np.std(scores)))
plt.boxplot(results, labels=names, showmeans=True)
plt.ylabel('Cross validation error',fontsize=15)
plt.xlabel('Depth of each tree',fontsize=15)
```

```
>1 9693.731 (810.090)
>2 7682.569 (489.841)
>3 6844.225 (536.792)
>4 5972.203 (538.693)
>5 5664.563 (497.882)
>6 5329.130 (404.330)
>7 5210.934 (461.038)
>8 5197.204 (494.957)
>9 5227.975 (478.789)
>10 5299.782 (446.509)
>11 5433.822 (451.673)
>12 5617.946 (509.797)
>13 5876.424 (542.981)
>14 6030.507 (560.447)
>15 6125.914 (643.852)
>16 6294.784 (672.646)
>17 6342.327 (677.050)
>18 6372.418 (791.068)
>19 6456.471 (741.693)
>20 6503.622 (759.193)
```

```
Text(0.5, 0, 'Depth of each tree')
```



11.2.3 Learning rate vs cross validation error

The optimal learning rate will depend on the number of trees, and vice-versa. If the learning rate is too low, it will take several trees to "learn" the response. If the learning rate is high, the response will be "learned" quickly (with fewer) trees. Learning too quickly will be prone to overfitting, while learning too slowly will be computationally expensive. Thus, there will be an optimal learning rate to minimize the prediction error.

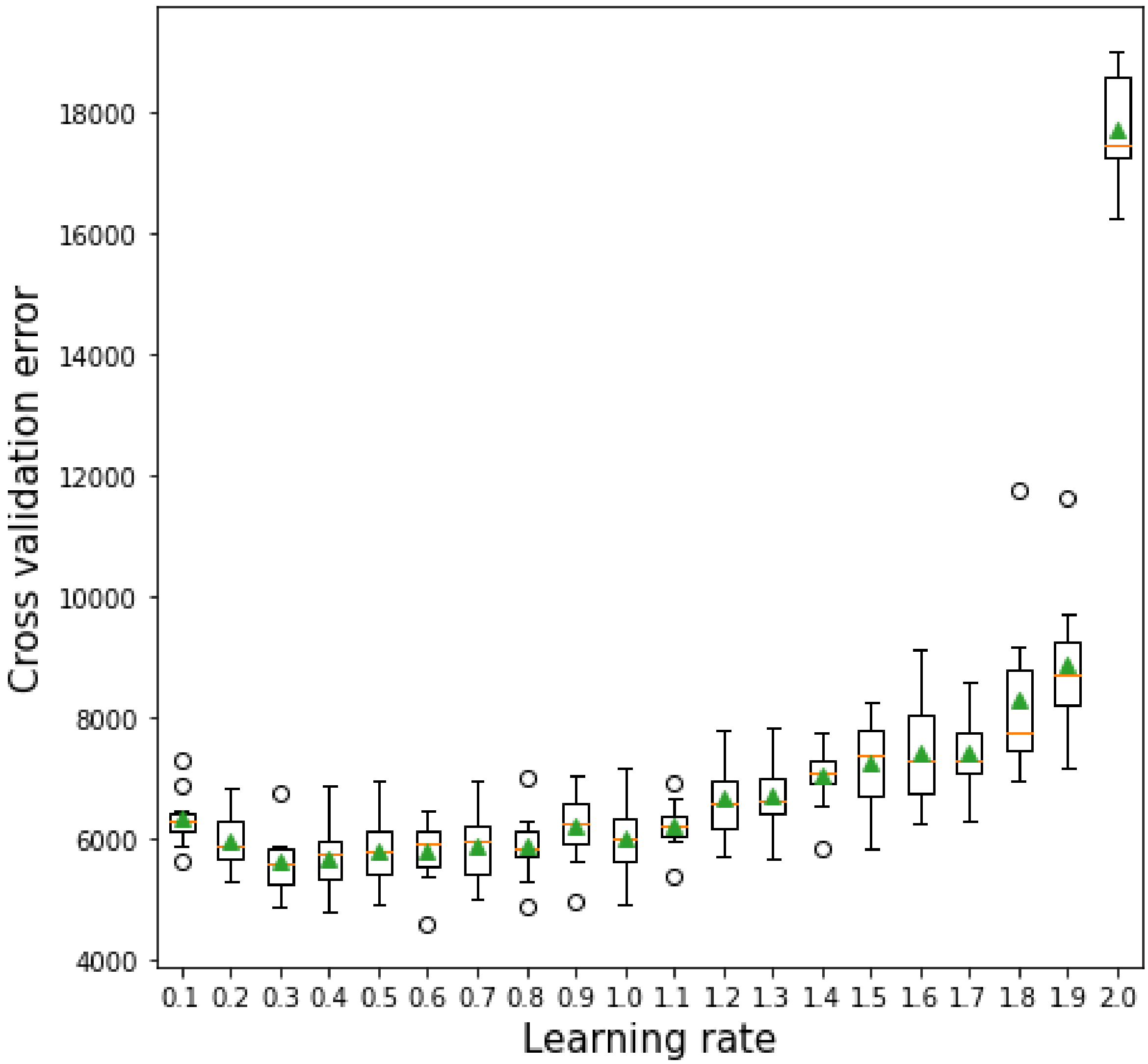
```
def get_models():
    models = dict()
    # explore learning rates from 0.1 to 2 in 0.1 increments
    for i in np.arange(0.1, 2.1, 0.1):
        key = '%.1f' % i
        models[key] = GradientBoostingRegressor(learning_rate=i,random_state=1,loss='huber')
    return models

# evaluate a given model using cross-validation
def evaluate_model(model, X, y):
```

```
    # define the evaluation procedure
    cv = KFold(n_splits=10, shuffle=True, random_state=1)
    # evaluate the model and collect the results
    scores = np.sqrt(-cross_val_score(model, X, y, scoring='neg_mean_squared_error', cv=cv, n
    return scores

# get the models to evaluate
models = get_models()
# evaluate the models and store results
results, names = list(), list()
for name, model in models.items():
    # evaluate the model
    scores = evaluate_model(model, X, y)
    # store the results
    results.append(scores)
    names.append(name)
    # summarize the performance along the way
    print('>%s %.1f (%.1f)' % (name, np.mean(scores), np.std(scores)))
# plot model performance for comparison
plt.figure(figsize=(7, 7))
plt.boxplot(results, labels=names, showmeans=True)
plt.ylabel('Cross validation error',fontsize=15)
plt.xlabel('Learning rate',fontsize=15)
```

```
>0.1 6329.8 (450.7)
>0.2 5942.9 (454.8)
>0.3 5618.4 (490.8)
>0.4 5665.9 (577.3)
>0.5 5783.5 (561.7)
>0.6 5773.8 (500.3)
>0.7 5875.5 (565.7)
>0.8 5878.5 (540.5)
>0.9 6214.4 (594.3)
>1.0 5986.1 (601.5)
>1.1 6216.5 (395.3)
>1.2 6667.5 (657.2)
>1.3 6717.4 (594.4)
>1.4 7048.4 (531.7)
>1.5 7265.0 (742.0)
>1.6 7404.4 (868.2)
>1.7 7425.8 (606.3)
>1.8 8283.0 (1345.3)
```

```
>1.9 8872.2 (1137.9)
>2.0 17713.3 (865.3)
```

```
Text(0.5, 0, 'Learning rate')
```

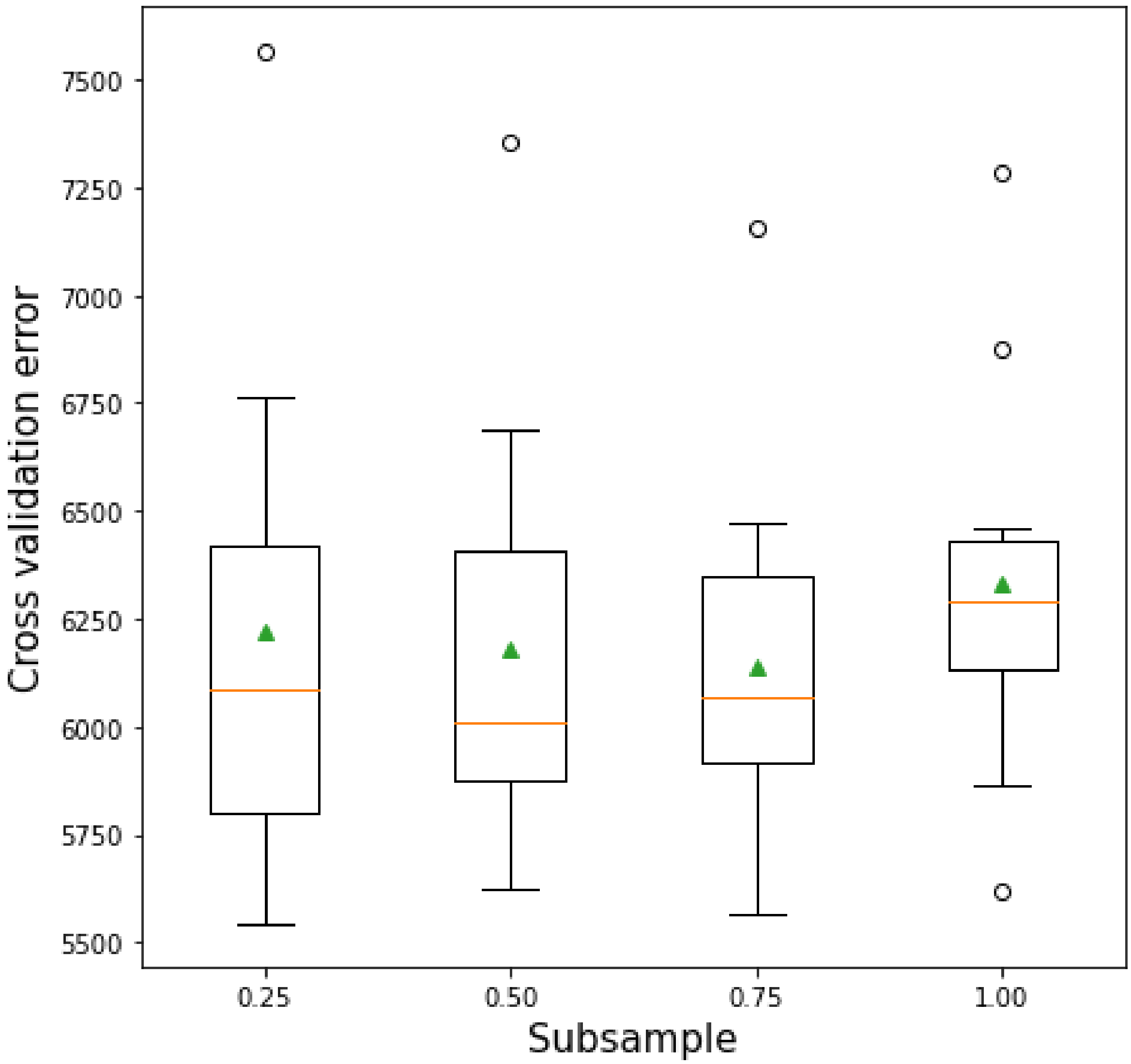


11.2.4 Subsampling vs cross validation error

```
def get_models():
    models = dict()
    # explore learning rates from 0.1 to 2 in 0.1 increments
    for s in np.arange(0.25, 1.1, 0.25):
        key = '%.2f' % s
        models[key] = GradientBoostingRegressor(random_state=1,subsample=s,loss='huber')
    return models

# evaluate a given model using cross-validation
def evaluate_model(model, X, y):
    # define the evaluation procedure
    cv = KFold(n_splits=10, shuffle=True, random_state=1)
    # evaluate the model and collect the results
    scores = np.sqrt(-cross_val_score(model, X, y, scoring='neg_mean_squared_error', cv=cv, n
    return scores

# get the models to evaluate
models = get_models()
# evaluate the models and store results
results, names = list(), list()
for name, model in models.items():
    # evaluate the model
    scores = evaluate_model(model, X, y)
    # store the results
    results.append(scores)
    names.append(name)
    # summarize the performance along the way
    print('>%s %.2f (%.2f)' % (name, np.mean(scores), np.std(scores)))
# plot model performance for comparison
plt.figure(figsize=(7, 7))
plt.boxplot(results, labels=names, showmeans=True)
plt.ylabel('Cross validation error',fontsize=15)
plt.xlabel('Subsample',fontsize=15)
```

```
>0.25 6219.59 (569.97)
>0.50 6178.28 (501.87)
>0.75 6141.96 (432.66)
>1.00 6329.79 (450.72)
```

```
Text(0.5, 0, 'Subsample')
```



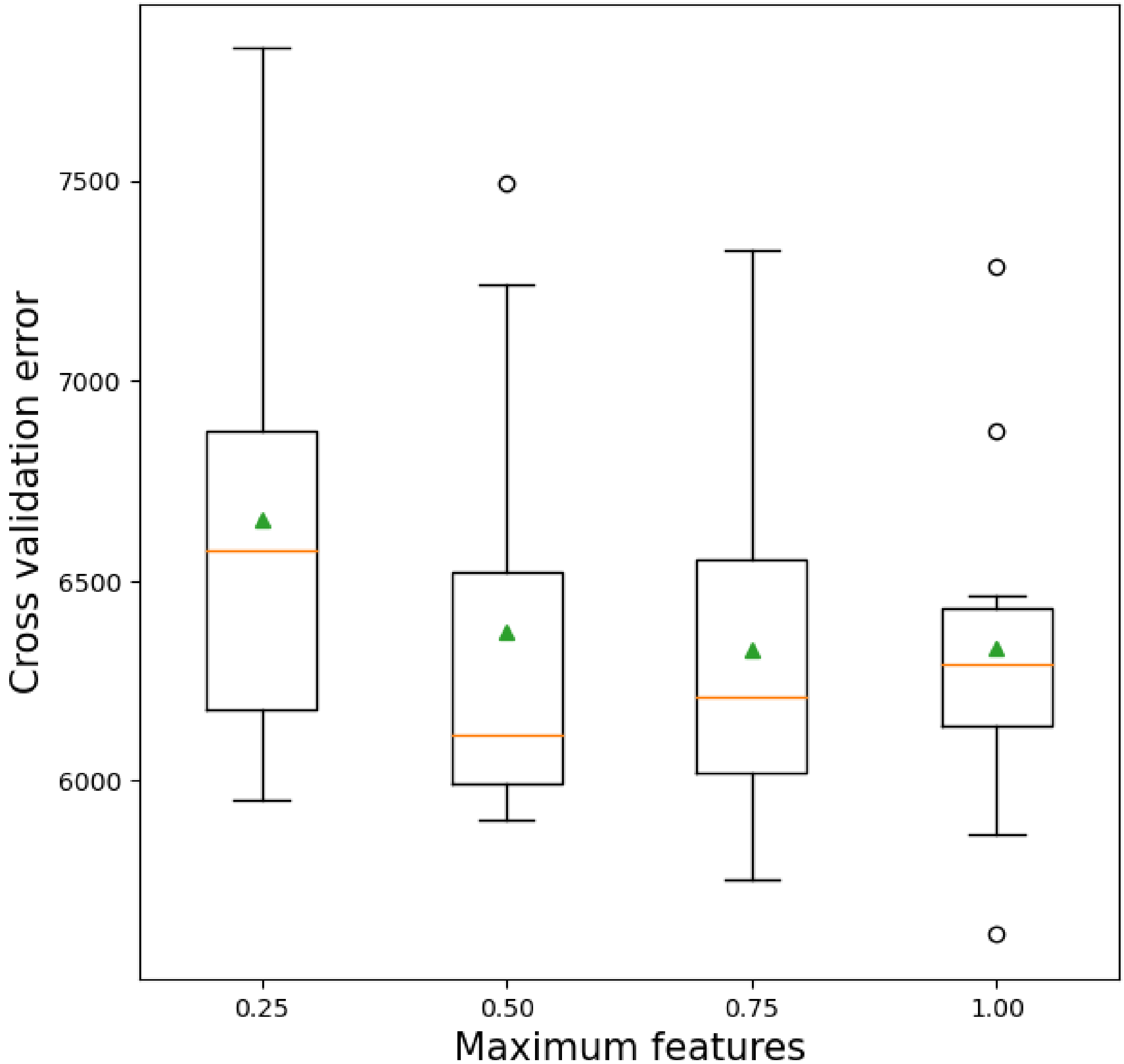
11.2.5 Maximum features vs cross-validation error

```
def get_models():
    models = dict()
    # explore learning rates from 0.1 to 2 in 0.1 increments
    for s in np.arange(0.25, 1.1, 0.25):
        key = '%.2f' % s
        models[key] = GradientBoostingRegressor(random_state=1,max_features=s,loss='huber')
    return models
```

```
# evaluate a given model using cross-validation
def evaluate_model(model, X, y):
    # define the evaluation procedure
    cv = KFold(n_splits=10, shuffle=True, random_state=1)
    # evaluate the model and collect the results
    scores = np.sqrt(-cross_val_score(model, X, y, scoring='neg_mean_squared_error', cv=cv, r
    return scores

# get the models to evaluate
models = get_models()
# evaluate the models and store results
results, names = list(), list()
for name, model in models.items():
    # evaluate the model
    scores = evaluate_model(model, X, y)
    # store the results
    results.append(scores)
    names.append(name)
    # summarize the performance along the way
    print('>%s %.2f (%.2f)' % (name, np.mean(scores), np.std(scores)))
# plot model performance for comparison
plt.figure(figsize=(7, 7))
plt.boxplot(results, labels=names, showmeans=True)
plt.ylabel('Cross validation error',fontsize=15)
plt.xlabel('Maximum features',fontsize=15)
```

```
>0.25 6654.27 (567.72)
>0.50 6373.92 (538.53)
>0.75 6325.55 (470.41)
>1.00 6329.79 (450.72)
```

```
Text(0.5, 0, 'Maximum features')
```



11.2.6 Tuning Gradient boosting for regression

As the optimal value of the parameters depend on each other, we need to optimize them simultaneously.

```
start_time = time.time()
model = GradientBoostingRegressor(random_state=1,loss='huber')
grid = dict()
grid['n_estimators'] = [10, 50, 100,200,500]
```

```
grid['learning_rate'] = [0.0001, 0.001, 0.01,0.1, 1.0]
grid['max_depth'] = [3,5,8,10,12,15]

# define the evaluation procedure
cv = KFold(n_splits=5, shuffle=True, random_state=1)
# define the grid search procedure
grid_search = GridSearchCV(estimator=model, param_grid=grid, n_jobs=-1, cv=cv, scoring='neg_r
                          verbose = True)
# execute the grid search
grid_result = grid_search.fit(X, y)
# summarize the best score and configuration
print("Best: %f using %s" % (np.sqrt(-grid_result.best_score_), grid_result.best_params_))
# summarize all scores that were evaluated
means = grid_result.cv_results_['mean_test_score']
stds = grid_result.cv_results_['std_test_score']
params = grid_result.cv_results_['params']
#for mean, stdev, param in zip(means, stds, params):
#    print("%f (%f) with: %r" % (mean, stdev, param)
print("Time taken = ",(time.time()-start_time)/60," minutes")
```

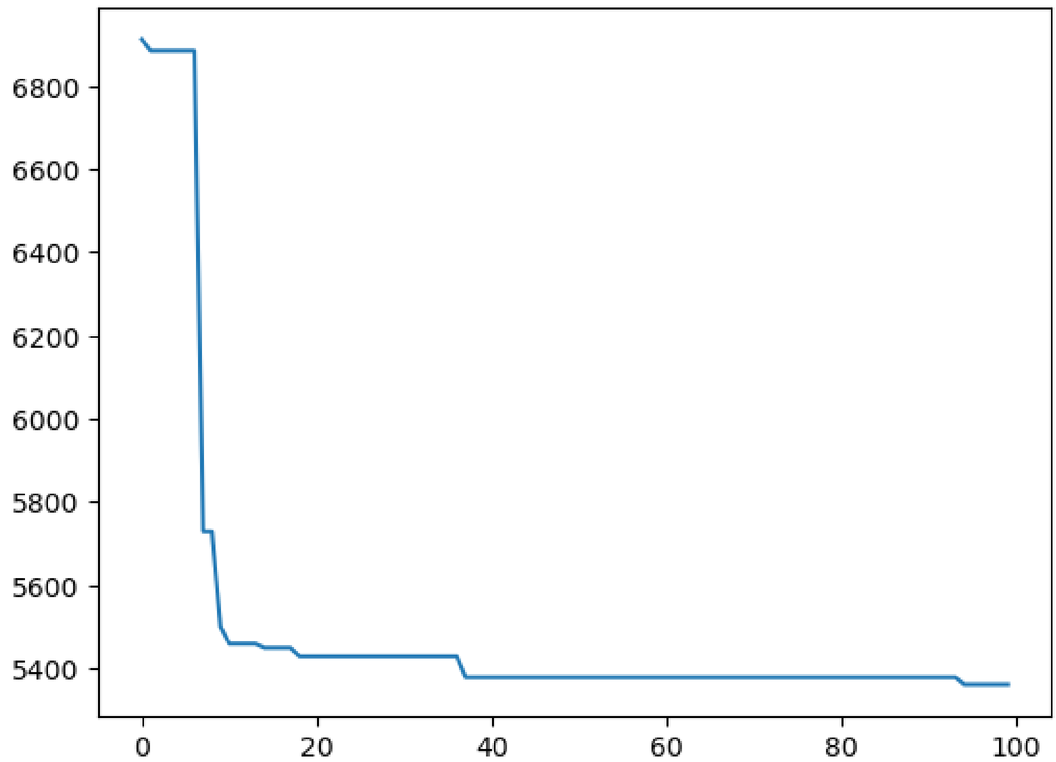
```
Best: 5190.765919 using {'learning_rate': 0.1, 'max_depth': 8, 'n_estimators': 100}
Time taken =  46.925597019990285  minutes
```

Note that the code takes 46 minutes to run. In case of a lot of hyperparameters, RandomizedSearchCV may be preferred to trade-off between optimality of the solution and computational cost.

```
model = GradientBoostingRegressor(random_state=1, loss='huber')
grid = dict()
grid['n_estimators'] = Integer(2, 1000)
grid['learning_rate'] = Real(0.0001, 1.0)
grid['max_leaf_nodes'] = Integer(4, 5000)
grid['subsample'] = Real(0.1, 1)
grid['max_features'] = Real(0.1, 1)

kfold = KFold(n_splits = 5, shuffle = True, random_state = 1)
gcv = BayesSearchCV(model, search_spaces = grid, cv = kfold, n_iter = 100, random_state = 1,
                         scoring = 'neg_root_mean_squared_error', n_jobs = -1)
paras = list(gcv.search_spaces.keys())
paras.sort()
start_time = time.time()
```

```
def monitor(optim_result):
    cv_values = pd.Series(optim_result['func_vals']).cummin()
    display.clear_output(wait = True)
    min_ind = pd.Series(optim_result['func_vals']).argmin()
    print(paras, "=", optim_result['x_iters'][min_ind], pd.Series(optim_result['func_vals'])
    print("Time so far = ", np.round((time.time()-start_time)/60), "minutes")
    sns.lineplot(cv_values)
    plt.show()
gcv.fit(X, y, callback = monitor)
```

```
['learning_rate', 'max_features', 'max_leaf_nodes', 'n_estimators', 'subsample'] = [0.2310208
Time so far =  21.0 minutes
```




```
BayesSearchCV(cv=KFold(n_splits=5, random_state=1, shuffle=True),
              estimator=GradientBoostingRegressor(loss='huber', random_state=1),
              n_iter=100, n_jobs=-1, random_state=1,
              scoring='neg_root_mean_squared_error',
              search_spaces={'learning_rate': Real(low=0.0001, high=1.0, prior='uniform', tra
```

```
                              'max_features': Real(low=0.1, high=1, prior='uniform', transfor
                              'max_leaf_nodes': Integer(low=4, high=5000, prior='uniform', tra
                              'n_estimators': Integer(low=2, high=1000, prior='uniform', trans
                              'subsample': Real(low=0.1, high=1, prior='uniform', transform='
```

```
#Model based on the optimal parameters
model = GradientBoostingRegressor(max_depth=8,n_estimators=100,learning_rate=0.1,
                         random_state=1,loss='huber').fit(X,y)
```

```
#RMSE of the optimized model on test data
print("Gradient boost RMSE = ",np.sqrt(mean_squared_error(model.predict(Xtest),ytest)))
```

```
Gradient boost RMSE =  5405.787029062213
```

```
#Model based on the optimal parameters
model_bayes = GradientBoostingRegressor(max_leaf_nodes=5000,n_estimators=817,learning_rate=0
                         random_state=1,subsample=1.0,loss='huber').fit(X,y)
```

```
#RMSE of the optimized model on test data
print("Gradient boost RMSE = ",np.sqrt(mean_squared_error(model_bayes.predict(Xtest),ytest))
```

```
Gradient boost RMSE =  5734.200307094321
```

```
#Let us combine the Gradient boost model with other models
model2 = AdaBoostRegressor(base_estimator=DecisionTreeRegressor(max_depth=10),n_estimators=5
                         random_state=1).fit(X,y)
print("AdaBoost RMSE = ",np.sqrt(mean_squared_error(model2.predict(Xtest),ytest)))
model3 = RandomForestRegressor(n_estimators=300, random_state=1,
                        n_jobs=-1, max_features=2).fit(X, y)
print("Random Forest RMSE = ",np.sqrt(mean_squared_error(model3.predict(Xtest),ytest)))
```

```
AdaBoost RMSE =  5693.165811600585
Random Forest RMSE =  5642.45839697972
```

```
#Ensemble model
pred1=model.predict(Xtest)#Gradient boost
pred2=model2.predict(Xtest)#Adaboost
pred3=model3.predict(Xtest)#Random forest
pred = 0.34*pred1+0.33*pred2+0.33*pred3 #Higher weight to the better model
print("Ensemble model RMSE = ", np.sqrt(mean_squared_error(pred,ytest)))
```

```
Ensemble model RMSE =  5364.478227748279
```

11.2.7 Ensemble modeling (for regression models)

```
#Ensemble model
pred1=model.predict(Xtest)#Gradient boost
pred2=model2.predict(Xtest)#Adaboost
pred3=model3.predict(Xtest)#Random forest
pred = 0.6*pred1+0.2*pred2+0.2*pred3 #Higher weight to the better model
print("Ensemble model RMSE = ", np.sqrt(mean_squared_error(pred,ytest)))
```

```
Ensemble model RMSE =  5323.119083375402
```

Combined, the random forest model, gradient boost and the Adaboost model do better than each of the individual models.

Note that ideally we should do K-fold cross validation to figure out the optimal weights. We'll learn about ensembling techniques later in the course.

11.3 Gradient boosting for classification

Below is the Gradient boost implementation on a classification problem. The takeaways are the same as that of the regression problem above.

```
train = pd.read_csv('./Datasets/diabetes_train.csv')
test = pd.read_csv('./Datasets/diabetes_test.csv')
```

```
X = train.drop(columns = 'Outcome')
Xtest = test.drop(columns = 'Outcome')
y = train['Outcome']
ytest = test['Outcome']
```

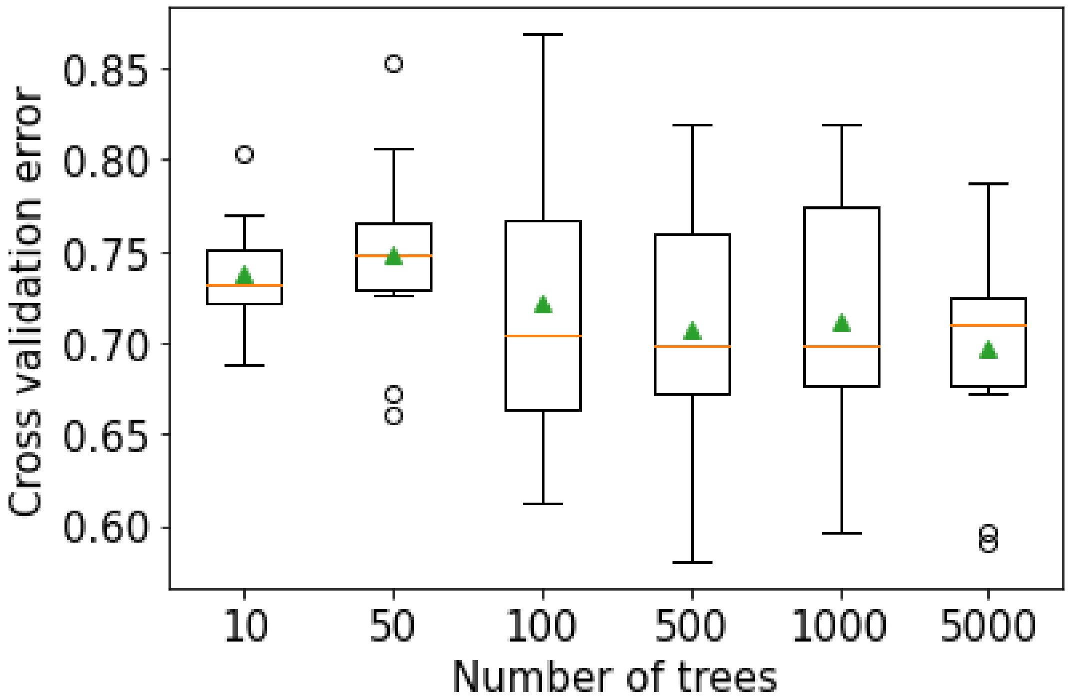
11.3.1 Number of trees vs cross validation accuracy

```
def get_models():
    models = dict()
    # define number of trees to consider
    n_trees = [10, 50, 100, 500, 1000, 5000]
    for n in n_trees:
```

```
        models[str(n)] = GradientBoostingClassifier(n_estimators=n,random_state=1)
    return models

# evaluate a given model using cross-validation
def evaluate_model(model, X, y):
    # define the evaluation procedure
    cv = StratifiedKFold(n_splits=10, shuffle=True, random_state=1)
    # evaluate the model and collect the results
    scores = cross_val_score(model, X, y, scoring='accuracy', cv=cv, n_jobs=-1)
    return scores

# get the models to evaluate
models = get_models()
# evaluate the models and store results
results, names = list(), list()
for name, model in models.items():
    # evaluate the model
    scores = evaluate_model(model, X, y)
    # store the results
    results.append(scores)
    names.append(name)
    # summarize the performance along the way
    print('>%s %.3f (%.3f)' % (name, np.mean(scores), np.std(scores)))
# plot model performance for comparison
plt.boxplot(results, labels=names, showmeans=True)
plt.ylabel('Cross validation error',fontsize=15)
plt.xlabel('Number of trees',fontsize=15)
```

```
>10 0.738 (0.031)
>50 0.748 (0.054)
>100 0.722 (0.075)
>500 0.707 (0.066)
>1000 0.712 (0.075)
>5000 0.697 (0.061)
```

```
Text(0.5, 0, 'Number of trees')
```



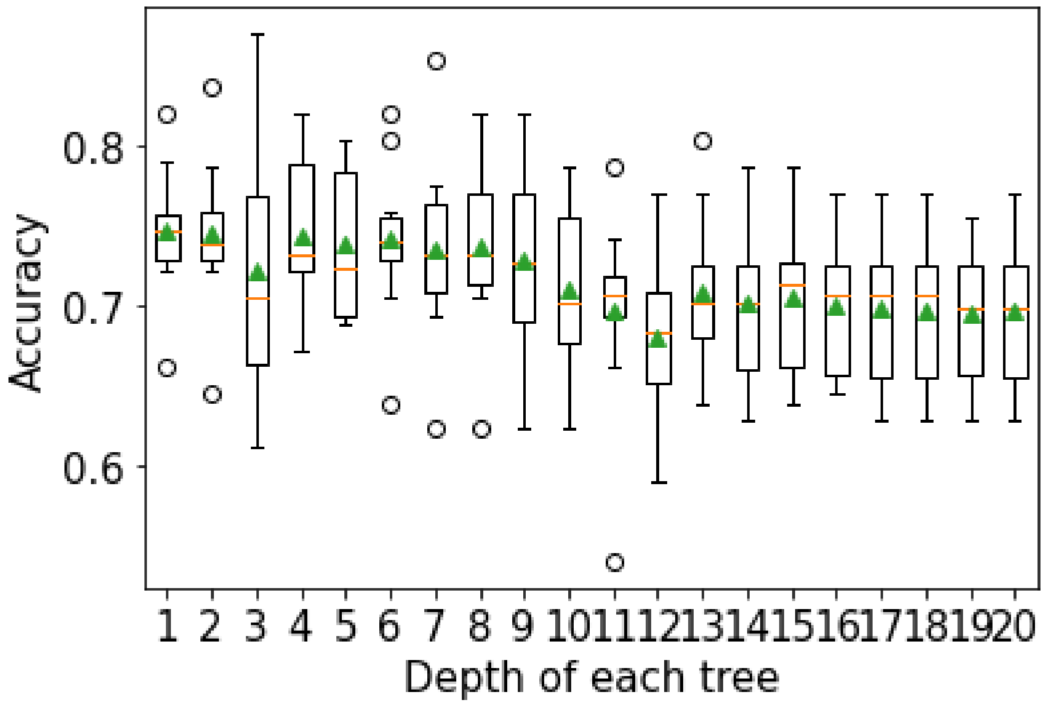
11.3.2 Depth of each tree vs cross validation accuracy

```
# get a list of models to evaluate
def get_models():
    models = dict()
    # explore depths from 1 to 10
    for i in range(1,21):
        # define ensemble model
        models[str(i)] = GradientBoostingClassifier(random_state=1,max_depth=i)
    return models

# evaluate a given model using cross-validation
def evaluate_model(model, X, y):
    # define the evaluation procedure
    cv = StratifiedKFold(n_splits=10, shuffle=True, random_state=1)
    # evaluate the model and collect the results
    scores = cross_val_score(model, X, y, scoring='accuracy', cv=cv, n_jobs=-1)
    return scores

# get the models to evaluate
```

```
models = get_models()
# evaluate the models and store results
results, names = list(), list()
for name, model in models.items():
    # evaluate the model
    scores = evaluate_model(model, X, y)
    # store the results
    results.append(scores)
    names.append(name)
    # summarize the performance along the way
    print('>%s %.3f (%.3f)' % (name, np.mean(scores), np.std(scores)))
plt.boxplot(results, labels=names, showmeans=True)
plt.ylabel('Accuracy',fontsize=15)
plt.xlabel('Depth of each tree',fontsize=15)
```

```
>1 0.746 (0.040)
>2 0.744 (0.046)
>3 0.722 (0.075)
>4 0.743 (0.049)
>5 0.738 (0.046)
>6 0.741 (0.047)
>7 0.735 (0.057)
>8 0.736 (0.051)
>9 0.728 (0.055)
>10 0.710 (0.050)
>11 0.697 (0.061)
>12 0.681 (0.056)
>13 0.709 (0.047)
>14 0.702 (0.048)
>15 0.705 (0.048)
>16 0.700 (0.042)
>17 0.699 (0.048)
>18 0.697 (0.050)
>19 0.696 (0.042)
>20 0.697 (0.048)
```

```
Text(0.5, 0, 'Depth of each tree')
```



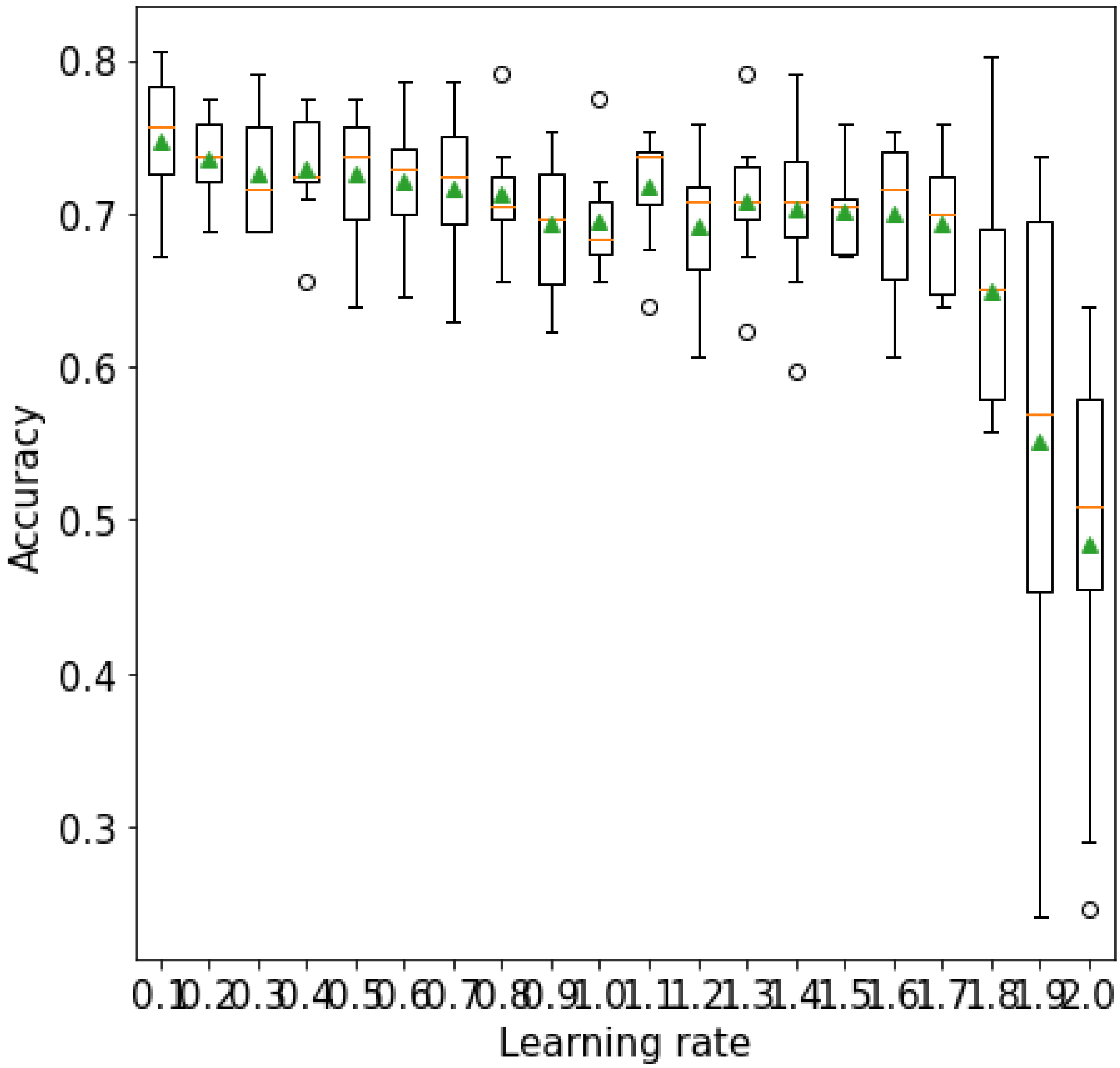
11.3.3 Learning rate vs cross validation accuracy

```
def get_models():
    models = dict()
    # explore learning rates from 0.1 to 2 in 0.1 increments
    for i in np.arange(0.1, 2.1, 0.1):
        key = '%.1f' % i
        models[key] = GradientBoostingClassifier(learning_rate=i,random_state=1)
    return models

# evaluate a given model using cross-validation
def evaluate_model(model, X, y):
    # define the evaluation procedure
    cv = KFold(n_splits=10, shuffle=True, random_state=1)
    # evaluate the model and collect the results
    scores = cross_val_score(model, X, y, scoring='accuracy', cv=cv, n_jobs=-1)
    return scores

# get the models to evaluate
models = get_models()
```

```
# evaluate the models and store results
results, names = list(), list()
for name, model in models.items():
    # evaluate the model
    scores = evaluate_model(model, X, y)
    # store the results
    results.append(scores)
    names.append(name)
    # summarize the performance along the way
    print('>%s %.3f (%.3f)' % (name, np.mean(scores), np.std(scores)))
# plot model performance for comparison
plt.figure(figsize=(7, 7))
plt.boxplot(results, labels=names, showmeans=True)
plt.ylabel('Accuracy',fontsize=15)
plt.xlabel('Learning rate',fontsize=15)
```

```
>0.1 0.747 (0.044)
>0.2 0.736 (0.028)
>0.3 0.726 (0.039)
>0.4 0.730 (0.034)
>0.5 0.726 (0.041)
>0.6 0.722 (0.043)
>0.7 0.717 (0.050)
>0.8 0.713 (0.033)
>0.9 0.694 (0.045)
>1.0 0.695 (0.032)
>1.1 0.718 (0.034)
>1.2 0.692 (0.045)
>1.3 0.708 (0.042)
>1.4 0.704 (0.050)
>1.5 0.702 (0.028)
>1.6 0.700 (0.050)
>1.7 0.694 (0.044)
>1.8 0.650 (0.075)
>1.9 0.551 (0.163)
>2.0 0.484 (0.123)
```

```
Text(0.5, 0, 'Learning rate')
```



11.3.4 Tuning Gradient boosting Classifier

```
start_time = time.time()
model = GradientBoostingClassifier(random_state=1)
grid = dict()
grid['n_estimators'] = [10, 50, 100,200,500]
grid['learning_rate'] = [0.0001, 0.001, 0.01,0.1, 1.0]
grid['max_depth'] = [1,2,3,4,5]
```

```
grid['subsample'] = [0.5,1.0]
# define the evaluation procedure
cv = StratifiedKFold(n_splits=5, shuffle=True, random_state=1)
# define the grid search procedure
grid_search = GridSearchCV(estimator=model, param_grid=grid, n_jobs=-1, cv=cv, verbose = True
# execute the grid search
grid_result = grid_search.fit(X, y)
# summarize the best score and configuration
print("Best: %f using %s" % (grid_result.best_score_, grid_result.best_params_))
print("Time taken = ", time.time() - start_time, "seconds")
```

```
Fitting 5 folds for each of 250 candidates, totalling 1250 fits
Best: 0.701045 using {'learning_rate': 1.0, 'max_depth': 3, 'n_estimators': 200, 'subsample'
Time taken =  32.46394085884094
```

```
#Model based on the optimal parameters
model = GradientBoostingClassifier(random_state=1,max_depth=3,learning_rate=0.1,subsample=0.5
                          n_estimators=200).fit(X,y)

# Note that we are using the cross-validated predicted probabilities, instead of directly usi
# predicted probabilities on train data, as the model may be overfitting on the train data, a
# may lead to misleading results
cross_val_ypred = cross_val_predict(GradientBoostingClassifier(random_state=1,max_depth=3,
                                                              learning_rate=0.1,subsample=0
                          n_estimators=200), X, y, cv = 5, method = 'predict_proba')

p, r, thresholds = precision_recall_curve(y, cross_val_ypred[:,1])
def plot_precision_recall_vs_threshold(precisions, recalls, thresholds):
    plt.figure(figsize=(8, 8))
    plt.title("Precision and Recall Scores as a function of the decision threshold")
    plt.plot(thresholds, precisions[:-1], "b--", label="Precision")
    plt.plot(thresholds, recalls[:-1], "g-", label="Recall")
    plt.plot(thresholds, precisions[:-1], "o", color = 'blue')
    plt.plot(thresholds, recalls[:-1], "o", color = 'green')
    plt.ylabel("Score")
    plt.xlabel("Decision Threshold")
    plt.legend(loc='best')
    plt.legend()
plot_precision_recall_vs_threshold(p, r, thresholds)
```


```
# Thresholds with precision and recall
all_thresholds = np.concatenate([thresholds.reshape(-1,1), p[:-1].reshape(-1,1), r[:-1].resha
recall_more_than_80 = all_thresholds[all_thresholds[:,2]>0.8,:]
# As the values in 'recall_more_than_80' are arranged in decreasing order of recall and incre
# the last value will provide the maximum threshold probability for the recall to be more tha
# We wish to find the maximum threshold probability to obtain the maximum possible precision
recall_more_than_80[recall_more_than_80.shape[0]-1]
```

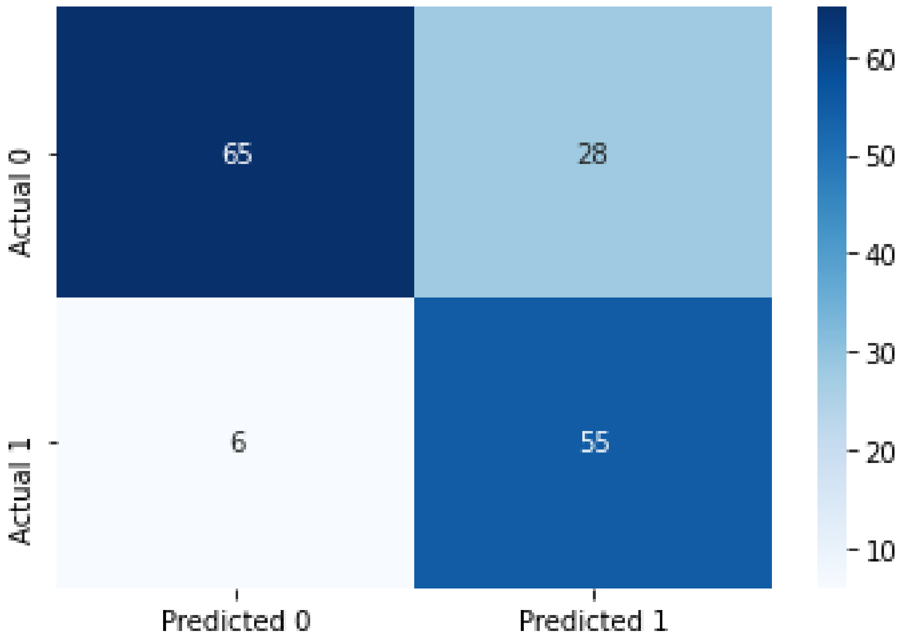
```
array([0.18497144, 0.53205128, 0.80193237])
```

```
#Optimal decision threshold probability
thres = recall_more_than_80[recall_more_than_80.shape[0]-1][0]
thres
```

```
0.18497143500912738
```

```
# Performance metrics computation for the optimum decision threshold probability
desired_threshold = thres

y_pred_prob = model.predict_proba(Xtest)[:,1]

# Classifying observations in the positive class (y = 1) if the predicted probability is grea
# than the desired decision threshold probability
y_pred = y_pred_prob > desired_threshold
y_pred = y_pred.astype(int)

#Computing the accuracy
print("Accuracy: ",accuracy_score(y_pred, ytest)*100)

#Computing the ROC-AUC
fpr, tpr, auc_thresholds = roc_curve(ytest, y_pred_prob)
print("ROC-AUC: ",auc(fpr, tpr))# AUC of ROC

#Computing the precision and recall
print("Precision: ", precision_score(ytest, y_pred))
print("Recall: ", recall_score(ytest, y_pred))

#Confusion matrix
cm = pd.DataFrame(confusion_matrix(ytest, y_pred),
                  columns=['Predicted 0', 'Predicted 1'], index = ['Actual 0', 'Actual 1'])
sns.heatmap(cm, annot=True, cmap='Blues', fmt='g');
```

```
Accuracy:  77.92207792207793
ROC-AUC:  0.8704389212057112
Precision:  0.6626506024096386
Recall:  0.9016393442622951
```



The model seems to be similar to the Adaboost model. However, gradient boosting algorithms with robust loss functions can perform better than Adaboost in the presence of outliers *(in terms of response)* in the data.

11.4 Faster algorithms and tuning tips

Check out `HistGradientBoostingRegressor()` and `HistGradientBoostingClassifier()` for a faster gradient boosting algorithm for big datasets *(more than 10,000 observations)*.

Check out tips for faster hyperparameter tuning, such as tuning `max_leaf_nodes` instead of `max_depth` here.

12 XGBoost

XGBoost is a very recently developed algorithm (2016). Thus, it's not yet there in standard textbooks. Here are some resources for it.

Documentation

Slides

Reference paper

Video by author (Tianqi Chen)

Video by StatQuest

12.1 Hyperparameters

The following are some of the important hyperparameters to tune in XGBoost:

1. Number of trees (`n_estimators`)
2. Depth of each tree (`max_depth`)
3. Learning rate (`learning_rate`)
4. Sampling observations / predictors (`subsample` for observations, `colsample_bytree` for predictors)
5. Regularization parameters (`reg_lambda` & `gamma`)

However, there are other hyperparameters that can be tuned as well. Check out the list of all hyperparameters in the XGBoost documentation.

```
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.metrics import mean_squared_error
from sklearn.model_selection import cross_val_score,train_test_split, KFold, cross_val_predi
from sklearn.metrics import mean_squared_error,r2_score,roc_curve,auc,precision_recall_curve
```

```
recall_score, precision_score, confusion_matrix
from sklearn.tree import DecisionTreeRegressor,DecisionTreeClassifier
from sklearn.model_selection import GridSearchCV, ParameterGrid, StratifiedKFold, RandomizedS
from sklearn.ensemble import VotingRegressor, VotingClassifier, StackingRegressor, StackingCl
from sklearn.linear_model import LinearRegression,LogisticRegression, LassoCV, RidgeCV, Elas
from sklearn.neighbors import KNeighborsRegressor
import itertools as it
import time as time
import xgboost as xgb
from skopt import BayesSearchCV
from skopt.space import Real, Categorical, Integer
from skopt.plots import plot_objective, plot_histogram, plot_convergence
import warnings
from IPython import display
```

```
#Using the same datasets as used for linear regression in STAT303-2,
#so that we can compare the non-linear models with linear regression
trainf = pd.read_csv('./Datasets/Car_features_train.csv')
trainp = pd.read_csv('./Datasets/Car_prices_train.csv')
testf = pd.read_csv('./Datasets/Car_features_test.csv')
testp = pd.read_csv('./Datasets/Car_prices_test.csv')
train = pd.merge(trainf,trainp)
test = pd.merge(testf,testp)
train.head()
```

	carID	brand	model	year	transmission	mileage	fuelType	tax	mpg	engineSize	price
0	18473	bmw	6 Series	2020	Semi-Auto	11	Diesel	145	53.3282	3.0	37980
1	15064	bmw	6 Series	2019	Semi-Auto	10813	Diesel	145	53.0430	3.0	33980
2	18268	bmw	6 Series	2020	Semi-Auto	6	Diesel	145	53.4379	3.0	36850
3	18480	bmw	6 Series	2017	Semi-Auto	18895	Diesel	145	51.5140	3.0	25998
4	18492	bmw	6 Series	2015	Automatic	62953	Diesel	160	51.4903	3.0	18990

```
X = train[['mileage','mpg','year','engineSize']]
Xtest = test[['mileage','mpg','year','engineSize']]
y = train['price']
ytest = test['price']
```

12.2 XGBoost for regression

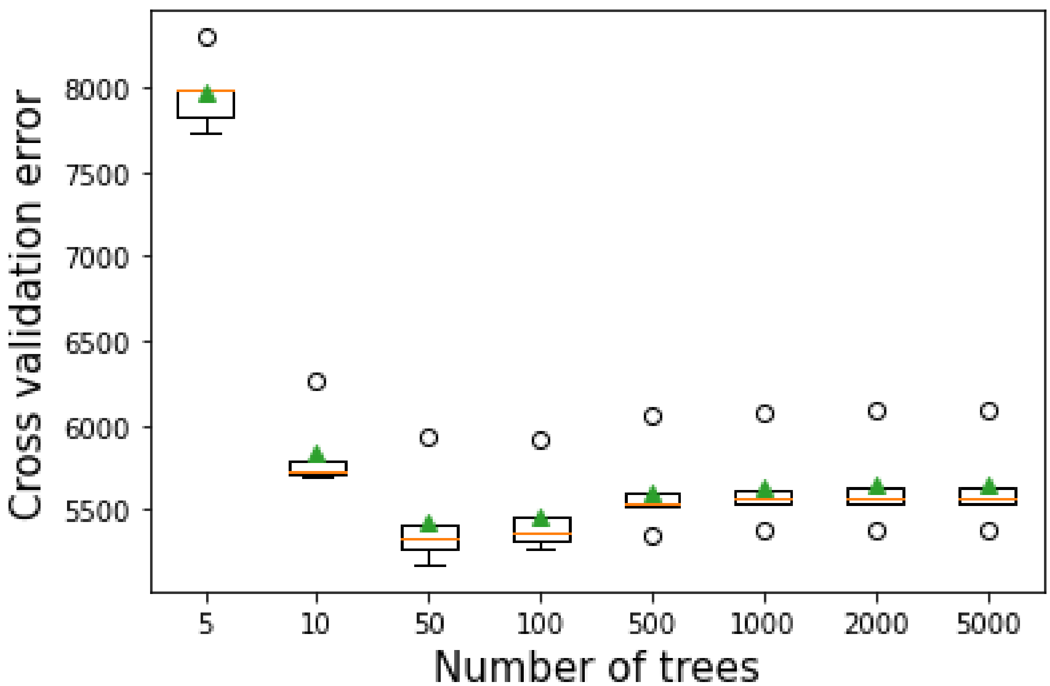
12.2.1 Number of trees vs cross validation error

As the number of trees increase, the prediction bias will decrease. Like gradient boosting is relatively robust *(as compared to AdaBoost)* to over-fitting (why?) so a large number usually results in better performance. Note that the number of trees still need to be tuned for optimal performance.

```
def get_models():
    models = dict()
    # define number of trees to consider
    n_trees = [5, 10, 50, 100, 500, 1000, 2000, 5000]
    for n in n_trees:
        models[str(n)] = xgb.XGBRegressor(n_estimators=n,random_state=1)
    return models

# evaluate a given model using cross-validation
def evaluate_model(model, X, y):
    # define the evaluation procedure
    cv = KFold(n_splits=5, shuffle=True, random_state=1)
    # evaluate the model and collect the results
    scores = np.sqrt(-cross_val_score(model, X, y, scoring='neg_mean_squared_error', cv=cv, n
    return scores

# get the models to evaluate
models = get_models()
# evaluate the models and store results
results, names = list(), list()
for name, model in models.items():
    # evaluate the model
    scores = evaluate_model(model, X, y)
    # store the results
    results.append(scores)
    names.append(name)
    # summarize the performance along the way
    print('>%s %.3f (%.3f)' % (name, np.mean(scores), np.std(scores)))
# plot model performance for comparison
plt.boxplot(results, labels=names, showmeans=True)
plt.ylabel('Cross validation error',fontsize=15)
plt.xlabel('Number of trees',fontsize=15)
```

```
>5 7961.485 (192.906)
>10 5837.134 (217.986)
>50 5424.788 (263.890)
>100 5465.396 (237.938)
>500 5608.350 (235.903)
>1000 5635.159 (236.664)
>2000 5642.669 (236.192)
>5000 5643.411 (236.074)
```

```
Text(0.5, 0, 'Number of trees')
```



12.2.2 Depth of tree vs cross validation error

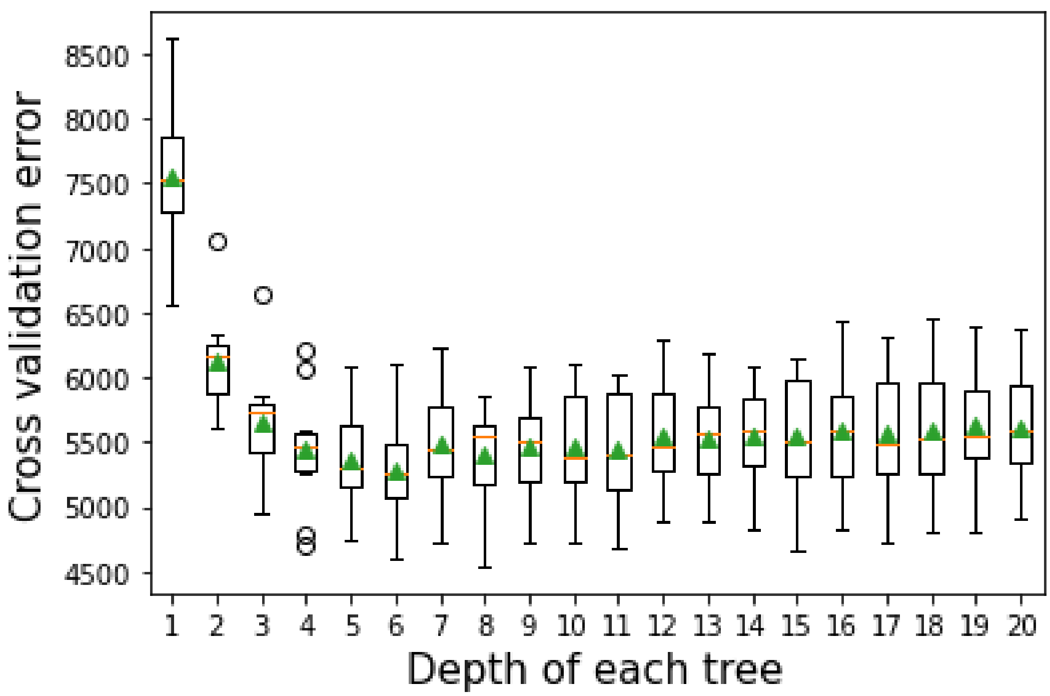
As the depth of each weak learner (decision tree) increases, the complexity of the weak learner will increase. As the complexity increases, the prediction bias will decrease, while the prediction variance will increase. Thus, there will be an optimal depth of each weak learner that minimizes the prediction error.

```
# get a list of models to evaluate
def get_models():
    models = dict()
    # explore depths from 1 to 10
    for i in range(1,21):
        # define ensemble model
        models[str(i)] = xgb.XGBRegressor(random_state=1,max_depth=i)
    return models

# evaluate a given model using cross-validation
def evaluate_model(model, X, y):
    # define the evaluation procedure
    cv = KFold(n_splits=10, shuffle=True, random_state=1)
    # evaluate the model and collect the results
    scores = np.sqrt(-cross_val_score(model, X, y, scoring='neg_mean_squared_error', cv=cv, r
    return scores

# get the models to evaluate
models = get_models()
# evaluate the models and store results
results, names = list(), list()
for name, model in models.items():
    # evaluate the model
    scores = evaluate_model(model, X, y)
    # store the results
    results.append(scores)
    names.append(name)
    # summarize the performance along the way
    print('>%s %.3f (%.3f)' % (name, np.mean(scores), np.std(scores)))
plt.boxplot(results, labels=names, showmeans=True)
plt.ylabel('Cross validation error',fontsize=15)
plt.xlabel('Depth of each tree',fontsize=15)
```

```
>1 7541.827 (545.951)
>2 6129.425 (393.357)
>3 5647.783 (454.318)
>4 5438.481 (453.726)
>5 5358.074 (379.431)
>6 5281.675 (383.848)
>7 5495.163 (459.356)
>8 5399.145 (380.437)
>9 5469.563 (384.004)
```

```
>10 5461.549 (416.630)
>11 5443.210 (432.863)
>12 5546.447 (412.097)
>13 5532.414 (369.131)
>14 5556.761 (362.746)
>15 5540.366 (452.612)
>16 5586.004 (451.199)
>17 5563.137 (464.344)
>18 5594.919 (480.221)
>19 5641.226 (451.713)
>20 5616.462 (417.405)
```

```
Text(0.5, 0, 'Depth of each tree')
```



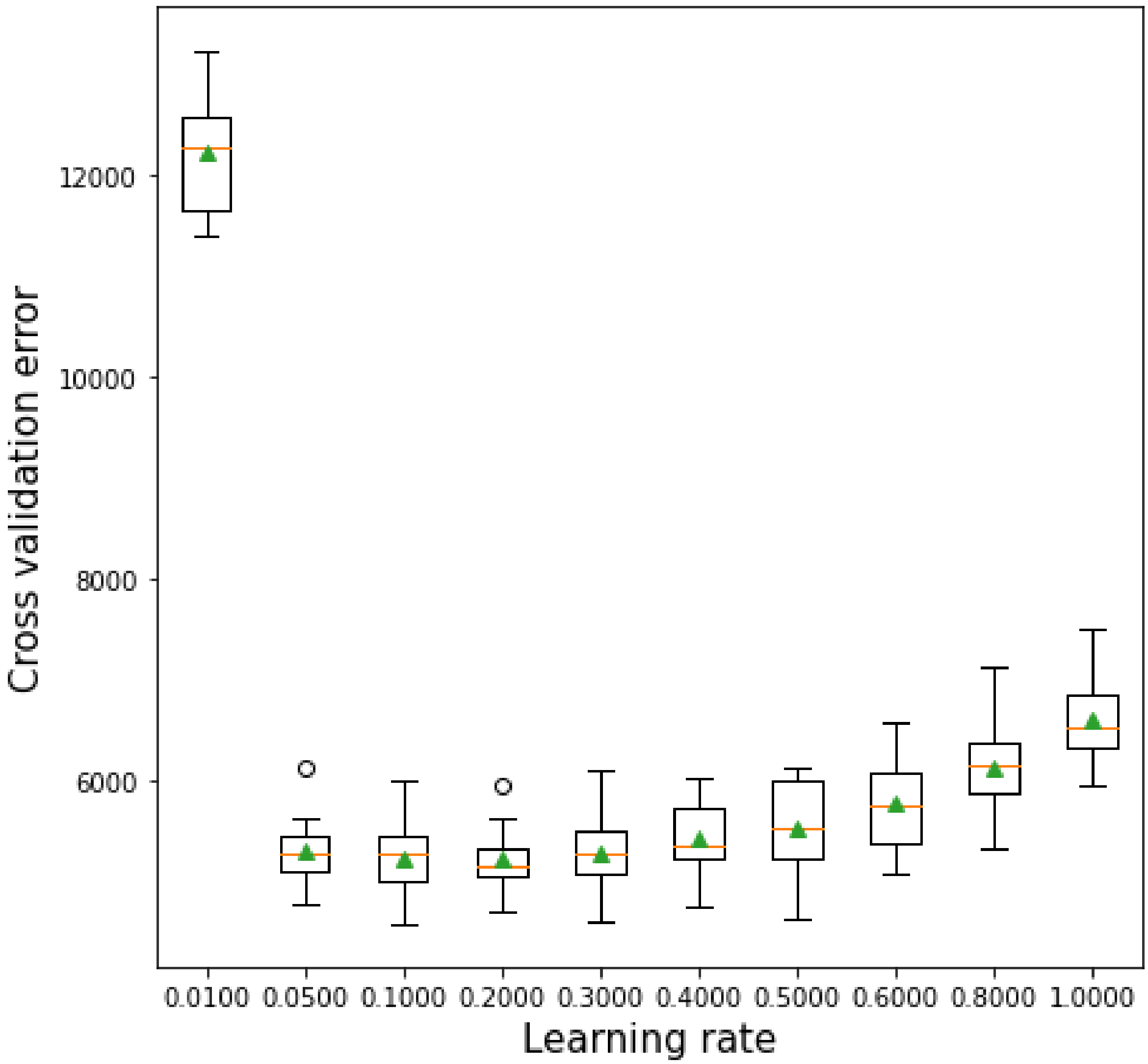
12.2.3 Learning rate vs cross validation error

The optimal learning rate will depend on the number of trees, and vice-versa. If the learning rate is too low, it will take several trees to "learn" the response. If the learning rate is high, the response will be "learned" quickly (with fewer) trees. Learning too quickly will be prone to overfitting, while learning too slowly will be computationally expensive. Thus, there will be an optimal learning rate to minimize the prediction error.

```
def get_models():
    models = dict()
    # explore learning rates from 0.1 to 2 in 0.1 increments
    for i in [0.01,0.05,0.1,0.2,0.3,0.4,0.5,0.6,0.8,1.0]:
        key = '%.4f' % i
        models[key] = xgb.XGBRegressor(learning_rate=i,random_state=1)
    return models

# evaluate a given model using cross-validation
def evaluate_model(model, X, y):
    # define the evaluation procedure
    cv = KFold(n_splits=10, shuffle=True, random_state=1)
    # evaluate the model and collect the results
    scores = np.sqrt(-cross_val_score(model, X, y, scoring='neg_mean_squared_error', cv=cv, r
    return scores

# get the models to evaluate
models = get_models()
# evaluate the models and store results
results, names = list(), list()
for name, model in models.items():
    # evaluate the model
    scores = evaluate_model(model, X, y)
    # store the results
    results.append(scores)
    names.append(name)
    # summarize the performance along the way
    print('>%s %.1f (%.1f)' % (name, np.mean(scores), np.std(scores)))
# plot model performance for comparison
plt.figure(figsize=(7, 7))
plt.boxplot(results, labels=names, showmeans=True)
plt.ylabel('Cross validation error',fontsize=15)
plt.xlabel('Learning rate',fontsize=15)
```

```
>0.0100 12223.8 (636.7)
>0.0500 5298.5 (383.5)
>0.1000 5236.3 (397.5)
>0.2000 5221.5 (347.5)
>0.3000 5281.7 (383.8)
>0.4000 5434.1 (364.6)
>0.5000 5537.0 (471.9)
>0.6000 5767.4 (478.5)
```

```
>0.8000 6132.7 (472.5)
>1.0000 6593.6 (408.9)

Text(0.5, 0, 'Learning rate')
```



12.2.4 Regularization (`reg_lambda`) vs cross validation error

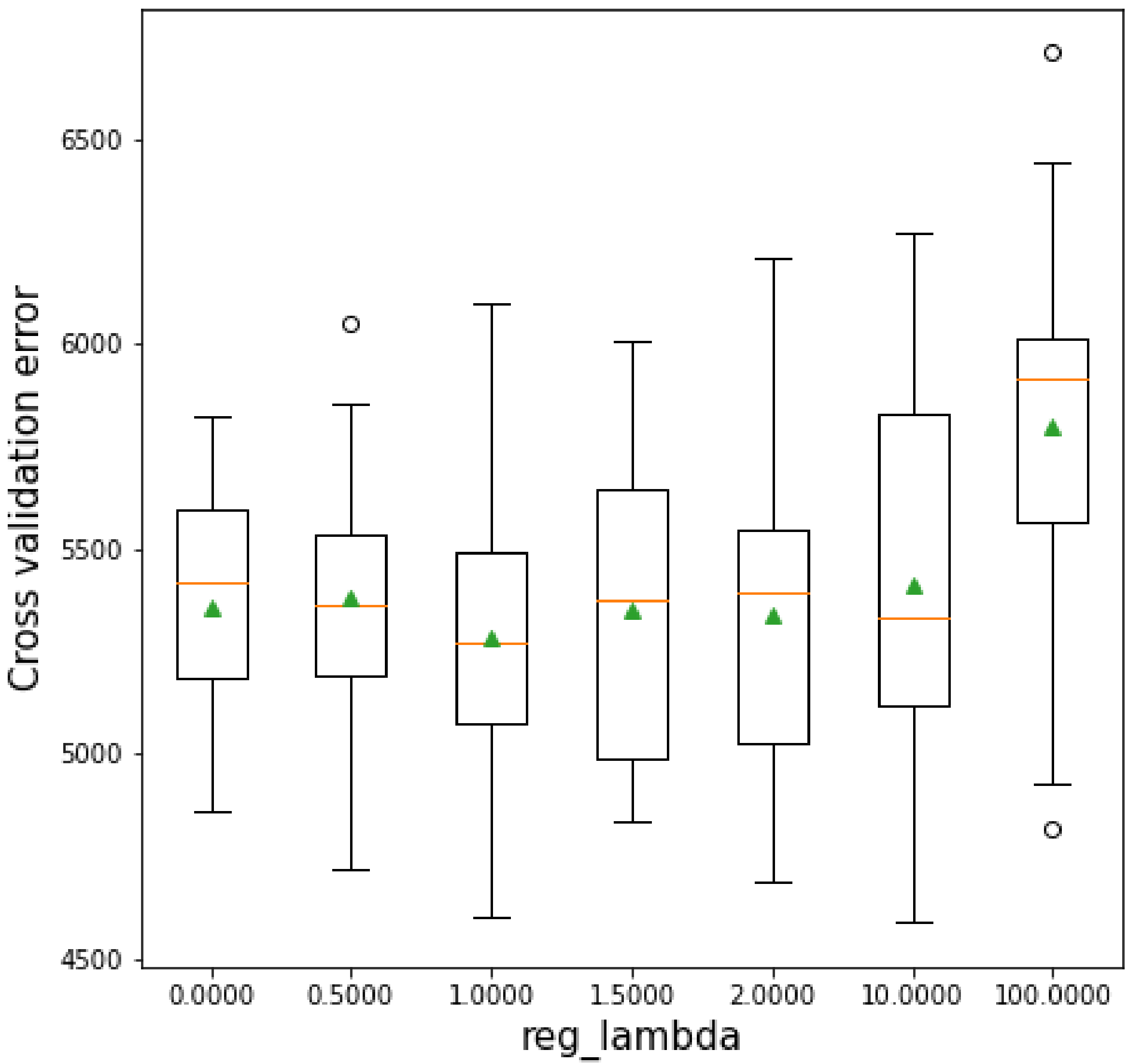
The parameter `reg_lambda` penalizes the *L2 norm* of the leaf scores. For example, in case of classification, it will penalize the summation of the square of log odds of the predicted probability. This penalization will tend to reduce the log odds, thereby reducing the tendency to overfit. "*Reducing the log odds*" in layman terms will mean not being overly sure about the prediction.

Without regularization, the algorithm will be closer to the gradient boosting algorithm. Regularization may provide some additional boost to prediction accuracy by reducing over-fitting. In the example below, regularization with *reg_lambda=1 turns out to be better than no regularization* (`reg_lambda=0`)*. Of course, too much regularization may increase bias so much such that it leads to a decrease in prediction accuracy.

```
def get_models():
    models = dict()
    # explore 'reg_lambda' from 0.1 to 2 in 0.1 increments
    for i in [0,0.5,1.0,1.5,2,10,100]:
        key = '%.4f' % i
        models[key] = xgb.XGBRegressor(reg_lambda=i,random_state=1)
    return models

# evaluate a given model using cross-validation
def evaluate_model(model, X, y):
    # define the evaluation procedure
    cv = KFold(n_splits=10, shuffle=True, random_state=1)
    # evaluate the model and collect the results
    scores = np.sqrt(-cross_val_score(model, X, y, scoring='neg_mean_squared_error', cv=cv,
    return scores

# get the models to evaluate
models = get_models()
# evaluate the models and store results
results, names = list(), list()
for name, model in models.items():
    # evaluate the model
    scores = evaluate_model(model, X, y)
    # store the results
    results.append(scores)
    names.append(name)
    # summarize the performance along the way
    print('>%s %.1f (%.1f)' % (name, np.mean(scores), np.std(scores)))
# plot model performance for comparison
plt.figure(figsize=(7, 7))
plt.boxplot(results, labels=names, showmeans=True)
plt.ylabel('Cross validation error',fontsize=15)
plt.xlabel('reg_lambda',fontsize=15)
```

```
>0.0000 5359.2 (317.0)
>0.5000 5382.7 (363.1)
>1.0000 5281.7 (383.8)
>1.5000 5348.0 (383.9)
>2.0000 5336.4 (426.6)
>10.0000 5410.9 (521.9)
>100.0000 5801.1 (563.7)
```

```
Text(0.5, 0, 'reg_lambda')
```



12.2.5 Regularization (`gamma`) vs cross validation error

The parameter `gamma` penalizes the tree based on the number of leaves. This is similar to the parameter `alpha` of cost complexity pruning. As `gamma` increases, more leaves will be pruned. Note that the previous parameter `reg_lambda` penalizes the leaf score, but does not prune the tree.

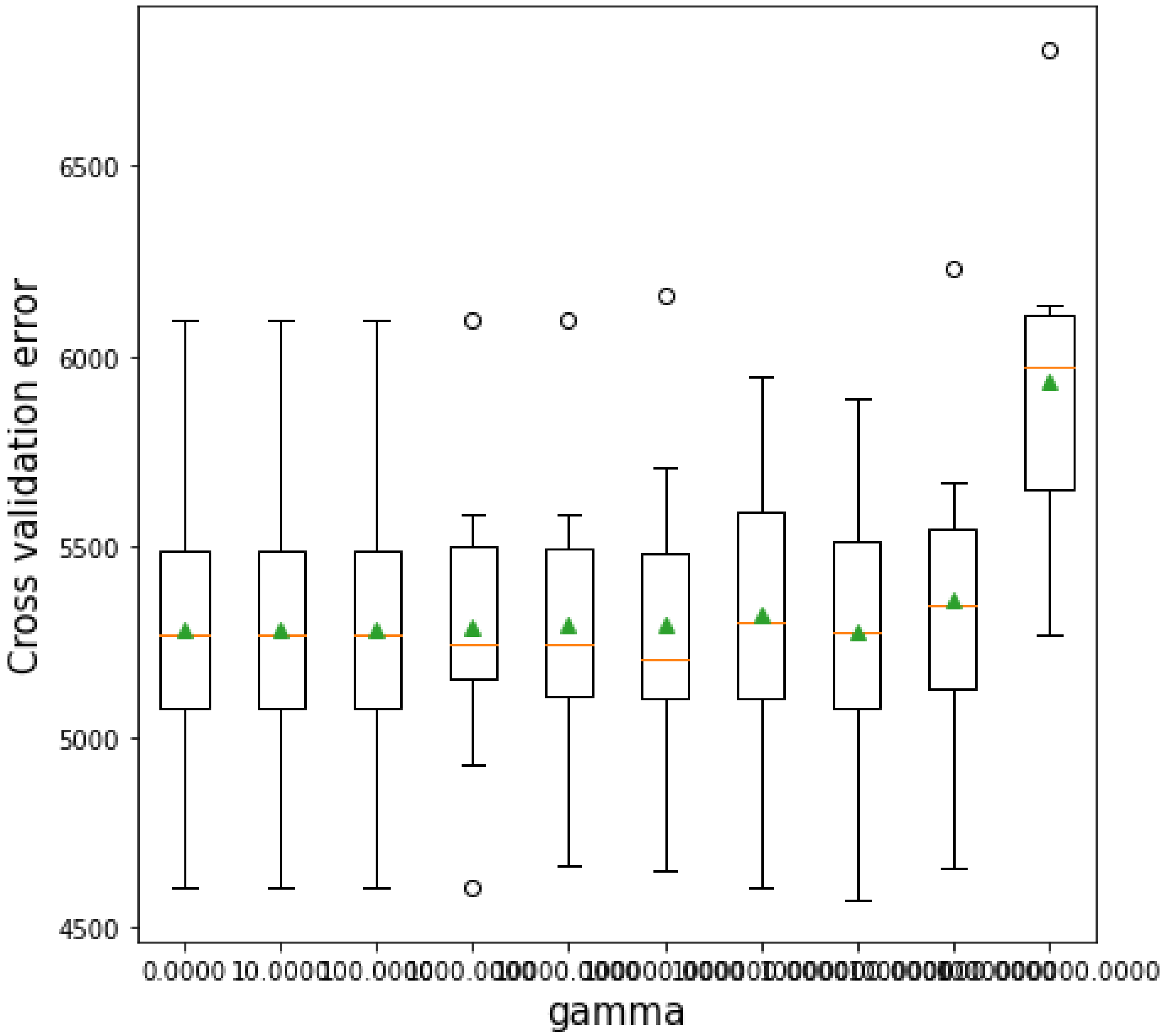
Without regularization, the algorithm will be closer to the gradient boosting algorithm. Regularization may provide some additional boost to prediction accuracy by reducing over-fitting. However, in the example below, no regularization (in terms of `gamma=0`) turns out to be better than a non-zero regularization. *(reg_lambda=0)*.

```
def get_models():
    models = dict()
    # explore gamma from 0.1 to 2 in 0.1 increments
    for i in [0,10,1e2,1e3,1e4,1e5,1e6,1e7,1e8,1e9]:
        key = '%.4f' % i
        models[key] = xgb.XGBRegressor(gamma=i,random_state=1)
    return models

# evaluate a given model using cross-validation
def evaluate_model(model, X, y):
    # define the evaluation procedure
    cv = KFold(n_splits=10, shuffle=True, random_state=1)
    # evaluate the model and collect the results
    scores = np.sqrt(-cross_val_score(model, X, y, scoring='neg_mean_squared_error', cv=cv, n
    return scores

# get the models to evaluate
models = get_models()
# evaluate the models and store results
results, names = list(), list()
for name, model in models.items():
    # evaluate the model
    scores = evaluate_model(model, X, y)
    # store the results
    results.append(scores)
    names.append(name)
    # summarize the performance along the way
    print('>%s %.1f (%.1f)' % (name, np.mean(scores), np.std(scores)))
# plot model performance for comparison
plt.figure(figsize=(7, 7))
plt.boxplot(results, labels=names, showmeans=True)
```

```python
plt.ylabel('Cross validation error',fontsize=15)
plt.xlabel('gamma',fontsize=15)
```

```
>0.0000 5281.7 (383.8)
>10.0000 5281.7 (383.8)
>100.0000 5281.7 (383.8)
>1000.0000 5291.8 (381.8)
>10000.0000 5295.7 (370.2)
>100000.0000 5293.0 (402.5)
>1000000.0000 5322.2 (368.9)
>10000000.0000 5273.7 (409.8)
>100000000.0000 5362.1 (407.8)
>1000000000.0000 5932.3 (397.6)
```

```
Text(0.5, 0, 'gamma')
```



12.2.6 Tuning XGboost regressor

Along with `max_depth`, `learning_rate`, and `n_estimators`, here we tune `reg_lambda` - the regularization parameter for penalizing the tree predictions.

```
#K-fold cross validation to find optimal parameters for XGBoost
start_time = time.time()
param_grid = {'max_depth': [4,6,8],
              'learning_rate': [0.01, 0.05, 0.1],
               'reg_lambda':[0, 1, 10],
                'n_estimators':[100, 500, 1000],
```

```
                'gamma': [0, 10, 100],
                'subsample': [0.5, 0.75, 1.0],
                'colsample_bytree': [0.5, 0.75, 1.0]}

cv = KFold(n_splits=5,shuffle=True,random_state=1)
optimal_params = RandomizedSearchCV(estimator=xgb.XGBRegressor(random_state=1),
                             param_distributions = param_grid, n_iter = 200,
                             verbose = 1,
                             n_jobs=-1,
                             cv = cv)
optimal_params.fit(X,y)
print("Optimal parameter values =", optimal_params.best_params_)
print("Optimal cross validation R-squared = ",optimal_params.best_score_)
print("Time taken = ", round((time.time()-start_time)/60), " minutes")
```

```
Fitting 5 folds for each of 200 candidates, totalling 1000 fits
Optimal parameter values = {'subsample': 0.75, 'reg_lambda': 1, 'n_estimators': 1000, 'max_de
Optimal cross validation R-squared =  0.9002580404500382
Time taken =  4  minutes
```

```
#RMSE based on the optimal parameter values
np.sqrt(mean_squared_error(optimal_params.best_estimator_.predict(Xtest),ytest))
```

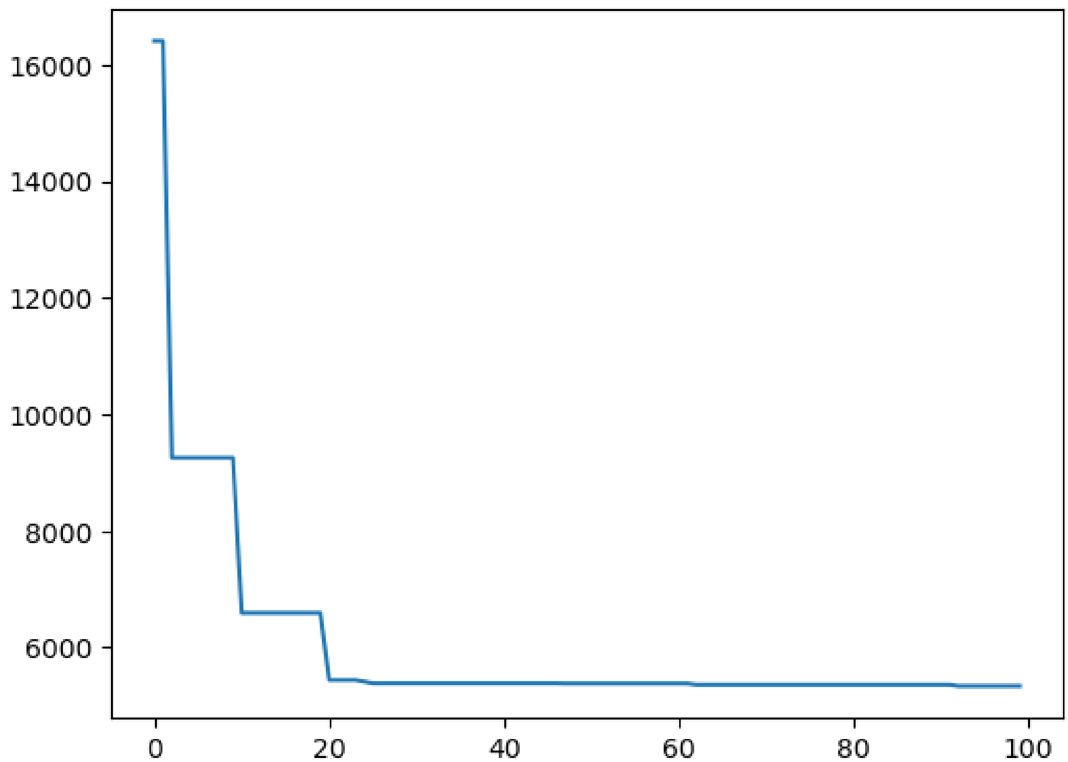
```
5497.553788113875
```

Let us use Bayes search to tune the model.

```
model = xgb.XGBRegressor(random_state = 1)

grid = {'max_leaves': Integer(4, 5000),
              'learning_rate': Real(0.0001, 1.0),
               'reg_lambda':Real(0, 1e4),
                'n_estimators':Integer(2, 2000),
                'gamma': Real(0, 1e11),
                'subsample': Real(0.1,1.0),
                'colsample_bytree': Real(0.1, 1.0)}

kfold = KFold(n_splits = 5, shuffle = True, random_state = 1)
gcv = BayesSearchCV(model, search_spaces = grid, cv = kfold, n_iter = 100, random_state = 1,
                         scoring = 'neg_root_mean_squared_error', n_jobs = -1)
```

```
paras = list(gcv.search_spaces.keys())
paras.sort()

def monitor(optim_result):
    cv_values = pd.Series(optim_result['func_vals']).cummin()
    display.clear_output(wait = True)
    min_ind = pd.Series(optim_result['func_vals']).argmin()
    print(paras, "=", optim_result['x_iters'][min_ind], pd.Series(optim_result['func_vals'])
    sns.lineplot(cv_values)
    plt.show()
gcv.fit(X, y, callback = monitor)
```

```
['colsample_bytree', 'gamma', 'learning_rate', 'max_leaves', 'n_estimators', 'reg_lambda', 's
```




```
BayesSearchCV(cv=KFold(n_splits=5, random_state=1, shuffle=True),
              estimator=XGBRegressor(base_score=None, booster=None,
                                     callbacks=None, colsample_bylevel=None,
                                     colsample_bynode=None,
```

```
                                    colsample_bytree=None,
                                    early_stopping_rounds=None,
                                    enable_categorical=False, eval_metric=None,
                                    feature_types=None, gamma=None,
                                    gpu_id=None, grow_policy=None,
                                    importance_type=None,
                                    inte...
                            'learning_rate': Real(low=0.0001, high=1.0, prior='uniform', tra
                            'max_leaves': Integer(low=4, high=5000, prior='uniform', transfo
                            'n_estimators': Integer(low=2, high=2000, prior='uniform', trans
                            'reg_lambda': Real(low=0, high=10000.0, prior='uniform', transfo
                            'subsample': Real(low=0.1, high=1.0, prior='uniform', transform=
```

```
model1 = xgb.XGBRegressor(random_state = 1, colsample_bytree = 0.85, gamma = 0, learning_rate
                          max_leaves = 802, n_estimators = 1023, reg_lambda = 1394, subsample
```

```
np.sqrt(mean_squared_error(model1.predict(Xtest),ytest))
```

```
5466.076861800755
```

We got a different set of optimal hyperparameters with Bayes search. Thus, ensembling the model based on the two sets of hyperparameters is likely to improve the accuracy over the individual models.

```
model2 = xgb.XGBRegressor(random_state = 1, colsample_bytree = 1.0, gamma = 100, learning_rat
                          max_depth = 8, n_estimators = 1000, reg_lambda = 1, subsample = 0.7
```

```
np.sqrt(mean_squared_error(0.5*model1.predict(Xtest)+0.5*model2.predict(Xtest),ytest))
```

```
5393.379834226845
```

12.2.7 Early stopping with XGBoost

If we have a test dataset *(or we can further split the train data into a smaller train and test data)*, we can use it with the `early_stopping_rounds` argument of XGBoost, where it will stop growing trees once the model accuracy fails to increase for a certain number of consecutive iterations, given as `early_stopping_rounds`.

```
X_train_sub, X_test_sub, y_train_sub, y_test_sub = \
train_test_split(X, y, test_size = 0.2, random_state = 45)
```

```
model = xgb.XGBRegressor(random_state = 1, max_depth = 8, learning_rate = 0.01,
                        n_estimators = 20000,reg_lambda = 1, gamma = 100, subsample = 0.75, c
model.fit(X_train_sub, y_train_sub, eval_set = ([(X_test_sub, y_test_sub)]), early_stopping_r
```

The results of the code are truncated to save space. A snapshot of the beginning and end of the results is below. The algorithm keeps adding trees to the model until the RMSE ceases to decrease for 10 consecutive iterations.

```
<IPython.core.display.Image object>
```

```
print("XGBoost RMSE = ",np.sqrt(mean_squared_error(model.predict(Xtest),ytest)))
```

```
XGBoost RMSE =  5508.787454011525
```

Let us further reduce the `learning rate` to `0.001` and see if the accuracy increases further on the test data. We'll use the `early_stopping_rounds` argument to stop growing trees once the accuracy fails to increase for 250 consecutive iterations.

```
model = xgb.XGBRegressor(random_state = 1, max_depth = 8, learning_rate = 0.001,
                        n_estimators = 20000,reg_lambda = 1, gamma = 100, subsample = 0.75, c
model.fit(X_train_sub, y_train_sub, eval_set = ([(X_test_sub, y_test_sub)]), early_stopping_r
```

```
<IPython.core.display.Image object>
```

```
print("XGBoost RMSE = ",np.sqrt(mean_squared_error(model.predict(Xtest),ytest)))
```

```
XGBoost RMSE =  5483.518711988693
```

Note that the accuracy on this test data has further increased with a lower learning rate.

#Let us combine the XGBoost model with other tuned models from earlier chapters.

```
#Tuned AdaBoost model from Section 7.2.4
model_ada = AdaBoostRegressor(base_estimator=DecisionTreeRegressor(max_depth=10),n_estimators
                         random_state=1).fit(X,y)
print("AdaBoost RMSE = ", np.sqrt(mean_squared_error(model_ada.predict(Xtest),ytest)))

#Tuned Random forest model from Section 6.1.2
model_rf = RandomForestRegressor(n_estimators=300, random_state=1,
                        n_jobs=-1, max_features=2).fit(X, y)
print("Random Forest RMSE = ",np.sqrt(mean_squared_error(model_rf.predict(Xtest),ytest)))

#Tuned gradient boosting model from Section 8.2.5
model_gb = GradientBoostingRegressor(max_depth=8,n_estimators=100,learning_rate=0.1,
                         random_state=1,loss='huber').fit(X,y)
print("Gradient boost RMSE = ",np.sqrt(mean_squared_error(model_gb.predict(Xtest),ytest)))
```

```
AdaBoost RMSE =  5693.165811600585
Random Forest RMSE =  5642.45839697972
Gradient boost RMSE =  5405.787029062213
```

```
#Ensemble model
pred_xgb = model.predict(Xtest)    #XGBoost
pred_ada = model_ada.predict(Xtest)#AdaBoost
pred_rf = model_rf.predict(Xtest)  #Random Forest
pred_gb = model_gb.predict(Xtest)  #Gradient boost
pred = 0.25*pred_xgb + 0.25*pred_ada + 0.25*pred_rf + 0.25*pred_gb #Option 1 - All models are
#pred = 0.15*pred1+0.15*pred2+0.15*pred3+0.55*pred4 #Option 2 - Higher weight to the better m
print("Ensemble model RMSE = ", np.sqrt(mean_squared_error(pred,ytest)))
```

```
Ensemble model RMSE =  5352.145010078119
```

Combined, the random forest model, gradient boost, XGBoost and the Adaboost model do better than each of the individual models.

12.3 XGBoost for classification

```
data = pd.read_csv('./Datasets/Heart.csv')
data.dropna(inplace = True)
data.head()
```

	Age	Sex	ChestPain	RestBP	Chol	Fbs	RestECG	MaxHR	ExAng	Oldpeak	Slope	Ca
0	63	1	typical	145	233	1	2	150	0	2.3	3	0.0
1	67	1	asymptomatic	160	286	0	2	108	1	1.5	2	3.0
2	67	1	asymptomatic	120	229	0	2	129	1	2.6	2	2.0
3	37	1	nonanginal	130	250	0	0	187	0	3.5	3	0.0
4	41	0	nontypical	130	204	0	2	172	0	1.4	1	0.0

```
#Response variable
y = pd.get_dummies(data['AHD'])['Yes']

#Creating a dataframe for predictors with dummy varibles replacing the categorical variables
X = data.drop(columns = ['AHD','ChestPain','Thal'])
X = pd.concat([X,pd.get_dummies(data['ChestPain']),pd.get_dummies(data['Thal'])],axis=1)
X.head()
```

	Age	Sex	RestBP	Chol	Fbs	RestECG	MaxHR	ExAng	Oldpeak	Slope	Ca	asymptomatic
0	63	1	145	233	1	2	150	0	2.3	3	0.0	0
1	67	1	160	286	0	2	108	1	1.5	2	3.0	1
2	67	1	120	229	0	2	129	1	2.6	2	2.0	1
3	37	1	130	250	0	0	187	0	3.5	3	0.0	0
4	41	0	130	204	0	2	172	0	1.4	1	0.0	0

```
#Creating train and test datasets
Xtrain,Xtest,ytrain,ytest = train_test_split(X,y,train_size = 0.5,random_state=1)
```

XGBoost has an additional parameter for classification: **`scale_pos_weight`**

Gradients are used as the basis for fitting subsequent trees added to boost or correct errors made by the existing state of the ensemble of decision trees.

The `scale_pos_weight` value is used to scale the gradient for the positive class.

This has the effect of scaling errors made by the model during training on the positive class and encourages the model to over-correct them. In turn, this can help the model achieve better performance when making predictions on the positive class. Pushed too far, it may result in the model overfitting the positive class at the cost of worse performance on the negative class or both classes.

As such, the scale_pos_weight can be used to train a class-weighted or cost-sensitive version of XGBoost for imbalanced classification.

A sensible default value to set for the scale_pos_weight hyperparameter is the inverse of the class distribution. For example, for a dataset with a 1 to 100 ratio for examples in the minority to majority classes, the scale_pos_weight can be set to 100. This will give classification errors made by the model on the minority class (positive class) 100 times more impact, and in turn, 100 times more correction than errors made on the majority class.

Ref:https://machinelearningmastery.com/xgboost-for-imbalanced-classification/#:~:text=The%20scale_pos_w

```
start_time = time.time()
param_grid = {'n_estimators':[25,100,500],
                'max_depth': [6,7,8],
              'learning_rate': [0.01,0.1,0.2],
               'gamma': [0.1,0.25,0.5],
               'reg_lambda':[0,0.01,0.001],
                'scale_pos_weight':[1.25,1.5,1.75]#Control the balance of positive and negati
             }

cv = StratifiedKFold(n_splits=5,shuffle=True,random_state=1)
optimal_params = GridSearchCV(estimator=xgb.XGBClassifier(objective = 'binary:logistic',rando
                                                          use_label_encoder=False),
                             param_grid = param_grid,
                             scoring = 'accuracy',
                             verbose = 1,
                             n_jobs=-1,
                             cv = cv)
optimal_params.fit(Xtrain,ytrain)
print(optimal_params.best_params_,optimal_params.best_score_)
print("Time taken = ", (time.time()-start_time)/60, " minutes")
```

```
Fitting 5 folds for each of 729 candidates, totalling 3645 fits
[22:00:02] WARNING: D:\bld\xgboost-split_1645118015404\work\src\learner.cc:1115: Starting in
{'gamma': 0.25, 'learning_rate': 0.2, 'max_depth': 6, 'n_estimators': 25, 'reg_lambda': 0.01
```

```
cv_results=pd.DataFrame(optimal_params.cv_results_)
cv_results.sort_values(by = 'mean_test_score',ascending=False)[0:5]
```

	mean_fit_time	std_fit_time	mean_score_time	std_score_time	param_gamma	param_learnin
409	0.111135	0.017064	0.005629	0.000737	0.25	0.2
226	0.215781	0.007873	0.005534	0.001615	0.1	0.2
290	1.391273	0.107808	0.007723	0.006286	0.25	0.01
266	1.247463	0.053597	0.006830	0.002728	0.25	0.01

	mean_fit_time	std_fit_time	mean_score_time	std_score_time	param_gamma	param_learnin
269	1.394361	0.087307	0.005530	0.001718	0.25	0.01

```
#Function to compute confusion matrix and prediction accuracy on test/train data
def confusion_matrix_data(data,actual_values,model,cutoff=0.5):
#Predict the values using the Logit model
    pred_values = model.predict_proba(data)[:,1]
# Specify the bins
    bins=np.array([0,cutoff,1])
#Confusion matrix
    cm = np.histogram2d(actual_values, pred_values, bins=bins)[0]
    cm_df = pd.DataFrame(cm)
    cm_df.columns = ['Predicted 0','Predicted 1']
    cm_df = cm_df.rename(index={0: 'Actual 0',1:'Actual 1'})
# Calculate the accuracy
    accuracy = 100*(cm[0,0]+cm[1,1])/cm.sum()
    fnr = 100*(cm[1,0])/(cm[1,0]+cm[1,1])
    precision = 100*(cm[1,1])/(cm[0,1]+cm[1,1])
    fpr = 100*(cm[0,1])/(cm[0,0]+cm[0,1])
    tpr = 100*(cm[1,1])/(cm[1,0]+cm[1,1])
    print("Accuracy = ", accuracy)
    print("Precision = ", precision)
    print("FNR = ", fnr)
    print("FPR = ", fpr)
    print("TPR or Recall = ", tpr)
    print("Confusion matrix = \n", cm_df)
    return (" ")
```

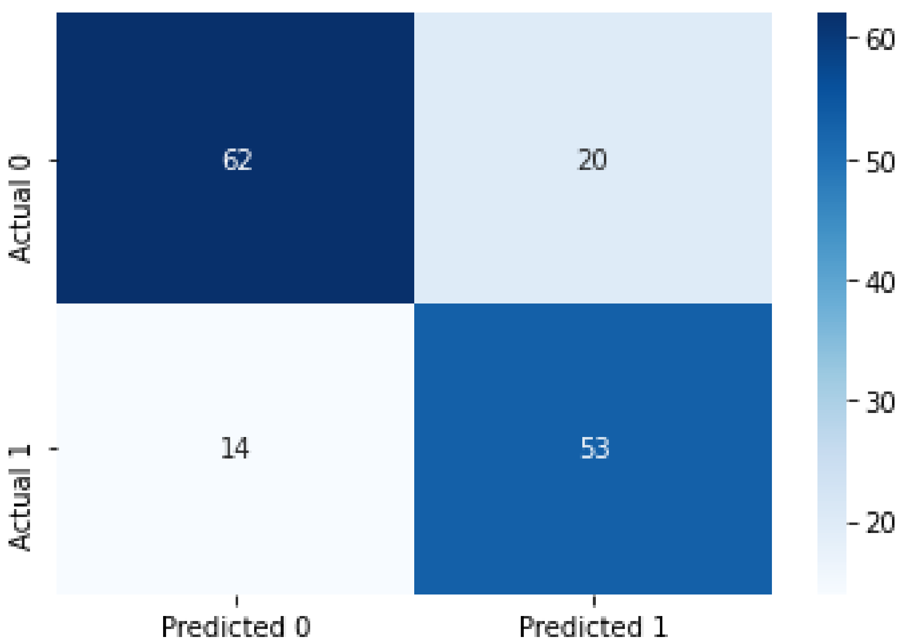
```
model4 = xgb.XGBClassifier(objective = 'binary:logistic',random_state=1,gamma=0.25,learning_r
                              n_estimators = 500,reg_lambda = 0.01,scale_pos_weight=1.75)
model4.fit(Xtrain,ytrain)
model4.score(Xtest,ytest)
```

```
0.7718120805369127
```

```
#Computing the accuracy
y_pred = model4.predict(Xtest)
print("Accuracy: ",accuracy_score(y_pred, ytest)*100)

#Computing the ROC-AUC
```

```
y_pred_prob = model4.predict_proba(Xtest)[:,1]
fpr, tpr, auc_thresholds = roc_curve(ytest, y_pred_prob)
print("ROC-AUC: ",auc(fpr, tpr))# AUC of ROC

#Computing the precision and recall
print("Precision: ", precision_score(ytest, y_pred))
print("Recall: ", recall_score(ytest, y_pred))

#Confusion matrix
cm = pd.DataFrame(confusion_matrix(ytest, y_pred), columns=['Predicted 0', 'Predicted 1'],
            index = ['Actual 0', 'Actual 1'])
sns.heatmap(cm, annot=True, cmap='Blues', fmt='g');
```

```
Accuracy:  77.18120805369128
ROC-AUC:  0.8815070986530761
Precision:  0.726027397260274
Recall:  0.7910447761194029
```



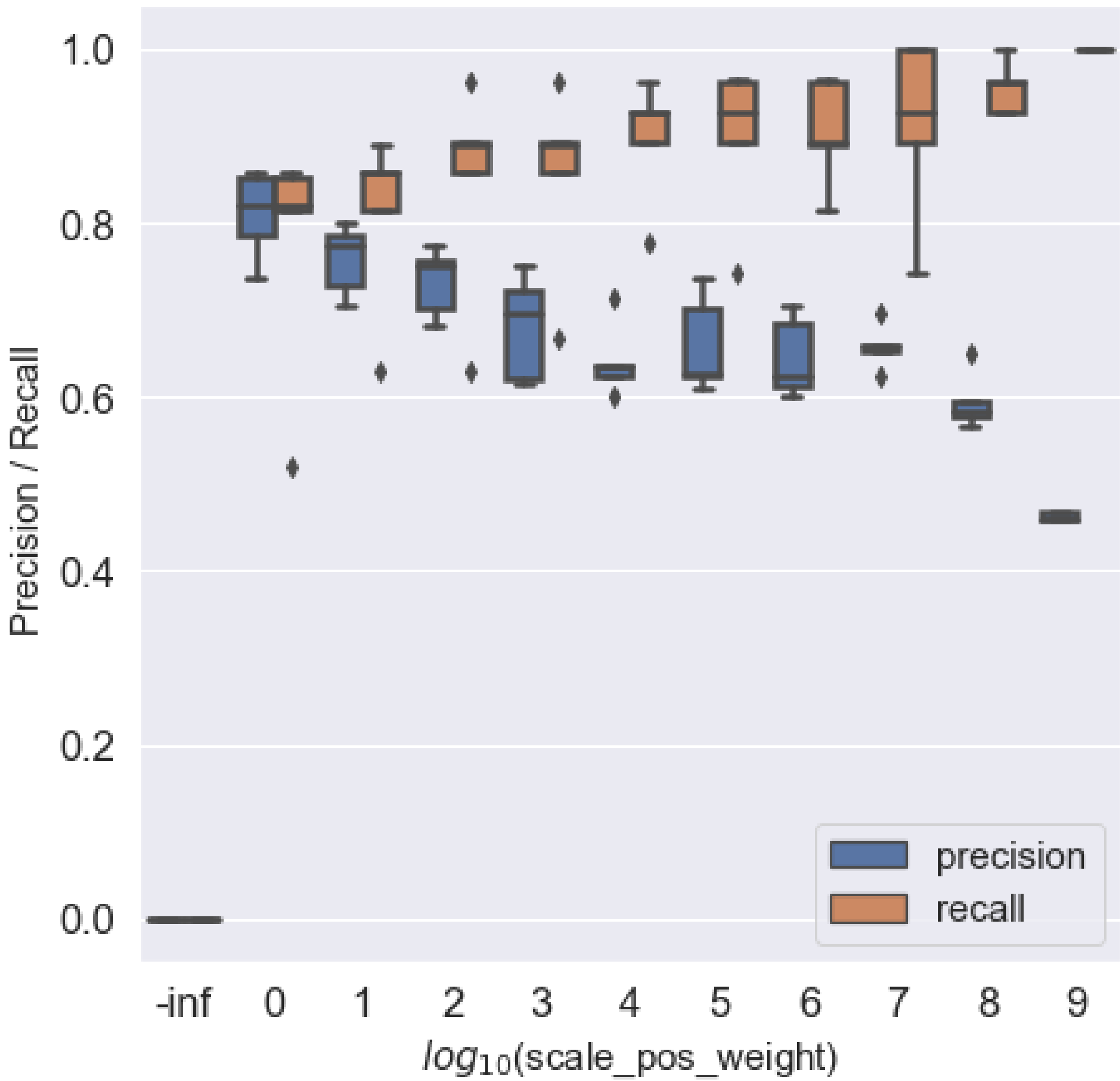
If we increase the value of `scale_pos_weight`, the model will focus on classifying positives more correctly. This will increase the recall (true positive rate) since the focus is on identifying all positives. However, this will lead to identifying positives aggressively, and observations 'similar' to observations of the positive class will also be predicted as positive resulting in an increase in false positives and a decrease in precision. See the trend below as we increase the value of scale_pos_weight.

12.3.1 Precision & recall vs scale_pos_weight

```
def get_models():
    models = dict()
    # explore 'scale_pos_weight' from 0.1 to 2 in 0.1 increments
    for i in [0,1,10,1e2,1e3,1e4,1e5,1e6,1e7,1e8,1e9]:
        key = '%.0f' % i
        models[key] = xgb.XGBClassifier(objective = 'binary:logistic',scale_pos_weight=i,ranc
    return models

# evaluate a given model using cross-validation
def evaluate_model(model, X, y):
    # define the evaluation procedure
    cv = StratifiedKFold(n_splits=5, shuffle=True, random_state=1)
    # evaluate the model and collect the results
    scores_recall = cross_val_score(model, X, y, scoring='recall', cv=cv, n_jobs=-1)
    scores_precision = cross_val_score(model, X, y, scoring='precision', cv=cv, n_jobs=-1)
    return list([scores_recall,scores_precision])

# get the models to evaluate
models = get_models()
# evaluate the models and store results
results_recall, results_precision, names = list(), list(), list()
for name, model in models.items():
    # evaluate the model
    scores = evaluate_model(model, X, y)
    scores_recall = scores[0]
    scores_precision = scores[1]
    # store the results
    results_recall.append(scores_recall)
    results_precision.append(scores_precision)
    names.append(name)
    # summarize the performance along the way
    print('>%s %.2f (%.2f)' % (name, np.mean(scores_recall), np.std(scores_recall)))
# plot model performance for comparison
plt.figure(figsize=(7, 7))
sns.set(font_scale = 1.5)
pdata = pd.DataFrame(results_precision)
```

```python
pdata.columns = list(['p1','p2','p3','p4','p5'])
pdata['metric'] = 'precision'
rdata = pd.DataFrame(results_recall)
rdata.columns = list(['p1','p2','p3','p4','p5'])
rdata['metric'] = 'recall'
pr_data = pd.concat([pdata,rdata])
pr_data.reset_index(drop=False,inplace= True)
#sns.boxplot(x="day", y="total_bill", hue="time",pr_data=tips, linewidth=2.5)
pr_data_melt=pr_data.melt(id_vars = ['index','metric'])
pr_data_melt['index']=pr_data_melt['index']-1
pr_data_melt['index'] = pr_data_melt['index'].astype('str')
pr_data_melt.replace(to_replace='-1',value =  '-inf',inplace=True)
sns.boxplot(x='index', y="value", hue="metric", data=pr_data_melt, linewidth=2.5)
plt.xlabel('$log_{10}$(scale_pos_weight)',fontsize=15)
plt.ylabel('Precision / Recall ',fontsize=15)
plt.legend(loc="lower right", frameon=True, fontsize=15)
```

```
>0 0.00 (0.00)
>1 0.77 (0.13)
>10 0.81 (0.09)
>100 0.85 (0.11)
>1000 0.85 (0.10)
>10000 0.90 (0.06)
>100000 0.90 (0.08)
>1000000 0.90 (0.06)
>10000000 0.91 (0.10)
>100000000 0.96 (0.03)
>1000000000 1.00 (0.00)
```


1.0
0.8
0.6
0.4
0.2
0.0
Precision / Recall
precision
recall
-inf
0
1
2
3
4
5
6
7
8
9
log_{10}(scale_pos_weight)

13 More boosting models

```
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.metrics import mean_squared_error
from sklearn.model_selection import cross_val_score,train_test_split, KFold, cross_val_predic
from sklearn.metrics import mean_squared_error,r2_score,roc_curve,auc,precision_recall_curve
recall_score, precision_score, confusion_matrix
from sklearn.tree import DecisionTreeRegressor,DecisionTreeClassifier
from sklearn.model_selection import GridSearchCV, ParameterGrid, StratifiedKFold, Randomized
from sklearn.ensemble import VotingRegressor, VotingClassifier, StackingRegressor, StackingCl
from sklearn.linear_model import LinearRegression,LogisticRegression, LassoCV, RidgeCV, Elas
from sklearn.neighbors import KNeighborsRegressor
import itertools as it
import time as time
import xgboost as xgb
from pyearth import Earth
from lightgbm import LGBMRegressor
from catboost import CatBoostRegressor
```

We'll continue to use the same datasets that we have been using throughout the course.

```
#Using the same datasets as used for linear regression in STAT303-2,
#so that we can compare the non-linear models with linear regression
trainf = pd.read_csv('./Datasets/Car_features_train.csv')
trainp = pd.read_csv('./Datasets/Car_prices_train.csv')
testf = pd.read_csv('./Datasets/Car_features_test.csv')
testp = pd.read_csv('./Datasets/Car_prices_test.csv')
train = pd.merge(trainf,trainp)
test = pd.merge(testf,testp)
train.head()
```

	carID	brand	model	year	transmission	mileage	fuelType	tax	mpg	engineSize	price
0	18473	bmw	6 Series	2020	Semi-Auto	11	Diesel	145	53.3282	3.0	37980
1	15064	bmw	6 Series	2019	Semi-Auto	10813	Diesel	145	53.0430	3.0	33980
2	18268	bmw	6 Series	2020	Semi-Auto	6	Diesel	145	53.4379	3.0	36850
3	18480	bmw	6 Series	2017	Semi-Auto	18895	Diesel	145	51.5140	3.0	25998
4	18492	bmw	6 Series	2015	Automatic	62953	Diesel	160	51.4903	3.0	18990

```
X = train[['mileage','mpg','year','engineSize']]
Xtest = test[['mileage','mpg','year','engineSize']]
y = train['price']
ytest = test['price']
```

13.1 LightGBM

LightGBM is a gradient boosting decision tree algorithm developed by Microsoft in 2017. LightGBM outperforms XGBoost in terms of compuational speed, and provides comparable accuracy in general. The following two key features in LightGBM that make it faster than XGBoost:

1. Gradient-based One-Side Sampling (GOSS): Recall, in gradient boosting, we fit trees on the gradient of the loss function *(refer the gradient boosting algorithm in section 10.10.2 of the book, Elements of Statistical Learning):*

$$r_m = -\left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)}\right]_{f=f_{m-1}}.$$

Observations that correspond to relatively larger gradients contribute more to minimizing the loss function as compared to observations with smaller gradients. The algorithm down-samples the observations with small gradients, while selecting all the observations with large gradients. As observations with large gradients contribute the most to the reduction in loss function when considering a split, the accuracy of loss reduction estimate is maintained even with a reduced sample size. This leads to similar performance in terms of prediction accuracy while reducing computation speed due to reduction in sample size to fit trees.

2. Exclusive feature bundling (EFB): This is useful when there are a lot of predictors, but the predictor space is sparse, i.e., most of the values are zero for several predictors, and the predictors rarely take non-zero values simultaneously. This can typically happen in case of a lot of dummy variables in the data. In such a case, the predictors are bundled to create a single predictor.

In the example below you can see that feature1 and feature2 are mutually exclusive. In order to achieve non overlapping buckets we add bundle size of feature1 to feature2. This makes sure that non zero data points of bundled features (feature1 and feature2) reside in different buckets. In feature_bundle buckets 1 to 4 contains non zero instances of feature1 and buckets 5,6 contain non zero instances of feature2 *(Reference)*.

feature1	feature2	feature_bundle
0	2	6
0	1	5
0	2	6
1	0	1
2	0	2
3	0	3
4	0	4

Read the LightGBM paper for more details.

13.1.1 LightGBM for regression

Let us tune a lightGBM model for regression for our problem of predicting car price. We'll use the function `LGBMRegressor`. For classification problems, `LGBMClassifier` can be used.

```
#K-fold cross validation to find optimal parameters for LightGBM regressor
start_time = time.time()
param_grid = {'max_depth': [4,6,8],
              'num_leaves': [20, 31, 40],
              'learning_rate': [0.01, 0.05, 0.1],
               'reg_lambda':[0, 10, 100],
                'n_estimators':[100, 500, 1000],
                'reg_alpha': [0, 10, 100],
                'subsample': [0.5, 0.75, 1.0],
                'colsample_bytree': [0.5, 0.75, 1.0]}

cv = KFold(n_splits=5,shuffle=True,random_state=1)
optimal_params = RandomizedSearchCV(estimator=LGBMRegressor(random_state=1),
                             param_distributions = param_grid, n_iter = 200,
                             verbose = 1,
                             n_jobs=-1,
                             cv = cv)
optimal_params.fit(X,y)
print("Optimal parameter values =", optimal_params.best_params_)
```

```
print("Optimal cross validation R-squared = ",optimal_params.best_score_)
print("Time taken = ", round((time.time()-start_time)/60), " minutes")
```

```
Fitting 5 folds for each of 200 candidates, totalling 1000 fits
Optimal parameter values = {'subsample': 0.75, 'reg_lambda': 0, 'reg_alpha': 100, 'num_leaves
Optimal cross validation R-squared =  0.8935432951824455
Time taken =  1  minutes
```

```
#RMSE based on the optimal parameter values of a LighGBM Regressor model
np.sqrt(mean_squared_error(optimal_params.best_estimator_.predict(Xtest),ytest))
```

```
5400.723918176313
```

13.1.2 LightGBM vs XGBoost

LightGBM model took 1 minute for a random search with 1000 fits as compared to 4 minutes for an XGBoost model with 1000 fits on the same data (as shown below). In terms of prediction accuracy, we observe that the accuracy of LightGBM on test *(unseen)* data is comparable to that of XGBoost.

```
#K-fold cross validation to find optimal parameters for XGBoost
start_time = time.time()
param_grid = {'max_depth': [4,6,8],
              'learning_rate': [0.01, 0.05, 0.1],
               'reg_lambda':[0, 1, 10],
                'n_estimators':[100, 500, 1000],
                'gamma': [0, 10, 100],
                'subsample': [0.5, 0.75, 1.0],
                'colsample_bytree': [0.5, 0.75, 1.0]}

cv = KFold(n_splits=5,shuffle=True,random_state=1)
optimal_params = RandomizedSearchCV(estimator=xgb.XGBRegressor(random_state=1),
                             param_distributions = param_grid, n_iter = 200,
                             verbose = 1,
                             n_jobs=-1,
                             cv = cv)
optimal_params.fit(X,y)
print("Optimal parameter values =", optimal_params.best_params_)
print("Optimal cross validation R-squared = ",optimal_params.best_score_)
print("Time taken = ", round((time.time()-start_time)/60), " minutes")
```

```
Fitting 5 folds for each of 200 candidates, totalling 1000 fits
Optimal parameter values = {'subsample': 0.75, 'reg_lambda': 1, 'n_estimators': 1000, 'max_de
Optimal cross validation R-squared =  0.9002580404500382
Time taken =  4  minutes
```

```
#RMSE based on the optimal parameter values
np.sqrt(mean_squared_error(optimal_params.best_estimator_.predict(Xtest),ytest))
```

```
5497.553788113875
```

13.2 CatBoost

CatBoost is a gradient boosting algorithm developed by Yandex *(Russian Google)* in 2017. Like LightGBM, CatBoost is also faster than XGBoost in training. However, unlike LightGBM, the authors have claimed that it outperforms both LightGBM and XGBoost in terms of prediction accuracy as well.

The key feature of CatBoost that address the issue with the gradient boosting procedure is the idea of ordered boosting. Classic boosting algorithms are prone to overfitting on small/noisy datasets due to a problem known as prediction shift. Recall, in gradient boosting, we fit trees on the gradient of the loss function *(refer the gradient boosting algorithm in section 10.10.2 of the book, Elements of Statistical Learning):*

$$r_m = -\left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)}\right]_{f=f_{m-1}}.$$

When calculating the gradient estimate of an observation, these algorithms use the same observations that the model was built with, thus having no chances of experiencing unseen data. CatBoost, on the other hand, uses the concept of ordered boosting, a permutation-driven approach to train model on a subset of data while calculating residuals on another subset, thus preventing "target leakage" and overfitting. The residuals of an observation are computed based on a model developed on the previous observations, where the observations are randomly shuffled at each iteration, i.e., for each tree.

Thus, the gradient of the loss function is based on test *(unseen)* data, instead of the data on which the model has been trained, which improves the generalizability of the model, and avoids overfitting on train data.

The authors have also shown that CatBoost performs better than XGBoost and LightGBM without tuning, i.e., with default hyperparameter settings.

Read the CatBoost paper for more details.

Here is a good blog listing the key features of CatBoost.

13.2.1 CatBoost for regression

We'll use the function CatBoostRegressor for regression. For classification problems CatBoost-Classifier can be used.

Let us check the performance of `CatBoostRegressor()` without tuning, i.e., with default hyperparameter settings.

```
model_cat = CatBoostRegressor().fit(X, y)
```

```
np.sqrt(mean_squared_error(model_cat.predict(Xtest),ytest))
```

```
5288.82153844634
```

Even with default hyperparameter settings, CatBoost has outperformed both XGBoost and LightGBM in terms of RMSE on test data for our example of predicting car prices.

13.2.2 CatBoost vs XGBoost

Let us see the performance of XGBoost with default hyperparameter settings.

```
model_xgb = xgb.XGBRFRegressor().fit(X, y)
np.sqrt(mean_squared_error(model_xgb.predict(Xtest),ytest))
```

```
6821.745153860935
```

XGBoost performance deteriorates showing that hyperparameter tuning is more important in XGBoost.

Let us see the performance of LightGBM with default hyperparameter settings.

```
model_lgbm = LGBMRegressor().fit(X, y)
np.sqrt(mean_squared_error(model_lgbm.predict(Xtest),ytest))
```

```
5494.0777923513515
```

LightGBM's default hyperparameter settings also seem to be more robust as compared to those of XGBoost.

13.2.3 Tuning CatBoostRegressor

The CatBoost hyperparameters can be tuned just like the XGBoost hyperparameters. However, there is some difference in the hyperparameters of both the packages. For example, `reg_alpha` *(the L1 penalization on weights of leaves)* and `colsample_bytree` *(subsample ratio of columns when constructing each tree)* hyperparameters are not there in CatBoost.

```
#K-fold cross validation to find optimal parameters for CatBoost regressor
start_time = time.time()
param_grid = {'max_depth': [4,6,8],
              'num_leaves': [20, 31, 40],
              'learning_rate': [0.01, 0.05, 0.1],
               'reg_lambda':[0, 10, 100],
                'n_estimators':[100, 500, 1000],
                'subsample': [0.5, 0.75, 1.0]}

cv = KFold(n_splits=5,shuffle=True,random_state=1)
optimal_params = RandomizedSearchCV(estimator=CatBoostRegressor(random_state=1, verbose=Fals
                             param_distributions = param_grid, n_iter = 200,
                             verbose = 1,random_state = 1,
                             n_jobs=-1,
                             cv = cv)
optimal_params.fit(X,y)
print("Optimal parameter values =", optimal_params.best_params_)
print("Optimal cross validation R-squared = ",optimal_params.best_score_)
print("Time taken = ", round((time.time()-start_time)/60), " minutes")
```

```
Fitting 5 folds for each of 200 candidates, totalling 1000 fits
Optimal parameter values = {'subsample': 0.75, 'reg_lambda': 0, 'num_leaves': 31, 'n_estimat
Optimal cross validation R-squared =  0.9068137174802073
Time taken =  2  minutes
```

```
C:\Users\akl0407\Anaconda3\lib\site-packages\sklearn\model_selection\_search.py:918: UserWarn
        nan 0.86528582        nan        nan 0.84104458 0.79227627
        nan        nan 0.84395413 0.89887462        nan        nan
        nan 0.90260407        nan        nan        nan        nan
        nan        nan 0.86545114        nan 0.84894322        nan
 0.8913253         nan        nan 0.90681372 0.90270419 0.84033192
        nan        nan        nan        nan        nan 0.89897627
        nan 0.75750273 0.63799634 0.82429155 0.8541958         nan
 0.85795537 0.84778687        nan 0.82552044 0.88776603        nan
 0.87183014        nan        nan        nan        nan        nan
```

```
        nan        nan        nan        nan 0.868381   0.88627774
        nan        nan        nan        nan 0.88302748        nan
        nan        nan 0.87173927 0.90364659        nan 0.68716329
 0.86810108        nan 0.90387934 0.86198    0.79482791        nan
 0.867492          nan        nan        nan 0.8681382         nan
        nan        nan        nan        nan        nan 0.82487077
 0.54242665        nan        nan        nan        nan        nan
        nan        nan 0.88919641        nan        nan        nan
 0.85336326        nan 0.8619873  0.83934649 0.90477081 0.79750609
 0.86543518        nan        nan        nan        nan 0.80115517
        nan        nan        nan        nan        nan 0.75434919
 0.60871141        nan        nan 0.79028956 0.66728925 0.89361737
        nan        nan        nan        nan        nan 0.89080628
        nan 0.75063605        nan 0.90090587        nan        nan
 0.82573579 0.90680318 0.85290443        nan        nan 0.89928321
        nan        nan        nan 0.86285405 0.8978184         nan
        nan 0.84783232        nan        nan        nan        nan
 0.86225177        nan        nan 0.8621329         nan        nan
 0.54359637        nan        nan 0.8994749  0.84800071        nan
        nan        nan        nan        nan        nan        nan
 0.63020005        nan 0.87308398        nan 0.86614844        nan
        nan        nan        nan        nan        nan        nan
 0.68846678 0.8406747         nan        nan        nan        nan
 0.88741464 0.86148835]
  warnings.warn(
```

```
#RMSE based on the optimal parameter values
np.sqrt(mean_squared_error(optimal_params.best_estimator_.predict(Xtest),ytest))
```

```
5254.902079026533
```

It takes 2 minutes to tune CatBoost, which is higher than LightGBM and lesser than XGBoost. CatBoost falls in between LightGBM and XGBoost in terms of speed. However, it is likely to be more accurate than XGBoost and LighGBM, and likely to require lesser tuning as compared to XGBoost.

Part III

Assignments

14 Assignment 1

Instructions

1. You may talk to a friend, discuss the questions and potential directions for solving them. However, you need to write your own solutions and code separately, and not as a group activity.

2. Write your code in the **Code cells** and your answers in the **Markdown cells** of the Jupyter notebook. Ensure that the solution is written neatly enough to for the graders to understand and follow.

3. Use Quarto to render the **.ipynb** file as HTML. You will need to open the command prompt, navigate to the directory containing the file, and use the command: `quarto render filename.ipynb --to html`. Submit the HTML file.

4. The assignment is worth 100 points, and is due on **Thursday, 11th April 2024 at 11:59 pm**.

5. **Five points are properly formatting the assignment**. The breakdown is as follows:

   - Must be an HTML file rendered using Quarto **(2 points)**. *If you have a Quarto issue, you must mention the issue & quote the error you get when rendering using Quarto in the comments section of Canvas, and submit the ipynb file.*
   - There aren't excessively long outputs of extraneous information (e.g. no printouts of entire data frames without good reason, there aren't long printouts of which iteration a loop is on, there aren't long sections of commented-out code, etc.) **(1 point)**
   - Final answers to each question are written in the Markdown cells. **(1 point)**
   - There is no piece of unnecessary / redundant code, and no unnecessary / redundant text. **(1 point)**

14.1 1) Bias-Variance Trade-off for Regression (32 points)

The main goal of this question is to understand and visualize the bias-variance trade-off in a regression model by performing repetitive simulations.

The conceptual clarity about bias and variance will help with the main logic behind creating many models that will come up later in the course.

14.1.1 a)

First, you need to implement the underlying function of the population you want to sample data from. Assume that the function is the Bukin function. Implement it as a user-defined function and run it with the test cases below to make sure it is implemented correctly. **(3 points)**

Note: It would be more useful to have only one input to the function. You can treat the input as an array of two elements.

```
print(Bukin(np.array([1,2]))) # The output should be 141.177
print(Bukin(np.array([6,-4]))) # The output should be 208.966
print(Bukin(np.array([0,1]))) # The output should be 100.1
```

14.1.2 b)

Using the following assumptions, sample a test dataset with 100 observations from the underlying function. Remember how the test dataset is supposed to be sampled for bias-variance calculations. **No loops are allowed for this question - .apply should be very useful and actually simpler to use. (4 points)**

Assumptions:

- The first predictor, x_1, comes from a uniform distribution between -15 and -5. ($U[-15,-5]$)
- The second predictor, x_2, comes from a uniform distribution between -3 and 3. ($U[-3,3]$)
- Use `np.random.seed(100)` for reproducibility.

14.1.3 c)

Create an empty DataFrame with columns named **degree**, **bias_sq** and **var**. This will be useful to store the analysis results in this question. **(1 point)**

14.1.4 d)

Sample 100 training datasets to calculate the bias and the variance of a Linear Regression model that predicts data coming from the underlying Bukin function. You need to repeat this process with polynomial transformations from degree 1 (which is the original predictors) to degree 7. For each degree, store the degree, bias-squared and variance values in the DataFrame. **(15 points)**

Note:

- For a linear regression model, bias refers to squared bias
- Assume that the noise in the population is a zero-mean Gaussian with a standard deviation of 10. ($N(0, 10)$)
- Keep the training data size the same as the test data size.
- You need both the interactions and the higher-order transformations in your polynomial predictors.
- For i^{th} training dataset, you can consider using `np.random.seed(i)` for reproducibility.

14.1.5 e)

Using the results stored in the DataFrame, plot the (1) expected mean squared error, (2) expected squared bias, (3) expected variance, and (4) the expected sum of squared bias, variance and noise variance *(i.e., summation of 2, 3, and noise variance)*, against the degree of the predictors in the model. **(5 points)**

Make sure you add a legend to label the four lineplots. **(1 point)**

14.1.6 f)

What is the degree of the optimal model? **(1 point)** What are the squared bias, variance and mean squared error for that degree? **(2 points)**

14.2 2) Low-Bias-Low-Variance Model via Regularization (25 points)

The main goal of this question is to further reduce the total error by regularization - in other words, to implement the low-bias-low-variance model for the underlying function and the data coming from it.

14.2.1 a)

First of all, explain why it is not guaranteed for the optimal model (with the optimal degree) in Question 1 to be the low-bias-low-variance model. **(2 points)** Why would regularization be necessary to achieve that model? **(2 points)**

14.2.2 b)

Before repeating the process in Question 1, you should see from the figure in 1e and the results in 1f that there is no point in trying some degrees again with regularization. Find out these degrees and explain why you should not use them for this question, **considering how regularization affects the bias and the variance of a model. (3 points)**

14.2.3 c)

Repeat 1c and 1d with Ridge regularization. **Exclude the degrees you found in 2b and also degree 7**. Use Leave-One-Out (LOO) cross-validation (CV) to tune the model hyperparameter and use `neg_root_mean_squared_error` as the scoring metric. **(7 points)**

Consider hyperparamter values in the range [1, 100].

14.2.4 d)

Repeat part 1e with Ridge regularization, using the results from 2c. **(2 points)**

14.2.5 e)

What is the degree of the optimal Ridge Regression model? **(1 point)** What are the bias-squared, variance and total error values for that degree? **(1 point)** How do they compare to the Linear Regression model results? **(2 points)**

14.2.6 f)

Is the regularization successful in reducing the total error of the regression model? **(2 points)** Explain the results in 2e in terms of how bias and variance change with regularization. **(3 points)**

14.3 3) Bias-Variance Trade-off for Classification (38 points)

Now, it is time to understand and visualize the bias-variance trade-off in a classification model. As we covered in class, the error calculations for classification are different than regression, so it is necessary to understand the bias-variance analysis for classification as well.

First of all, you need to visualize the underlying boundary between the classes in the population. Run the given code that implements the following:

- 2000 test observations are sampled from a population with two predictors.
- Each predictor is uniformly distributed between -15 and 15. ($U[-15, 15]$)
- The underlying boundary between the classes is a circle with radius 10.
- The noise in the population is a 30% chance that the observation is misclassified.

```
# Number of observations
n = 2000

np.random.seed(111)

# Test predictors
x1 = np.random.uniform(-15, 15, n)
x2 = np.random.uniform(-15, 15, n)
X_test = pd.DataFrame({'x1': x1, 'x2': x2})

# Underlying boundary
boundary = (x1**2) + (x2**2)

# Test response (no noise!)
y_test_wo_noise = (boundary < 100).astype(int)

# Test response with noise (for comparison)
noise_prob = 0.3
num_noisy_obs = int(noise_prob*n)

y_test_w_noise = y_test_wo_noise.copy()
noise_indices = np.random.choice(range(len(y_test_w_noise)), num_noisy_obs, replace = False)
y_test_w_noise[noise_indices] = 1 - y_test_wo_noise[noise_indices]
```

```
sns.scatterplot(x = x1, y = x2, hue=y_test_wo_noise)
plt.title('Sample without the noise')
plt.show()
```

```
<IPython.core.display.Image object>
```

```
sns.scatterplot(x = x1, y = x2, hue=y_test_w_noise)
plt.title('Sample with the noise')
plt.show()
```

```
<IPython.core.display.Image object>
```

14.3.1 a)

Create an empty DataFrame with columns named **K**, **bias**, **var** and **noise**. This will be useful to store the analysis results in this question. **(1 point)**

14.3.2 b)

Sample 100 training datasets to calculate the bias and the variance of a K-Nearest Neighbors (KNN) Classifier that predicts data coming from the population with the circular underlying boundary. You need to repeat this process with a K value **from 10 to 150, with a stepsize of 10**. For each K, store the following values in the DataFrame:

(1) K,

(2) bias,

(3) variance,

(4) expected loss computed directly using the true response and predictions,

(5) expected loss computed as (expected Bias) + (c_2 expected variance) + (c_1 expected noise)

(20 points)

Note:

- Keep the training data size the same as the test data size.
- The given code should help you both with sampling the training data and adding noise to the training responses.
- For i^{th} training dataset, you can consider using `np.random.seed(i)` for reproducibility.
- To check the progress of the code while running, a simple but efficient method is to add a `print(K)` line in the loop.

14.3.3 c)

Using the results stored in the DataFrame, plot the bias and the variance against the K value on one figure, and the expected loss (computed directly) & expected loss computed as (expected Bias) + ($c_2$expected variance) + ($c_1$expected noise) against the K value **on a separate figure**. **(5 points)** Make sure you add a legend to label the lineplots in the first figure. **(1 point)**

14.3.4 d)

What is the K of the optimal model? **(1 point)** What are the bias, variance and expected loss (computed either way) for that K? **(2 points)**

14.3.5 e)

In part c, you should see the variance leveling off after a certain K value. Explain why this is the case, considering the effect of the K value on a KNN model. **(2 points)**

14.3.6 f)

Lastly, visualize the decision boundary of a KNN Classifier with **high-bias-low-variance (option 1)** and **low-bias-high-variance (option 2)**, using data from the same population.

- For each option, pick a K value (1 and 90 would be good numbers.) **You are expected to know which number belongs to which option.**
- Sample a training dataset. (Use `np.random.seed(1)`.)
- Using the training dataset, train a KNN model with the K value you picked.
- The rest of the code is given below for you.

Note that you need to produce two figures. **(2x2 = 4 points)** Put titles on the figures to describe which figure is which option. **(2 points)**

```
# Develop and save the model as the 'model' object before using the code
xx, yy = np.meshgrid(np.linspace(-15, 15, 100), np.linspace(-15, 15, 100))
Z = model.predict(np.c_[xx.ravel(), yy.ravel()])
Z = Z.reshape(xx.shape)
sns.scatterplot(x = x1, y = x2, hue=y_train, legend=False);
plt.contour(xx, yy, Z, levels=[0.5], linewidths=2)

plt.title('____-bias-____-variance Model')
```

15 Assignment 2 (Section 21)

Instructions

1. You may talk to a friend, discuss the questions and potential directions for solving them. However, you need to write your own solutions and code separately, and not as a group activity.
2. Write your code in the **Code cells** and your answers in the **Markdown cells** of the Jupyter notebook. Ensure that the solution is written neatly enough to for the graders to understand and follow.
3. Use Quarto to render the **.ipynb** file as HTML. You will need to open the command prompt, navigate to the directory containing the file, and use the command: `quarto render filename.ipynb --to html`. Submit the HTML file.
4. The assignment is worth 100 points, and is due on **Monday, 22nd April 2024 at 11:59 pm**.
5. **Five points are properly formatting the assignment**. The breakdown is as follows:
   - Must be an HTML file rendered using Quarto **(2 points)**. *If you have a Quarto issue, you must mention the issue & quote the error you get when rendering using Quarto in the comments section of Canvas, and submit the ipynb file.*
   - There aren't excessively long outputs of extraneous information (e.g. no printouts of entire data frames without good reason, there aren't long printouts of which iteration a loop is on, there aren't long sections of commented-out code, etc.) **(1 point)**
   - Final answers to each question are written in the Markdown cells. **(1 point)**
   - There is no piece of unnecessary / redundant code, and no unnecessary / redundant text. **(1 point)**

15.1 1) Tuning a KNN Classifier with Sklearn Tools (40 points)

In this question, you will use **classification_data.csv**. Each row is a loan and the each column represents some financial information as follows:

- `hi_int_prncp_pd`: Indicates if a high percentage of the repayments went to interest rather than principal. **This is the classification response.**
- `out_prncp_inv`: Remaining outstanding principal for portion of total amount funded by investors
- `loan_amnt`: The listed amount of the loan applied for by the borrower. If at some point in time, the credit department reduces the loan amount, then it will be reflected in this value.
- `int_rate`: Interest Rate on the loan
- `term`: The number of payments on the loan. Values are in months and can be either 36 or 60.
- `mort_acc`: The number of mortgage accounts
- `application_type_Individual`: 1 if the loan is an individual application or a joint application with two co-borrowers
- `tot_cur_bal`: Total current balance of all accounts
- `pub_rec`: Number of derogatory public records

As indicated above, `hi_int_prncp_pd` is the response and all the remaining columns are predictors. You will tune and train a K-Nearest Neighbors (KNN) classifier throughout this question.

15.1.1 1a)

Read the dataset. Create the predictor and the response variables.

Create the training and the test data with the following specifications: - The split should be 75%-25%. - You need to ensure that the class ratio is preserved in the training and the test datasets. i.e. **the data is stratified.** - Use `random_state=45`.

Print the class ratios of the entire dataset, the training set and the test set to check if the ratio is kept the same.

(1 point)

15.1.2 1b)

Scale the datasets. The data is ready for modeling at this point.

Before creating and tuning a model, you need to create a sklearn cross-validation object to ensure the most accurate representation of the data among all the folds.

Use the following specifications for your cross-validation settings: - Make sure the data is stratified in all the folds *(Use `StratifiedKFold()`)*. - Use 5 folds. - Shuffle the data for more randomness. - Use `random_state=14`.

(1 point)

Note that you need to use these settings for the rest of this question (Q1) for consistency.

Cross-validate a KNN Classifier with the following specifications: - Use every odd K value between 1 and 50. (including 1) - Fix the weights at "uniform", which is default. - Use the cv object you created in part 1(c). - Use accuracy as metric.

(4 points)

Print the best average cross-validation accuracy and the K value that corresponds to it. *(2 points)*

15.1.3 1c)

Using the optimal K value you found in part 1(b), find the threshold that maximizes the cross-validation accuracy with the following specifications:

- Use all the possible threshold values with a stepsize of 0.01.
- Use the cross-validation settings you created in part f.
- Use accuracy as metric, which is default.

(4 points)

Print the best cross-validation accuracy *(1 point)* and the threshold value that corresponds to it. *(1 points)*

15.1.4 1d)

Is the method we used in parts 1(b) and 1(c) guaranteed to find the best K & threshold combination, i.e. tune the classifier to its best values? *(1 point)* Why or why not? *(1 point)*

15.1.5 1e)

Use the tuned classifier and threshold to find the test accuracy. *(2 points)* .

How does it compare to the cross-validation accuracy, i.e. is the model generalizing well? *(1 point)*

15.1.6 1f)

Now, you need to tune K and the threshold **at the same time**. Use the following specifications: - Use every odd K value between 1 and 50. (including 1) - Fix the weights at "uniform". - Use all the possible threshold values with a stepsize of 0.01. - Use accuracy as metric.

(5 points)

Print the best cross-validation accuracy, and the K and threshold values that correspond to it. *(1 point)*

15.1.7 1g)

How does the best cross-validation accuracy in part 1(f) compare to parts 1(b) and 1(c)? *(1 point)* Did the K and threshold value change? *(1 point)* Explain why or why not. *(2 points)*

15.1.8 1h)

Use the tuned classifier and threshold from part 1(f) to find the test accuracy. *(1 point)*

15.1.9 1i)

Compare the methods you used in parts 1(b) & 1(c) with the method you used in part 1(f) in terms of computational power. How many K & threshold pairs did you try in both? *(2 points)* Combining your answer with the answer in part 1(i), explain the main trade-off while tuning a model. *(2 points)*

15.1.10 1j)

Cross-validate a KNN classifier with the following specifications: - Use every odd K value between 1 and 50. (including 1) - Fix the weights at "uniform" - Use accuracy, precision and recall as three metrics **at the same time.**

Find the K value that maximizes recall **while having a precision above 75%.** *(3 points)* Print the average cross-validation results of that K value. *(1 point)*

Which metric *(among precision, recall, and accuracy)* seems to be the least sensitive to the value of 'K'. Why? *(3 points)*

15.2 2) Tuning a KNN Regressor with Sklearn Tools (55 points)

In this question, you will use **bank_loan_train_data.csv** to tune *(the model hyperparameters)* and train the model. Each row is a loan and the each column represents some financial information as follows:

- `money_made_inv`: Indicates the amount of money made by the bank on the loan. **This is the regression response.**
- `out_prncp_inv`: Remaining outstanding principal for portion of total amount funded by investors
- `loan_amnt`: The listed amount of the loan applied for by the borrower. If at some point in time, the credit department reduces the loan amount, then it will be reflected in this value.
- `int_rate`: Interest Rate on the loan
- `term`: The number of payments on the loan. Values are in months and can be either 36 or 60
- `mort_acc`: The number of mortgage accounts
- `application_type_Individual`: 1 if the loan is an individual application or a joint application with two co-borrowers
- `tot_cur_bal`: Total current balance of all accounts
- `pub_rec`: Number of derogatory public records

As indicated above, `money_made_inv` is the response and all the remaining columns are predictors. You will tune and train a K-Nearest Neighbors (KNN) regressor throughout this question.

15.2.1 2a)

Find the optimal hyperparameter values and the corresponging optimal cross-validated RMSE. The hyperparameters that you must consider are

1. Number of nearest neighbors,
2. Weight of the neighbor, and
3. the power `p` of the Minkowski distance.

For the `weights` hyperparameter, in addition to `uniform` and `distance`, consider 3 custom weights as well. The custom weights to consider are weight inversely proportional to distance squared, weight inversely proportional to distance cube, and weight inversely proportional to distance raised to the power of 4. Mathematically, these weights can be written as:

$weight \propto 1$,

$weight \propto \frac{1}{distance}$,

$weight \propto \frac{1}{distance^2}$

$weight \propto \frac{1}{distance^3}$

$weight \propto \frac{1}{distance^4}$

Show all the 3 search approaches - grid search, random search, and Bayes search. As this is a simple problem, all the 3 approaches should yield the same result.

For Bayes search, show the implementation of real-time monitoring of cross-validation error.

None of the cross-validation approaches should take more than a minute as this is a simlpe problem.

Hint:

Create three different user-defined functions. The functions should take **one input**, named **distance** and return `1/(1e-10+distance**n)`, where n is 2, 3, and 4, respectively. Note that the `1e-10` is to avoid computational overflow.

Name your functions, `dist_power_n`, where n is 2, 3, and 4, respectively. You can use these function names as the weights input to a KNN model.

(15 points)

15.2.2 2b)

Based on the optimal model in 2(a), find the RMSE on test data *(bank_loan_test_data.csv)*. It must be less than $1400.

Note: You will achieve the test RMSE if you tuned the hyperparameters well in 2(a). If you did not, redo 2(a). You are not allowed to use test data for tuning the hyperparameter values.

(2 points)

15.2.3 2c)

KNN performance may deteriorate significantly if irrelevant predictors are included. We'll add variable selection as well in the cross-validation procedure along with tuning of the hyperparameters for those variables.

Use a variable selection method to consider the best 'r' predictors, optimize the hyperparameters specified in 2(a), and compute the cross-validation error for those 'r' predictors. Note that 'r' will vary from 1 to 7, thus you will need to do 7 cross-validations - one for each 'r'.

Report the optimal value of 'r', the 'r' predictors, the optimal hyperparameter values, and the optimal cross-validated RMSE.

You are free to use any search method.

Hint: You may use Lasso to consider the best 'r' predictors as that is the only variable selection you have learned so far.

(20 points)

15.2.4 2d)

Find the RMSE on test data based on the optimal model in 2(c). Your test RMSE must be less than $800.

Note: You will achieve the test RMSE if you tuned the hyperparameters well in 2(c). If you did not, redo 2(c). You are not allowed to use test data for tuning the hyperparameter values.

(2 points)

15.2.5 2e)

How did you decide the range of hyperparameter values to consider in this question? Discuss for `p` and `n_neighbors`.

(4 points)

15.2.6 2f)

Is it possible to futher improve the results if we also optimize the `metric` hyperparameter along with the hyperparameters specified in 2(a)? Why or why not?

(4 points)

15.2.7 2g)

What is the benefit of using the `RepeatedKFold()` function over the `KFold()` function of the `model_selection` module of the `sklearn` library? Explain in terms of bias-variance of test error. Did you observe any benefit of using `RepeatedKFold()` over `KFold()` in Q2? Why or why not?

(4 + 4 points)

16 Assignment 3 (Sections 21 & 22)

Instructions

1. You may talk to a friend, discuss the questions and potential directions for solving them. However, you need to write your own solutions and code separately, and not as a group activity.
2. Write your code in the *Code* cells and your answer in the *Markdown* cells of the Jupyter notebook. Ensure that the solution is written neatly enough to understand and grade.
3. Use Quarto to print the *.ipynb* file as HTML. You will need to open the command prompt, navigate to the directory containing the file, and use the command: `quarto render filename.ipynb --to html`. Submit the HTML file.
4. The assignment is worth 100 points, and is due on **Wednesday, 8th May 2024 at 11:59 pm**.
5. **Five points are properly formatting the assignment**. The breakdown is as follows:

- Must be an HTML file rendered using Quarto (2 pts). *If you have a Quarto issue, you must mention the issue & quote the error you get when rendering using Quarto in the comments section of Canvas, and submit the ipynb file. If your issue doesn't seem genuine, you will lose points.*
- There aren't excessively long outputs of extraneous information (e.g. no printouts of entire data frames without good reason, there aren't long printouts of which iteration a loop is on, there aren't long sections of commented-out code, etc.) (1 pt)
- Final answers of each question are written in Markdown cells (1 pt).
- There is no piece of unnecessary / redundant code, and no unnecessary / redundant text (1 pt)

16.1 1) Regression Problem - Miami housing

16.1.1 1a) Data preparation

Read the data *miami-housing.csv*. Check the description of the variables here. Split the data into 60% train and 40% test. Use `random_state = 45`. The response is `SALE_PRC`, and the rest of the columns are predictors, except `PARCELNO`. Print the shape of the predictors dataframe of the train data.

(2 points)

16.1.2 1b) Decision tree

Develop a decision tree model to predict `SALE_PRC` based on all the predictors. Use `random_state = 45`. Use the default hyperparameter values. What is the MAE (mean absolute error) on test data, and the cross-validated MAE?

(3 points)

16.1.3 1c) Tuning decision tree

Tune the hyperparameters of the decision tree model developed in the previous question, and compute the MAE on test data. You must tune the hyperparameters in the following manner:

The cross-validated MAE obtained must be less than $68,000. You must show the optimal values of the hyperparameters obtained, and the find the test MAE with the tuned model.

Hint:

1. BayesSearchCV() may take less than a minute with `max_depth` and `max_features`
2. You are free to decide which hyperparameters to tune.

(9 points)

16.1.4 1d) Bagging decision trees

Bag decision trees, and compute the out-of-bag MAE. Use enough number of trees, such that the MAE stabilizes. Other than `n_estimators`, use default values of hyperparameters.

The out-of-bag cross-validated MAE must be less than $48,000.

(4 points)

16.1.5 1e) Bagging without bootstrapping

Bag decision trees without bootstrapping, i.e., put `bootstrap = False` while bagging the trees, and compute the cross-valdiated MAE. Why is the MAE obtained much higher than that in the previous question, but lower than that obtained in 1(b)?

(1 point for code, 3 + 3 points for reasoning)

16.1.6 1f) Bagging without bootstrapping samples, but bootstrapping features

Bag decision trees without bootstrapping samplse, but bootstrapping features, i.e., put `bootstrap = False`, and `bootstrap_features = True` while bagging the trees, and compute the cross-validated MAE. Why is the MAE obtained much lower than that in the previous question?

(1 point for code, 3 points for reasoning)

16.1.7 1g) Tuning bagged tree model

16.1.7.1 1g)i) Approaches

There are two approaches for tuning a bagged tree model:

1. Out of bag prediction
2. K-fold cross validation using `GridSearchCV`.

What is the advantage of each approach over the other, i.e., what is the advantage of the out-of-bag approach over K-fold cross validation, and what is the advantage of K-fold cross validation over the out-of-bag approach?

(3 + 3 points)

16.1.7.2 1g)ii) Tuning the hyperparameters

Tune the hyperparameters of the bagged tree model developed in 1(d). You may use either of the approaches mentioned in the previous question. Show the optimal values of the hyperparameters obtained. Compute the MAE on test data with the tuned model. Your cross-validated MAE must be less than the cross-validate MAE ontained in the previous question.

It is up to you to pick the hyperparameters and their values in the grid.

Hint:

`GridSearchCV()` may work better than `BayesSearchCV()` in this case. Why?

(9 points)

16.1.8 1h) Random forest

16.1.8.1 1h)(i) Tuning random forest

Tune a random forest model to predict `SALE_PRC`, and compute the MAE on test data. The cross-validated MAE must be less than $46,000.

It is up to you to pick the hyperparameters and their values in the grid.

Hint: OOB approach will take less than a minute.

(9 points)

16.1.8.2 1h)(ii) Feature importance

Arrange and print the predictors in decreasing order of importance.

(4 points)

16.1.8.3 1h)(iii) Feature selection

Drop the least important predictor, and find the cross-validated MAE of the tuned model again. You may need to adjust the `max_features` hyperparameter to account for the dropped predictor. Did the cross-validate MAE reduce?

(4 points)

16.1.8.4 1h)(iv) Random forest vs bagging: `max_features`

Note that the `max_features` hyperparameter is there both in the `RandomForestRegressor()` function and the `BaggingRegressor()` function. Does it have the same meaning in both the functions? If not, then what is the difference?

Hint: Check scikit-learn documentation

(1 + 3 points)

16.2 2) Classification - Term deposit

The data for this question is related with direct marketing campaigns of a Portuguese banking institution. The marketing campaigns were based on phone calls, where bank clients were called to subscribe for a term deposit.

There is a train data - *train.csv*, which you will use to develop a model. There is a test data - *test.csv*, which you will use to test your model. Each dataset has the following attributes about the clients called in the marketing campaign:

1. `age`: Age of the client
2. `education`: Education level of the client
3. `day`: Day of the month the call is made
4. `month`: Month of the call
5. `y`: did the client subscribe to a term deposit?
6. `duration`: Call duration, in seconds. This attribute highly affects the output target (e.g., if `duration`=0 then `y`='no'). Yet, the duration is not known before a call is performed. Also, after the end of the call `y` is obviously known. Thus, this input should only be included for inference purposes and should be discarded if the intention is to have a realistic predictive model.

(Raw data source: Source. Do not use the raw data source for this assignment. It is just for reference.)

16.2.1 2a) Data preparation

Convert all the categorical predictors in the data to dummy variables. Note that `month` and `education` are categorical variables.

(2 points)

16.2.2 2b) Random forest

Develop and tune a **random forest model** to predict the probability of a client subscribing to a term deposit based on `age`, `education`, `day` and `month`. The model must have:

(a) **Minimum overall classification accuracy of 75%** among the classification accuracies on *train.csv*, and *test.csv*.

(b) **Minimum recall of 60%** among the recall on *train.csv*, and *test.csv*.

Print the accuracy and recall for both the datasets - *train.csv*, and *test.csv*.

Note that:

i. You cannot use `duration` as a predictor. The predictor is not useful for prediction because its value is determined after the marketing call ends. However, after the call ends, we already know whether the client responded positively or negatively.

ii. You are free to choose any value of threshold probability for classifying observations. However, you must use the same threshold on both the datasets.

iii. Use cross-validation on train data to optimize the model hyperparameters.

iv. Using the optimal model hyperparameters obtained in (iii), develop the decision tree model. Plot the cross-validated accuracy and recall against decision threshold probability. Tune the decision threshold probability based on the plot, or the data underlying the plot to achieve the required trade-off between recall and accuracy.

v. Evaluate the accuracy and recall of the developed model with the tuned decision threshold probability on both the datasets. Note that the test dataset must only be used to evaluate performance metrics, and not optimize any hyperparameters or decision threshold probability.

(22 points - 8 points for tuning the hyperparameters, 5 points for making the plot, 5 points for tuning the decision threshold probability based on the plot, and 4 points for printing the accuracy & recall on both the datasets)

Hint:

1. Restrict the search for `max_depth` to a maximum of 25, and `max_leaf_nodes` to a maximum of 45. Without this restriction, you may get a better recall for threshold probability = 0.5, but are likely to get a worse trade-off between recall and accuracy. Tune `max_features`, `max_depth`, and `max_leaf_nodes` with OOB cross-validation.

2. Use `oob_decision_function_` for OOB cross-validated probabilities.

It is up to you to pick the hyperparameters and their values in the grid.

16.3 3) Predictor transformations in trees

Can a non-linear monotonic transformation of predictors (such as *log(), sqrt()* etc.) be useful in improving the accuracy of decision tree models?

(4 points for answer)

A Stratified splitting (classification problem)

A.1 Stratified splitting with respect to response

Q: When splitting data into train and test for developing and assessing a classification model, it is recommended to stratify the split with respect to the response. Why?

A: The main advantage of stratified splitting is that it can help ensure that the training and testing sets have similar distributions of the target variable, which can lead to more accurate and reliable model performance estimates.

In many real-world datasets, the target variable may be imbalanced, meaning that one class is more prevalent than the other(s). For example, in a medical dataset, the majority of patients may not have a particular disease, while only a small fraction may have the disease. If a random split is used to divide the dataset into training and testing sets, there is a risk that the testing set may not have enough samples from the minority class, which can lead to biased model performance estimates.

Stratified splitting addresses this issue by ensuring that both the training and testing sets have similar proportions of the target variable. This can lead to more accurate model performance estimates, especially for imbalanced datasets, by ensuring that the testing set contains enough samples from each class to make reliable predictions.

Another advantage of stratified splitting is that it can help ensure that the model is not overfitting to a particular class. If a random split is used and one class is overrepresented in the training set, the model may learn to predict that class well but perform poorly on the other class(es). Stratified splitting can help ensure that the model is exposed to a representative sample of all classes during training, which can improve its generalization performance on new, unseen data.

In summary, the advantages of stratified splitting are that it can lead to more accurate and reliable model performance estimates, especially for imbalanced datasets, and can help prevent overfitting to a particular class.

A.2 Stratified splitting with respect to response and categorical predictors

Q: Will it be better to stratify the split with respect to the response as well as categorical predictors, instead of only the response? In that case, the train and test datasets will be even more representative of the complete data.

A: It is not recommended to stratify with respect to both the response and categorical predictors simultaneously, while splitting a dataset into train and test, because doing so may result in the test data being very similar to train data, thereby defeating the purpose of assessing the model on unseen data. This kind of a stratified splitting will tend to make the relationships between the response and predictors in train data also appear in test data, which will result in the performance on test data being very similar to that in train data. Thus, in this case, the ability of the model to generalize to new, unseen data won't be assessed by test data.

Therefore, it is generally recommended to only stratify the response variable when splitting the data for model training, and to use random sampling for the predictor variables. This helps to ensure that the model is able to capture the underlying relationships between the predictor variables and the response variable, while still being able to generalize well to new, unseen data.

In the extreme scenario, when there are no continuous predictors, and there are enough observations for stratification with respect to the response and the categorical predictors, the train and test datasets may turn out to be exactly the same. Example 1 below illustrates this scenario.

A.3 Example 1

The example below shows that the train and test data can be exactly the same if we stratify the split with respect to response and the categorical predictors.

```
# Importing necessary libraries
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import train_test_split, cross_val_predict, cross_val_score
from sklearn.metrics import accuracy_score
from itertools import product
sns.set(font_scale=1.35)
```

Let us simulate a dataset with 8 observations, two categorical predictors `x1` and `x2` and the the binary response `y`.

```
#Setting a seed for reproducible results
np.random.seed(9)

# 8 observations
n = 8

#Simulating the categorical predictors
x1 = pd.Series(np.random.randint(0,2,n), name = 'x1')
x2 = pd.Series(np.random.randint(0,2,n), name = 'x2')

#Simulating the response
pr = (x1==1)*0.7+(x2==0)*0.3# + (x3*0.1>0.1)*0.1
y = pd.Series(1*(np.random.uniform(size = n) < pr), name = 'y')

#Defining the predictor object 'X'
X = pd.concat([x1, x2], axis = 1)

#Stratified splitting with respect to the response and predictors to create 50% train and tes
X_train_stratified, X_test_stratified, y_train_stratified,\
y_test_stratified = train_test_split(X, y, test_size = 0.5, random_state = 45, stratify=data

#Train and test data resulting from the above stratified splitting
data_train = pd.concat([X_train_stratified, y_train_stratified], axis = 1)
data_test = pd.concat([X_test_stratified, y_test_stratified], axis = 1)
```

Let us check the train and test datasets created with stratified splitting with respect to both the predictors and the response.

```
data_train
```

	x1	x2	y
2	0	0	1
7	0	1	0
3	1	0	1
1	0	1	0

```
data_test
```

	x1	x2	y
4	0	1	0
6	1	0	1
0	0	1	0
5	0	0	1

Note that the train and test datasets are exactly the same! Stratified splitting tends to have the same proportion of observations corresponding to each strata in both the train and test datasets, where each strata is a unique combination of values of `x1`, `x2`, and `y`. This will tend to make the train and test datasets quite similar!

A.4 Example 2: Simulation results

The example below shows that train and test set performance will tend to be quite similar if we stratify the datasets with respect to the predictors and the response.

We'll simulate a dataset consisting of 1000 observations, 2 categorical predictors `x1` and `x2`, a continuous predictor `x3`, and a binary response `y`.

```
#Setting a seed for reproducible results
np.random.seed(99)

# 1000 Observations
n = 1000

#Simulating categorical predictors x1 and x2
x1 = pd.Series(np.random.randint(0,2,n), name = 'x1')
x2 = pd.Series(np.random.randint(0,2,n), name = 'x2')

#Simulating continuous predictor x3
x3 = pd.Series(np.random.normal(0,1,n), name = 'x3')

#Simulating the response
pr = (x1==1)*0.7+(x2==0)*0.3 + (x3*0.1>0.1)*0.1
y = pd.Series(1*(np.random.uniform(size = n) < pr), name = 'y')

#Defining the predictor object 'X'
X = pd.concat([x1, x2, x3], axis = 1)
```

We'll comparing model performance metrics when the data is split into train and test by performing stratified splitting

1. Only with respect to the response
2. With respect to the response and categorical predictors

We'll perform 1000 simulations, where the data is split using a different seed in each simulation.

```
#Creating an empty dataframe to store simulation results of 1000 simulations
accuracy_iter = pd.DataFrame(columns = {'train_y_stratified','test_y_stratified',
                                        'train_y_CatPredictors_stratified','test_y_CatPredict
```

```
# Comparing model performance metrics when the data is split into train and test by performin
# (1) only with respect to the response
# (2) with respect to the response and categorical predictors

# Stratified splitting is performed 1000 times and the results are compared
for i in np.arange(1,1000):

    #--------Case 1-------------------#
    # Stratified splitting with respect to response only to create train and test data
    X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.2, random_state =
    model = LogisticRegression()
    model.fit(X_train, y_train)

    # Model accuracy on train and test data, with stratification only on response while split
    # the complete data into train and test
    accuracy_iter.loc[(i-1), 'train_y_stratified'] = model.score(X_train, y_train)
    accuracy_iter.loc[(i-1), 'test_y_stratified'] = model.score(X_test, y_test)

    #--------Case 2-------------------#
    # Stratified splitting with respect to response and categorical predictors to create trai
    # and test data
    X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.2, random_state =
                                                        stratify=pd.concat([x1, x2, y], axis
    model.fit(X_train, y_train)

    # Model accuracy on train and test data, with stratification on response and predictors w
    # splitting the complete data into train and test
    accuracy_iter.loc[(i-1), 'train_y_CatPredictors_stratified'] = model.score(X_train, y_tra
    accuracy_iter.loc[(i-1), 'test_y_CatPredictors_stratified'] = model.score(X_test, y_test)
```

```
# Converting accuracy to numeric
accuracy_iter = accuracy_iter.apply(lambda x:x.astype(float), axis = 1)
```

Distribution of train and test accuracies

The table below shows the distribution of train and test accuracies when the data is split into train and test by performing stratified splitting:

1. Only with respect to the response (see `train_y_stratified` and `test_y_stratified`)
2. With respect to the response and categorical predictors (see `train_y_CatPredictors_stratified` and `test_y_CatPredictors_stratified`)

```
accuracy_iter.describe()
```

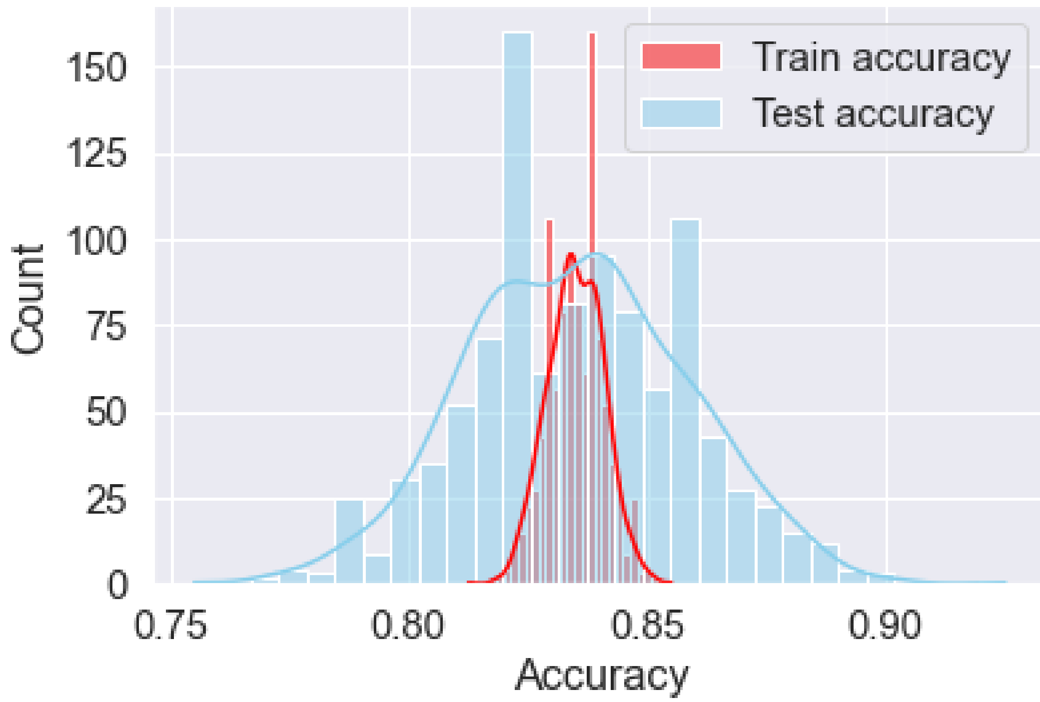
	train_y_stratified	test_y_stratified	train_y_CatPredictors_stratified	test_y_CatPredictors_st
count	999.000000	999.000000	9.990000e+02	9.990000e+02
mean	0.834962	0.835150	8.350000e-01	8.350000e-01
std	0.005833	0.023333	8.552999e-15	8.552999e-15
min	0.812500	0.755000	8.350000e-01	8.350000e-01
25%	0.831250	0.820000	8.350000e-01	8.350000e-01
50%	0.835000	0.835000	8.350000e-01	8.350000e-01
75%	0.838750	0.850000	8.350000e-01	8.350000e-01
max	0.855000	0.925000	8.350000e-01	8.350000e-01

Let us visualize the distribution of these accuracies.

A.4.1 Stratified splitting only with respect to the response

```
sns.histplot(data=accuracy_iter, x="train_y_stratified", color="red", label="Train accuracy"
sns.histplot(data=accuracy_iter, x="test_y_stratified", color="skyblue", label="Test accurac
plt.legend()
plt.xlabel('Accuracy')
```

```
Text(0.5, 0, 'Accuracy')
```

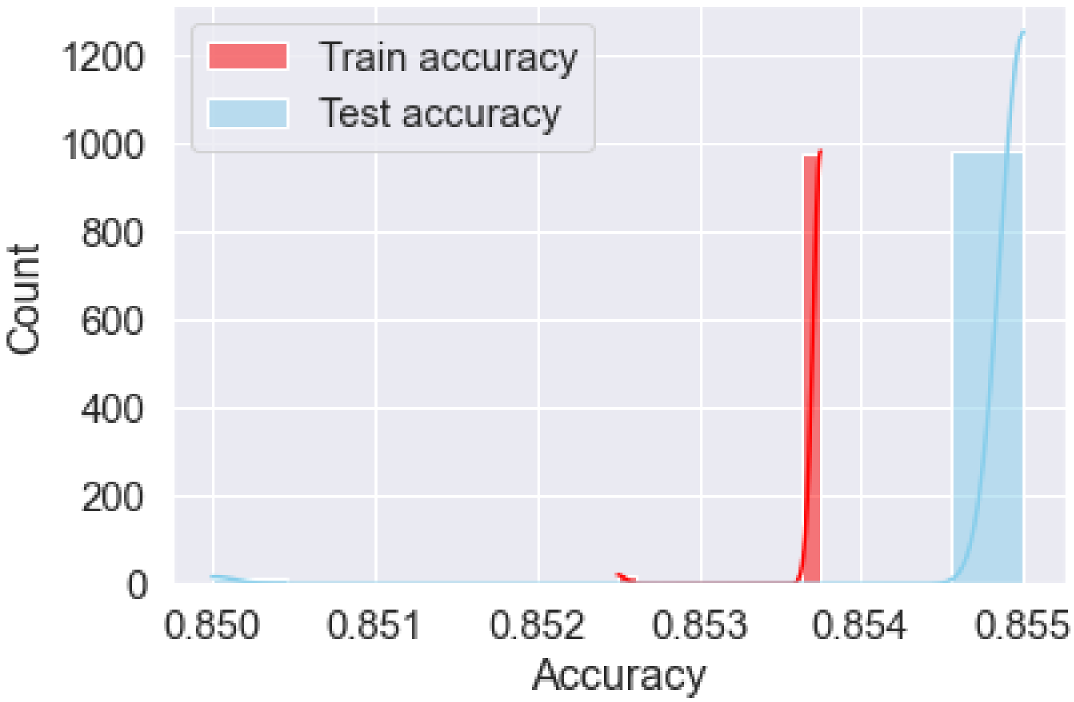


Note the variability in train and test accuracies when the data is stratified only with respect to the response. The train accuracy varies between 81.2% and 85.5%, while the test accuracy varies between 75.5% and 92.5%.

A.4.2 Stratified splitting with respect to the response and categorical predictors

```
sns.histplot(data=accuracy_iter, x="train_y_CatPredictors_stratified", color="red", label="Tr
sns.histplot(data=accuracy_iter, x="test_y_CatPredictors_stratified", color="skyblue", label=
plt.legend()
plt.xlabel('Accuracy')
```

```
Text(0.5, 0, 'Accuracy')
```



The train and test accuracies are between 85% and 85.5% for all the simulations. As a results of stratifying the splitting with respect to both the response and the categorical predictors, the train and test datasets are almost the same because the datasets are engineered to be quite similar, thereby making the test dataset inappropriate for assessing accuracy on unseen data. Thus, it is recommended to stratify the splitting only with respect to the response.

B Parallel processing bonus Q

```
import numpy as np
import pandas as pd
from sklearn.model_selection import train_test_split, cross_val_score, cross_val_predict, \
cross_validate, GridSearchCV, RandomizedSearchCV, KFold, StratifiedKFold, RepeatedKFold, Repe
from sklearn.neighbors import KNeighborsClassifier, KNeighborsRegressor
from sklearn.preprocessing import StandardScaler
from sklearn.metrics import accuracy_score, recall_score, mean_squared_error
from scipy.stats import uniform
from skopt import BayesSearchCV
from skopt.space import Real, Categorical, Integer
import seaborn as sns
from skopt.plots import plot_objective
import matplotlib.pyplot as plt
import warnings
import time as tm
```

```
#Using the same datasets as used for linear regression in STAT303-2,
#so that we can compare the non-linear models with linear regression
trainf = pd.read_csv('./Datasets/Car_features_train.csv')
trainp = pd.read_csv('./Datasets/Car_prices_train.csv')
testf = pd.read_csv('./Datasets/Car_features_test.csv')
testp = pd.read_csv('./Datasets/Car_prices_test.csv')
train = pd.merge(trainf,trainp)
test = pd.merge(testf,testp)
train.head()
predictors = ['mpg', 'engineSize', 'year', 'mileage']
X_train = train[predictors]
y_train = train['price']
X_test = test[predictors]
y_test = test['price']

# Scale
sc = StandardScaler()
```

```
sc.fit(X_train)
X_train_scaled = sc.transform(X_train)
X_test_scaled = sc.transform(X_test)
```

C Case 1: No parallelization

```
time_taken_case1 = []
for i in range(50):
    start_time = tm.time()
    Ks = range(1, 20)
    kfold = KFold(n_splits=5, shuffle=True, random_state=1)
    cross_val_error = []
    for k in Ks:
        cross_val_error.append(-cross_val_score(KNeighborsRegressor(n_neighbors=k),
                            X_train_scaled, y_train, cv = kfold,
                             scoring="neg_root_mean_squared_error").mean())
    time_taken_case1.append(tm.time() - start_time)
```

D Case 2: Parallelization in cross_val_score()

```
time_taken_case2 = []
for i in range(50):
    start_time = tm.time()
    Ks = range(1, 20)
    kfold = KFold(n_splits=5, shuffle=True, random_state=1)
    cross_val_error = []
    for k in Ks:
        cross_val_error.append(-cross_val_score(KNeighborsRegressor(n_neighbors=k),
                                 X_train_scaled, y_train, cv = kfold, n_jobs = -1,
                                           scoring="neg_root_mean_squared_error").mean())
    time_taken_case2.append(tm.time() - start_time)
```

E Case 3: Parallelization in `KNeighborsRegressor()`

```
time_taken_case3 = []
for i in range(50):
    start_time = tm.time()
    Ks = range(1, 20)
    kfold = KFold(n_splits=5, shuffle=True, random_state=1)
    cross_val_error = []
    for k in Ks:
        cross_val_error.append(-cross_val_score(KNeighborsRegressor(n_neighbors=k,
                n_jobs= -1), X_train_scaled, y_train, cv = kfold,
                                  scoring="neg_root_mean_squared_error").mean())
    time_taken_case3.append(tm.time() - start_time)
```

F Case 4: Nested parallelization: Both `cross_val_score()` and `KNeighborsRegressor()`

```
time_taken_case4 = []
for i in range(50):
    start_time = tm.time()
    Ks = range(1, 20)
    kfold = KFold(n_splits=5, shuffle=True, random_state=1)
    cross_val_error = []
    for k in Ks:
        cross_val_error.append(-cross_val_score(KNeighborsRegressor(n_neighbors=k,
                n_jobs= -1), X_train_scaled, y_train, cv = kfold, n_jobs = -1,
                scoring="neg_root_mean_squared_error").mean())
    time_taken_case4.append(tm.time() - start_time)
```

```
sns.boxplot([time_taken_case1, time_taken_case2, time_taken_case3, time_taken_case4])
plt.xticks([0, 1, 2, 3], ['Case 1', 'Case 2', 'Case 3', 'Case 4']);
plt.ylabel('Time');
```

```
<IPython.core.display.Image object>
```

G Q1

Case 1 is without parallelization. Why is Case 3 with parallelization of `KNeighborsRegressor()` taking more time than case 1?

H Q2

If nested parallelization is worse than parallelization, why is case 4 with nested parallelization taking less time than case 3 with parallelization of KNeighborsRegressor()?

I Q3

If nested parallelization is worse than no parallelization, why is case 4 with nested parallelization taking less time than case 1 with no parallelization?

J Q4

If nested parallelization is the best scenario, why is case 4 with nested parallelization taking more time than case 2 with with parallelization in `cross_val_score()`?

K Miscellaneous questions

K.1 Q1

Why is boosting inappropriate for linear Regression, but appropriate for decision trees?

The question has been well answered in the post. The intuitive explanation is that the weighted average of a sequence of linear regression models will also be a single linear regression model. However, if the weighted average of the sequence of linear regression models results in a linear regression model (say `boosted_linear_regression`) that is different from the linear regression model that is obtained by fitting directly to the data (say `regular_linear_regression`), then the `boosted_linear_regression` model will have a higher bias than the `regular_linear_regression` model as the `regular_linear_regression` model minimizes the sum of squared errors (SSE). Thus, the `boosted_linear_regression` model should be the same as the `regular_linear_regression` model for the optimal hyperparameter values of the boosting algorithm. Thus, all the hard-work of tuning the boosting model will at best lead to the linear regression model that can be obtained by fitting a linear regression model directly to the train data!

However, a sequence of shallow regression trees will not lead to the same regression tree that can be developed directly. A sequence of shallow trees will continuously reduce bias with relative less increase in variance. A single decision tree is likely to have a relatively high variance, and thus boosting with shallow trees may provide a better performance. Boosting aims to reduce bias by using low variance models, while a single decision tree has almost zero bias at the cost of having a high variance.

The second response in the post provides a mathematical explanation, which is more convincing.

L Datasets, assignment and project files

Datasets used in the book, assignment files, project files, and prediction problems report tempate can be found here