

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 validation
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 (different ways)
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 large
# 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 different
# of magn., scaling is necessary. This is to enable the training algo. which we did not cover
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 transform
```

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.py:1181:
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=1)
#The 2nd column in the output of predict_proba() consists of the probability of the observation
#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=['Predicted', 'Actual'],
                  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.

```

# 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 greater
# 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 greater
# 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_scaled,
                                         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=['Predicted 0', 'Predicted 1'],
                  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_stratified,
                                              y_train_stratified, cv = 5, method = 'predicted_proba')

    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 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)

# 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 greater
# 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=['P', '1'])
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 decision 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 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)
```

```
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_s  
    cv_scores.append(score)
```

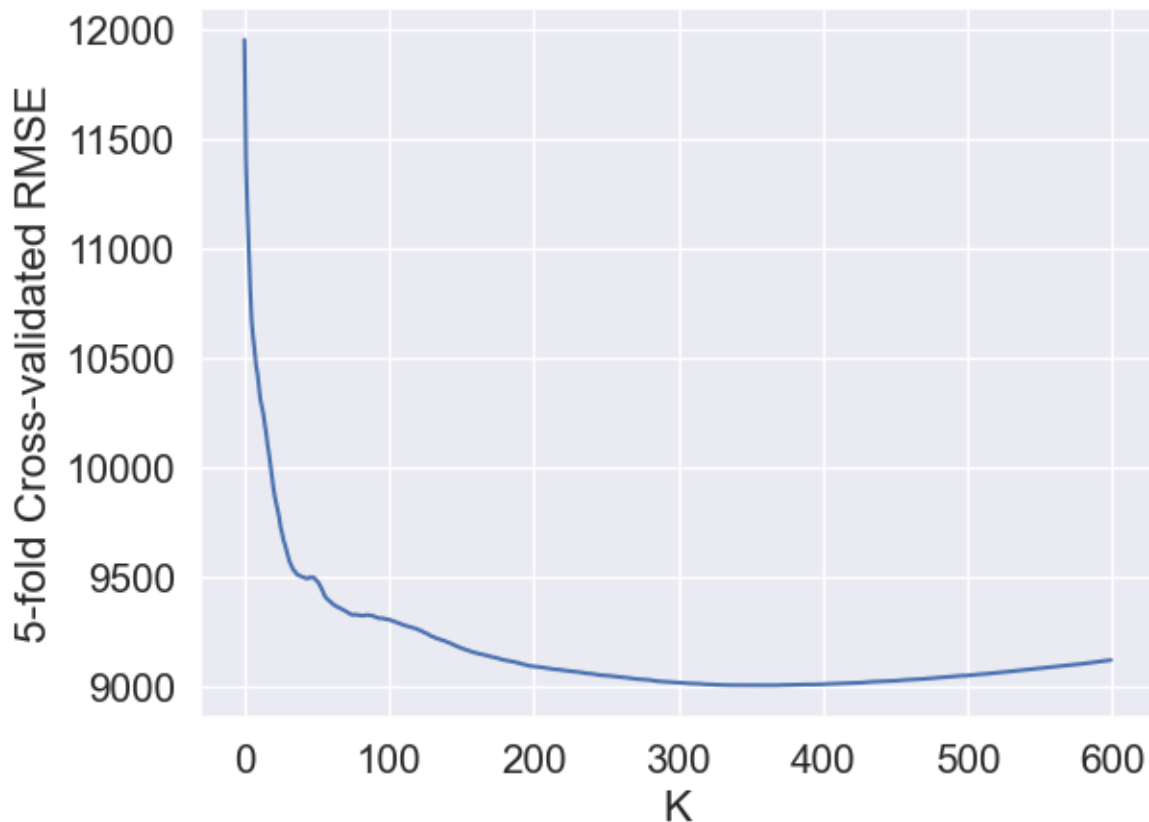
```
np.array(cv_scores).shape  
# Each row is a K
```

```
(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)
```

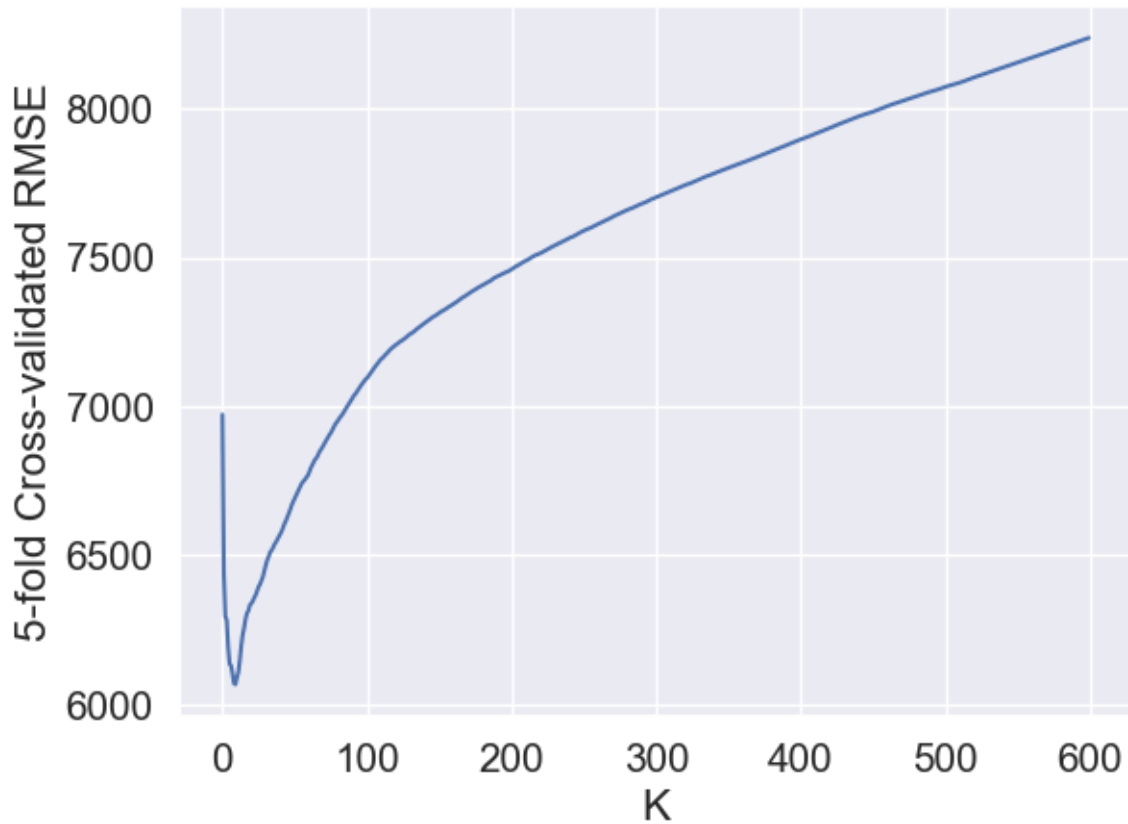
Now, let us again try to find the optimal K for KNN, using the new folds, based on shuffled data.

```
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_mean_squared_error')
    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 v
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_me
```

```
    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 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)
```

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, Rep
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 grid
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, 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 GridSearchCV
gcv = GridSearchCV(model, grid, cv = kfold, scoring = 'neg_root_mean_squared_error', n_jobs=5)

# 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 chapter](#). 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_train_scaled, y_train_scaled)
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_train_scaled, y_train_scaled)
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 computationally 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 hyperparameters

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

# 3) Create the Kfold object (Using RepeatedKfold will be more robust, but more expensive, use it if budget allows)
# 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
gcv = RandomizedSearchCV(model, param_distributions = grid, cv = kfold, n_iter = 180, random_state=10,
                        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 object>,
                                      '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 hyperparameters, 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 distribution 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 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 Diagnosis 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 frequency 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 optimal 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:

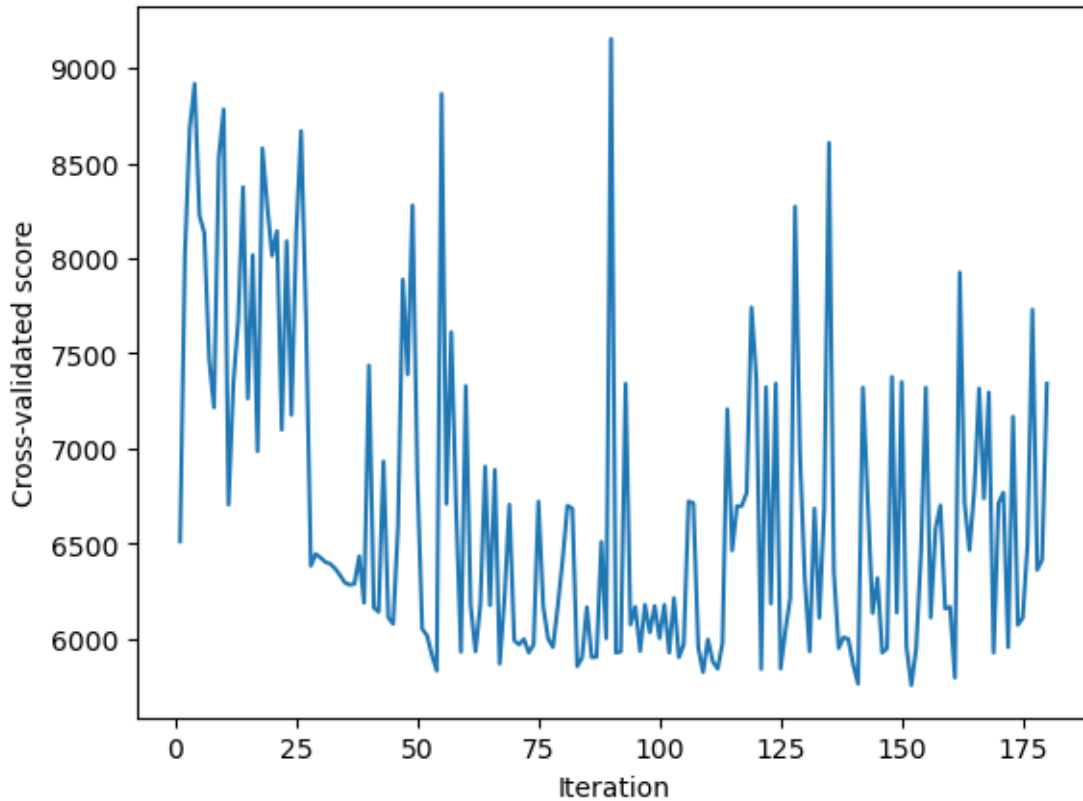
```
gcv.optimizer_results_[0]['x_iters'][53]
```

```
[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 exploiting 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 `BayesSearchCV()` 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', transform='log'),
                              'p': Real(low=1, high=10, prior='uniform', transform='normalize'),
                              'weights': Categorical(categories=('uniform', 'distance'), prior='uniform')})
```

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, stratify=y)
```

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

```
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 = 'precision')  
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 = 'accuracy')  
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

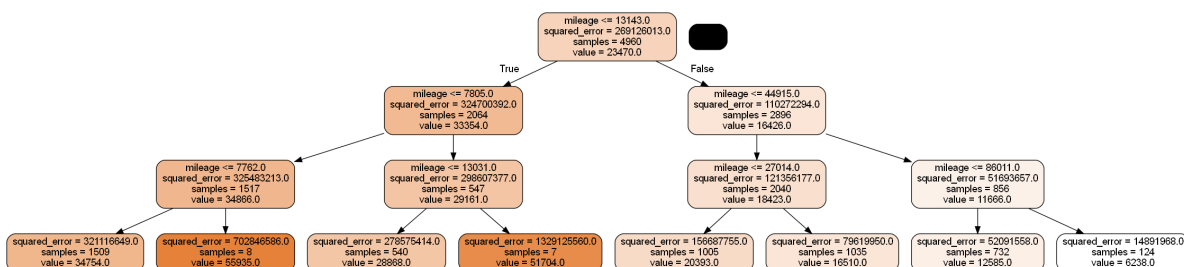
```
X = train['mileage']
y = train['price']
```

```
#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

```

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.

```
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,
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,
                     scoring=['neg_root_mean_squared_error', 'r2'], refit = 'neg_root_mean_squared_error')
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_error))
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,
                    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 optimize 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.DecisionTreeRegressor](https://scikit-learn.org/stable/modules/generated/sklearn.tree.DecisionTreeRegressor.html)*

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 than 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-
```

```
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

```

time = 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 z
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]

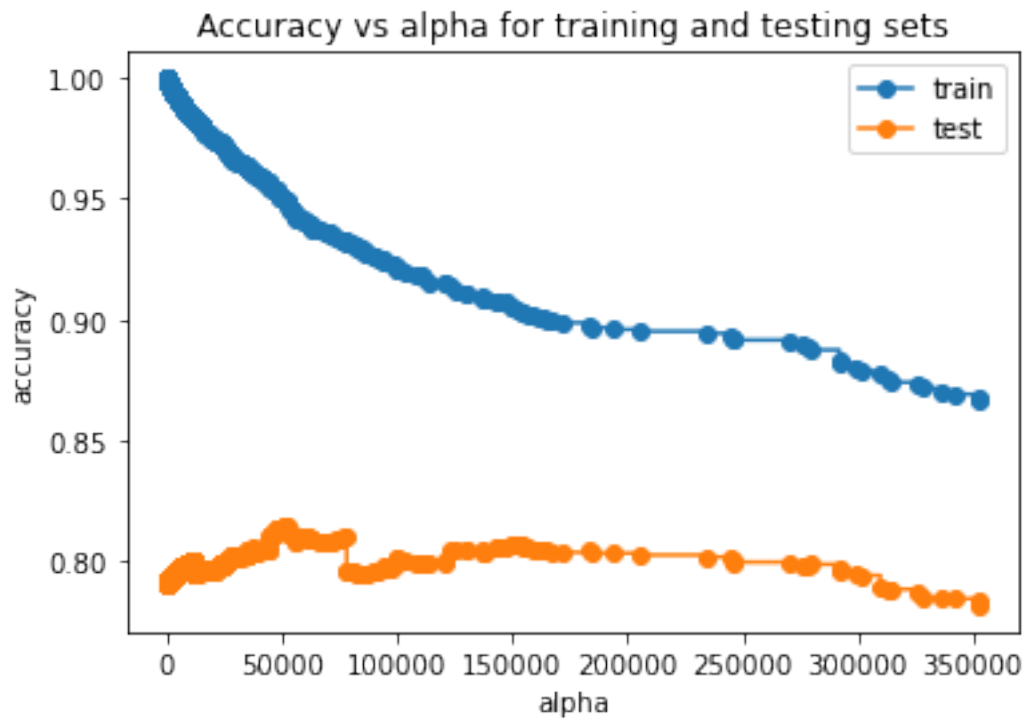
```



```

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-post")
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 nodes (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

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

14

```
#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
                                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.

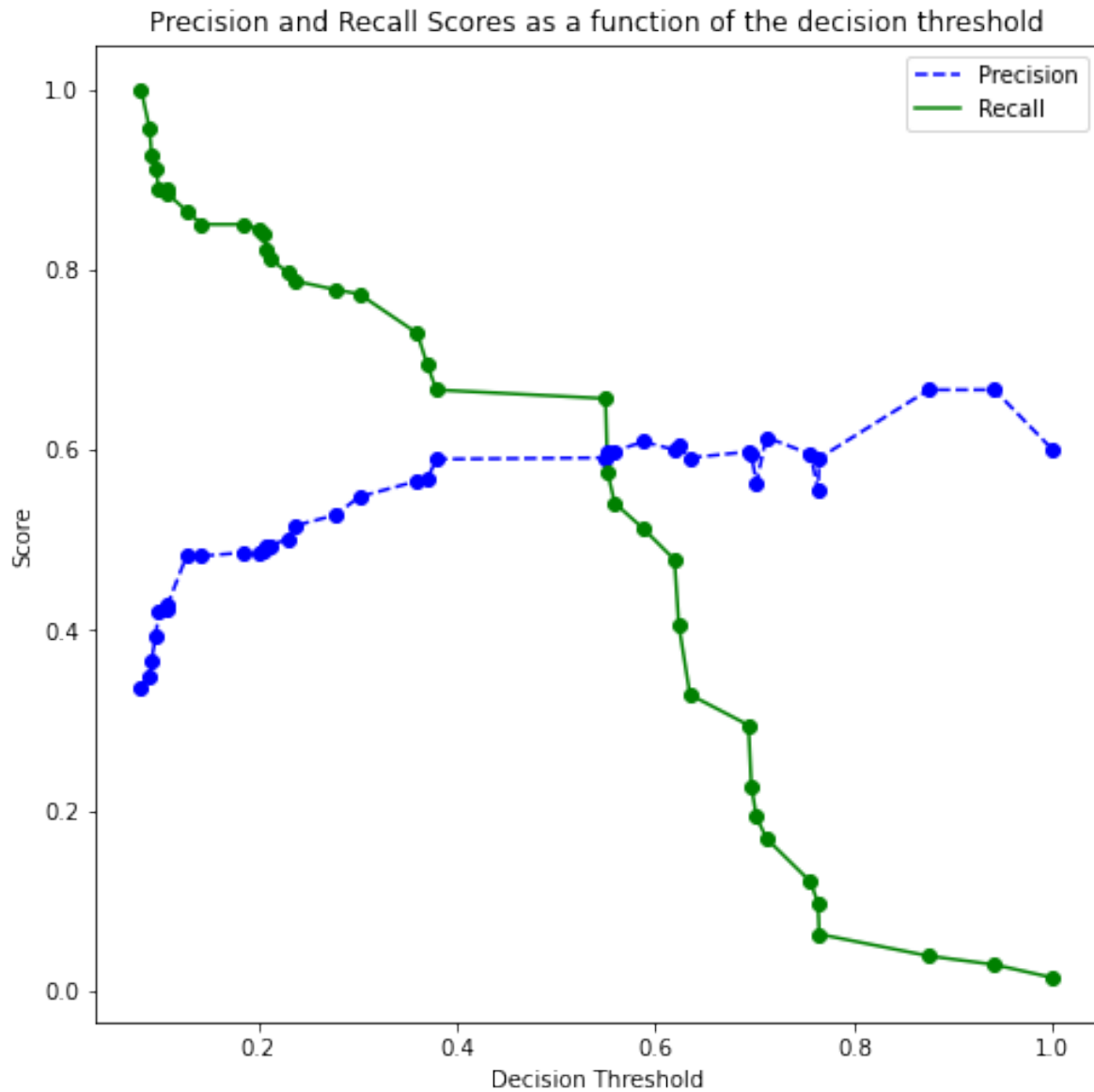
6.3.1 Balancing recall with precision

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 us
# 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 greater
# 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))

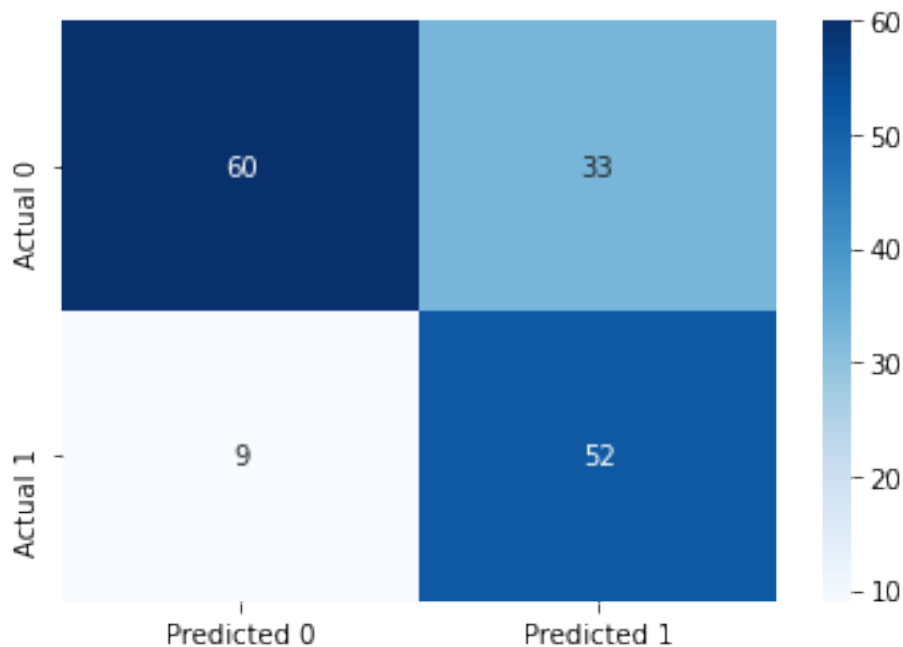
#Confusion matrix
cm = pd.DataFrame(confusion_matrix(ytest, y_pred),
                  columns=['Predicted 0', 'Predicted 1'], index = ['Actual 0', 'Actual 1'])
sns.heatmap(cm, annot=True, cmap='Blues', fmt='g');

```

```

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(-1,1)])
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 decreasing order of FPR,
# the first value will provide the maximum threshold probability for the recall to be more than 80%
# 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 greater
# 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-
```

```
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=10)

grid_search.fit(X, y)
```



```
# 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}

```
# 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,
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_error
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.

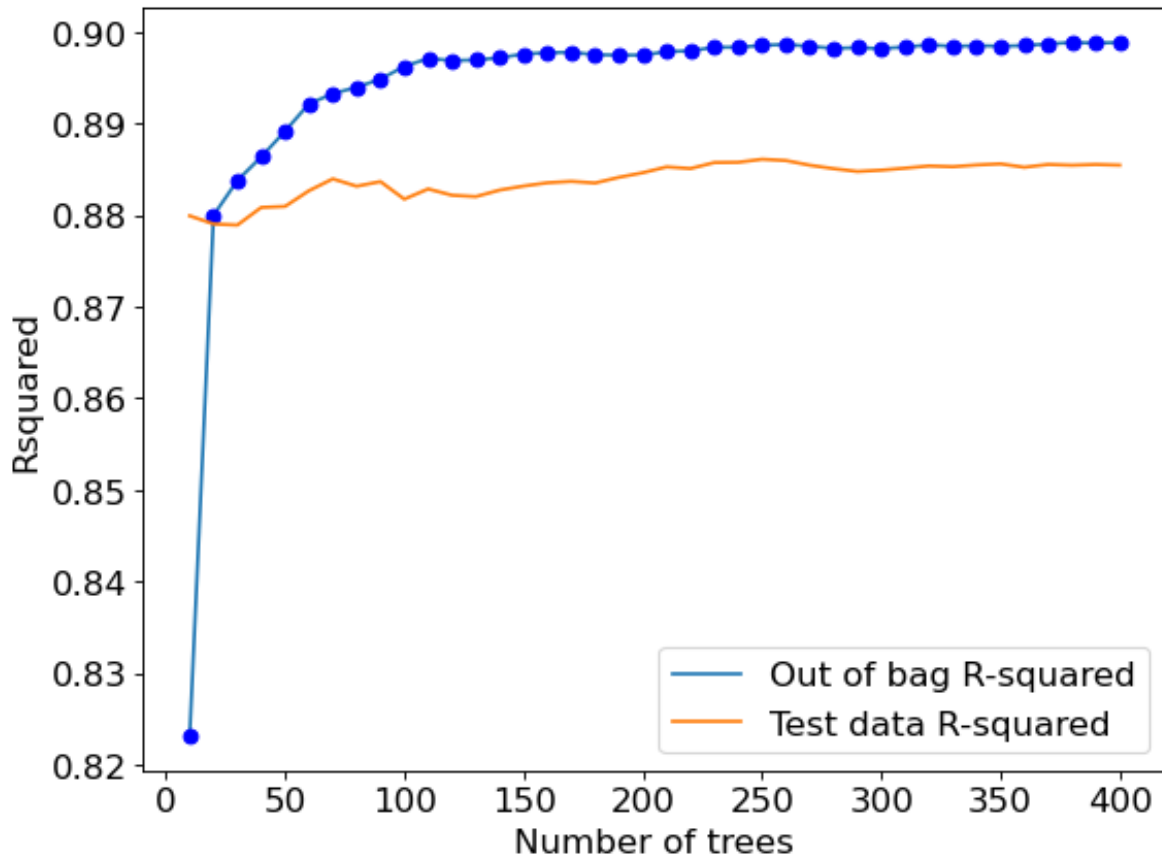
```
#Finding model accuracy vs number of trees
warnings.filterwarnings("ignore")
oob_rsquared={};test_rsquared={};oob_rmse={};test_rmse = {}
for i in np.linspace(10,400,40, dtype=int):
    model = BaggingRegressor(estimator=DecisionTreeRegressor(), n_estimators=i, random_state=
                           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_state=42,
                          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 negligible.

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

params = {'base_estimator': [DecisionTreeRegressor(random_state = 1), LinearRegression()], #Cor
        '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': Tr

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_state=0,
                        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_state=0,
                        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 greater
# 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)

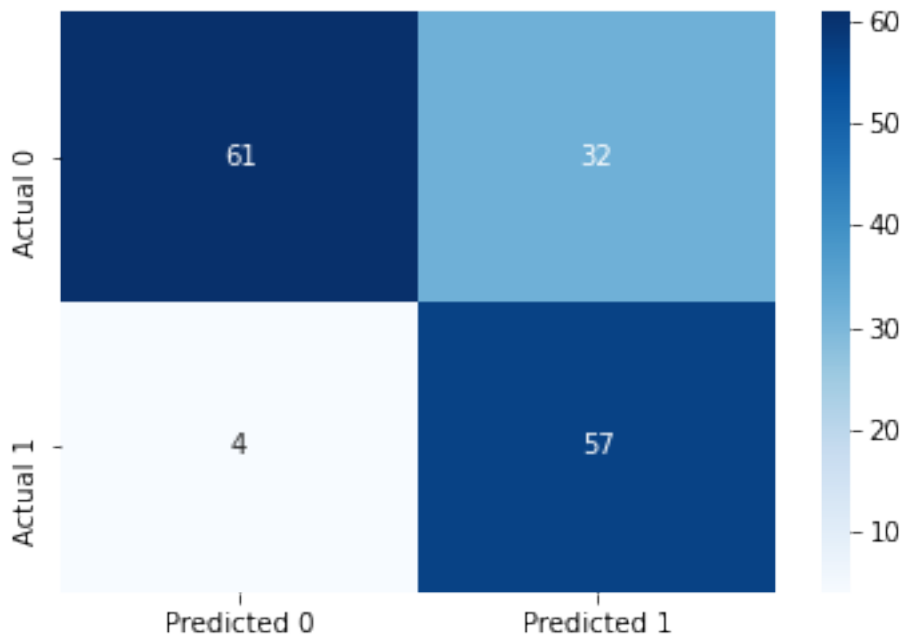
#Computing the ROC-AUC
fpr, tpr, auc_thresholds = roc_curve(ytest, y_pred_prob)
print("ROC-AUC: ",auc(fpr, tpr))# AUC of ROC

#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 probability 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.

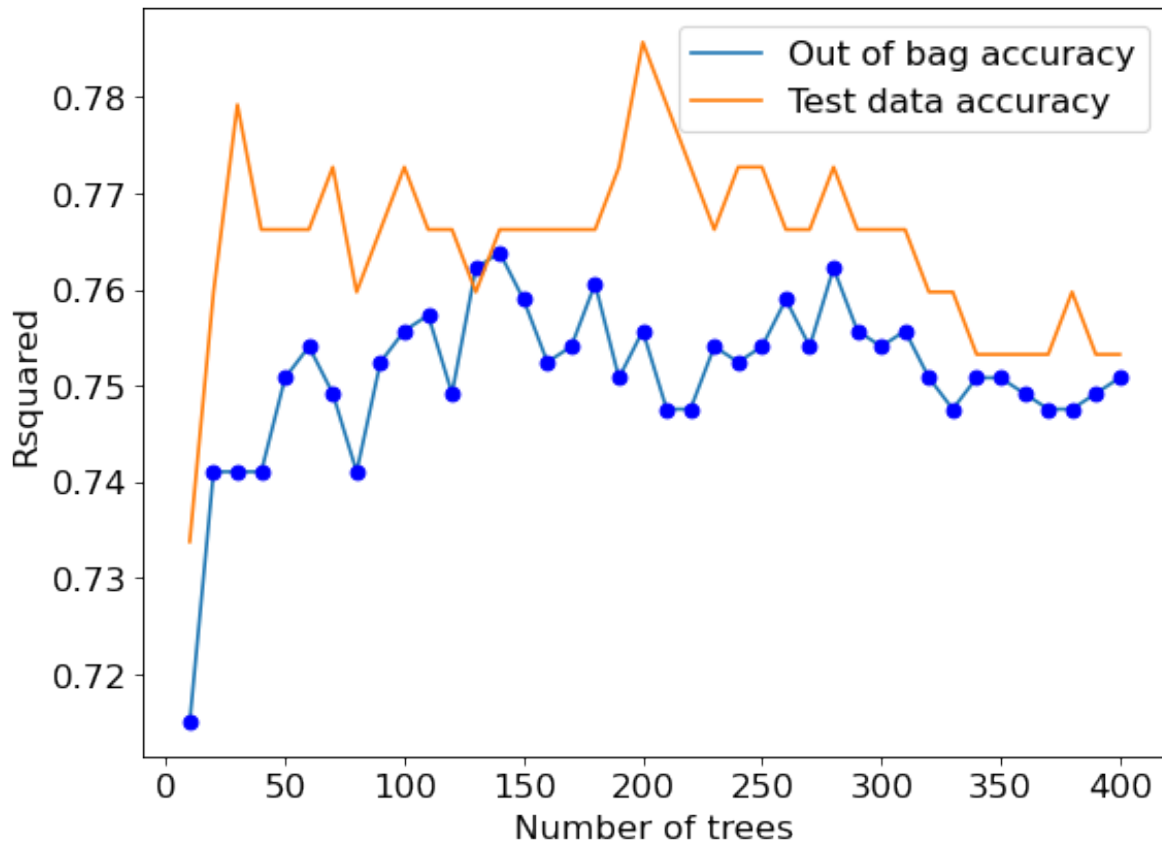
7.2.1 Model accuracy vs number of trees

```
#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, random
                             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: 
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 $\text{ROC-AUC} = 1$. 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': True}

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_estimators=
                          random_state=1, max_features=1.0, oob_score=True,
                          max_samples=1.0, n_jobs=-1, bootstrap=True, bootstrap_features=False).fit(X, y)

```

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.

```

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)

```


Precision and Recall Scores as a function of the decision threshold



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)
```

Precision and Recall Scores as a function of the decision threshold



```
# Thresholds with precision and recall
all_thresholds = np.concatenate([thresholds.reshape(-1,1), p[:-1].reshape(-1,1), r[:-1].reshape(-1,1)])
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 increasing order of precision, the last value will provide the maximum threshold probability for the recall to be more than 0.8.

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 greater
# 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, 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_log_error
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

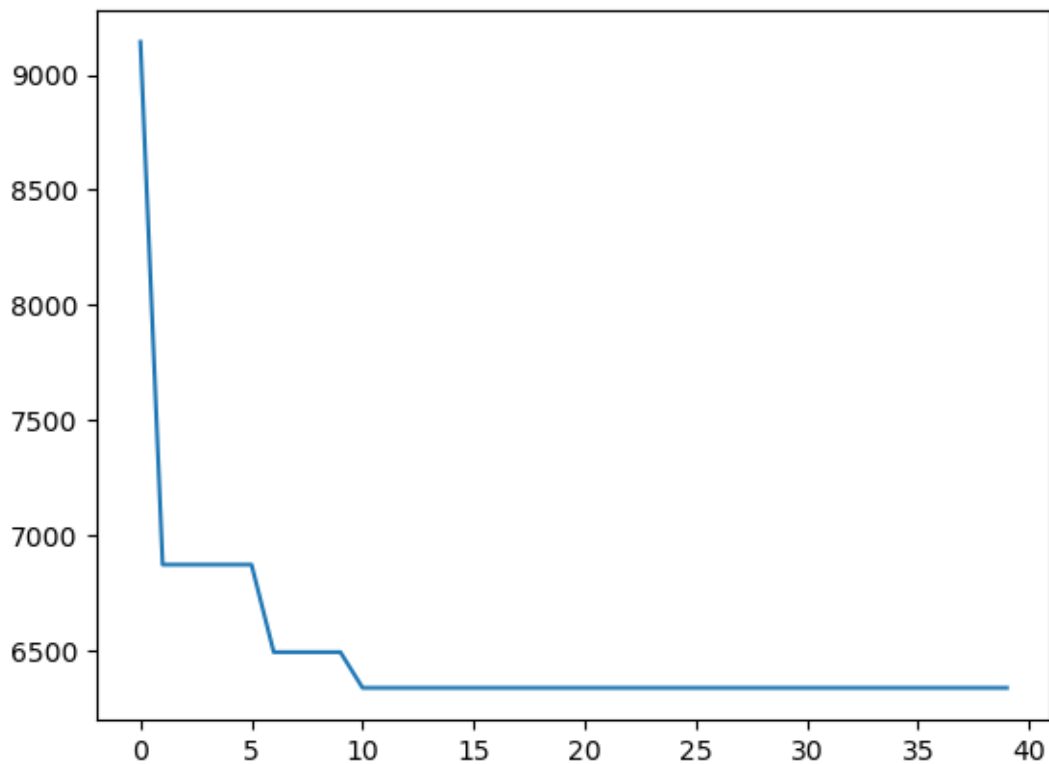
```

param_grid = {'max_depth': Integer(2, 30)}
gcv = BayesSearchCV(model, search_spaces = param_grid, cv = cv, n_iter = 40, random_state = 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)

```

['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 increase in bias of individual trees. Bagging trees only reduces the variance, but not the bias of the individual 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_estimators=100)
    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 sampling 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]
```

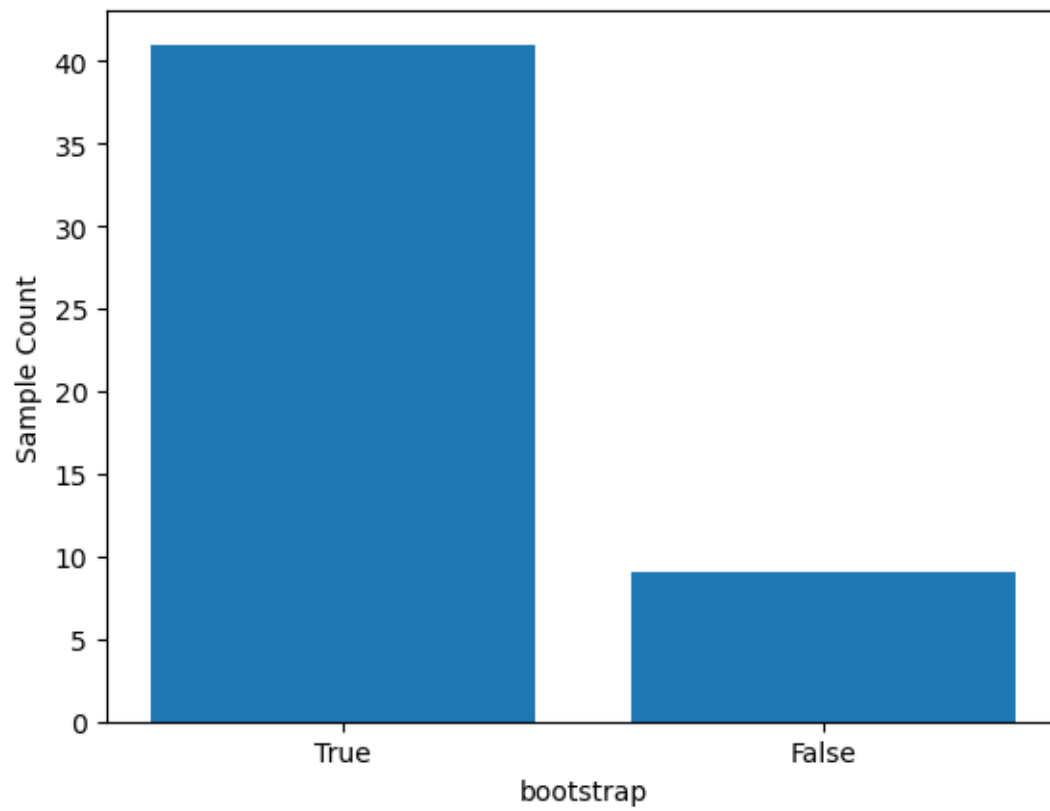


```

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', transform=None),
                              'max_samples': Real(low=0.2, high=1.0, prior='uniform', transform=None)},
               verbose=1)

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 neighbors
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)
```



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, RandomForestClassifier
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()
```

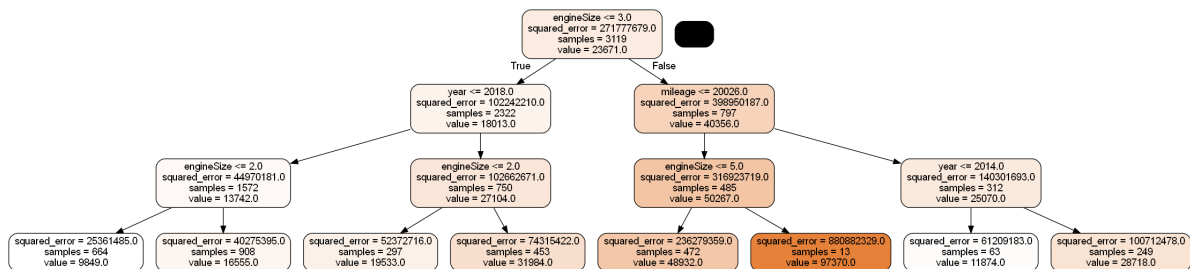
	carID	brand	model	year	transmission	mileage	fuelType	tax	mpg	engineSize	price
0	18473	bmw	6 Series	2020	Semi-Auto	11	Diesel	145	53.3282	3.0	37980
1	15064	bmw	6 Series	2019	Semi-Auto	10813	Diesel	145	53.0430	3.0	33980
2	18268	bmw	6 Series	2020	Semi-Auto	6	Diesel	145	53.4379	3.0	36850
3	18480	bmw	6 Series	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, random_state=42,
                        n_jobs=-1).fit(X, y)
```

```
#Change the index of model.estimators_[index] to visualize the 10 bagged trees, one at a time
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])
```

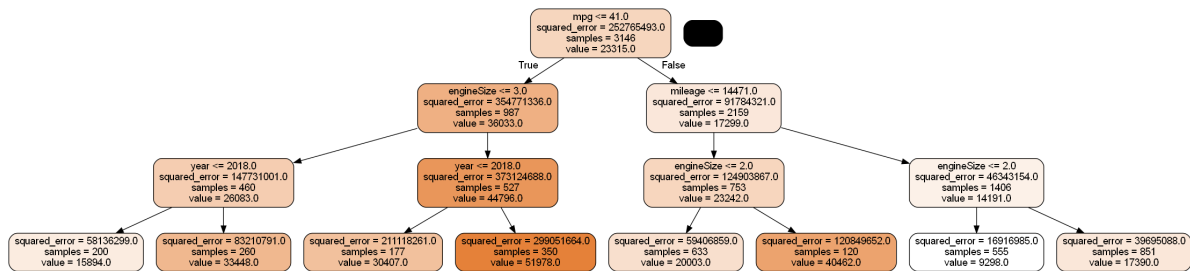
We can see that `engineSize` has the highest importance among predictors, supporting the visualization that it dominates the trees.

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=5,
                             n_jobs=-1).fit(X, y)
```

```
#Change the index of model.estimators_[index] to visualize the 10 random forest trees, one at a time
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

```

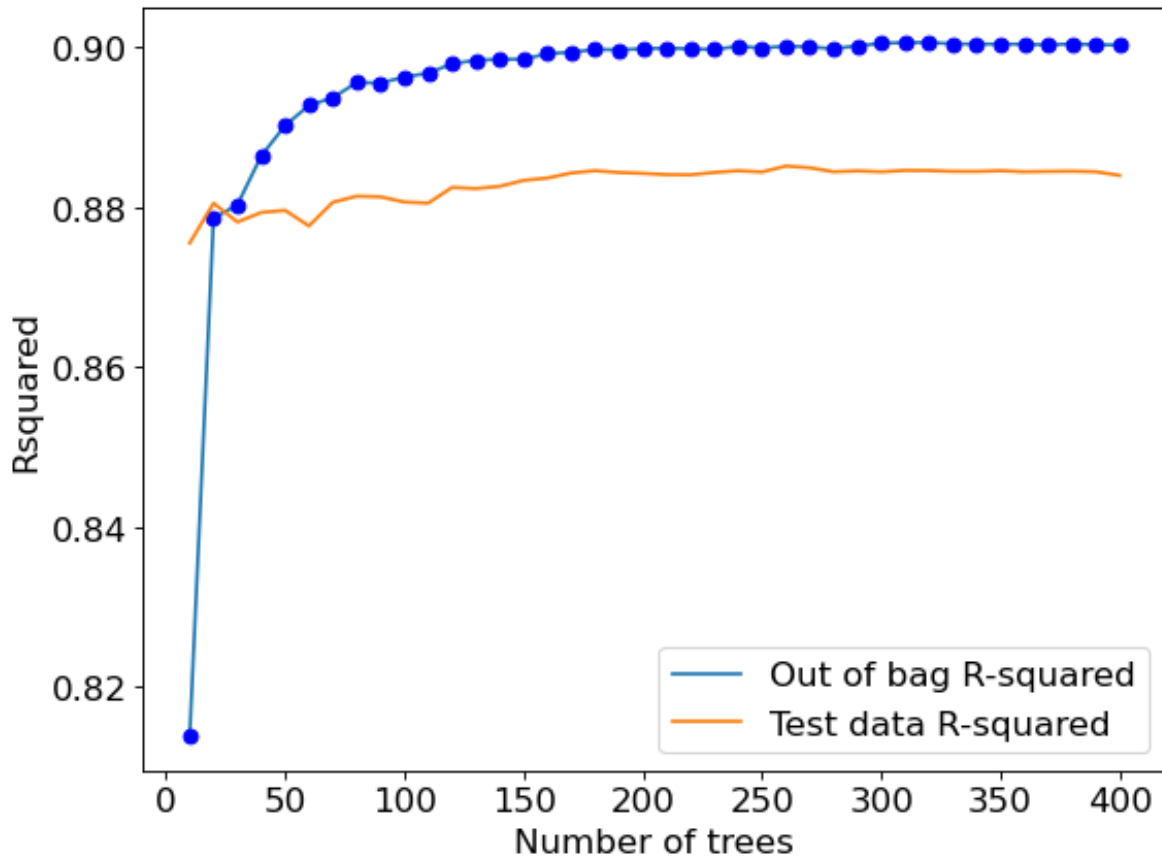
As we are ensemble only 10 trees in the first iteration, some of the observations are selected in every bootstrapped sample, and thus they don't have an out-of-bag error, which is producing the warning. For every observation to have an out-of-bag error, the number of trees must be sufficiently large.

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 hyperparameter 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 developed with cross validation.
#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=-1)
```

```
#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 greater
# than the desired decision threshold probability
```

```
y_pred = y_pred_prob > desired_threshold
y_pred = y_pred.astype(int)
```

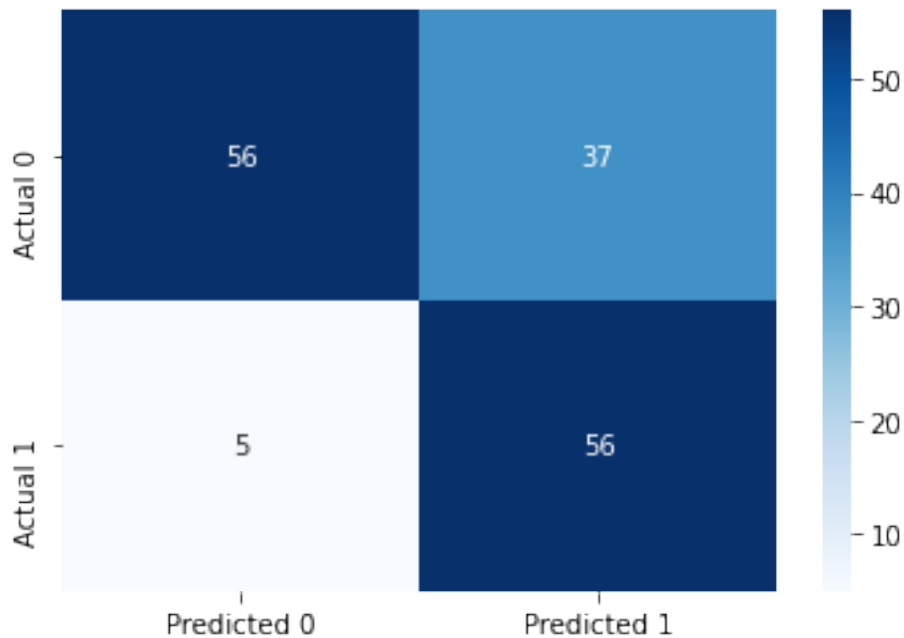
```
#Computing the accuracy
print("Accuracy: ",accuracy_score(y_pred, ytest)*100)
```

```
#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 greater
# 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

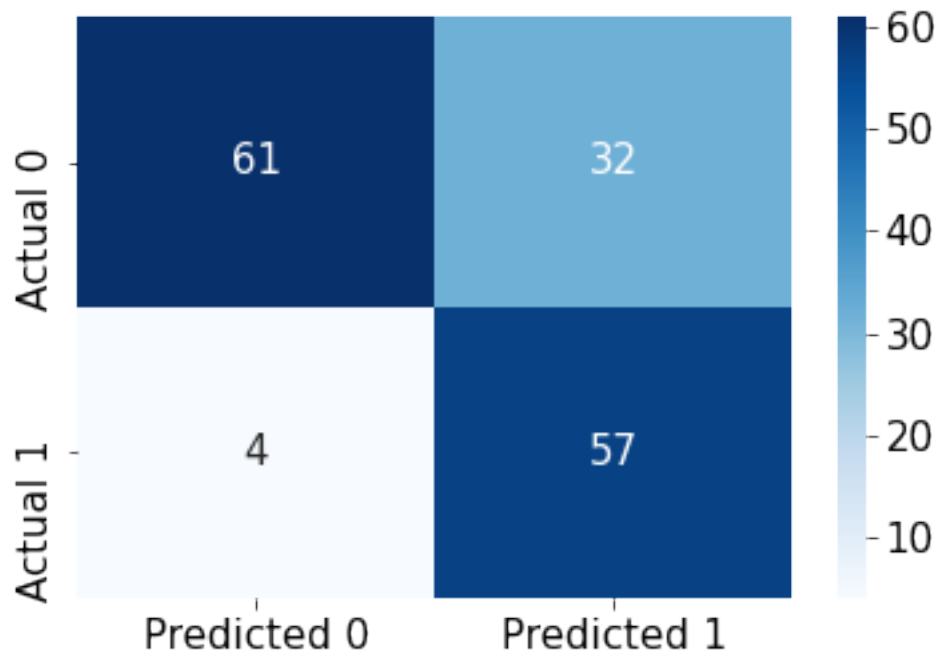
#Computing the precision and recall
print("Precision: ", precision_score(ytest, y_pred))
print("Recall: ", recall_score(ytest, y_pred))

#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 = 100,
                                   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_accuracy2={};

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

    #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 the model
    test_accuracy2[i]=model2.score(Xtest,ytest) #Returns the classification accuracy of the model
```

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

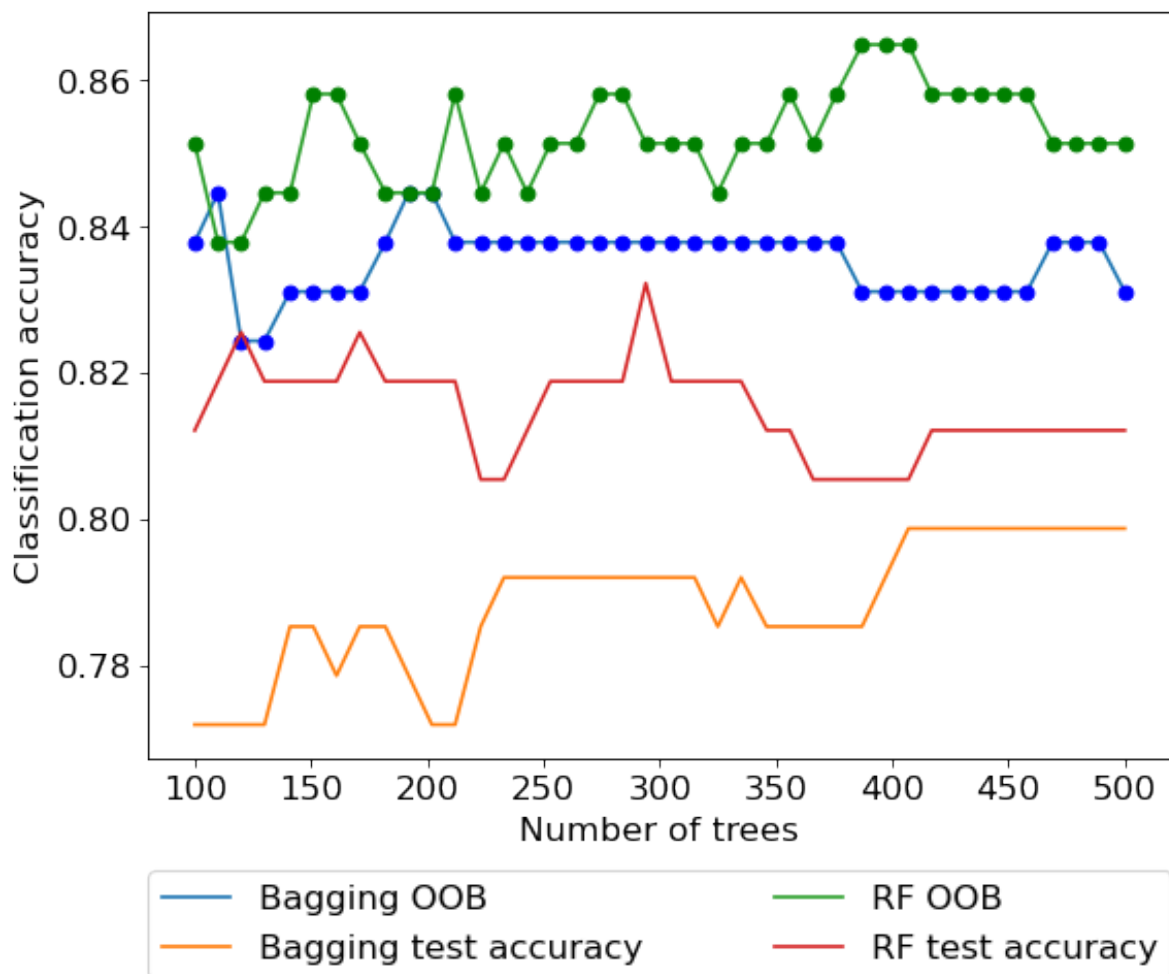
```
array([0.04381883, 0.05913479, 0.08585651, 0.07165678, 0.00302965,
       0.00903484, 0.05890448, 0.01223421, 0.072461  , 0.01337919,
       0.17495662, 0.18224651, 0.00527156, 0.00953965, 0.00396654,
       0.00163193, 0.09955286, 0.09332406])
```

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_accuracy2.keys(),test_accuracy2.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_predict
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, AdaBoostClassifier
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_jobs=5)
    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_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('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_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 %.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_depth=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_mean_squared_error')
# 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': 0.001}

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': 500}

The BayesSearchCV() approach also covers 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



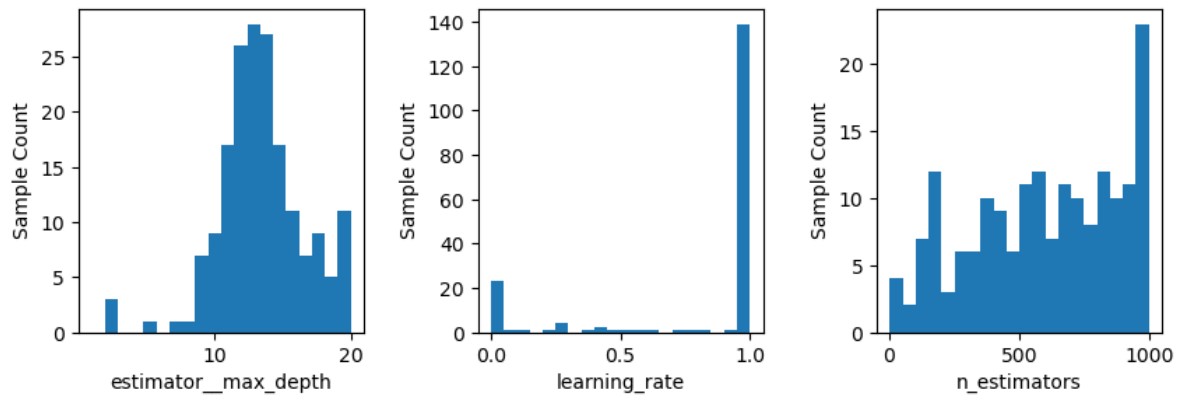
```

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',
                                                               '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=10,
plt.show();

```



```
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,learning_rate=0.1,
                           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,learning_rate=0.1,
                           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
```

```

# 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()
```



```

# 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),
                           n_estimators=200).fit(X,y)

# Note that we are using the cross-validated predicted probabilities, instead of directly using
# predicted probabilities on train data, as the model may be overfitting on the train data, and
# may lead to misleading results
cross_val_ypred = cross_val_predict(AdaBoostClassifier(random_state=1,base_estimator = DecisionTreeClassifier(max_depth=3),
                                                         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].reshape(-1,1)])
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 increasing order of precision,
# the last value will provide the maximum threshold probability for the recall to be more than 80%
# 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 greater
# 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
```

RDC-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_predict
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, BaggingRegressor
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_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)

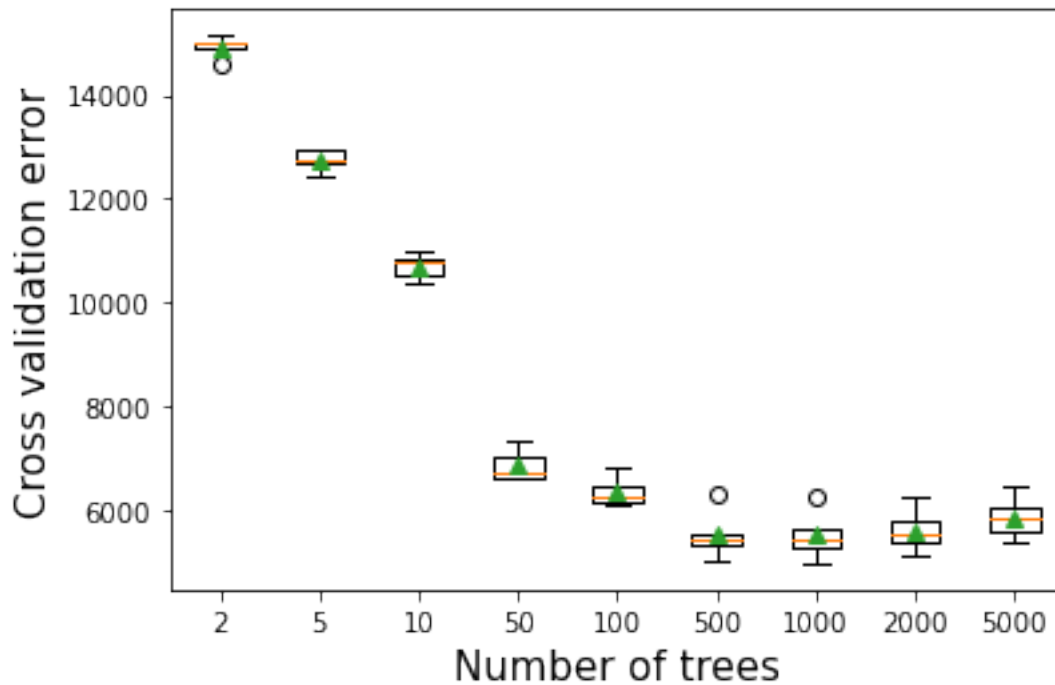
```

```

>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=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, 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('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_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 %.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)

```

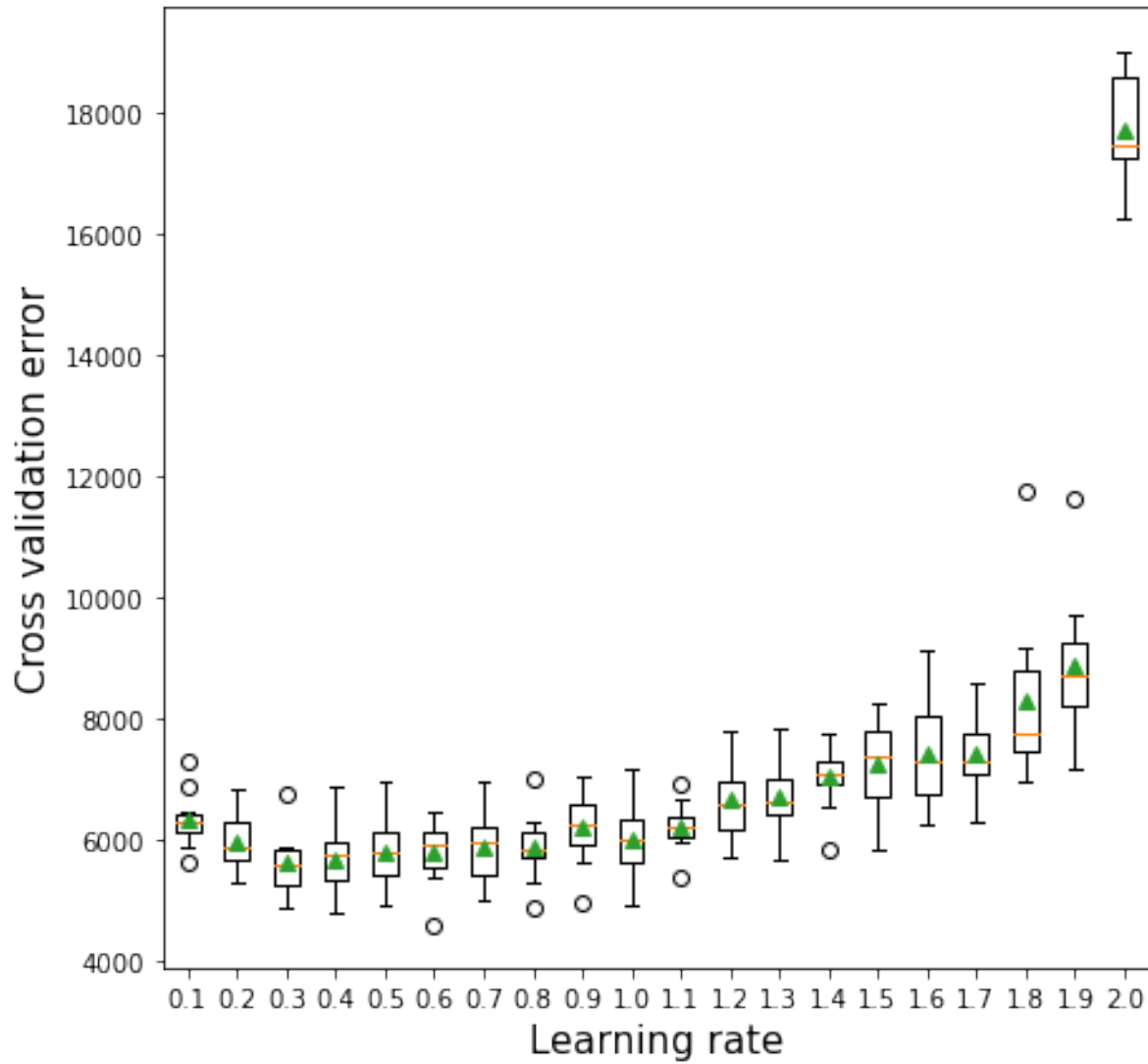
```

>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_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 %.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)

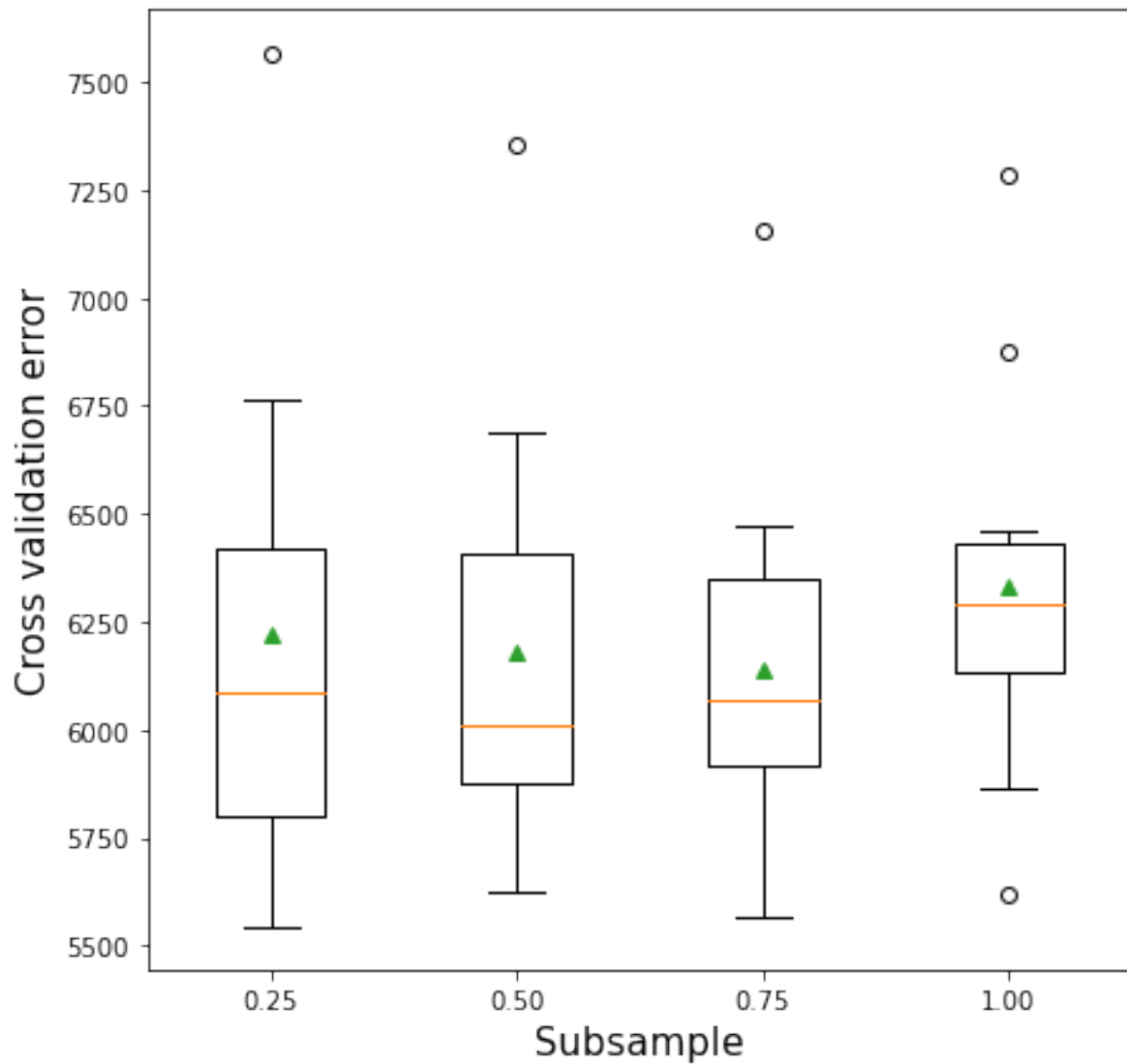
```

```

>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, 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 %.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'] = [0.231020
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', tr
```

```
'max_features': Real(low=0.1, high=1, prior='uniform', transform='log'),
'max_leaf_nodes': Integer(low=4, high=5000, prior='uniform', transform='log'),
'n_estimators': Integer(low=2, high=1000, prior='uniform', transform='log'),
'subsample': Real(low=0.1, high=1, prior='uniform', transform='log')
```

```
#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=0.1,
                                       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=500,
                           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)

```

```

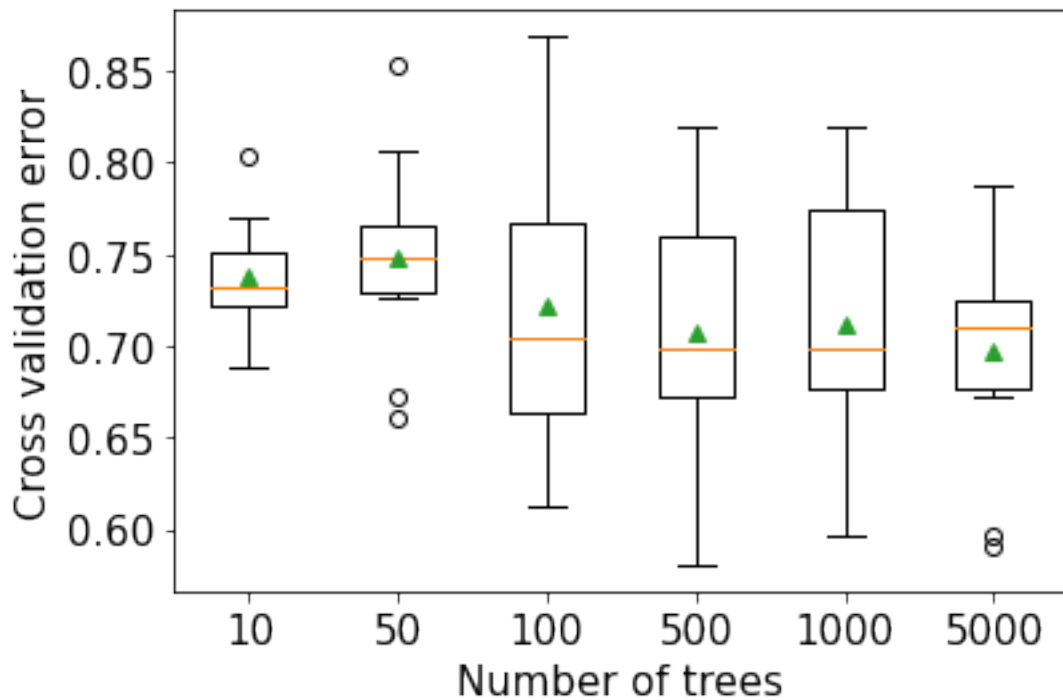
>10 0.738 (0.031)
>50 0.748 (0.054)
>100 0.722 (0.075)
>500 0.707 (0.066)
>1000 0.712 (0.075)
>5000 0.697 (0.061)

```

```

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)

```

```

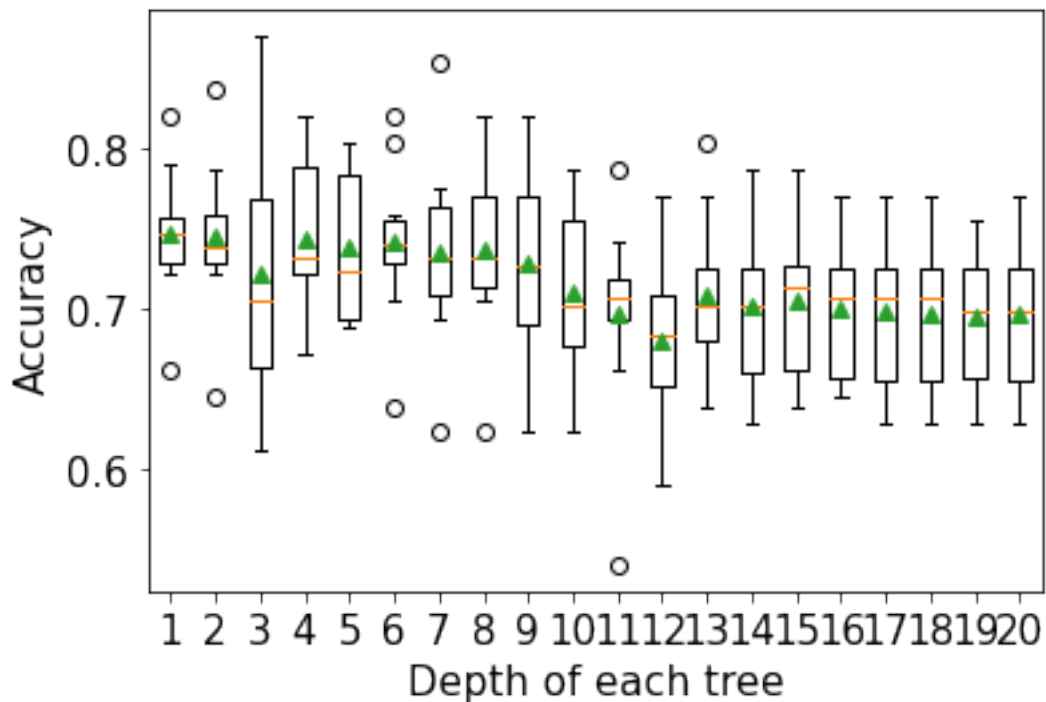
>1 0.746 (0.040)
>2 0.744 (0.046)
>3 0.722 (0.075)
>4 0.743 (0.049)
>5 0.738 (0.046)
>6 0.741 (0.047)
>7 0.735 (0.057)
>8 0.736 (0.051)
>9 0.728 (0.055)
>10 0.710 (0.050)
>11 0.697 (0.061)
>12 0.681 (0.056)
>13 0.709 (0.047)
>14 0.702 (0.048)
>15 0.705 (0.048)
>16 0.700 (0.042)
>17 0.699 (0.048)
>18 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': 1.0}

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 using
# predicted probabilities on train data, as the model may be overfitting on the train data, and
# may lead to misleading results
cross_val_ypred = cross_val_predict(GradientBoostingClassifier(random_state=1,max_depth=3,
                                                                learning_rate=0.1,subsample=0.5,
                                                                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].reshape(-1,1)])
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 increasing order of precision,
# the last value will provide the maximum threshold probability for the recall to be more than 0.8.
# 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 greater
# 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_predict
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, RandomizedSearchCV
from sklearn.ensemble import VotingRegressor, VotingClassifier, StackingRegressor, StackingClassifier
from sklearn.linear_model import LinearRegression, LogisticRegression, LassoCV, RidgeCV, ElasticNetCV
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_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)
```

```

>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, 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('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, 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 %.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, 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 %.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_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 %.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('gamma',fontsize=15)
#ax.set_xticklabels(x.astype(int))
plt.xticks(ticks=plt.xticks()[0].astype(int), labels=np.round([0,10,1e2,1e3,1e4,1e5,1e6,1e7,
rotation = 30);
```

```
>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 5345.4 (373.9)
>1000000000.0000 5932.3 (397.6)
```



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_d

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)}

```

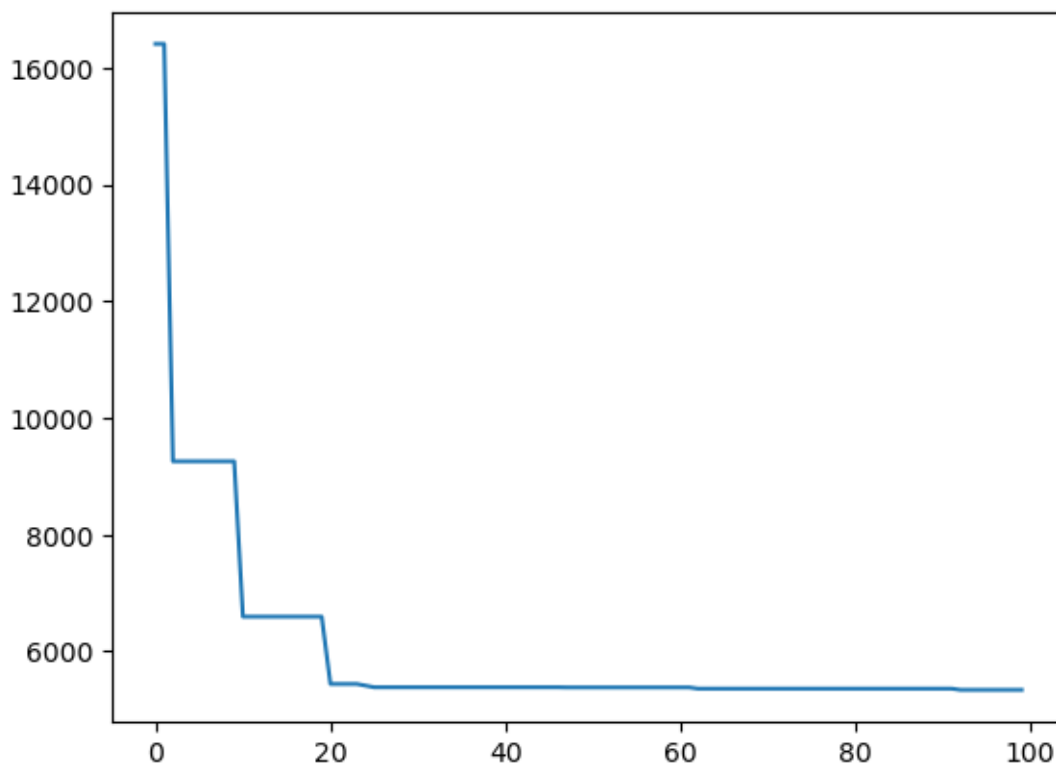
```

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', '...



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', tr
                        'max_leaves': Integer(low=4, high=5000, prior='uniform', transf
                        '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 = 0.1,
                           max_leaves = 802, n_estimators = 1023, reg_lambda = 1394, subsample = 0.8)

```

```

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_rate = 0.1,
                           max_depth = 8, n_estimators = 1000, reg_lambda = 1, subsample = 0.8)

```

```

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,
model.fit(X_train_sub, y_train_sub, eval_set = ((X_test_sub, y_test_sub))), early_stopping_
```

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 250 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,
model.fit(X_train_sub, y_train_sub, eval_set = ((X_test_sub, y_test_sub))), early_stopping_
```

```
<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=100,
                             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 given equal weight
#pred = 0.15*pred1+0.15*pred2+0.15*pred3+0.55*pred4 #Option 2 - Higher weight to the better model
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 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
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** hyperparameter 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.

Reference

```
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 negative
            }

cv = StratifiedKFold(n_splits=5, shuffle=True, random_state=1)
optimal_params = GridSearchCV(estimator=xgb.XGBClassifier(objective = 'binary:logistic', random_state=1,
                                                         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_learning_rate
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_learning_rate
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_rate=0.01,
                           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,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=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)
```

```

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)

```




13 LightGBM and CatBoost

```
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_predict
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, RandomizedSearchCV
from sklearn.ensemble import VotingRegressor, VotingClassifier, StackingRegressor, StackingClassifier
from sklearn.linear_model import LinearRegression, LogisticRegression, LassoCV, RidgeCV, ElasticNetCV
from sklearn.neighbors import KNeighborsRegressor
import itertools as it
import time as time
import xgboost as xgb
from lightgbm import LGBMRegressor
from catboost import CatBoostRegressor
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
```

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 computational 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. Note that we are using the GOSS algorithm to downsample observations with smaller gradients.

```
#K-fold cross validation to find optimal parameters for LightGBM regressor
start_time = time.time()
param_grid = {'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(boosting_type = 'goss'),
                                   param_distributions = param_grid, n_iter = 200,
                                   verbose = 1, scoring='neg_root_mean_squared_error',
```

```

n_jobs=-1,random_state=1,
cv = cv)

optimal_params.fit(X,y)
print("Optimal parameter values =", optimal_params.best_params_)
print("Optimal cross validation RMSE = ",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': 1.0, 'reg_lambda': 10, 'reg_alpha': 0, 'num_leaves':

Optimal cross validation R-squared = -5670.309021679375

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))

```

5614.374498193448

Note that downsampling of small-gradient observations leads to faster execution time, but potentially by compromising some accuracy. We can expect to improve the accuracy by increasing the `top_rate` or the `other_rate` hyperparameters, but at an increased computational cost. In the cross-validation below, we have increased the `top_rate` to 0.5 from the default value of 0.2.

```

#K-fold cross validation to find optimal parameters for LightGBM regressor
start_time = time.time()
param_grid = {'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(boosting_type = 'goss', top_rate
                                param_distributions = param_grid, n_iter = 200,
                                verbose = 1, scoring='neg_root_mean_squared_error',
                                n_jobs=-1,random_state=1,
                                cv = cv)

optimal_params.fit(X,y)

```

```
print("Optimal parameter values =", optimal_params.best_params_)
print("Optimal cross validation RMSE = ", 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': 0.5, 'reg_lambda': 0, 'reg_alpha': 100, 'num_leaves': 100}

Optimal cross validation R-squared = -5436.062435616846

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))
```

5355.964600884197

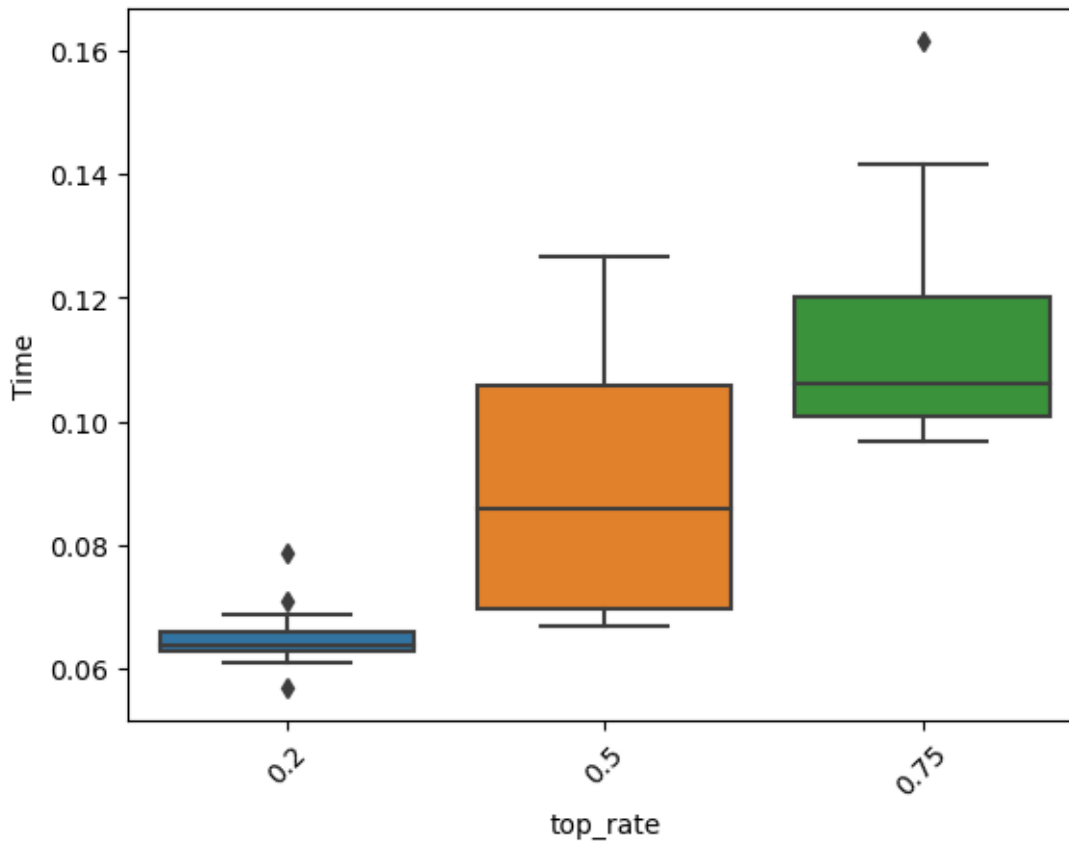
Note that the cross-validated RMSE has reduced. However, this is at an increased computational expense. In the simulations below, we compare the time taken to train models with increasing values of the `top_rate` hyperparameter.

```
time_list = []
for i in range(50):
    start_time = time.time()
    model = LGBMRegressor(boosting_type = 'goss', top_rate = 0.2, n_jobs=-1).fit(X, y)
    time_list.append(time.time()-start_time)
```

```
time_list2 = []
for i in range(50):
    start_time = time.time()
    model = LGBMRegressor(boosting_type = 'goss', top_rate = 0.5, n_jobs=-1).fit(X, y)
    time_list2.append(time.time()-start_time)
```

```
time_list3 = []
for i in range(50):
    start_time = time.time()
    model = LGBMRegressor(boosting_type = 'goss', top_rate = 0.8, n_jobs=-1).fit(X, y)
    time_list3.append(time.time()-start_time)
```

```
ax = sns.boxplot([time_list, time_list2, time_list3]);
ax.set_xticklabels([0.2, 0.5, 0.75]);
plt.ylabel('Time');
plt.xlabel('top_rate');
plt.xticks(rotation = 45);
```



13.1.2 LightGBM vs XGBoost

LightGBM model took 2 minutes for a random search with 1000 fits as compared to 7 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(),
                                   param_distributions = param_grid, n_iter = 200,
                                   verbose = 1, scoring = 'neg_root_mean_squared_error',
                                   n_jobs=-1,random_state = 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_d

Optimal cross validation R-squared = -5178.8689594137295

Time taken = 7 minutes

#RMSE based on the optimal parameter values

```
np.sqrt(mean_squared_error(optimal_params.best_estimator_.predict(Xtest),ytest))
```

5420.661056398766

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 [CatBoostClassifier](#) can be used.

Let us check the performance of `CatBoostRegressor()` without tuning, i.e., with default hyperparameter settings.

```
model_cat = CatBoostRegressor(verbose=0).fit(X, y)

cv = KFold(n_splits=5, shuffle=True, random_state=1)
np.mean(-cross_val_score(CatBoostRegressor(verbose=0), X, y, cv = cv, n_jobs = -1,
                          scoring='neg_root_mean_squared_error'))
```

```
5035.972129299527
```

```
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 cross-validated RMSE, and 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.mean(-cross_val_score(xgb.XGBRFRegressor(), X, y, cv = cv, n_jobs = -1,
                        scoring='neg_root_mean_squared_error'))
```

6273.043859096154

```
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.mean(-cross_val_score(LGBMRegressor(), X, y, cv = cv, n_jobs = -1,
                        scoring='neg_root_mean_squared_error'))
```

5562.149251902867

```
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, 10],
              'num_leaves': [20, 31, 40, 60],
              'learning_rate': [0.01, 0.05, 0.1],
              'reg_lambda': [0, 10, 100],
              'n_estimators': [500, 1000, 1500],
              'subsample': [0.5, 0.75, 1.0],
              'colsample_bylevel': [0.25, 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=False),
                                   grow_policy='Lossguide'),
                                   param_distributions = param_grid, n_iter = 200,
                                   verbose = 1,random_state = 1, scoring='neg_root_mean_squared_error',
                                   n_jobs=-1,
                                   cv = cv)

optimal_params.fit(X,y)
print("Optimal parameter values =", optimal_params.best_params_)
print("Optimal cross validation RMSE = ",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': 0.5, 'reg_lambda': 0, 'num_leaves': 40, 'n_estimators': 1500}
 Optimal cross validation RMSE = -4993.129407810791
 Time taken = 23 minutes

```

#RMSE based on the optimal parameter values
np.sqrt(mean_squared_error(optimal_params.best_estimator_.predict(Xtest),ytest))

```

5249.434282204398

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 LightGBM, and likely to require lesser tuning as compared to XGBoost.

```

model = CatBoostRegressor(grow_policy='Lossguide')

grid = {'num_leaves': Integer(4, 64),

```

```

        'learning_rate': Real(0.0001, 1.0),
        'reg_lambda': Real(0, 1e4),
        'n_estimators': Integer(2, 2000),
        'subsample': Real(0.1, 1.0),
        'colsample_bylevel': 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 = 200, 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_bylevel', 'learning_rate', 'n_estimators', 'num_leaves', 'reg_lambda', 'subsample']
0: learn: 15586.6547227 total: 7.88ms remaining: 15.8s
1: learn: 14594.4802869 total: 16.4ms remaining: 16.4s
2: learn: 14594.4802869 total: 17.2ms remaining: 11.5s
3: learn: 13743.4503923 total: 20.1ms remaining: 10s
4: learn: 13266.2414822 total: 24.9ms remaining: 9.94s
5: learn: 12498.3369959 total: 28.1ms remaining: 9.33s
6: learn: 12129.2561319 total: 30.3ms remaining: 8.63s
7: learn: 11505.6411010 total: 32.3ms remaining: 8.03s
8: learn: 11505.6411010 total: 32.7ms remaining: 7.23s
9: learn: 11021.2139091 total: 34.6ms remaining: 6.89s
10: learn: 10442.9678139 total: 37ms remaining: 6.69s
11: learn: 9947.6741148 total: 39.3ms remaining: 6.51s
12: learn: 9619.4595819 total: 41ms remaining: 6.27s
13: learn: 9259.8855899 total: 42.9ms remaining: 6.08s
14: learn: 9259.8855899 total: 43.4ms remaining: 5.74s
15: learn: 8939.7710703 total: 45.3ms remaining: 5.62s
16: learn: 8711.0852634 total: 47.3ms remaining: 5.52s
17: learn: 8604.6071027 total: 49.1ms remaining: 5.41s
18: learn: 8438.7728051 total: 50.8ms remaining: 5.3s
19: learn: 8274.7829809 total: 53.2ms remaining: 5.26s

```

20: learn: 8042.3020027 total: 55.9ms remaining: 5.27s
21: learn: 7876.9560283 total: 57.5ms remaining: 5.17s
22: learn: 7710.6772232 total: 59.5ms remaining: 5.12s
23: learn: 7571.7455782 total: 61.1ms remaining: 5.03s
24: learn: 7440.8874033 total: 63ms remaining: 4.98s
25: learn: 7316.5070355 total: 65ms remaining: 4.93s
26: learn: 7190.4998886 total: 66.8ms remaining: 4.88s
27: learn: 7126.4859430 total: 68.2ms remaining: 4.8s
28: learn: 7126.4859430 total: 68.6ms remaining: 4.66s
29: learn: 7016.0377180 total: 70.1ms remaining: 4.6s
30: learn: 7000.1845553 total: 70.7ms remaining: 4.49s
31: learn: 6884.2153374 total: 72.3ms remaining: 4.45s
32: learn: 6884.2153374 total: 72.7ms remaining: 4.33s
33: learn: 6859.6936709 total: 74.3ms remaining: 4.29s
34: learn: 6859.6936709 total: 74.7ms remaining: 4.19s
35: learn: 6784.1411674 total: 76.4ms remaining: 4.17s
36: learn: 6784.1411674 total: 76.9ms remaining: 4.08s
37: learn: 6759.2775251 total: 77.8ms remaining: 4.01s
38: learn: 6699.5901664 total: 79.7ms remaining: 4.01s
39: learn: 6618.8189493 total: 81.6ms remaining: 4s
40: learn: 6588.5585061 total: 83.2ms remaining: 3.97s
41: learn: 6576.3802378 total: 84.1ms remaining: 3.92s
42: learn: 6576.3802378 total: 84.5ms remaining: 3.85s
43: learn: 6576.3802378 total: 84.9ms remaining: 3.77s
44: learn: 6576.3802378 total: 85.3ms remaining: 3.71s
45: learn: 6554.9758286 total: 86.5ms remaining: 3.67s
46: learn: 6525.5802913 total: 88.1ms remaining: 3.66s
47: learn: 6466.1035176 total: 89.1ms remaining: 3.62s
48: learn: 6436.3855462 total: 90.1ms remaining: 3.59s
49: learn: 6425.6798093 total: 91.3ms remaining: 3.56s
50: learn: 6415.6723682 total: 92.3ms remaining: 3.53s
51: learn: 6370.9376356 total: 95ms remaining: 3.56s
52: learn: 6362.2269483 total: 96.1ms remaining: 3.53s
53: learn: 6270.8381417 total: 97.5ms remaining: 3.51s
54: learn: 6224.2584318 total: 98.8ms remaining: 3.49s
55: learn: 6196.9126269 total: 100ms remaining: 3.48s
56: learn: 6159.9795842 total: 102ms remaining: 3.48s
57: learn: 6095.2640049 total: 104ms remaining: 3.48s
58: learn: 6068.5568780 total: 105ms remaining: 3.47s
59: learn: 6045.8539265 total: 107ms remaining: 3.45s
60: learn: 6014.2089991 total: 108ms remaining: 3.44s
61: learn: 6014.2089991 total: 109ms remaining: 3.4s
62: learn: 5991.4276619 total: 110ms remaining: 3.4s

63:	learn:	5960.8755319	total:	112ms	remaining:	3.4s
64:	learn:	5939.4519328	total:	114ms	remaining:	3.39s
65:	learn:	5937.5977651	total:	114ms	remaining:	3.35s
66:	learn:	5914.5991789	total:	116ms	remaining:	3.34s
67:	learn:	5893.7012597	total:	117ms	remaining:	3.34s
68:	learn:	5881.6048683	total:	119ms	remaining:	3.33s
69:	learn:	5857.2384791	total:	121ms	remaining:	3.33s
70:	learn:	5856.3744823	total:	121ms	remaining:	3.3s
71:	learn:	5844.6720134	total:	123ms	remaining:	3.29s
72:	learn:	5808.4057279	total:	125ms	remaining:	3.29s
73:	learn:	5796.1301234	total:	126ms	remaining:	3.29s
74:	learn:	5774.0161859	total:	128ms	remaining:	3.29s
75:	learn:	5771.0218306	total:	129ms	remaining:	3.27s
76:	learn:	5771.0218306	total:	129ms	remaining:	3.23s
77:	learn:	5754.9516948	total:	131ms	remaining:	3.23s
78:	learn:	5753.1841839	total:	132ms	remaining:	3.22s
79:	learn:	5750.6624545	total:	134ms	remaining:	3.21s
80:	learn:	5730.0398718	total:	136ms	remaining:	3.21s
81:	learn:	5730.0398718	total:	136ms	remaining:	3.18s
82:	learn:	5724.0710370	total:	138ms	remaining:	3.18s
83:	learn:	5709.8421847	total:	139ms	remaining:	3.18s
84:	learn:	5695.5072261	total:	141ms	remaining:	3.18s
85:	learn:	5681.9956673	total:	143ms	remaining:	3.18s
86:	learn:	5660.6016053	total:	145ms	remaining:	3.18s
87:	learn:	5643.4061588	total:	147ms	remaining:	3.18s
88:	learn:	5635.8928486	total:	148ms	remaining:	3.18s
89:	learn:	5614.4729570	total:	149ms	remaining:	3.17s
90:	learn:	5607.0906414	total:	151ms	remaining:	3.17s
91:	learn:	5606.5748917	total:	151ms	remaining:	3.14s
92:	learn:	5593.2044205	total:	153ms	remaining:	3.14s
93:	learn:	5581.7260489	total:	154ms	remaining:	3.13s
94:	learn:	5568.1299183	total:	156ms	remaining:	3.12s
95:	learn:	5568.1299183	total:	156ms	remaining:	3.1s
96:	learn:	5568.1299183	total:	157ms	remaining:	3.07s
97:	learn:	5547.7453457	total:	158ms	remaining:	3.07s
98:	learn:	5536.8538716	total:	160ms	remaining:	3.07s
99:	learn:	5533.3512293	total:	162ms	remaining:	3.07s
100:	learn:	5531.6988001	total:	163ms	remaining:	3.06s
101:	learn:	5521.6827472	total:	164ms	remaining:	3.06s
102:	learn:	5512.1275625	total:	166ms	remaining:	3.05s
103:	learn:	5501.2710735	total:	167ms	remaining:	3.04s
104:	learn:	5483.1332945	total:	169ms	remaining:	3.04s
105:	learn:	5468.6932573	total:	170ms	remaining:	3.04s

106:	learn: 5468.6932573	total: 171ms	remaining: 3.02s
107:	learn: 5466.3196454	total: 172ms	remaining: 3.01s
108:	learn: 5466.3196454	total: 173ms	remaining: 2.99s
109:	learn: 5450.8555079	total: 174ms	remaining: 2.99s
110:	learn: 5450.5222911	total: 175ms	remaining: 2.98s
111:	learn: 5444.9363205	total: 176ms	remaining: 2.98s
112:	learn: 5434.7455852	total: 178ms	remaining: 2.98s
113:	learn: 5434.7455852	total: 179ms	remaining: 2.96s
114:	learn: 5433.5957428	total: 180ms	remaining: 2.94s
115:	learn: 5415.6597932	total: 181ms	remaining: 2.94s
116:	learn: 5415.6597932	total: 181ms	remaining: 2.92s
117:	learn: 5401.1008140	total: 183ms	remaining: 2.92s
118:	learn: 5391.8658503	total: 185ms	remaining: 2.92s
119:	learn: 5380.7927393	total: 186ms	remaining: 2.92s
120:	learn: 5365.7813769	total: 188ms	remaining: 2.92s
121:	learn: 5365.7813769	total: 188ms	remaining: 2.9s
122:	learn: 5354.1319730	total: 191ms	remaining: 2.91s
123:	learn: 5354.1319730	total: 191ms	remaining: 2.89s
124:	learn: 5342.7838789	total: 193ms	remaining: 2.89s
125:	learn: 5342.7838789	total: 193ms	remaining: 2.87s
126:	learn: 5327.8897475	total: 195ms	remaining: 2.88s
127:	learn: 5310.2941871	total: 197ms	remaining: 2.88s
128:	learn: 5306.9281433	total: 198ms	remaining: 2.87s
129:	learn: 5294.2149974	total: 200ms	remaining: 2.87s
130:	learn: 5291.2189448	total: 202ms	remaining: 2.88s
131:	learn: 5285.4079447	total: 203ms	remaining: 2.87s
132:	learn: 5276.3888293	total: 205ms	remaining: 2.88s
133:	learn: 5253.7966160	total: 206ms	remaining: 2.88s
134:	learn: 5242.4363346	total: 208ms	remaining: 2.87s
135:	learn: 5234.7617159	total: 210ms	remaining: 2.87s
136:	learn: 5230.7299511	total: 211ms	remaining: 2.87s
137:	learn: 5228.9494984	total: 212ms	remaining: 2.86s
138:	learn: 5220.7658686	total: 213ms	remaining: 2.86s
139:	learn: 5220.7658686	total: 214ms	remaining: 2.84s
140:	learn: 5220.3928102	total: 214ms	remaining: 2.83s
141:	learn: 5216.5111017	total: 216ms	remaining: 2.82s
142:	learn: 5213.4217372	total: 217ms	remaining: 2.82s
143:	learn: 5211.7652831	total: 218ms	remaining: 2.81s
144:	learn: 5193.0346592	total: 220ms	remaining: 2.81s
145:	learn: 5185.9448931	total: 221ms	remaining: 2.81s
146:	learn: 5182.0516815	total: 223ms	remaining: 2.81s
147:	learn: 5174.6829049	total: 225ms	remaining: 2.81s
148:	learn: 5174.6829049	total: 225ms	remaining: 2.79s

149:	learn: 5166.2911738	total: 226ms	remaining: 2.79s
150:	learn: 5159.8205215	total: 229ms	remaining: 2.8s
151:	learn: 5156.3185114	total: 230ms	remaining: 2.8s
152:	learn: 5156.3185114	total: 231ms	remaining: 2.78s
153:	learn: 5147.4051798	total: 232ms	remaining: 2.79s
154:	learn: 5147.4051798	total: 233ms	remaining: 2.77s
155:	learn: 5147.2407560	total: 234ms	remaining: 2.76s
156:	learn: 5146.4759564	total: 235ms	remaining: 2.75s
157:	learn: 5137.3716292	total: 236ms	remaining: 2.75s
158:	learn: 5121.4193275	total: 238ms	remaining: 2.75s
159:	learn: 5115.5018273	total: 239ms	remaining: 2.75s
160:	learn: 5115.5018273	total: 240ms	remaining: 2.74s
161:	learn: 5110.2699403	total: 242ms	remaining: 2.74s
162:	learn: 5109.9847477	total: 242ms	remaining: 2.73s
163:	learn: 5101.1792661	total: 244ms	remaining: 2.73s
164:	learn: 5094.6570018	total: 246ms	remaining: 2.73s
165:	learn: 5087.8982851	total: 247ms	remaining: 2.73s
166:	learn: 5075.5065415	total: 249ms	remaining: 2.73s
167:	learn: 5073.0923568	total: 250ms	remaining: 2.73s
168:	learn: 5059.3039228	total: 252ms	remaining: 2.73s
169:	learn: 5052.5169956	total: 254ms	remaining: 2.73s
170:	learn: 5048.6517154	total: 255ms	remaining: 2.73s
171:	learn: 5044.5398469	total: 257ms	remaining: 2.73s
172:	learn: 5042.2657789	total: 258ms	remaining: 2.73s
173:	learn: 5027.5698491	total: 260ms	remaining: 2.73s
174:	learn: 5018.2624339	total: 262ms	remaining: 2.73s
175:	learn: 5015.4207674	total: 263ms	remaining: 2.73s
176:	learn: 5004.4326005	total: 265ms	remaining: 2.73s
177:	learn: 5002.2042902	total: 267ms	remaining: 2.73s
178:	learn: 4991.5613784	total: 268ms	remaining: 2.73s
179:	learn: 4986.5919903	total: 270ms	remaining: 2.73s
180:	learn: 4983.2524252	total: 272ms	remaining: 2.73s
181:	learn: 4983.0495780	total: 273ms	remaining: 2.72s
182:	learn: 4972.3553519	total: 274ms	remaining: 2.72s
183:	learn: 4963.4540764	total: 276ms	remaining: 2.72s
184:	learn: 4959.3484378	total: 277ms	remaining: 2.72s
185:	learn: 4953.8290305	total: 278ms	remaining: 2.71s
186:	learn: 4948.8512443	total: 280ms	remaining: 2.71s
187:	learn: 4942.0173436	total: 282ms	remaining: 2.71s
188:	learn: 4935.2163749	total: 283ms	remaining: 2.71s
189:	learn: 4927.8308601	total: 285ms	remaining: 2.71s
190:	learn: 4922.7874103	total: 286ms	remaining: 2.71s
191:	learn: 4921.8930548	total: 287ms	remaining: 2.71s

192:	learn: 4921.8930548	total: 288ms	remaining: 2.69s
193:	learn: 4916.1740670	total: 289ms	remaining: 2.69s
194:	learn: 4910.6747951	total: 291ms	remaining: 2.69s
195:	learn: 4901.7995007	total: 292ms	remaining: 2.69s
196:	learn: 4901.7821460	total: 293ms	remaining: 2.68s
197:	learn: 4897.4539465	total: 295ms	remaining: 2.68s
198:	learn: 4894.9567494	total: 296ms	remaining: 2.68s
199:	learn: 4891.2982974	total: 298ms	remaining: 2.68s
200:	learn: 4886.1187451	total: 299ms	remaining: 2.67s
201:	learn: 4877.8813207	total: 301ms	remaining: 2.67s
202:	learn: 4875.4244708	total: 302ms	remaining: 2.67s
203:	learn: 4870.3140418	total: 304ms	remaining: 2.67s
204:	learn: 4870.3140418	total: 304ms	remaining: 2.66s
205:	learn: 4856.6381725	total: 306ms	remaining: 2.66s
206:	learn: 4856.6381725	total: 306ms	remaining: 2.65s
207:	learn: 4852.3702566	total: 307ms	remaining: 2.65s
208:	learn: 4851.5158620	total: 309ms	remaining: 2.64s
209:	learn: 4847.0222783	total: 310ms	remaining: 2.64s
210:	learn: 4842.1138566	total: 312ms	remaining: 2.64s
211:	learn: 4838.7635392	total: 313ms	remaining: 2.64s
212:	learn: 4826.0451253	total: 315ms	remaining: 2.64s
213:	learn: 4819.7240280	total: 316ms	remaining: 2.64s
214:	learn: 4811.2169173	total: 318ms	remaining: 2.64s
215:	learn: 4811.2169173	total: 319ms	remaining: 2.63s
216:	learn: 4807.9718531	total: 320ms	remaining: 2.63s
217:	learn: 4806.7792354	total: 322ms	remaining: 2.63s
218:	learn: 4804.2533811	total: 323ms	remaining: 2.63s
219:	learn: 4799.5793423	total: 325ms	remaining: 2.63s
220:	learn: 4792.8584914	total: 326ms	remaining: 2.63s
221:	learn: 4787.4430082	total: 328ms	remaining: 2.63s
222:	learn: 4781.1207856	total: 330ms	remaining: 2.63s
223:	learn: 4773.1142514	total: 331ms	remaining: 2.62s
224:	learn: 4771.3835507	total: 332ms	remaining: 2.62s
225:	learn: 4769.0205967	total: 334ms	remaining: 2.62s
226:	learn: 4769.0205967	total: 334ms	remaining: 2.61s
227:	learn: 4765.8353863	total: 336ms	remaining: 2.61s
228:	learn: 4765.1621035	total: 337ms	remaining: 2.61s
229:	learn: 4761.9525642	total: 339ms	remaining: 2.61s
230:	learn: 4760.0450712	total: 341ms	remaining: 2.61s
231:	learn: 4755.1246652	total: 342ms	remaining: 2.61s
232:	learn: 4753.8217625	total: 343ms	remaining: 2.6s
233:	learn: 4747.5145731	total: 345ms	remaining: 2.6s
234:	learn: 4747.5145731	total: 345ms	remaining: 2.59s

235:	learn: 4744.6301998	total: 347ms	remaining: 2.59s
236:	learn: 4738.8864864	total: 348ms	remaining: 2.59s
237:	learn: 4736.5714509	total: 350ms	remaining: 2.59s
238:	learn: 4735.0890903	total: 352ms	remaining: 2.59s
239:	learn: 4728.3682935	total: 354ms	remaining: 2.59s
240:	learn: 4721.9886699	total: 355ms	remaining: 2.59s
241:	learn: 4717.3702814	total: 357ms	remaining: 2.59s
242:	learn: 4714.6835057	total: 359ms	remaining: 2.59s
243:	learn: 4712.3286406	total: 360ms	remaining: 2.59s
244:	learn: 4710.3755007	total: 362ms	remaining: 2.59s
245:	learn: 4710.3755007	total: 362ms	remaining: 2.58s
246:	learn: 4710.3279402	total: 363ms	remaining: 2.57s
247:	learn: 4708.7320386	total: 364ms	remaining: 2.57s
248:	learn: 4708.5308039	total: 365ms	remaining: 2.57s
249:	learn: 4708.4446512	total: 366ms	remaining: 2.56s
250:	learn: 4704.9778190	total: 368ms	remaining: 2.56s
251:	learn: 4703.1372636	total: 369ms	remaining: 2.56s
252:	learn: 4698.4459674	total: 371ms	remaining: 2.56s
253:	learn: 4698.4309104	total: 371ms	remaining: 2.55s
254:	learn: 4696.1765101	total: 373ms	remaining: 2.55s
255:	learn: 4693.9238815	total: 374ms	remaining: 2.55s
256:	learn: 4689.8119640	total: 377ms	remaining: 2.56s
257:	learn: 4689.8119640	total: 378ms	remaining: 2.55s
258:	learn: 4686.5896296	total: 380ms	remaining: 2.55s
259:	learn: 4680.2191721	total: 382ms	remaining: 2.56s
260:	learn: 4675.0591879	total: 385ms	remaining: 2.56s
261:	learn: 4671.5328062	total: 386ms	remaining: 2.56s
262:	learn: 4669.4746102	total: 388ms	remaining: 2.56s
263:	learn: 4666.6833477	total: 389ms	remaining: 2.56s
264:	learn: 4665.4037114	total: 391ms	remaining: 2.56s
265:	learn: 4663.4051577	total: 392ms	remaining: 2.56s
266:	learn: 4663.3353224	total: 393ms	remaining: 2.55s
267:	learn: 4660.7525508	total: 394ms	remaining: 2.55s
268:	learn: 4657.2685203	total: 396ms	remaining: 2.54s
269:	learn: 4657.2685203	total: 396ms	remaining: 2.54s
270:	learn: 4656.1503206	total: 397ms	remaining: 2.53s
271:	learn: 4652.0533288	total: 399ms	remaining: 2.54s
272:	learn: 4648.9435674	total: 401ms	remaining: 2.54s
273:	learn: 4645.7461085	total: 403ms	remaining: 2.54s
274:	learn: 4642.4289709	total: 404ms	remaining: 2.53s
275:	learn: 4635.8782081	total: 406ms	remaining: 2.53s
276:	learn: 4629.6954381	total: 407ms	remaining: 2.53s
277:	learn: 4627.1516605	total: 409ms	remaining: 2.53s

278:	learn: 4620.0534128	total: 410ms	remaining: 2.53s
279:	learn: 4620.0534128	total: 411ms	remaining: 2.52s
280:	learn: 4617.4583624	total: 412ms	remaining: 2.52s
281:	learn: 4615.3063600	total: 413ms	remaining: 2.52s
282:	learn: 4615.3063600	total: 414ms	remaining: 2.51s
283:	learn: 4615.3063600	total: 414ms	remaining: 2.5s
284:	learn: 4615.2984525	total: 415ms	remaining: 2.5s
285:	learn: 4611.3120573	total: 416ms	remaining: 2.5s
286:	learn: 4602.2423954	total: 418ms	remaining: 2.5s
287:	learn: 4600.2687023	total: 420ms	remaining: 2.5s
288:	learn: 4600.2687023	total: 420ms	remaining: 2.49s
289:	learn: 4596.0500378	total: 422ms	remaining: 2.49s
290:	learn: 4596.0500378	total: 422ms	remaining: 2.48s
291:	learn: 4594.3298144	total: 424ms	remaining: 2.48s
292:	learn: 4594.3298144	total: 424ms	remaining: 2.47s
293:	learn: 4591.3635862	total: 426ms	remaining: 2.47s
294:	learn: 4591.3400551	total: 426ms	remaining: 2.46s
295:	learn: 4591.3400551	total: 427ms	remaining: 2.46s
296:	learn: 4587.7544912	total: 428ms	remaining: 2.46s
297:	learn: 4582.6753402	total: 429ms	remaining: 2.45s
298:	learn: 4581.1496820	total: 431ms	remaining: 2.45s
299:	learn: 4580.8360346	total: 432ms	remaining: 2.45s
300:	learn: 4580.6042904	total: 433ms	remaining: 2.44s
301:	learn: 4577.5019033	total: 435ms	remaining: 2.44s
302:	learn: 4577.5019033	total: 435ms	remaining: 2.44s
303:	learn: 4577.4991453	total: 436ms	remaining: 2.43s
304:	learn: 4574.0774804	total: 438ms	remaining: 2.43s
305:	learn: 4567.1656172	total: 440ms	remaining: 2.44s
306:	learn: 4567.1656172	total: 440ms	remaining: 2.43s
307:	learn: 4567.1656172	total: 441ms	remaining: 2.42s
308:	learn: 4563.1270449	total: 442ms	remaining: 2.42s
309:	learn: 4556.4082285	total: 444ms	remaining: 2.42s
310:	learn: 4549.4002934	total: 446ms	remaining: 2.42s
311:	learn: 4548.6445542	total: 447ms	remaining: 2.42s
312:	learn: 4548.6445542	total: 447ms	remaining: 2.41s
313:	learn: 4548.6445542	total: 448ms	remaining: 2.4s
314:	learn: 4543.7698643	total: 449ms	remaining: 2.4s
315:	learn: 4537.5322728	total: 450ms	remaining: 2.4s
316:	learn: 4537.5322728	total: 451ms	remaining: 2.39s
317:	learn: 4535.8866669	total: 452ms	remaining: 2.39s
318:	learn: 4534.0177274	total: 454ms	remaining: 2.39s
319:	learn: 4534.0177274	total: 454ms	remaining: 2.38s
320:	learn: 4532.6563239	total: 456ms	remaining: 2.38s

321:	learn: 4532.5713131	total: 457ms	remaining: 2.38s
322:	learn: 4530.5122706	total: 458ms	remaining: 2.38s
323:	learn: 4530.0043105	total: 460ms	remaining: 2.38s
324:	learn: 4530.0043105	total: 460ms	remaining: 2.37s
325:	learn: 4521.2667630	total: 462ms	remaining: 2.37s
326:	learn: 4521.2667630	total: 462ms	remaining: 2.37s
327:	learn: 4514.9759966	total: 464ms	remaining: 2.36s
328:	learn: 4514.5353565	total: 465ms	remaining: 2.36s
329:	learn: 4514.5353565	total: 466ms	remaining: 2.35s
330:	learn: 4514.2251824	total: 467ms	remaining: 2.35s
331:	learn: 4513.4657797	total: 468ms	remaining: 2.35s
332:	learn: 4508.6585143	total: 469ms	remaining: 2.35s
333:	learn: 4506.4620472	total: 471ms	remaining: 2.35s
334:	learn: 4505.0540337	total: 472ms	remaining: 2.35s
335:	learn: 4501.2064750	total: 474ms	remaining: 2.35s
336:	learn: 4501.2064750	total: 474ms	remaining: 2.34s
337:	learn: 4496.9533102	total: 476ms	remaining: 2.34s
338:	learn: 4495.3477163	total: 478ms	remaining: 2.34s
339:	learn: 4495.0865050	total: 478ms	remaining: 2.33s
340:	learn: 4495.0865050	total: 479ms	remaining: 2.33s
341:	learn: 4494.8878363	total: 480ms	remaining: 2.33s
342:	learn: 4494.8878363	total: 481ms	remaining: 2.32s
343:	learn: 4493.9972375	total: 482ms	remaining: 2.32s
344:	learn: 4487.6187148	total: 483ms	remaining: 2.32s
345:	learn: 4485.1605053	total: 485ms	remaining: 2.32s
346:	learn: 4483.9053796	total: 486ms	remaining: 2.31s
347:	learn: 4483.9053796	total: 486ms	remaining: 2.31s
348:	learn: 4483.9051133	total: 487ms	remaining: 2.3s
349:	learn: 4483.6219873	total: 489ms	remaining: 2.3s
350:	learn: 4478.6575151	total: 490ms	remaining: 2.3s
351:	learn: 4478.1207406	total: 492ms	remaining: 2.3s
352:	learn: 4472.9000386	total: 493ms	remaining: 2.3s
353:	learn: 4472.8453202	total: 494ms	remaining: 2.3s
354:	learn: 4471.0678218	total: 496ms	remaining: 2.3s
355:	learn: 4468.5441814	total: 497ms	remaining: 2.29s
356:	learn: 4465.5049818	total: 498ms	remaining: 2.29s
357:	learn: 4461.3387165	total: 500ms	remaining: 2.29s
358:	learn: 4459.7424491	total: 501ms	remaining: 2.29s
359:	learn: 4455.5656117	total: 503ms	remaining: 2.29s
360:	learn: 4452.7121694	total: 504ms	remaining: 2.29s
361:	learn: 4447.3890000	total: 506ms	remaining: 2.29s
362:	learn: 4447.0423543	total: 507ms	remaining: 2.29s
363:	learn: 4445.7774126	total: 508ms	remaining: 2.29s

364:	learn: 4445.7774126	total: 509ms	remaining: 2.28s
365:	learn: 4444.5254579	total: 511ms	remaining: 2.28s
366:	learn: 4442.4085722	total: 512ms	remaining: 2.28s
367:	learn: 4441.9445764	total: 513ms	remaining: 2.27s
368:	learn: 4439.0150744	total: 514ms	remaining: 2.27s
369:	learn: 4435.2123964	total: 516ms	remaining: 2.27s
370:	learn: 4433.5067182	total: 517ms	remaining: 2.27s
371:	learn: 4425.5447245	total: 519ms	remaining: 2.27s
372:	learn: 4425.5447245	total: 520ms	remaining: 2.27s
373:	learn: 4423.8261031	total: 521ms	remaining: 2.26s
374:	learn: 4423.3283440	total: 522ms	remaining: 2.26s
375:	learn: 4423.3283440	total: 523ms	remaining: 2.26s
376:	learn: 4420.3203928	total: 524ms	remaining: 2.26s
377:	learn: 4419.5474976	total: 526ms	remaining: 2.25s
378:	learn: 4414.1595475	total: 527ms	remaining: 2.25s
379:	learn: 4412.2039198	total: 529ms	remaining: 2.25s
380:	learn: 4403.8910365	total: 530ms	remaining: 2.25s
381:	learn: 4403.2953039	total: 532ms	remaining: 2.25s
382:	learn: 4399.9196106	total: 533ms	remaining: 2.25s
383:	learn: 4398.9201818	total: 535ms	remaining: 2.25s
384:	learn: 4398.2316231	total: 536ms	remaining: 2.25s
385:	learn: 4398.2316231	total: 536ms	remaining: 2.24s
386:	learn: 4397.1150817	total: 538ms	remaining: 2.24s
387:	learn: 4396.4216007	total: 540ms	remaining: 2.24s
388:	learn: 4391.6969293	total: 541ms	remaining: 2.24s
389:	learn: 4389.9434594	total: 543ms	remaining: 2.24s
390:	learn: 4387.7026310	total: 544ms	remaining: 2.24s
391:	learn: 4385.6624572	total: 546ms	remaining: 2.24s
392:	learn: 4384.3285328	total: 547ms	remaining: 2.24s
393:	learn: 4381.9411758	total: 549ms	remaining: 2.24s
394:	learn: 4377.9349406	total: 550ms	remaining: 2.23s
395:	learn: 4375.2340793	total: 552ms	remaining: 2.23s
396:	learn: 4375.2338690	total: 552ms	remaining: 2.23s
397:	learn: 4374.5378448	total: 553ms	remaining: 2.23s
398:	learn: 4374.5378448	total: 554ms	remaining: 2.22s
399:	learn: 4374.0246587	total: 556ms	remaining: 2.22s
400:	learn: 4373.0983116	total: 557ms	remaining: 2.22s
401:	learn: 4371.7726903	total: 558ms	remaining: 2.22s
402:	learn: 4371.7726903	total: 559ms	remaining: 2.21s
403:	learn: 4367.9188809	total: 561ms	remaining: 2.22s
404:	learn: 4367.3837471	total: 563ms	remaining: 2.22s
405:	learn: 4367.3837471	total: 563ms	remaining: 2.21s
406:	learn: 4366.3383986	total: 565ms	remaining: 2.21s

407:	learn: 4364.9695002	total: 566ms	remaining: 2.21s
408:	learn: 4364.5791148	total: 567ms	remaining: 2.21s
409:	learn: 4364.5791148	total: 567ms	remaining: 2.2s
410:	learn: 4360.6650300	total: 569ms	remaining: 2.2s
411:	learn: 4358.8850197	total: 570ms	remaining: 2.2s
412:	learn: 4358.0952260	total: 572ms	remaining: 2.2s
413:	learn: 4358.0952260	total: 572ms	remaining: 2.19s
414:	learn: 4358.0952260	total: 573ms	remaining: 2.19s
415:	learn: 4353.9406626	total: 574ms	remaining: 2.19s
416:	learn: 4353.9406626	total: 574ms	remaining: 2.18s
417:	learn: 4353.9406626	total: 575ms	remaining: 2.17s
418:	learn: 4350.8582602	total: 576ms	remaining: 2.17s
419:	learn: 4348.7656427	total: 578ms	remaining: 2.17s
420:	learn: 4348.7654323	total: 579ms	remaining: 2.17s
421:	learn: 4347.2057659	total: 580ms	remaining: 2.17s
422:	learn: 4345.8380325	total: 582ms	remaining: 2.17s
423:	learn: 4340.0889391	total: 583ms	remaining: 2.17s
424:	learn: 4337.3466418	total: 585ms	remaining: 2.17s
425:	learn: 4333.1806959	total: 586ms	remaining: 2.16s
426:	learn: 4332.8557929	total: 587ms	remaining: 2.16s
427:	learn: 4332.8557929	total: 588ms	remaining: 2.16s
428:	learn: 4331.0378307	total: 589ms	remaining: 2.16s
429:	learn: 4325.1923800	total: 591ms	remaining: 2.16s
430:	learn: 4319.7524581	total: 592ms	remaining: 2.16s
431:	learn: 4316.9973772	total: 594ms	remaining: 2.16s
432:	learn: 4315.3920928	total: 596ms	remaining: 2.15s
433:	learn: 4313.5095488	total: 597ms	remaining: 2.15s
434:	learn: 4312.0378766	total: 599ms	remaining: 2.15s
435:	learn: 4309.9677471	total: 600ms	remaining: 2.15s
436:	learn: 4307.8543156	total: 602ms	remaining: 2.15s
437:	learn: 4306.3912379	total: 603ms	remaining: 2.15s
438:	learn: 4304.0146016	total: 605ms	remaining: 2.15s
439:	learn: 4304.0146016	total: 605ms	remaining: 2.15s
440:	learn: 4304.0146016	total: 606ms	remaining: 2.14s
441:	learn: 4296.2066898	total: 607ms	remaining: 2.14s
442:	learn: 4296.2066898	total: 608ms	remaining: 2.13s
443:	learn: 4296.2066898	total: 608ms	remaining: 2.13s
444:	learn: 4293.7742302	total: 610ms	remaining: 2.13s
445:	learn: 4290.6682497	total: 611ms	remaining: 2.13s
446:	learn: 4290.6682497	total: 612ms	remaining: 2.13s
447:	learn: 4290.6659104	total: 612ms	remaining: 2.12s
448:	learn: 4290.6659104	total: 613ms	remaining: 2.12s
449:	learn: 4290.6659104	total: 613ms	remaining: 2.11s

450:	learn: 4289.4314861	total: 615ms	remaining: 2.11s
451:	learn: 4287.6019761	total: 616ms	remaining: 2.11s
452:	learn: 4284.1460191	total: 618ms	remaining: 2.11s
453:	learn: 4283.1275688	total: 619ms	remaining: 2.11s
454:	learn: 4283.1275688	total: 620ms	remaining: 2.1s
455:	learn: 4282.2886315	total: 621ms	remaining: 2.1s
456:	learn: 4282.2886315	total: 622ms	remaining: 2.1s
457:	learn: 4281.3414277	total: 623ms	remaining: 2.1s
458:	learn: 4280.9302933	total: 624ms	remaining: 2.1s
459:	learn: 4280.2722045	total: 625ms	remaining: 2.09s
460:	learn: 4278.2675356	total: 627ms	remaining: 2.09s
461:	learn: 4276.8834771	total: 628ms	remaining: 2.09s
462:	learn: 4276.8162392	total: 629ms	remaining: 2.09s
463:	learn: 4271.9664215	total: 631ms	remaining: 2.09s
464:	learn: 4268.1650630	total: 633ms	remaining: 2.09s
465:	learn: 4261.3143626	total: 634ms	remaining: 2.09s
466:	learn: 4261.3143592	total: 635ms	remaining: 2.08s
467:	learn: 4255.8005291	total: 636ms	remaining: 2.08s
468:	learn: 4250.4214698	total: 638ms	remaining: 2.08s
469:	learn: 4248.4840035	total: 640ms	remaining: 2.08s
470:	learn: 4247.4707012	total: 642ms	remaining: 2.08s
471:	learn: 4244.9999349	total: 643ms	remaining: 2.08s
472:	learn: 4244.8961803	total: 644ms	remaining: 2.08s
473:	learn: 4243.5136900	total: 646ms	remaining: 2.08s
474:	learn: 4240.5620812	total: 647ms	remaining: 2.08s
475:	learn: 4237.5068841	total: 649ms	remaining: 2.08s
476:	learn: 4235.7372353	total: 650ms	remaining: 2.08s
477:	learn: 4235.5684329	total: 652ms	remaining: 2.07s
478:	learn: 4235.2638310	total: 653ms	remaining: 2.07s
479:	learn: 4234.8174553	total: 655ms	remaining: 2.07s
480:	learn: 4234.0613475	total: 657ms	remaining: 2.07s
481:	learn: 4234.0612821	total: 657ms	remaining: 2.07s
482:	learn: 4230.8662841	total: 659ms	remaining: 2.07s
483:	learn: 4228.3535703	total: 660ms	remaining: 2.07s
484:	learn: 4227.2170785	total: 662ms	remaining: 2.07s
485:	learn: 4227.2037809	total: 663ms	remaining: 2.07s
486:	learn: 4225.3901041	total: 665ms	remaining: 2.06s
487:	learn: 4224.7331910	total: 667ms	remaining: 2.06s
488:	learn: 4218.3517171	total: 668ms	remaining: 2.06s
489:	learn: 4218.3517171	total: 669ms	remaining: 2.06s
490:	learn: 4217.8187895	total: 670ms	remaining: 2.06s
491:	learn: 4215.5984258	total: 671ms	remaining: 2.06s
492:	learn: 4215.5984258	total: 672ms	remaining: 2.05s

493:	learn: 4213.8364336	total: 674ms	remaining: 2.05s
494:	learn: 4213.8364336	total: 674ms	remaining: 2.05s
495:	learn: 4213.0051294	total: 676ms	remaining: 2.05s
496:	learn: 4212.8201871	total: 677ms	remaining: 2.05s
497:	learn: 4210.8474431	total: 678ms	remaining: 2.04s
498:	learn: 4208.3847884	total: 680ms	remaining: 2.05s
499:	learn: 4207.8647287	total: 682ms	remaining: 2.04s
500:	learn: 4205.4937402	total: 683ms	remaining: 2.04s
501:	learn: 4201.6181630	total: 685ms	remaining: 2.04s
502:	learn: 4199.5545731	total: 686ms	remaining: 2.04s
503:	learn: 4199.5545731	total: 687ms	remaining: 2.04s
504:	learn: 4194.7013059	total: 688ms	remaining: 2.04s
505:	learn: 4194.7012736	total: 689ms	remaining: 2.03s
506:	learn: 4194.2513690	total: 690ms	remaining: 2.03s
507:	learn: 4193.7391858	total: 692ms	remaining: 2.03s
508:	learn: 4192.8297057	total: 694ms	remaining: 2.03s
509:	learn: 4192.3261240	total: 695ms	remaining: 2.03s
510:	learn: 4188.6361916	total: 696ms	remaining: 2.03s
511:	learn: 4184.1036666	total: 698ms	remaining: 2.03s
512:	learn: 4176.3244783	total: 700ms	remaining: 2.03s
513:	learn: 4176.3244783	total: 700ms	remaining: 2.02s
514:	learn: 4172.9846817	total: 701ms	remaining: 2.02s
515:	learn: 4168.9849081	total: 703ms	remaining: 2.02s
516:	learn: 4167.2190260	total: 704ms	remaining: 2.02s
517:	learn: 4167.2190260	total: 705ms	remaining: 2.02s
518:	learn: 4166.9911886	total: 706ms	remaining: 2.01s
519:	learn: 4162.8150043	total: 707ms	remaining: 2.01s
520:	learn: 4162.4234461	total: 709ms	remaining: 2.01s
521:	learn: 4161.6787564	total: 711ms	remaining: 2.01s
522:	learn: 4161.6787564	total: 711ms	remaining: 2.01s
523:	learn: 4159.0877863	total: 713ms	remaining: 2.01s
524:	learn: 4158.1609903	total: 714ms	remaining: 2.01s
525:	learn: 4154.6942835	total: 716ms	remaining: 2.01s
526:	learn: 4151.0966275	total: 718ms	remaining: 2s
527:	learn: 4149.3851416	total: 719ms	remaining: 2s
528:	learn: 4148.7633600	total: 721ms	remaining: 2s
529:	learn: 4148.2950844	total: 722ms	remaining: 2s
530:	learn: 4147.3736223	total: 724ms	remaining: 2s
531:	learn: 4147.3736223	total: 725ms	remaining: 2s
532:	learn: 4147.3596110	total: 725ms	remaining: 2s
533:	learn: 4145.0761992	total: 727ms	remaining: 2s
534:	learn: 4138.0181778	total: 729ms	remaining: 2s
535:	learn: 4136.2533307	total: 730ms	remaining: 1.99s

536:	learn: 4135.3564180	total: 732ms	remaining: 1.99s
537:	learn: 4135.3564180	total: 733ms	remaining: 1.99s
538:	learn: 4134.6207875	total: 734ms	remaining: 1.99s
539:	learn: 4130.3626163	total: 736ms	remaining: 1.99s
540:	learn: 4127.8526230	total: 738ms	remaining: 1.99s
541:	learn: 4127.8526230	total: 738ms	remaining: 1.99s
542:	learn: 4126.9499016	total: 740ms	remaining: 1.99s
543:	learn: 4124.4222877	total: 742ms	remaining: 1.99s
544:	learn: 4124.4093974	total: 744ms	remaining: 1.99s
545:	learn: 4120.4906474	total: 745ms	remaining: 1.98s
546:	learn: 4120.1085313	total: 747ms	remaining: 1.98s
547:	learn: 4118.5497982	total: 748ms	remaining: 1.98s
548:	learn: 4118.5497982	total: 749ms	remaining: 1.98s
549:	learn: 4116.7736360	total: 750ms	remaining: 1.98s
550:	learn: 4114.8590115	total: 752ms	remaining: 1.98s
551:	learn: 4113.8718524	total: 754ms	remaining: 1.98s
552:	learn: 4113.6509912	total: 755ms	remaining: 1.97s
553:	learn: 4112.7943829	total: 756ms	remaining: 1.97s
554:	learn: 4112.7943829	total: 757ms	remaining: 1.97s
555:	learn: 4111.8971678	total: 758ms	remaining: 1.97s
556:	learn: 4108.7174163	total: 760ms	remaining: 1.97s
557:	learn: 4108.0979840	total: 762ms	remaining: 1.97s
558:	learn: 4107.4667399	total: 763ms	remaining: 1.97s
559:	learn: 4107.0891159	total: 765ms	remaining: 1.97s
560:	learn: 4106.3886713	total: 767ms	remaining: 1.97s
561:	learn: 4106.3851242	total: 768ms	remaining: 1.96s
562:	learn: 4106.3797848	total: 768ms	remaining: 1.96s
563:	learn: 4106.3797848	total: 769ms	remaining: 1.96s
564:	learn: 4106.3797848	total: 769ms	remaining: 1.95s
565:	learn: 4106.3797848	total: 770ms	remaining: 1.95s
566:	learn: 4104.3466739	total: 772ms	remaining: 1.95s
567:	learn: 4102.6349434	total: 773ms	remaining: 1.95s
568:	learn: 4093.9566800	total: 775ms	remaining: 1.95s
569:	learn: 4089.1688460	total: 777ms	remaining: 1.95s
570:	learn: 4088.2412857	total: 778ms	remaining: 1.95s
571:	learn: 4088.2412857	total: 779ms	remaining: 1.94s
572:	learn: 4087.4126865	total: 781ms	remaining: 1.94s
573:	learn: 4087.3246347	total: 784ms	remaining: 1.95s
574:	learn: 4079.1728530	total: 786ms	remaining: 1.95s
575:	learn: 4076.9756189	total: 788ms	remaining: 1.95s
576:	learn: 4074.5129417	total: 790ms	remaining: 1.95s
577:	learn: 4073.6434006	total: 792ms	remaining: 1.95s
578:	learn: 4073.6434006	total: 793ms	remaining: 1.95s

579:	learn: 4073.1058334	total: 795ms	remaining: 1.95s
580:	learn: 4070.4631078	total: 797ms	remaining: 1.95s
581:	learn: 4068.7561071	total: 799ms	remaining: 1.95s
582:	learn: 4067.6543142	total: 801ms	remaining: 1.95s
583:	learn: 4064.0010837	total: 802ms	remaining: 1.95s
584:	learn: 4062.6699329	total: 804ms	remaining: 1.95s
585:	learn: 4061.8289513	total: 806ms	remaining: 1.95s
586:	learn: 4058.8888104	total: 808ms	remaining: 1.94s
587:	learn: 4057.5685823	total: 810ms	remaining: 1.94s
588:	learn: 4056.3428995	total: 812ms	remaining: 1.94s
589:	learn: 4051.0984948	total: 814ms	remaining: 1.94s
590:	learn: 4050.7321529	total: 816ms	remaining: 1.94s
591:	learn: 4048.6650531	total: 818ms	remaining: 1.95s
592:	learn: 4047.2165603	total: 820ms	remaining: 1.95s
593:	learn: 4043.7914684	total: 822ms	remaining: 1.94s
594:	learn: 4043.2525797	total: 823ms	remaining: 1.94s
595:	learn: 4043.2525797	total: 824ms	remaining: 1.94s
596:	learn: 4042.6610138	total: 826ms	remaining: 1.94s
597:	learn: 4039.9999717	total: 828ms	remaining: 1.94s
598:	learn: 4034.3252839	total: 830ms	remaining: 1.94s
599:	learn: 4034.3252839	total: 830ms	remaining: 1.94s
600:	learn: 4034.3252839	total: 831ms	remaining: 1.93s
601:	learn: 4034.2830758	total: 832ms	remaining: 1.93s
602:	learn: 4033.9653700	total: 834ms	remaining: 1.93s
603:	learn: 4033.9606019	total: 834ms	remaining: 1.93s
604:	learn: 4028.7695295	total: 836ms	remaining: 1.93s
605:	learn: 4028.4370609	total: 838ms	remaining: 1.93s
606:	learn: 4026.1362055	total: 840ms	remaining: 1.93s
607:	learn: 4025.1194150	total: 842ms	remaining: 1.93s
608:	learn: 4021.1161232	total: 844ms	remaining: 1.93s
609:	learn: 4020.5508077	total: 846ms	remaining: 1.93s
610:	learn: 4020.5508077	total: 846ms	remaining: 1.92s
611:	learn: 4020.3832148	total: 847ms	remaining: 1.92s
612:	learn: 4016.1194956	total: 849ms	remaining: 1.92s
613:	learn: 4013.4009443	total: 851ms	remaining: 1.92s
614:	learn: 4012.3927298	total: 853ms	remaining: 1.92s
615:	learn: 4012.3875832	total: 853ms	remaining: 1.92s
616:	learn: 4012.2092547	total: 855ms	remaining: 1.92s
617:	learn: 4010.9373855	total: 856ms	remaining: 1.91s
618:	learn: 4010.6712533	total: 858ms	remaining: 1.91s
619:	learn: 4007.0184514	total: 859ms	remaining: 1.91s
620:	learn: 4007.0184514	total: 860ms	remaining: 1.91s
621:	learn: 4006.3237895	total: 862ms	remaining: 1.91s

622:	learn: 4004.8793407	total: 864ms	remaining: 1.91s
623:	learn: 4003.9471214	total: 865ms	remaining: 1.91s
624:	learn: 4000.7887982	total: 867ms	remaining: 1.91s
625:	learn: 4000.4795677	total: 868ms	remaining: 1.91s
626:	learn: 4000.3438616	total: 870ms	remaining: 1.9s
627:	learn: 3999.1296902	total: 871ms	remaining: 1.9s
628:	learn: 3998.0867078	total: 873ms	remaining: 1.9s
629:	learn: 3998.0867078	total: 873ms	remaining: 1.9s
630:	learn: 3995.4813310	total: 875ms	remaining: 1.9s
631:	learn: 3995.4813310	total: 876ms	remaining: 1.9s
632:	learn: 3994.7973506	total: 878ms	remaining: 1.9s
633:	learn: 3994.4255478	total: 879ms	remaining: 1.89s
634:	learn: 3993.8426501	total: 881ms	remaining: 1.89s
635:	learn: 3992.4595577	total: 883ms	remaining: 1.89s
636:	learn: 3991.2065592	total: 885ms	remaining: 1.89s
637:	learn: 3990.5372097	total: 887ms	remaining: 1.89s
638:	learn: 3990.5313149	total: 887ms	remaining: 1.89s
639:	learn: 3989.2375720	total: 889ms	remaining: 1.89s
640:	learn: 3987.6399593	total: 891ms	remaining: 1.89s
641:	learn: 3986.0680229	total: 893ms	remaining: 1.89s
642:	learn: 3986.0680229	total: 893ms	remaining: 1.89s
643:	learn: 3985.3611248	total: 895ms	remaining: 1.88s
644:	learn: 3984.9141762	total: 897ms	remaining: 1.88s
645:	learn: 3978.4243745	total: 899ms	remaining: 1.88s
646:	learn: 3978.0748821	total: 900ms	remaining: 1.88s
647:	learn: 3975.0948892	total: 902ms	remaining: 1.88s
648:	learn: 3973.7336182	total: 904ms	remaining: 1.88s
649:	learn: 3973.5694895	total: 906ms	remaining: 1.88s
650:	learn: 3973.5694895	total: 906ms	remaining: 1.88s
651:	learn: 3973.2035512	total: 908ms	remaining: 1.88s
652:	learn: 3971.3748963	total: 910ms	remaining: 1.88s
653:	learn: 3970.8273230	total: 912ms	remaining: 1.88s
654:	learn: 3970.6661701	total: 913ms	remaining: 1.87s
655:	learn: 3970.3188222	total: 915ms	remaining: 1.87s
656:	learn: 3967.7537638	total: 917ms	remaining: 1.87s
657:	learn: 3965.3162844	total: 919ms	remaining: 1.87s
658:	learn: 3963.3457135	total: 922ms	remaining: 1.88s
659:	learn: 3960.6737011	total: 924ms	remaining: 1.88s
660:	learn: 3957.5551840	total: 927ms	remaining: 1.88s
661:	learn: 3954.5284019	total: 928ms	remaining: 1.88s
662:	learn: 3954.2685083	total: 930ms	remaining: 1.88s
663:	learn: 3953.7975769	total: 936ms	remaining: 1.88s
664:	learn: 3952.5579480	total: 939ms	remaining: 1.89s

665:	learn:	3952.5579480	total:	940ms	remaining:	1.88s
666:	learn:	3952.5579480	total:	941ms	remaining:	1.88s
667:	learn:	3952.0530212	total:	943ms	remaining:	1.88s
668:	learn:	3951.0236652	total:	946ms	remaining:	1.88s
669:	learn:	3948.8482121	total:	948ms	remaining:	1.88s
670:	learn:	3948.1039576	total:	950ms	remaining:	1.88s
671:	learn:	3948.1039576	total:	951ms	remaining:	1.88s
672:	learn:	3947.8466720	total:	952ms	remaining:	1.88s
673:	learn:	3944.7760408	total:	954ms	remaining:	1.88s
674:	learn:	3944.3794626	total:	956ms	remaining:	1.88s
675:	learn:	3943.8828460	total:	959ms	remaining:	1.88s
676:	learn:	3939.4803751	total:	962ms	remaining:	1.88s
677:	learn:	3937.0226901	total:	964ms	remaining:	1.88s
678:	learn:	3935.6062093	total:	966ms	remaining:	1.88s
679:	learn:	3931.6908549	total:	968ms	remaining:	1.88s
680:	learn:	3931.6908549	total:	969ms	remaining:	1.88s
681:	learn:	3931.4780236	total:	970ms	remaining:	1.88s
682:	learn:	3931.4780236	total:	971ms	remaining:	1.87s
683:	learn:	3930.1802631	total:	973ms	remaining:	1.87s
684:	learn:	3930.1802631	total:	974ms	remaining:	1.87s
685:	learn:	3930.1802631	total:	974ms	remaining:	1.87s
686:	learn:	3929.9546359	total:	975ms	remaining:	1.86s
687:	learn:	3929.9546359	total:	976ms	remaining:	1.86s
688:	learn:	3929.5200873	total:	978ms	remaining:	1.86s
689:	learn:	3924.1504149	total:	980ms	remaining:	1.86s
690:	learn:	3924.1504149	total:	981ms	remaining:	1.86s
691:	learn:	3924.1504149	total:	981ms	remaining:	1.85s
692:	learn:	3923.3728173	total:	984ms	remaining:	1.86s
693:	learn:	3923.3728173	total:	985ms	remaining:	1.85s
694:	learn:	3921.6096814	total:	987ms	remaining:	1.85s
695:	learn:	3920.3917066	total:	989ms	remaining:	1.85s
696:	learn:	3919.1748239	total:	991ms	remaining:	1.85s
697:	learn:	3918.6781013	total:	993ms	remaining:	1.85s
698:	learn:	3915.5786090	total:	995ms	remaining:	1.85s
699:	learn:	3914.9386661	total:	997ms	remaining:	1.85s
700:	learn:	3914.1044266	total:	999ms	remaining:	1.85s
701:	learn:	3914.1044266	total:	1000ms	remaining:	1.85s
702:	learn:	3911.5461909	total:	1s	remaining:	1.85s
703:	learn:	3909.7858547	total:	1s	remaining:	1.85s
704:	learn:	3908.5848398	total:	1s	remaining:	1.85s
705:	learn:	3908.5846612	total:	1.01s	remaining:	1.84s
706:	learn:	3906.3544545	total:	1.01s	remaining:	1.84s
707:	learn:	3902.5421111	total:	1.01s	remaining:	1.84s

708:	learn: 3900.6794103	total: 1.01s	remaining: 1.84s
709:	learn: 3900.1145635	total: 1.01s	remaining: 1.84s
710:	learn: 3898.7988768	total: 1.02s	remaining: 1.84s
711:	learn: 3897.7890023	total: 1.02s	remaining: 1.84s
712:	learn: 3897.3063669	total: 1.02s	remaining: 1.84s
713:	learn: 3896.0709359	total: 1.02s	remaining: 1.84s
714:	learn: 3893.2716970	total: 1.03s	remaining: 1.84s
715:	learn: 3893.2716970	total: 1.03s	remaining: 1.84s
716:	learn: 3892.7696855	total: 1.03s	remaining: 1.84s
717:	learn: 3891.8609727	total: 1.03s	remaining: 1.84s
718:	learn: 3891.8609727	total: 1.03s	remaining: 1.84s
719:	learn: 3886.5432527	total: 1.03s	remaining: 1.84s
720:	learn: 3885.5890724	total: 1.03s	remaining: 1.84s
721:	learn: 3885.2509517	total: 1.04s	remaining: 1.83s
722:	learn: 3884.8683416	total: 1.04s	remaining: 1.83s
723:	learn: 3883.8658058	total: 1.04s	remaining: 1.83s
724:	learn: 3882.8769674	total: 1.04s	remaining: 1.83s
725:	learn: 3880.1551434	total: 1.04s	remaining: 1.83s
726:	learn: 3878.8486183	total: 1.05s	remaining: 1.83s
727:	learn: 3878.0455602	total: 1.05s	remaining: 1.83s
728:	learn: 3878.0455602	total: 1.05s	remaining: 1.83s
729:	learn: 3875.8100129	total: 1.05s	remaining: 1.83s
730:	learn: 3875.8100129	total: 1.05s	remaining: 1.83s
731:	learn: 3874.7519439	total: 1.05s	remaining: 1.82s
732:	learn: 3873.0181722	total: 1.05s	remaining: 1.82s
733:	learn: 3872.6475110	total: 1.06s	remaining: 1.82s
734:	learn: 3870.6422449	total: 1.06s	remaining: 1.82s
735:	learn: 3869.4474087	total: 1.06s	remaining: 1.82s
736:	learn: 3867.0168014	total: 1.06s	remaining: 1.82s
737:	learn: 3865.3121541	total: 1.06s	remaining: 1.82s
738:	learn: 3864.3253068	total: 1.07s	remaining: 1.82s
739:	learn: 3863.3321651	total: 1.07s	remaining: 1.82s
740:	learn: 3863.0244965	total: 1.07s	remaining: 1.82s
741:	learn: 3861.8958492	total: 1.07s	remaining: 1.82s
742:	learn: 3861.7968837	total: 1.07s	remaining: 1.82s
743:	learn: 3861.7962967	total: 1.07s	remaining: 1.81s
744:	learn: 3860.4491412	total: 1.08s	remaining: 1.81s
745:	learn: 3860.4491412	total: 1.08s	remaining: 1.81s
746:	learn: 3859.3516675	total: 1.08s	remaining: 1.81s
747:	learn: 3858.3562986	total: 1.08s	remaining: 1.81s
748:	learn: 3858.3562986	total: 1.08s	remaining: 1.8s
749:	learn: 3858.3490771	total: 1.08s	remaining: 1.8s
750:	learn: 3858.2502493	total: 1.08s	remaining: 1.8s

751:	learn:	3857.4697682	total:	1.08s	remaining:	1.8s
752:	learn:	3857.4659809	total:	1.08s	remaining:	1.8s
753:	learn:	3856.9435214	total:	1.09s	remaining:	1.8s
754:	learn:	3856.9435214	total:	1.09s	remaining:	1.79s
755:	learn:	3856.2765714	total:	1.09s	remaining:	1.79s
756:	learn:	3855.7600481	total:	1.09s	remaining:	1.79s
757:	learn:	3852.6969291	total:	1.09s	remaining:	1.79s
758:	learn:	3852.6730764	total:	1.09s	remaining:	1.79s
759:	learn:	3852.2047553	total:	1.09s	remaining:	1.79s
760:	learn:	3851.5653409	total:	1.1s	remaining:	1.79s
761:	learn:	3851.5508266	total:	1.1s	remaining:	1.78s
762:	learn:	3848.7387610	total:	1.1s	remaining:	1.78s
763:	learn:	3847.7080161	total:	1.1s	remaining:	1.78s
764:	learn:	3847.7080161	total:	1.1s	remaining:	1.78s
765:	learn:	3847.6293776	total:	1.1s	remaining:	1.78s
766:	learn:	3847.6293776	total:	1.1s	remaining:	1.77s
767:	learn:	3847.6289207	total:	1.1s	remaining:	1.77s
768:	learn:	3845.8710962	total:	1.11s	remaining:	1.77s
769:	learn:	3845.3032079	total:	1.11s	remaining:	1.77s
770:	learn:	3844.5649758	total:	1.11s	remaining:	1.77s
771:	learn:	3843.7347054	total:	1.11s	remaining:	1.77s
772:	learn:	3841.6978237	total:	1.11s	remaining:	1.77s
773:	learn:	3841.0971126	total:	1.12s	remaining:	1.77s
774:	learn:	3837.4084642	total:	1.12s	remaining:	1.77s
775:	learn:	3837.0934050	total:	1.12s	remaining:	1.76s
776:	learn:	3836.7762376	total:	1.12s	remaining:	1.76s
777:	learn:	3836.2799013	total:	1.12s	remaining:	1.76s
778:	learn:	3834.5565153	total:	1.12s	remaining:	1.76s
779:	learn:	3832.9932344	total:	1.13s	remaining:	1.76s
780:	learn:	3829.3338033	total:	1.13s	remaining:	1.76s
781:	learn:	3828.5601788	total:	1.13s	remaining:	1.76s
782:	learn:	3828.5601788	total:	1.13s	remaining:	1.76s
783:	learn:	3828.5601744	total:	1.13s	remaining:	1.75s
784:	learn:	3827.5366664	total:	1.13s	remaining:	1.75s
785:	learn:	3826.4151057	total:	1.13s	remaining:	1.75s
786:	learn:	3825.7586832	total:	1.14s	remaining:	1.75s
787:	learn:	3825.0938251	total:	1.14s	remaining:	1.75s
788:	learn:	3824.9906903	total:	1.14s	remaining:	1.75s
789:	learn:	3824.5655529	total:	1.14s	remaining:	1.75s
790:	learn:	3822.6288381	total:	1.14s	remaining:	1.75s
791:	learn:	3822.3783984	total:	1.15s	remaining:	1.75s
792:	learn:	3820.2943393	total:	1.15s	remaining:	1.75s
793:	learn:	3820.0646286	total:	1.15s	remaining:	1.74s

794:	learn:	3819.9664245	total:	1.15s	remaining:	1.74s
795:	learn:	3818.9084625	total:	1.15s	remaining:	1.74s
796:	learn:	3818.5750938	total:	1.15s	remaining:	1.74s
797:	learn:	3817.5402599	total:	1.16s	remaining:	1.74s
798:	learn:	3816.2278347	total:	1.16s	remaining:	1.74s
799:	learn:	3812.7380606	total:	1.16s	remaining:	1.74s
800:	learn:	3812.7380606	total:	1.16s	remaining:	1.74s
801:	learn:	3812.7380606	total:	1.16s	remaining:	1.73s
802:	learn:	3811.5718740	total:	1.16s	remaining:	1.73s
803:	learn:	3811.3369065	total:	1.16s	remaining:	1.73s
804:	learn:	3811.1293690	total:	1.16s	remaining:	1.73s
805:	learn:	3811.1183005	total:	1.17s	remaining:	1.73s
806:	learn:	3808.8433205	total:	1.17s	remaining:	1.73s
807:	learn:	3808.6095214	total:	1.17s	remaining:	1.72s
808:	learn:	3807.7139243	total:	1.17s	remaining:	1.72s
809:	learn:	3807.5754253	total:	1.17s	remaining:	1.72s
810:	learn:	3807.4133638	total:	1.17s	remaining:	1.72s
811:	learn:	3805.7109740	total:	1.18s	remaining:	1.72s
812:	learn:	3804.7089862	total:	1.18s	remaining:	1.72s
813:	learn:	3802.8930509	total:	1.18s	remaining:	1.72s
814:	learn:	3802.2797474	total:	1.18s	remaining:	1.72s
815:	learn:	3800.9263311	total:	1.18s	remaining:	1.72s
816:	learn:	3796.9644567	total:	1.19s	remaining:	1.72s
817:	learn:	3796.9644567	total:	1.19s	remaining:	1.71s
818:	learn:	3794.6321824	total:	1.19s	remaining:	1.71s
819:	learn:	3793.7138810	total:	1.19s	remaining:	1.71s
820:	learn:	3793.4292740	total:	1.19s	remaining:	1.71s
821:	learn:	3793.4255576	total:	1.19s	remaining:	1.71s
822:	learn:	3792.1343626	total:	1.19s	remaining:	1.71s
823:	learn:	3790.4684901	total:	1.2s	remaining:	1.71s
824:	learn:	3790.0355937	total:	1.2s	remaining:	1.71s
825:	learn:	3789.5560775	total:	1.2s	remaining:	1.7s
826:	learn:	3787.8915354	total:	1.2s	remaining:	1.7s
827:	learn:	3787.5419872	total:	1.2s	remaining:	1.7s
828:	learn:	3784.9113968	total:	1.2s	remaining:	1.7s
829:	learn:	3784.9113968	total:	1.21s	remaining:	1.7s
830:	learn:	3784.5295880	total:	1.21s	remaining:	1.7s
831:	learn:	3784.5061352	total:	1.21s	remaining:	1.7s
832:	learn:	3783.9559552	total:	1.21s	remaining:	1.7s
833:	learn:	3783.2083733	total:	1.21s	remaining:	1.69s
834:	learn:	3782.5879048	total:	1.21s	remaining:	1.69s
835:	learn:	3778.7531050	total:	1.22s	remaining:	1.69s
836:	learn:	3778.3606445	total:	1.22s	remaining:	1.69s

837:	learn: 3777.5169044	total: 1.22s	remaining: 1.69s
838:	learn: 3776.0781037	total: 1.22s	remaining: 1.69s
839:	learn: 3774.1576914	total: 1.22s	remaining: 1.69s
840:	learn: 3773.0961327	total: 1.23s	remaining: 1.69s
841:	learn: 3769.1849336	total: 1.23s	remaining: 1.69s
842:	learn: 3769.1849336	total: 1.23s	remaining: 1.69s
843:	learn: 3768.5544138	total: 1.23s	remaining: 1.68s
844:	learn: 3767.0540299	total: 1.23s	remaining: 1.68s
845:	learn: 3766.5195021	total: 1.23s	remaining: 1.68s
846:	learn: 3766.5195021	total: 1.23s	remaining: 1.68s
847:	learn: 3766.4835237	total: 1.23s	remaining: 1.68s
848:	learn: 3766.3146637	total: 1.24s	remaining: 1.68s
849:	learn: 3766.3146637	total: 1.24s	remaining: 1.67s
850:	learn: 3760.7193853	total: 1.24s	remaining: 1.67s
851:	learn: 3760.2822988	total: 1.24s	remaining: 1.67s
852:	learn: 3760.2822988	total: 1.24s	remaining: 1.67s
853:	learn: 3760.1005594	total: 1.24s	remaining: 1.67s
854:	learn: 3758.8854406	total: 1.24s	remaining: 1.67s
855:	learn: 3758.2299296	total: 1.25s	remaining: 1.67s
856:	learn: 3755.6860428	total: 1.25s	remaining: 1.66s
857:	learn: 3754.4660145	total: 1.25s	remaining: 1.66s
858:	learn: 3753.1371758	total: 1.25s	remaining: 1.66s
859:	learn: 3752.4535790	total: 1.25s	remaining: 1.66s
860:	learn: 3752.2871783	total: 1.25s	remaining: 1.66s
861:	learn: 3751.5256924	total: 1.26s	remaining: 1.66s
862:	learn: 3751.5209414	total: 1.26s	remaining: 1.66s
863:	learn: 3751.2839240	total: 1.26s	remaining: 1.66s
864:	learn: 3750.8896543	total: 1.26s	remaining: 1.65s
865:	learn: 3748.9138530	total: 1.26s	remaining: 1.65s
866:	learn: 3748.7446691	total: 1.26s	remaining: 1.65s
867:	learn: 3748.2933914	total: 1.27s	remaining: 1.65s
868:	learn: 3747.7771132	total: 1.27s	remaining: 1.65s
869:	learn: 3747.4756519	total: 1.27s	remaining: 1.65s
870:	learn: 3746.8798693	total: 1.27s	remaining: 1.65s
871:	learn: 3746.3395775	total: 1.27s	remaining: 1.65s
872:	learn: 3746.1296952	total: 1.27s	remaining: 1.65s
873:	learn: 3743.5685571	total: 1.28s	remaining: 1.65s
874:	learn: 3741.4152266	total: 1.28s	remaining: 1.64s
875:	learn: 3741.2402215	total: 1.28s	remaining: 1.64s
876:	learn: 3741.0882207	total: 1.28s	remaining: 1.64s
877:	learn: 3740.1415409	total: 1.28s	remaining: 1.64s
878:	learn: 3740.1413814	total: 1.28s	remaining: 1.64s
879:	learn: 3738.9862194	total: 1.29s	remaining: 1.64s

880:	learn: 3737.5337821	total: 1.29s	remaining: 1.64s
881:	learn: 3737.5337821	total: 1.29s	remaining: 1.63s
882:	learn: 3737.1581488	total: 1.29s	remaining: 1.63s
883:	learn: 3736.7844566	total: 1.29s	remaining: 1.63s
884:	learn: 3736.7844566	total: 1.29s	remaining: 1.63s
885:	learn: 3736.7841652	total: 1.29s	remaining: 1.63s
886:	learn: 3736.5406219	total: 1.3s	remaining: 1.63s
887:	learn: 3736.1152642	total: 1.3s	remaining: 1.63s
888:	learn: 3734.4118333	total: 1.3s	remaining: 1.62s
889:	learn: 3733.9724930	total: 1.3s	remaining: 1.62s
890:	learn: 3733.8000485	total: 1.3s	remaining: 1.62s
891:	learn: 3733.4601714	total: 1.3s	remaining: 1.62s
892:	learn: 3733.1641953	total: 1.31s	remaining: 1.62s
893:	learn: 3733.0912557	total: 1.31s	remaining: 1.62s
894:	learn: 3731.9732853	total: 1.31s	remaining: 1.62s
895:	learn: 3731.4078934	total: 1.31s	remaining: 1.62s
896:	learn: 3730.4823594	total: 1.31s	remaining: 1.62s
897:	learn: 3730.4018892	total: 1.32s	remaining: 1.61s
898:	learn: 3729.7012273	total: 1.32s	remaining: 1.61s
899:	learn: 3729.2725886	total: 1.32s	remaining: 1.61s
900:	learn: 3728.4962656	total: 1.32s	remaining: 1.61s
901:	learn: 3728.2322230	total: 1.32s	remaining: 1.61s
902:	learn: 3727.5962340	total: 1.32s	remaining: 1.61s
903:	learn: 3726.0272566	total: 1.33s	remaining: 1.61s
904:	learn: 3725.9333842	total: 1.33s	remaining: 1.61s
905:	learn: 3724.8243608	total: 1.33s	remaining: 1.6s
906:	learn: 3724.2181171	total: 1.33s	remaining: 1.6s
907:	learn: 3724.2181171	total: 1.33s	remaining: 1.6s
908:	learn: 3724.1997717	total: 1.33s	remaining: 1.6s
909:	learn: 3722.5087637	total: 1.33s	remaining: 1.6s
910:	learn: 3722.5087637	total: 1.33s	remaining: 1.6s
911:	learn: 3722.3746981	total: 1.34s	remaining: 1.59s
912:	learn: 3722.0076978	total: 1.34s	remaining: 1.59s
913:	learn: 3721.3351238	total: 1.34s	remaining: 1.59s
914:	learn: 3721.3351238	total: 1.34s	remaining: 1.59s
915:	learn: 3719.7788144	total: 1.34s	remaining: 1.59s
916:	learn: 3718.5757182	total: 1.34s	remaining: 1.59s
917:	learn: 3717.0143275	total: 1.35s	remaining: 1.59s
918:	learn: 3716.7013645	total: 1.35s	remaining: 1.58s
919:	learn: 3716.7013645	total: 1.35s	remaining: 1.58s
920:	learn: 3716.1538803	total: 1.35s	remaining: 1.58s
921:	learn: 3715.6253818	total: 1.35s	remaining: 1.58s
922:	learn: 3715.0529522	total: 1.35s	remaining: 1.58s

923:	learn: 3714.5005523	total: 1.36s	remaining: 1.58s
924:	learn: 3712.1508975	total: 1.36s	remaining: 1.58s
925:	learn: 3711.6039564	total: 1.36s	remaining: 1.58s
926:	learn: 3710.1385822	total: 1.36s	remaining: 1.58s
927:	learn: 3708.9893699	total: 1.36s	remaining: 1.57s
928:	learn: 3708.9768362	total: 1.36s	remaining: 1.57s
929:	learn: 3708.9709846	total: 1.36s	remaining: 1.57s
930:	learn: 3708.4679536	total: 1.37s	remaining: 1.57s
931:	learn: 3707.2311610	total: 1.37s	remaining: 1.57s
932:	learn: 3707.0972053	total: 1.37s	remaining: 1.57s
933:	learn: 3706.8547678	total: 1.37s	remaining: 1.57s
934:	learn: 3704.6011174	total: 1.37s	remaining: 1.56s
935:	learn: 3702.5238173	total: 1.38s	remaining: 1.56s
936:	learn: 3702.4828780	total: 1.38s	remaining: 1.56s
937:	learn: 3702.4828780	total: 1.38s	remaining: 1.56s
938:	learn: 3702.3967813	total: 1.38s	remaining: 1.56s
939:	learn: 3702.0342639	total: 1.38s	remaining: 1.56s
940:	learn: 3701.1780133	total: 1.38s	remaining: 1.55s
941:	learn: 3700.7531695	total: 1.38s	remaining: 1.55s
942:	learn: 3700.4658106	total: 1.39s	remaining: 1.55s
943:	learn: 3699.2095210	total: 1.39s	remaining: 1.55s
944:	learn: 3699.0562756	total: 1.39s	remaining: 1.55s
945:	learn: 3699.0562756	total: 1.39s	remaining: 1.55s
946:	learn: 3698.2595417	total: 1.39s	remaining: 1.55s
947:	learn: 3695.5636725	total: 1.39s	remaining: 1.55s
948:	learn: 3694.5819843	total: 1.4s	remaining: 1.55s
949:	learn: 3694.3462767	total: 1.4s	remaining: 1.54s
950:	learn: 3693.6615322	total: 1.4s	remaining: 1.54s
951:	learn: 3692.5638974	total: 1.4s	remaining: 1.54s
952:	learn: 3692.5638974	total: 1.4s	remaining: 1.54s
953:	learn: 3685.4910277	total: 1.4s	remaining: 1.54s
954:	learn: 3685.2059786	total: 1.4s	remaining: 1.54s
955:	learn: 3684.2455121	total: 1.41s	remaining: 1.54s
956:	learn: 3683.7580229	total: 1.41s	remaining: 1.53s
957:	learn: 3681.9457611	total: 1.41s	remaining: 1.53s
958:	learn: 3681.5652050	total: 1.41s	remaining: 1.53s
959:	learn: 3681.5652050	total: 1.41s	remaining: 1.53s
960:	learn: 3680.2135370	total: 1.41s	remaining: 1.53s
961:	learn: 3680.1767027	total: 1.42s	remaining: 1.53s
962:	learn: 3679.8473836	total: 1.42s	remaining: 1.53s
963:	learn: 3677.4207960	total: 1.42s	remaining: 1.52s
964:	learn: 3677.4207960	total: 1.42s	remaining: 1.52s
965:	learn: 3677.4188338	total: 1.42s	remaining: 1.52s

966:	learn: 3677.4188338	total: 1.42s	remaining: 1.52s
967:	learn: 3676.9216619	total: 1.42s	remaining: 1.52s
968:	learn: 3675.3089857	total: 1.42s	remaining: 1.51s
969:	learn: 3675.2688544	total: 1.43s	remaining: 1.51s
970:	learn: 3674.0677886	total: 1.43s	remaining: 1.51s
971:	learn: 3673.5915745	total: 1.43s	remaining: 1.51s
972:	learn: 3673.3693200	total: 1.43s	remaining: 1.51s
973:	learn: 3672.7873480	total: 1.43s	remaining: 1.51s
974:	learn: 3671.8253357	total: 1.43s	remaining: 1.51s
975:	learn: 3668.8709628	total: 1.44s	remaining: 1.51s
976:	learn: 3668.8709628	total: 1.44s	remaining: 1.5s
977:	learn: 3668.7627721	total: 1.44s	remaining: 1.5s
978:	learn: 3667.4786633	total: 1.44s	remaining: 1.5s
979:	learn: 3666.5861168	total: 1.44s	remaining: 1.5s
980:	learn: 3666.3023313	total: 1.44s	remaining: 1.5s
981:	learn: 3666.1529594	total: 1.44s	remaining: 1.5s
982:	learn: 3664.1631253	total: 1.45s	remaining: 1.5s
983:	learn: 3663.8921268	total: 1.45s	remaining: 1.5s
984:	learn: 3663.5891686	total: 1.45s	remaining: 1.49s
985:	learn: 3663.3478513	total: 1.45s	remaining: 1.49s
986:	learn: 3663.3443644	total: 1.45s	remaining: 1.49s
987:	learn: 3662.4739468	total: 1.45s	remaining: 1.49s
988:	learn: 3659.7979207	total: 1.46s	remaining: 1.49s
989:	learn: 3656.7774930	total: 1.46s	remaining: 1.49s
990:	learn: 3655.5815035	total: 1.46s	remaining: 1.49s
991:	learn: 3655.3199530	total: 1.46s	remaining: 1.48s
992:	learn: 3653.0603803	total: 1.46s	remaining: 1.48s
993:	learn: 3653.0603803	total: 1.46s	remaining: 1.48s
994:	learn: 3652.4369568	total: 1.46s	remaining: 1.48s
995:	learn: 3651.9836020	total: 1.47s	remaining: 1.48s
996:	learn: 3649.7055373	total: 1.47s	remaining: 1.48s
997:	learn: 3649.3310304	total: 1.47s	remaining: 1.48s
998:	learn: 3648.6113397	total: 1.47s	remaining: 1.47s
999:	learn: 3648.1952207	total: 1.47s	remaining: 1.47s
1000:	learn: 3647.6434249	total: 1.48s	remaining: 1.47s
1001:	learn: 3647.4992176	total: 1.48s	remaining: 1.47s
1002:	learn: 3647.4992176	total: 1.48s	remaining: 1.47s
1003:	learn: 3645.5814467	total: 1.48s	remaining: 1.47s
1004:	learn: 3645.1610774	total: 1.48s	remaining: 1.47s
1005:	learn: 3645.1130043	total: 1.48s	remaining: 1.47s
1006:	learn: 3643.9491608	total: 1.48s	remaining: 1.46s
1007:	learn: 3641.4554180	total: 1.49s	remaining: 1.46s
1008:	learn: 3640.8504319	total: 1.49s	remaining: 1.46s

1009:	learn:	3640.7715577	total:	1.49s	remaining:	1.46s
1010:	learn:	3640.6094922	total:	1.49s	remaining:	1.46s
1011:	learn:	3638.4023054	total:	1.49s	remaining:	1.46s
1012:	learn:	3636.7756918	total:	1.49s	remaining:	1.46s
1013:	learn:	3635.7462844	total:	1.5s	remaining:	1.45s
1014:	learn:	3635.4468132	total:	1.5s	remaining:	1.45s
1015:	learn:	3635.3983898	total:	1.5s	remaining:	1.45s
1016:	learn:	3635.1676270	total:	1.5s	remaining:	1.45s
1017:	learn:	3634.6068208	total:	1.5s	remaining:	1.45s
1018:	learn:	3633.7610803	total:	1.5s	remaining:	1.45s
1019:	learn:	3632.7942984	total:	1.51s	remaining:	1.45s
1020:	learn:	3630.7096665	total:	1.51s	remaining:	1.45s
1021:	learn:	3629.6153402	total:	1.51s	remaining:	1.45s
1022:	learn:	3629.5740763	total:	1.51s	remaining:	1.44s
1023:	learn:	3629.3666657	total:	1.51s	remaining:	1.44s
1024:	learn:	3628.5367924	total:	1.51s	remaining:	1.44s
1025:	learn:	3627.3209578	total:	1.52s	remaining:	1.44s
1026:	learn:	3627.0698097	total:	1.52s	remaining:	1.44s
1027:	learn:	3624.6297907	total:	1.52s	remaining:	1.44s
1028:	learn:	3624.2137850	total:	1.52s	remaining:	1.44s
1029:	learn:	3623.3317266	total:	1.52s	remaining:	1.43s
1030:	learn:	3623.0141339	total:	1.52s	remaining:	1.43s
1031:	learn:	3622.7357887	total:	1.53s	remaining:	1.43s
1032:	learn:	3622.3153971	total:	1.53s	remaining:	1.43s
1033:	learn:	3621.7364889	total:	1.53s	remaining:	1.43s
1034:	learn:	3621.2690431	total:	1.53s	remaining:	1.43s
1035:	learn:	3619.7498802	total:	1.53s	remaining:	1.43s
1036:	learn:	3617.4767168	total:	1.54s	remaining:	1.43s
1037:	learn:	3617.4767168	total:	1.54s	remaining:	1.42s
1038:	learn:	3616.3999831	total:	1.54s	remaining:	1.42s
1039:	learn:	3616.3999831	total:	1.54s	remaining:	1.42s
1040:	learn:	3616.3999831	total:	1.54s	remaining:	1.42s
1041:	learn:	3615.6974691	total:	1.54s	remaining:	1.42s
1042:	learn:	3613.3498141	total:	1.54s	remaining:	1.42s
1043:	learn:	3613.3498141	total:	1.54s	remaining:	1.41s
1044:	learn:	3612.5324436	total:	1.55s	remaining:	1.41s
1045:	learn:	3611.6863959	total:	1.55s	remaining:	1.41s
1046:	learn:	3611.6110633	total:	1.55s	remaining:	1.41s
1047:	learn:	3611.3409241	total:	1.55s	remaining:	1.41s
1048:	learn:	3609.1333550	total:	1.55s	remaining:	1.41s
1049:	learn:	3607.2325683	total:	1.55s	remaining:	1.41s
1050:	learn:	3606.8956123	total:	1.56s	remaining:	1.41s
1051:	learn:	3606.0445751	total:	1.56s	remaining:	1.4s

1052:	learn:	3604.8280679	total:	1.56s	remaining:	1.4s
1053:	learn:	3603.0442265	total:	1.56s	remaining:	1.4s
1054:	learn:	3603.0414058	total:	1.56s	remaining:	1.4s
1055:	learn:	3602.5215798	total:	1.56s	remaining:	1.4s
1056:	learn:	3601.7869199	total:	1.57s	remaining:	1.4s
1057:	learn:	3601.4903778	total:	1.57s	remaining:	1.4s
1058:	learn:	3601.4903778	total:	1.57s	remaining:	1.39s
1059:	learn:	3600.3736078	total:	1.57s	remaining:	1.39s
1060:	learn:	3599.3800476	total:	1.57s	remaining:	1.39s
1061:	learn:	3599.1596399	total:	1.57s	remaining:	1.39s
1062:	learn:	3598.7990757	total:	1.57s	remaining:	1.39s
1063:	learn:	3597.4087900	total:	1.58s	remaining:	1.39s
1064:	learn:	3597.2450173	total:	1.58s	remaining:	1.39s
1065:	learn:	3596.9727837	total:	1.58s	remaining:	1.39s
1066:	learn:	3596.3506297	total:	1.58s	remaining:	1.38s
1067:	learn:	3595.2715205	total:	1.58s	remaining:	1.38s
1068:	learn:	3593.1006259	total:	1.59s	remaining:	1.38s
1069:	learn:	3592.5959892	total:	1.59s	remaining:	1.38s
1070:	learn:	3592.5883966	total:	1.59s	remaining:	1.38s
1071:	learn:	3592.5343152	total:	1.59s	remaining:	1.38s
1072:	learn:	3592.4848819	total:	1.59s	remaining:	1.38s
1073:	learn:	3592.4848819	total:	1.59s	remaining:	1.38s
1074:	learn:	3591.5370427	total:	1.6s	remaining:	1.37s
1075:	learn:	3591.1534654	total:	1.6s	remaining:	1.37s
1076:	learn:	3591.0191414	total:	1.6s	remaining:	1.37s
1077:	learn:	3590.7011409	total:	1.6s	remaining:	1.37s
1078:	learn:	3590.3736424	total:	1.6s	remaining:	1.37s
1079:	learn:	3589.1039583	total:	1.61s	remaining:	1.37s
1080:	learn:	3588.7743905	total:	1.61s	remaining:	1.37s
1081:	learn:	3588.5977644	total:	1.61s	remaining:	1.36s
1082:	learn:	3588.2087809	total:	1.61s	remaining:	1.36s
1083:	learn:	3587.7235973	total:	1.61s	remaining:	1.36s
1084:	learn:	3587.3342363	total:	1.62s	remaining:	1.36s
1085:	learn:	3587.2197299	total:	1.62s	remaining:	1.36s
1086:	learn:	3587.2138956	total:	1.62s	remaining:	1.36s
1087:	learn:	3586.5718200	total:	1.62s	remaining:	1.36s
1088:	learn:	3586.3580947	total:	1.62s	remaining:	1.36s
1089:	learn:	3585.3864547	total:	1.62s	remaining:	1.36s
1090:	learn:	3581.8700961	total:	1.63s	remaining:	1.35s
1091:	learn:	3581.4482743	total:	1.63s	remaining:	1.35s
1092:	learn:	3581.4247096	total:	1.63s	remaining:	1.35s
1093:	learn:	3581.0372065	total:	1.63s	remaining:	1.35s
1094:	learn:	3579.1062612	total:	1.63s	remaining:	1.35s

1095:	learn:	3579.1062612	total:	1.63s	remaining:	1.35s
1096:	learn:	3578.4765793	total:	1.64s	remaining:	1.35s
1097:	learn:	3578.2423896	total:	1.64s	remaining:	1.35s
1098:	learn:	3578.1712965	total:	1.64s	remaining:	1.34s
1099:	learn:	3575.3026950	total:	1.64s	remaining:	1.34s
1100:	learn:	3575.1259486	total:	1.64s	remaining:	1.34s
1101:	learn:	3573.3194123	total:	1.65s	remaining:	1.34s
1102:	learn:	3573.3081655	total:	1.65s	remaining:	1.34s
1103:	learn:	3573.2685013	total:	1.65s	remaining:	1.34s
1104:	learn:	3573.2685013	total:	1.65s	remaining:	1.34s
1105:	learn:	3572.4575298	total:	1.65s	remaining:	1.33s
1106:	learn:	3571.8274230	total:	1.65s	remaining:	1.33s
1107:	learn:	3571.6342525	total:	1.66s	remaining:	1.33s
1108:	learn:	3571.0126053	total:	1.66s	remaining:	1.33s
1109:	learn:	3569.9617541	total:	1.66s	remaining:	1.33s
1110:	learn:	3569.7106094	total:	1.66s	remaining:	1.33s
1111:	learn:	3569.5235690	total:	1.66s	remaining:	1.33s
1112:	learn:	3566.0157600	total:	1.66s	remaining:	1.33s
1113:	learn:	3564.8566264	total:	1.67s	remaining:	1.32s
1114:	learn:	3563.8169358	total:	1.67s	remaining:	1.32s
1115:	learn:	3563.1418067	total:	1.67s	remaining:	1.32s
1116:	learn:	3562.7999182	total:	1.67s	remaining:	1.32s
1117:	learn:	3562.6120048	total:	1.67s	remaining:	1.32s
1118:	learn:	3561.7899379	total:	1.68s	remaining:	1.32s
1119:	learn:	3561.5663789	total:	1.68s	remaining:	1.32s
1120:	learn:	3561.5653418	total:	1.68s	remaining:	1.32s
1121:	learn:	3560.3072786	total:	1.68s	remaining:	1.31s
1122:	learn:	3559.8587073	total:	1.68s	remaining:	1.31s
1123:	learn:	3559.8570120	total:	1.68s	remaining:	1.31s
1124:	learn:	3559.6594204	total:	1.69s	remaining:	1.31s
1125:	learn:	3557.8153776	total:	1.69s	remaining:	1.31s
1126:	learn:	3557.6496824	total:	1.69s	remaining:	1.31s
1127:	learn:	3557.6496824	total:	1.69s	remaining:	1.31s
1128:	learn:	3557.6496824	total:	1.69s	remaining:	1.3s
1129:	learn:	3557.2345494	total:	1.69s	remaining:	1.3s
1130:	learn:	3556.5439816	total:	1.7s	remaining:	1.3s
1131:	learn:	3555.8897573	total:	1.7s	remaining:	1.3s
1132:	learn:	3555.5143977	total:	1.7s	remaining:	1.3s
1133:	learn:	3554.2410994	total:	1.7s	remaining:	1.3s
1134:	learn:	3554.0107634	total:	1.71s	remaining:	1.3s
1135:	learn:	3553.9615743	total:	1.71s	remaining:	1.3s
1136:	learn:	3551.0941172	total:	1.71s	remaining:	1.3s
1137:	learn:	3550.3466574	total:	1.71s	remaining:	1.3s

1138:	learn:	3550.0225315	total:	1.72s	remaining:	1.3s
1139:	learn:	3550.0225315	total:	1.72s	remaining:	1.29s
1140:	learn:	3548.6873160	total:	1.72s	remaining:	1.29s
1141:	learn:	3547.3571996	total:	1.72s	remaining:	1.29s
1142:	learn:	3546.2323811	total:	1.73s	remaining:	1.29s
1143:	learn:	3545.2744841	total:	1.73s	remaining:	1.29s
1144:	learn:	3545.1597357	total:	1.73s	remaining:	1.29s
1145:	learn:	3545.1597357	total:	1.73s	remaining:	1.29s
1146:	learn:	3544.9196089	total:	1.73s	remaining:	1.29s
1147:	learn:	3542.6693975	total:	1.74s	remaining:	1.29s
1148:	learn:	3542.6693975	total:	1.74s	remaining:	1.29s
1149:	learn:	3542.0170374	total:	1.74s	remaining:	1.29s
1150:	learn:	3541.9987886	total:	1.74s	remaining:	1.29s
1151:	learn:	3541.4564659	total:	1.75s	remaining:	1.29s
1152:	learn:	3537.7902406	total:	1.75s	remaining:	1.29s
1153:	learn:	3535.9440933	total:	1.75s	remaining:	1.29s
1154:	learn:	3535.3618591	total:	1.76s	remaining:	1.29s
1155:	learn:	3534.0038064	total:	1.76s	remaining:	1.29s
1156:	learn:	3528.8624480	total:	1.77s	remaining:	1.29s
1157:	learn:	3528.8624480	total:	1.77s	remaining:	1.28s
1158:	learn:	3528.8624480	total:	1.77s	remaining:	1.28s
1159:	learn:	3528.5705897	total:	1.77s	remaining:	1.28s
1160:	learn:	3527.7039807	total:	1.77s	remaining:	1.28s
1161:	learn:	3526.8718806	total:	1.78s	remaining:	1.28s
1162:	learn:	3525.2002199	total:	1.78s	remaining:	1.28s
1163:	learn:	3524.7384686	total:	1.78s	remaining:	1.28s
1164:	learn:	3521.6204101	total:	1.78s	remaining:	1.28s
1165:	learn:	3521.0234755	total:	1.8s	remaining:	1.29s
1166:	learn:	3516.6497800	total:	1.8s	remaining:	1.29s
1167:	learn:	3516.0855787	total:	1.81s	remaining:	1.29s
1168:	learn:	3515.7976760	total:	1.81s	remaining:	1.29s
1169:	learn:	3515.5704574	total:	1.81s	remaining:	1.29s
1170:	learn:	3515.1427513	total:	1.82s	remaining:	1.29s
1171:	learn:	3515.0602849	total:	1.82s	remaining:	1.28s
1172:	learn:	3514.7638701	total:	1.82s	remaining:	1.28s
1173:	learn:	3513.5698655	total:	1.82s	remaining:	1.28s
1174:	learn:	3513.0935427	total:	1.82s	remaining:	1.28s
1175:	learn:	3512.7069115	total:	1.83s	remaining:	1.28s
1176:	learn:	3512.2088626	total:	1.83s	remaining:	1.28s
1177:	learn:	3511.8630839	total:	1.83s	remaining:	1.28s
1178:	learn:	3510.1118571	total:	1.83s	remaining:	1.28s
1179:	learn:	3509.9803469	total:	1.84s	remaining:	1.28s
1180:	learn:	3509.6869391	total:	1.84s	remaining:	1.27s

1181:	learn:	3507.4650152	total:	1.84s	remaining:	1.27s
1182:	learn:	3506.7078692	total:	1.84s	remaining:	1.27s
1183:	learn:	3504.7656726	total:	1.85s	remaining:	1.27s
1184:	learn:	3503.8159906	total:	1.85s	remaining:	1.27s
1185:	learn:	3503.8159906	total:	1.85s	remaining:	1.27s
1186:	learn:	3503.6273305	total:	1.85s	remaining:	1.27s
1187:	learn:	3503.6273305	total:	1.85s	remaining:	1.27s
1188:	learn:	3502.9832157	total:	1.85s	remaining:	1.26s
1189:	learn:	3502.7191578	total:	1.86s	remaining:	1.26s
1190:	learn:	3501.7102875	total:	1.86s	remaining:	1.26s
1191:	learn:	3501.6303065	total:	1.86s	remaining:	1.26s
1192:	learn:	3501.6303065	total:	1.86s	remaining:	1.26s
1193:	learn:	3500.2342721	total:	1.86s	remaining:	1.26s
1194:	learn:	3498.5046870	total:	1.87s	remaining:	1.26s
1195:	learn:	3497.4228105	total:	1.87s	remaining:	1.26s
1196:	learn:	3497.4228105	total:	1.87s	remaining:	1.25s
1197:	learn:	3496.7478212	total:	1.87s	remaining:	1.25s
1198:	learn:	3495.8283729	total:	1.88s	remaining:	1.25s
1199:	learn:	3495.8227030	total:	1.88s	remaining:	1.25s
1200:	learn:	3495.8195457	total:	1.88s	remaining:	1.25s
1201:	learn:	3495.8111827	total:	1.88s	remaining:	1.25s
1202:	learn:	3495.3319656	total:	1.88s	remaining:	1.25s
1203:	learn:	3494.7155581	total:	1.88s	remaining:	1.25s
1204:	learn:	3494.7155581	total:	1.88s	remaining:	1.24s
1205:	learn:	3494.4485050	total:	1.89s	remaining:	1.24s
1206:	learn:	3493.8914014	total:	1.89s	remaining:	1.24s
1207:	learn:	3493.4939211	total:	1.89s	remaining:	1.24s
1208:	learn:	3493.3499219	total:	1.89s	remaining:	1.24s
1209:	learn:	3492.0621516	total:	1.89s	remaining:	1.24s
1210:	learn:	3491.9988867	total:	1.9s	remaining:	1.24s
1211:	learn:	3491.9983620	total:	1.9s	remaining:	1.23s
1212:	learn:	3489.3417180	total:	1.9s	remaining:	1.23s
1213:	learn:	3489.1380101	total:	1.9s	remaining:	1.23s
1214:	learn:	3489.1380101	total:	1.9s	remaining:	1.23s
1215:	learn:	3489.1380101	total:	1.9s	remaining:	1.23s
1216:	learn:	3489.1340465	total:	1.91s	remaining:	1.23s
1217:	learn:	3489.1340465	total:	1.91s	remaining:	1.22s
1218:	learn:	3489.1340465	total:	1.91s	remaining:	1.22s
1219:	learn:	3489.0039633	total:	1.91s	remaining:	1.22s
1220:	learn:	3489.0039633	total:	1.91s	remaining:	1.22s
1221:	learn:	3488.9564392	total:	1.91s	remaining:	1.22s
1222:	learn:	3488.9564392	total:	1.92s	remaining:	1.22s
1223:	learn:	3488.9564392	total:	1.92s	remaining:	1.21s

1224:	learn: 3487.9908790	total: 1.92s	remaining: 1.21s
1225:	learn: 3487.7033151	total: 1.92s	remaining: 1.21s
1226:	learn: 3487.4716292	total: 1.92s	remaining: 1.21s
1227:	learn: 3487.4421957	total: 1.93s	remaining: 1.21s
1228:	learn: 3487.4417232	total: 1.93s	remaining: 1.21s
1229:	learn: 3486.1161129	total: 1.93s	remaining: 1.21s
1230:	learn: 3485.3868887	total: 1.93s	remaining: 1.21s
1231:	learn: 3485.0605288	total: 1.94s	remaining: 1.21s
1232:	learn: 3485.0067723	total: 1.94s	remaining: 1.21s
1233:	learn: 3483.1809236	total: 1.94s	remaining: 1.2s
1234:	learn: 3481.3149412	total: 1.94s	remaining: 1.2s
1235:	learn: 3481.1425501	total: 1.95s	remaining: 1.2s
1236:	learn: 3481.1425501	total: 1.95s	remaining: 1.2s
1237:	learn: 3480.8921921	total: 1.95s	remaining: 1.2s
1238:	learn: 3480.3199413	total: 1.95s	remaining: 1.2s
1239:	learn: 3480.3199413	total: 1.96s	remaining: 1.2s
1240:	learn: 3479.3737682	total: 1.96s	remaining: 1.2s
1241:	learn: 3478.0905011	total: 1.96s	remaining: 1.2s
1242:	learn: 3476.7956632	total: 1.96s	remaining: 1.2s
1243:	learn: 3476.3331213	total: 1.97s	remaining: 1.2s
1244:	learn: 3476.0137821	total: 1.97s	remaining: 1.2s
1245:	learn: 3473.3929457	total: 1.97s	remaining: 1.19s
1246:	learn: 3473.3929457	total: 1.97s	remaining: 1.19s
1247:	learn: 3468.8674239	total: 1.98s	remaining: 1.19s
1248:	learn: 3468.5034134	total: 1.98s	remaining: 1.19s
1249:	learn: 3468.5034134	total: 1.98s	remaining: 1.19s
1250:	learn: 3468.3679050	total: 1.98s	remaining: 1.19s
1251:	learn: 3468.3679050	total: 1.98s	remaining: 1.18s
1252:	learn: 3467.6336042	total: 1.98s	remaining: 1.18s
1253:	learn: 3466.0650105	total: 1.99s	remaining: 1.18s
1254:	learn: 3465.5514242	total: 1.99s	remaining: 1.18s
1255:	learn: 3464.7760892	total: 1.99s	remaining: 1.18s
1256:	learn: 3464.7760892	total: 1.99s	remaining: 1.18s
1257:	learn: 3464.7052528	total: 1.99s	remaining: 1.17s
1258:	learn: 3464.2389179	total: 1.99s	remaining: 1.17s
1259:	learn: 3464.2389179	total: 1.99s	remaining: 1.17s
1260:	learn: 3463.7080189	total: 2s	remaining: 1.17s
1261:	learn: 3463.6448661	total: 2s	remaining: 1.17s
1262:	learn: 3463.4723039	total: 2s	remaining: 1.17s
1263:	learn: 3463.4214435	total: 2s	remaining: 1.17s
1264:	learn: 3462.4528015	total: 2.01s	remaining: 1.17s
1265:	learn: 3462.3418798	total: 2.01s	remaining: 1.16s
1266:	learn: 3461.0735834	total: 2.01s	remaining: 1.16s

1267:	learn:	3460.9924441	total:	2.01s	remaining:	1.16s
1268:	learn:	3460.8876125	total:	2.02s	remaining:	1.16s
1269:	learn:	3460.4933662	total:	2.02s	remaining:	1.16s
1270:	learn:	3460.4919842	total:	2.02s	remaining:	1.16s
1271:	learn:	3460.4035048	total:	2.02s	remaining:	1.16s
1272:	learn:	3460.4035048	total:	2.02s	remaining:	1.15s
1273:	learn:	3459.3359575	total:	2.02s	remaining:	1.15s
1274:	learn:	3457.8199183	total:	2.02s	remaining:	1.15s
1275:	learn:	3457.4863670	total:	2.03s	remaining:	1.15s
1276:	learn:	3455.8452690	total:	2.03s	remaining:	1.15s
1277:	learn:	3455.0689443	total:	2.03s	remaining:	1.15s
1278:	learn:	3455.0689443	total:	2.03s	remaining:	1.14s
1279:	learn:	3454.6749412	total:	2.03s	remaining:	1.14s
1280:	learn:	3453.5278084	total:	2.04s	remaining:	1.14s
1281:	learn:	3453.3104756	total:	2.04s	remaining:	1.14s
1282:	learn:	3453.0127466	total:	2.04s	remaining:	1.14s
1283:	learn:	3452.9312517	total:	2.04s	remaining:	1.14s
1284:	learn:	3452.6055727	total:	2.04s	remaining:	1.14s
1285:	learn:	3451.5120403	total:	2.04s	remaining:	1.13s
1286:	learn:	3450.9189052	total:	2.04s	remaining:	1.13s
1287:	learn:	3450.9154103	total:	2.05s	remaining:	1.13s
1288:	learn:	3449.6982402	total:	2.05s	remaining:	1.13s
1289:	learn:	3449.0524982	total:	2.05s	remaining:	1.13s
1290:	learn:	3448.8385412	total:	2.05s	remaining:	1.13s
1291:	learn:	3448.8385412	total:	2.05s	remaining:	1.12s
1292:	learn:	3448.6875173	total:	2.05s	remaining:	1.12s
1293:	learn:	3447.7991746	total:	2.06s	remaining:	1.12s
1294:	learn:	3446.8332555	total:	2.06s	remaining:	1.12s
1295:	learn:	3446.7066740	total:	2.06s	remaining:	1.12s
1296:	learn:	3446.7066740	total:	2.06s	remaining:	1.12s
1297:	learn:	3440.0124138	total:	2.06s	remaining:	1.11s
1298:	learn:	3439.1136582	total:	2.06s	remaining:	1.11s
1299:	learn:	3438.8334759	total:	2.06s	remaining:	1.11s
1300:	learn:	3437.5049112	total:	2.07s	remaining:	1.11s
1301:	learn:	3436.4869249	total:	2.07s	remaining:	1.11s
1302:	learn:	3436.3743441	total:	2.07s	remaining:	1.11s
1303:	learn:	3436.3743441	total:	2.07s	remaining:	1.1s
1304:	learn:	3436.3743441	total:	2.07s	remaining:	1.1s
1305:	learn:	3436.3743441	total:	2.07s	remaining:	1.1s
1306:	learn:	3435.9674258	total:	2.07s	remaining:	1.1s
1307:	learn:	3435.7246142	total:	2.07s	remaining:	1.1s
1308:	learn:	3435.6276167	total:	2.08s	remaining:	1.09s
1309:	learn:	3434.9562900	total:	2.08s	remaining:	1.09s

1310:	learn:	3433.9987724	total:	2.08s	remaining:	1.09s
1311:	learn:	3433.6087305	total:	2.08s	remaining:	1.09s
1312:	learn:	3433.4416265	total:	2.08s	remaining:	1.09s
1313:	learn:	3433.4416265	total:	2.08s	remaining:	1.09s
1314:	learn:	3432.1607968	total:	2.08s	remaining:	1.08s
1315:	learn:	3432.1607968	total:	2.08s	remaining:	1.08s
1316:	learn:	3431.2901737	total:	2.09s	remaining:	1.08s
1317:	learn:	3429.9883872	total:	2.09s	remaining:	1.08s
1318:	learn:	3429.9284206	total:	2.09s	remaining:	1.08s
1319:	learn:	3429.8485066	total:	2.09s	remaining:	1.08s
1320:	learn:	3429.8485066	total:	2.09s	remaining:	1.07s
1321:	learn:	3428.8791224	total:	2.09s	remaining:	1.07s
1322:	learn:	3428.1362123	total:	2.1s	remaining:	1.07s
1323:	learn:	3426.5251308	total:	2.1s	remaining:	1.07s
1324:	learn:	3426.2746341	total:	2.1s	remaining:	1.07s
1325:	learn:	3426.2746341	total:	2.1s	remaining:	1.07s
1326:	learn:	3426.2746341	total:	2.1s	remaining:	1.06s
1327:	learn:	3425.9170980	total:	2.1s	remaining:	1.06s
1328:	learn:	3425.3611482	total:	2.1s	remaining:	1.06s
1329:	learn:	3424.4659138	total:	2.1s	remaining:	1.06s
1330:	learn:	3423.9350526	total:	2.1s	remaining:	1.06s
1331:	learn:	3422.9492344	total:	2.11s	remaining:	1.06s
1332:	learn:	3421.7893589	total:	2.11s	remaining:	1.05s
1333:	learn:	3421.5134698	total:	2.11s	remaining:	1.05s
1334:	learn:	3421.2251437	total:	2.11s	remaining:	1.05s
1335:	learn:	3420.8226376	total:	2.11s	remaining:	1.05s
1336:	learn:	3420.5664151	total:	2.12s	remaining:	1.05s
1337:	learn:	3420.5664151	total:	2.12s	remaining:	1.05s
1338:	learn:	3420.5664151	total:	2.12s	remaining:	1.04s
1339:	learn:	3420.5664151	total:	2.12s	remaining:	1.04s
1340:	learn:	3419.8780256	total:	2.12s	remaining:	1.04s
1341:	learn:	3419.0746453	total:	2.12s	remaining:	1.04s
1342:	learn:	3419.0746453	total:	2.12s	remaining:	1.04s
1343:	learn:	3419.0734552	total:	2.12s	remaining:	1.03s
1344:	learn:	3418.4145722	total:	2.12s	remaining:	1.03s
1345:	learn:	3418.1149355	total:	2.12s	remaining:	1.03s
1346:	learn:	3417.9532152	total:	2.13s	remaining:	1.03s
1347:	learn:	3417.5387633	total:	2.13s	remaining:	1.03s
1348:	learn:	3416.8310578	total:	2.13s	remaining:	1.03s
1349:	learn:	3416.8310578	total:	2.13s	remaining:	1.02s
1350:	learn:	3416.8310578	total:	2.13s	remaining:	1.02s
1351:	learn:	3416.8310578	total:	2.13s	remaining:	1.02s
1352:	learn:	3416.2403108	total:	2.13s	remaining:	1.02s

1353:	learn:	3415.5193738	total:	2.13s	remaining:	1.02s
1354:	learn:	3414.9793795	total:	2.13s	remaining:	1.02s
1355:	learn:	3414.8846548	total:	2.14s	remaining:	1.01s
1356:	learn:	3414.6135055	total:	2.14s	remaining:	1.01s
1357:	learn:	3414.4637963	total:	2.14s	remaining:	1.01s
1358:	learn:	3414.1424451	total:	2.14s	remaining:	1.01s
1359:	learn:	3414.1235906	total:	2.14s	remaining:	1.01s
1360:	learn:	3413.8978249	total:	2.15s	remaining:	1.01s
1361:	learn:	3413.8978249	total:	2.15s	remaining:	1s
1362:	learn:	3413.2717749	total:	2.15s	remaining:	1s
1363:	learn:	3413.1662130	total:	2.15s	remaining:	1s
1364:	learn:	3413.1662130	total:	2.15s	remaining:	1s
1365:	learn:	3412.5539553	total:	2.15s	remaining:	999ms
1366:	learn:	3412.5539553	total:	2.15s	remaining:	997ms
1367:	learn:	3412.2162145	total:	2.15s	remaining:	995ms
1368:	learn:	3411.7199549	total:	2.16s	remaining:	994ms
1369:	learn:	3410.7213858	total:	2.16s	remaining:	992ms
1370:	learn:	3410.7213858	total:	2.16s	remaining:	990ms
1371:	learn:	3410.7130116	total:	2.16s	remaining:	989ms
1372:	learn:	3409.6714120	total:	2.16s	remaining:	987ms
1373:	learn:	3407.0469234	total:	2.16s	remaining:	985ms
1374:	learn:	3406.8334734	total:	2.16s	remaining:	984ms
1375:	learn:	3405.7944436	total:	2.17s	remaining:	982ms
1376:	learn:	3404.3862481	total:	2.17s	remaining:	981ms
1377:	learn:	3404.1123839	total:	2.17s	remaining:	979ms
1378:	learn:	3403.9273859	total:	2.17s	remaining:	978ms
1379:	learn:	3403.8005365	total:	2.17s	remaining:	976ms
1380:	learn:	3403.4403922	total:	2.17s	remaining:	975ms
1381:	learn:	3402.6081195	total:	2.17s	remaining:	973ms
1382:	learn:	3402.1766047	total:	2.18s	remaining:	971ms
1383:	learn:	3402.0382933	total:	2.18s	remaining:	970ms
1384:	learn:	3401.9022868	total:	2.18s	remaining:	968ms
1385:	learn:	3401.9022868	total:	2.18s	remaining:	966ms
1386:	learn:	3401.4068753	total:	2.18s	remaining:	965ms
1387:	learn:	3400.9534708	total:	2.18s	remaining:	963ms
1388:	learn:	3400.0592208	total:	2.19s	remaining:	962ms
1389:	learn:	3399.9068631	total:	2.19s	remaining:	960ms
1390:	learn:	3399.7704808	total:	2.19s	remaining:	959ms
1391:	learn:	3398.3180640	total:	2.19s	remaining:	957ms
1392:	learn:	3398.1779493	total:	2.19s	remaining:	955ms
1393:	learn:	3397.4052751	total:	2.19s	remaining:	954ms
1394:	learn:	3397.3551202	total:	2.19s	remaining:	952ms
1395:	learn:	3397.3551202	total:	2.2s	remaining:	950ms

1396: learn: 3397.3032297 total: 2.2s remaining: 949ms
1397: learn: 3396.4413072 total: 2.2s remaining: 947ms
1398: learn: 3396.1246833 total: 2.2s remaining: 946ms
1399: learn: 3396.1246833 total: 2.2s remaining: 944ms
1400: learn: 3393.3386727 total: 2.2s remaining: 943ms
1401: learn: 3393.0818296 total: 2.21s remaining: 941ms
1402: learn: 3392.3444709 total: 2.21s remaining: 940ms
1403: learn: 3392.3188682 total: 2.21s remaining: 938ms
1404: learn: 3392.3180694 total: 2.21s remaining: 936ms
1405: learn: 3391.6507938 total: 2.21s remaining: 934ms
1406: learn: 3391.3211071 total: 2.21s remaining: 933ms
1407: learn: 3391.3199251 total: 2.21s remaining: 931ms
1408: learn: 3390.2805332 total: 2.22s remaining: 930ms
1409: learn: 3389.8258158 total: 2.22s remaining: 928ms
1410: learn: 3388.7130263 total: 2.22s remaining: 927ms
1411: learn: 3386.4266049 total: 2.22s remaining: 925ms
1412: learn: 3385.1734910 total: 2.22s remaining: 924ms
1413: learn: 3381.9668231 total: 2.23s remaining: 923ms
1414: learn: 3381.3037243 total: 2.23s remaining: 921ms
1415: learn: 3381.2345977 total: 2.23s remaining: 920ms
1416: learn: 3380.8300046 total: 2.23s remaining: 919ms
1417: learn: 3377.9959849 total: 2.23s remaining: 917ms
1418: learn: 3377.2197494 total: 2.24s remaining: 916ms
1419: learn: 3377.0327590 total: 2.24s remaining: 914ms
1420: learn: 3377.0327590 total: 2.24s remaining: 912ms
1421: learn: 3376.5109946 total: 2.24s remaining: 911ms
1422: learn: 3376.5038494 total: 2.24s remaining: 909ms
1423: learn: 3375.7564955 total: 2.24s remaining: 908ms
1424: learn: 3375.6156596 total: 2.25s remaining: 906ms
1425: learn: 3375.4890280 total: 2.25s remaining: 905ms
1426: learn: 3375.1804910 total: 2.25s remaining: 904ms
1427: learn: 3375.1536405 total: 2.25s remaining: 903ms
1428: learn: 3375.0401643 total: 2.25s remaining: 901ms
1429: learn: 3374.4391521 total: 2.26s remaining: 899ms
1430: learn: 3374.1964831 total: 2.26s remaining: 898ms
1431: learn: 3374.1497595 total: 2.26s remaining: 897ms
1432: learn: 3374.1493869 total: 2.26s remaining: 895ms
1433: learn: 3373.8020310 total: 2.26s remaining: 893ms
1434: learn: 3373.8020310 total: 2.26s remaining: 891ms
1435: learn: 3373.8020310 total: 2.26s remaining: 889ms
1436: learn: 3373.8020310 total: 2.26s remaining: 887ms
1437: learn: 3373.7951891 total: 2.27s remaining: 886ms
1438: learn: 3373.7019291 total: 2.27s remaining: 884ms

1439:	learn:	3371.3433288	total:	2.27s	remaining:	883ms
1440:	learn:	3371.3234119	total:	2.27s	remaining:	881ms
1441:	learn:	3371.0762139	total:	2.27s	remaining:	880ms
1442:	learn:	3370.8838681	total:	2.28s	remaining:	879ms
1443:	learn:	3370.1963553	total:	2.28s	remaining:	877ms
1444:	learn:	3369.8998741	total:	2.28s	remaining:	876ms
1445:	learn:	3368.6938579	total:	2.28s	remaining:	875ms
1446:	learn:	3368.4789147	total:	2.28s	remaining:	873ms
1447:	learn:	3368.3351815	total:	2.29s	remaining:	871ms
1448:	learn:	3366.8936917	total:	2.29s	remaining:	870ms
1449:	learn:	3366.8388420	total:	2.29s	remaining:	868ms
1450:	learn:	3366.7271114	total:	2.29s	remaining:	867ms
1451:	learn:	3366.7271114	total:	2.29s	remaining:	865ms
1452:	learn:	3366.7271114	total:	2.29s	remaining:	863ms
1453:	learn:	3366.7261233	total:	2.29s	remaining:	861ms
1454:	learn:	3366.5542195	total:	2.29s	remaining:	860ms
1455:	learn:	3366.4240616	total:	2.3s	remaining:	858ms
1456:	learn:	3365.8210886	total:	2.3s	remaining:	857ms
1457:	learn:	3364.7499193	total:	2.3s	remaining:	855ms
1458:	learn:	3364.7499193	total:	2.3s	remaining:	853ms
1459:	learn:	3364.4529790	total:	2.3s	remaining:	852ms
1460:	learn:	3363.8600341	total:	2.3s	remaining:	850ms
1461:	learn:	3363.7260588	total:	2.31s	remaining:	849ms
1462:	learn:	3362.7257758	total:	2.31s	remaining:	847ms
1463:	learn:	3361.8405663	total:	2.31s	remaining:	845ms
1464:	learn:	3361.3130622	total:	2.31s	remaining:	844ms
1465:	learn:	3361.3130622	total:	2.31s	remaining:	842ms
1466:	learn:	3360.9499820	total:	2.31s	remaining:	840ms
1467:	learn:	3358.8757138	total:	2.31s	remaining:	839ms
1468:	learn:	3358.8757138	total:	2.31s	remaining:	837ms
1469:	learn:	3358.4843122	total:	2.32s	remaining:	835ms
1470:	learn:	3358.1180199	total:	2.32s	remaining:	834ms
1471:	learn:	3357.6770658	total:	2.32s	remaining:	832ms
1472:	learn:	3357.5197320	total:	2.32s	remaining:	830ms
1473:	learn:	3357.2766382	total:	2.32s	remaining:	829ms
1474:	learn:	3356.2353078	total:	2.32s	remaining:	827ms
1475:	learn:	3355.3662159	total:	2.33s	remaining:	826ms
1476:	learn:	3355.1446737	total:	2.33s	remaining:	824ms
1477:	learn:	3355.1446737	total:	2.33s	remaining:	822ms
1478:	learn:	3355.1440713	total:	2.33s	remaining:	820ms
1479:	learn:	3355.1400279	total:	2.33s	remaining:	819ms
1480:	learn:	3355.1400279	total:	2.33s	remaining:	817ms
1481:	learn:	3354.4871633	total:	2.33s	remaining:	815ms

1482:	learn:	3354.4270963	total:	2.33s	remaining:	814ms
1483:	learn:	3354.4181495	total:	2.33s	remaining:	812ms
1484:	learn:	3354.1594655	total:	2.34s	remaining:	810ms
1485:	learn:	3353.2292466	total:	2.34s	remaining:	809ms
1486:	learn:	3353.2292466	total:	2.34s	remaining:	807ms
1487:	learn:	3353.1014820	total:	2.34s	remaining:	805ms
1488:	learn:	3353.0987823	total:	2.34s	remaining:	803ms
1489:	learn:	3353.0761911	total:	2.34s	remaining:	801ms
1490:	learn:	3353.0761911	total:	2.34s	remaining:	800ms
1491:	learn:	3352.9010122	total:	2.34s	remaining:	798ms
1492:	learn:	3352.6327161	total:	2.35s	remaining:	796ms
1493:	learn:	3351.5962084	total:	2.35s	remaining:	795ms
1494:	learn:	3351.5962084	total:	2.35s	remaining:	793ms
1495:	learn:	3350.1006470	total:	2.35s	remaining:	791ms
1496:	learn:	3350.1006470	total:	2.35s	remaining:	790ms
1497:	learn:	3350.0253032	total:	2.35s	remaining:	788ms
1498:	learn:	3349.5414000	total:	2.35s	remaining:	787ms
1499:	learn:	3349.4987197	total:	2.35s	remaining:	785ms
1500:	learn:	3349.2979973	total:	2.36s	remaining:	783ms
1501:	learn:	3349.1114527	total:	2.36s	remaining:	782ms
1502:	learn:	3348.9814439	total:	2.36s	remaining:	780ms
1503:	learn:	3348.2336001	total:	2.36s	remaining:	779ms
1504:	learn:	3348.2336001	total:	2.36s	remaining:	777ms
1505:	learn:	3348.2336001	total:	2.36s	remaining:	775ms
1506:	learn:	3347.9761559	total:	2.36s	remaining:	773ms
1507:	learn:	3345.8139572	total:	2.37s	remaining:	772ms
1508:	learn:	3344.4834264	total:	2.37s	remaining:	770ms
1509:	learn:	3344.0163725	total:	2.37s	remaining:	769ms
1510:	learn:	3344.0163725	total:	2.37s	remaining:	767ms
1511:	learn:	3343.9811918	total:	2.37s	remaining:	765ms
1512:	learn:	3343.8073597	total:	2.37s	remaining:	764ms
1513:	learn:	3343.5492516	total:	2.37s	remaining:	762ms
1514:	learn:	3343.5492516	total:	2.37s	remaining:	760ms
1515:	learn:	3343.0367120	total:	2.38s	remaining:	758ms
1516:	learn:	3341.9384454	total:	2.38s	remaining:	757ms
1517:	learn:	3341.2393729	total:	2.38s	remaining:	755ms
1518:	learn:	3340.1546795	total:	2.38s	remaining:	754ms
1519:	learn:	3340.1546795	total:	2.38s	remaining:	752ms
1520:	learn:	3339.2131062	total:	2.38s	remaining:	751ms
1521:	learn:	3338.8641810	total:	2.38s	remaining:	749ms
1522:	learn:	3338.8641810	total:	2.38s	remaining:	747ms
1523:	learn:	3338.8441572	total:	2.39s	remaining:	745ms
1524:	learn:	3338.7404088	total:	2.39s	remaining:	744ms

1525:	learn:	3338.5734868	total:	2.39s	remaining:	742ms
1526:	learn:	3338.1755709	total:	2.39s	remaining:	741ms
1527:	learn:	3338.1263132	total:	2.39s	remaining:	740ms
1528:	learn:	3336.8059586	total:	2.4s	remaining:	738ms
1529:	learn:	3336.7759575	total:	2.4s	remaining:	737ms
1530:	learn:	3333.9289410	total:	2.4s	remaining:	736ms
1531:	learn:	3333.9082217	total:	2.4s	remaining:	734ms
1532:	learn:	3333.2865190	total:	2.4s	remaining:	732ms
1533:	learn:	3332.0903192	total:	2.41s	remaining:	731ms
1534:	learn:	3332.0516926	total:	2.41s	remaining:	729ms
1535:	learn:	3331.9876738	total:	2.41s	remaining:	728ms
1536:	learn:	3331.9876738	total:	2.41s	remaining:	726ms
1537:	learn:	3331.9876738	total:	2.41s	remaining:	725ms
1538:	learn:	3325.7763364	total:	2.41s	remaining:	723ms
1539:	learn:	3325.5592471	total:	2.42s	remaining:	722ms
1540:	learn:	3324.5254327	total:	2.42s	remaining:	720ms
1541:	learn:	3323.4979834	total:	2.42s	remaining:	719ms
1542:	learn:	3323.4979834	total:	2.42s	remaining:	717ms
1543:	learn:	3323.2673846	total:	2.42s	remaining:	715ms
1544:	learn:	3323.1182052	total:	2.42s	remaining:	714ms
1545:	learn:	3323.0203677	total:	2.43s	remaining:	712ms
1546:	learn:	3323.0203677	total:	2.43s	remaining:	711ms
1547:	learn:	3322.3440984	total:	2.43s	remaining:	709ms
1548:	learn:	3321.0069035	total:	2.43s	remaining:	708ms
1549:	learn:	3320.0109679	total:	2.43s	remaining:	706ms
1550:	learn:	3319.6187768	total:	2.43s	remaining:	705ms
1551:	learn:	3318.7561915	total:	2.44s	remaining:	703ms
1552:	learn:	3317.9903066	total:	2.44s	remaining:	701ms
1553:	learn:	3317.6085681	total:	2.44s	remaining:	700ms
1554:	learn:	3317.3450224	total:	2.44s	remaining:	698ms
1555:	learn:	3316.8069448	total:	2.44s	remaining:	697ms
1556:	learn:	3316.8069448	total:	2.44s	remaining:	695ms
1557:	learn:	3316.7241953	total:	2.44s	remaining:	693ms
1558:	learn:	3316.6687696	total:	2.44s	remaining:	692ms
1559:	learn:	3316.5287101	total:	2.45s	remaining:	690ms
1560:	learn:	3315.8917801	total:	2.45s	remaining:	688ms
1561:	learn:	3312.5867515	total:	2.45s	remaining:	687ms
1562:	learn:	3312.1214123	total:	2.45s	remaining:	685ms
1563:	learn:	3312.1214123	total:	2.45s	remaining:	683ms
1564:	learn:	3312.0073329	total:	2.45s	remaining:	682ms
1565:	learn:	3311.9389137	total:	2.45s	remaining:	680ms
1566:	learn:	3310.6658293	total:	2.46s	remaining:	679ms
1567:	learn:	3309.9400964	total:	2.46s	remaining:	677ms

1568:	learn:	3308.8312949	total:	2.46s	remaining:	675ms
1569:	learn:	3308.7929726	total:	2.46s	remaining:	674ms
1570:	learn:	3308.3089963	total:	2.46s	remaining:	672ms
1571:	learn:	3308.3089963	total:	2.46s	remaining:	670ms
1572:	learn:	3308.1719911	total:	2.46s	remaining:	669ms
1573:	learn:	3308.1719876	total:	2.46s	remaining:	667ms
1574:	learn:	3307.5168749	total:	2.46s	remaining:	665ms
1575:	learn:	3307.2858943	total:	2.47s	remaining:	664ms
1576:	learn:	3307.1156302	total:	2.47s	remaining:	662ms
1577:	learn:	3305.3260678	total:	2.47s	remaining:	661ms
1578:	learn:	3304.6730614	total:	2.47s	remaining:	659ms
1579:	learn:	3304.2796680	total:	2.47s	remaining:	658ms
1580:	learn:	3303.7745689	total:	2.48s	remaining:	656ms
1581:	learn:	3303.6877004	total:	2.48s	remaining:	654ms
1582:	learn:	3302.7013801	total:	2.48s	remaining:	653ms
1583:	learn:	3302.6610349	total:	2.48s	remaining:	651ms
1584:	learn:	3302.4571914	total:	2.48s	remaining:	650ms
1585:	learn:	3302.3956629	total:	2.48s	remaining:	648ms
1586:	learn:	3302.3956629	total:	2.48s	remaining:	646ms
1587:	learn:	3302.3749386	total:	2.48s	remaining:	645ms
1588:	learn:	3302.3163183	total:	2.49s	remaining:	643ms
1589:	learn:	3300.9251761	total:	2.49s	remaining:	642ms
1590:	learn:	3300.7916655	total:	2.49s	remaining:	640ms
1591:	learn:	3300.2545046	total:	2.49s	remaining:	639ms
1592:	learn:	3300.0773203	total:	2.49s	remaining:	637ms
1593:	learn:	3300.0773203	total:	2.49s	remaining:	635ms
1594:	learn:	3299.7183538	total:	2.5s	remaining:	634ms
1595:	learn:	3299.5508090	total:	2.5s	remaining:	632ms
1596:	learn:	3299.4992761	total:	2.5s	remaining:	631ms
1597:	learn:	3299.0124633	total:	2.5s	remaining:	629ms
1598:	learn:	3298.1226298	total:	2.5s	remaining:	628ms
1599:	learn:	3298.1226298	total:	2.5s	remaining:	626ms
1600:	learn:	3298.1226298	total:	2.5s	remaining:	624ms
1601:	learn:	3297.9845713	total:	2.51s	remaining:	623ms
1602:	learn:	3297.9165567	total:	2.51s	remaining:	621ms
1603:	learn:	3297.8466098	total:	2.51s	remaining:	620ms
1604:	learn:	3297.8466098	total:	2.51s	remaining:	618ms
1605:	learn:	3297.6440647	total:	2.51s	remaining:	616ms
1606:	learn:	3297.3682602	total:	2.51s	remaining:	615ms
1607:	learn:	3296.5167491	total:	2.52s	remaining:	613ms
1608:	learn:	3296.5167491	total:	2.52s	remaining:	612ms
1609:	learn:	3295.8563649	total:	2.52s	remaining:	610ms
1610:	learn:	3295.8494358	total:	2.52s	remaining:	608ms

1611:	learn:	3294.8414772	total:	2.52s	remaining:	607ms
1612:	learn:	3294.7052746	total:	2.52s	remaining:	606ms
1613:	learn:	3292.9427939	total:	2.52s	remaining:	604ms
1614:	learn:	3290.8777820	total:	2.53s	remaining:	603ms
1615:	learn:	3290.2602050	total:	2.53s	remaining:	601ms
1616:	learn:	3290.1507549	total:	2.53s	remaining:	600ms
1617:	learn:	3289.8034961	total:	2.53s	remaining:	598ms
1618:	learn:	3287.2757282	total:	2.54s	remaining:	597ms
1619:	learn:	3286.3824528	total:	2.54s	remaining:	595ms
1620:	learn:	3286.0591981	total:	2.54s	remaining:	593ms
1621:	learn:	3285.7938179	total:	2.54s	remaining:	592ms
1622:	learn:	3285.7938179	total:	2.54s	remaining:	590ms
1623:	learn:	3285.7938179	total:	2.54s	remaining:	588ms
1624:	learn:	3285.7921888	total:	2.54s	remaining:	587ms
1625:	learn:	3285.7808692	total:	2.54s	remaining:	585ms
1626:	learn:	3285.7808692	total:	2.54s	remaining:	583ms
1627:	learn:	3285.6991139	total:	2.54s	remaining:	582ms
1628:	learn:	3285.6384378	total:	2.55s	remaining:	580ms
1629:	learn:	3285.6384378	total:	2.55s	remaining:	578ms
1630:	learn:	3284.5288549	total:	2.55s	remaining:	577ms
1631:	learn:	3284.1414311	total:	2.55s	remaining:	575ms
1632:	learn:	3284.0838173	total:	2.55s	remaining:	574ms
1633:	learn:	3284.0065353	total:	2.56s	remaining:	572ms
1634:	learn:	3284.0065353	total:	2.56s	remaining:	571ms
1635:	learn:	3283.8020325	total:	2.56s	remaining:	569ms
1636:	learn:	3279.9206222	total:	2.56s	remaining:	568ms
1637:	learn:	3279.9206222	total:	2.56s	remaining:	566ms
1638:	learn:	3279.8859464	total:	2.56s	remaining:	564ms
1639:	learn:	3279.8859464	total:	2.56s	remaining:	563ms
1640:	learn:	3279.8832386	total:	2.56s	remaining:	561ms
1641:	learn:	3279.0485989	total:	2.56s	remaining:	559ms
1642:	learn:	3278.8821714	total:	2.57s	remaining:	558ms
1643:	learn:	3278.8711028	total:	2.57s	remaining:	556ms
1644:	learn:	3277.1513013	total:	2.57s	remaining:	555ms
1645:	learn:	3275.8510292	total:	2.57s	remaining:	553ms
1646:	learn:	3275.6650452	total:	2.57s	remaining:	552ms
1647:	learn:	3275.6650452	total:	2.57s	remaining:	550ms
1648:	learn:	3275.3498004	total:	2.58s	remaining:	548ms
1649:	learn:	3274.9740567	total:	2.58s	remaining:	547ms
1650:	learn:	3274.7822665	total:	2.58s	remaining:	545ms
1651:	learn:	3274.6167592	total:	2.58s	remaining:	544ms
1652:	learn:	3274.3646848	total:	2.58s	remaining:	542ms
1653:	learn:	3274.1047843	total:	2.58s	remaining:	541ms

1654:	learn:	3273.1818950	total:	2.59s	remaining:	539ms
1655:	learn:	3273.1252249	total:	2.59s	remaining:	538ms
1656:	learn:	3273.1252249	total:	2.59s	remaining:	536ms
1657:	learn:	3271.8492413	total:	2.59s	remaining:	534ms
1658:	learn:	3271.8492413	total:	2.59s	remaining:	533ms
1659:	learn:	3271.6288756	total:	2.59s	remaining:	531ms
1660:	learn:	3270.5058777	total:	2.6s	remaining:	530ms
1661:	learn:	3270.2210417	total:	2.6s	remaining:	528ms
1662:	learn:	3270.1062275	total:	2.6s	remaining:	527ms
1663:	learn:	3268.8241585	total:	2.6s	remaining:	525ms
1664:	learn:	3266.3782201	total:	2.6s	remaining:	524ms
1665:	learn:	3266.1759854	total:	2.6s	remaining:	522ms
1666:	learn:	3265.9703532	total:	2.61s	remaining:	521ms
1667:	learn:	3265.8494761	total:	2.61s	remaining:	519ms
1668:	learn:	3265.4209061	total:	2.61s	remaining:	518ms
1669:	learn:	3265.4095181	total:	2.61s	remaining:	516ms
1670:	learn:	3265.3124921	total:	2.61s	remaining:	514ms
1671:	learn:	3265.1019024	total:	2.61s	remaining:	513ms
1672:	learn:	3265.1019024	total:	2.61s	remaining:	511ms
1673:	learn:	3264.8856079	total:	2.62s	remaining:	510ms
1674:	learn:	3264.1545710	total:	2.62s	remaining:	508ms
1675:	learn:	3263.4951654	total:	2.62s	remaining:	507ms
1676:	learn:	3263.3284898	total:	2.62s	remaining:	505ms
1677:	learn:	3263.0894233	total:	2.62s	remaining:	504ms
1678:	learn:	3261.6791751	total:	2.63s	remaining:	502ms
1679:	learn:	3261.6382914	total:	2.63s	remaining:	500ms
1680:	learn:	3260.9623079	total:	2.63s	remaining:	499ms
1681:	learn:	3260.5195101	total:	2.63s	remaining:	497ms
1682:	learn:	3260.5195101	total:	2.63s	remaining:	496ms
1683:	learn:	3260.4429661	total:	2.63s	remaining:	494ms
1684:	learn:	3259.2850353	total:	2.63s	remaining:	493ms
1685:	learn:	3259.1184729	total:	2.64s	remaining:	491ms
1686:	learn:	3257.4318582	total:	2.64s	remaining:	490ms
1687:	learn:	3256.3432607	total:	2.64s	remaining:	488ms
1688:	learn:	3256.1738614	total:	2.64s	remaining:	487ms
1689:	learn:	3256.0401169	total:	2.64s	remaining:	485ms
1690:	learn:	3256.0141182	total:	2.64s	remaining:	483ms
1691:	learn:	3255.6800659	total:	2.65s	remaining:	482ms
1692:	learn:	3255.3824190	total:	2.65s	remaining:	480ms
1693:	learn:	3255.3824190	total:	2.65s	remaining:	479ms
1694:	learn:	3255.3198326	total:	2.65s	remaining:	477ms
1695:	learn:	3255.0116992	total:	2.65s	remaining:	476ms
1696:	learn:	3254.4885471	total:	2.65s	remaining:	474ms

1697:	learn:	3253.9981370	total:	2.66s	remaining:	472ms
1698:	learn:	3253.7226823	total:	2.66s	remaining:	471ms
1699:	learn:	3252.0418807	total:	2.66s	remaining:	469ms
1700:	learn:	3251.9126909	total:	2.66s	remaining:	468ms
1701:	learn:	3251.7482284	total:	2.66s	remaining:	466ms
1702:	learn:	3251.7482284	total:	2.66s	remaining:	465ms
1703:	learn:	3251.4825436	total:	2.67s	remaining:	463ms
1704:	learn:	3251.4825436	total:	2.67s	remaining:	461ms
1705:	learn:	3251.0752854	total:	2.67s	remaining:	460ms
1706:	learn:	3251.0323167	total:	2.67s	remaining:	458ms
1707:	learn:	3250.9870171	total:	2.67s	remaining:	457ms
1708:	learn:	3250.9870171	total:	2.67s	remaining:	455ms
1709:	learn:	3250.8926521	total:	2.67s	remaining:	454ms
1710:	learn:	3250.8926521	total:	2.67s	remaining:	452ms
1711:	learn:	3250.6317391	total:	2.68s	remaining:	450ms
1712:	learn:	3250.2868656	total:	2.68s	remaining:	449ms
1713:	learn:	3247.8370753	total:	2.68s	remaining:	447ms
1714:	learn:	3247.5119753	total:	2.68s	remaining:	446ms
1715:	learn:	3247.4487605	total:	2.69s	remaining:	444ms
1716:	learn:	3247.2618348	total:	2.69s	remaining:	443ms
1717:	learn:	3246.1160185	total:	2.69s	remaining:	441ms
1718:	learn:	3246.0611944	total:	2.69s	remaining:	440ms
1719:	learn:	3245.9436964	total:	2.69s	remaining:	438ms
1720:	learn:	3245.8172996	total:	2.69s	remaining:	437ms
1721:	learn:	3245.5221004	total:	2.69s	remaining:	435ms
1722:	learn:	3244.7470276	total:	2.7s	remaining:	434ms
1723:	learn:	3244.5450469	total:	2.7s	remaining:	432ms
1724:	learn:	3244.3835899	total:	2.7s	remaining:	431ms
1725:	learn:	3243.7042952	total:	2.7s	remaining:	429ms
1726:	learn:	3242.7265075	total:	2.7s	remaining:	428ms
1727:	learn:	3242.7265036	total:	2.71s	remaining:	426ms
1728:	learn:	3242.6212553	total:	2.71s	remaining:	424ms
1729:	learn:	3242.6212553	total:	2.71s	remaining:	423ms
1730:	learn:	3242.6212553	total:	2.71s	remaining:	421ms
1731:	learn:	3242.5020831	total:	2.71s	remaining:	419ms
1732:	learn:	3242.2354098	total:	2.71s	remaining:	418ms
1733:	learn:	3242.1319816	total:	2.71s	remaining:	416ms
1734:	learn:	3239.9598138	total:	2.71s	remaining:	415ms
1735:	learn:	3239.9598138	total:	2.71s	remaining:	413ms
1736:	learn:	3239.9598138	total:	2.71s	remaining:	411ms
1737:	learn:	3238.4933588	total:	2.72s	remaining:	410ms
1738:	learn:	3238.4090395	total:	2.72s	remaining:	408ms
1739:	learn:	3237.9460828	total:	2.72s	remaining:	407ms

1740:	learn:	3237.9460828	total:	2.72s	remaining:	405ms
1741:	learn:	3237.5741813	total:	2.72s	remaining:	403ms
1742:	learn:	3237.5731105	total:	2.72s	remaining:	402ms
1743:	learn:	3236.6579709	total:	2.73s	remaining:	400ms
1744:	learn:	3236.6579709	total:	2.73s	remaining:	398ms
1745:	learn:	3236.6004231	total:	2.73s	remaining:	397ms
1746:	learn:	3236.5989813	total:	2.73s	remaining:	395ms
1747:	learn:	3235.7497974	total:	2.73s	remaining:	394ms
1748:	learn:	3235.6559333	total:	2.73s	remaining:	392ms
1749:	learn:	3235.6559333	total:	2.73s	remaining:	390ms
1750:	learn:	3235.6559333	total:	2.73s	remaining:	389ms
1751:	learn:	3234.7204734	total:	2.73s	remaining:	387ms
1752:	learn:	3234.0974067	total:	2.74s	remaining:	386ms
1753:	learn:	3232.7146744	total:	2.74s	remaining:	384ms
1754:	learn:	3232.0895286	total:	2.74s	remaining:	383ms
1755:	learn:	3231.0815741	total:	2.74s	remaining:	381ms
1756:	learn:	3230.3141273	total:	2.74s	remaining:	379ms
1757:	learn:	3230.1224354	total:	2.75s	remaining:	378ms
1758:	learn:	3229.9339115	total:	2.75s	remaining:	377ms
1759:	learn:	3227.6837115	total:	2.75s	remaining:	375ms
1760:	learn:	3227.1989900	total:	2.75s	remaining:	374ms
1761:	learn:	3227.1208964	total:	2.75s	remaining:	372ms
1762:	learn:	3227.1208964	total:	2.75s	remaining:	370ms
1763:	learn:	3227.1208964	total:	2.75s	remaining:	369ms
1764:	learn:	3227.1208964	total:	2.76s	remaining:	367ms
1765:	learn:	3226.9229197	total:	2.76s	remaining:	366ms
1766:	learn:	3226.8221035	total:	2.76s	remaining:	364ms
1767:	learn:	3226.8221035	total:	2.76s	remaining:	362ms
1768:	learn:	3226.8221035	total:	2.76s	remaining:	361ms
1769:	learn:	3226.7462898	total:	2.77s	remaining:	359ms
1770:	learn:	3226.6427809	total:	2.77s	remaining:	358ms
1771:	learn:	3226.5801495	total:	2.77s	remaining:	356ms
1772:	learn:	3225.3617666	total:	2.77s	remaining:	355ms
1773:	learn:	3225.1428621	total:	2.77s	remaining:	354ms
1774:	learn:	3224.9591976	total:	2.78s	remaining:	352ms
1775:	learn:	3224.9591976	total:	2.78s	remaining:	350ms
1776:	learn:	3224.6700894	total:	2.78s	remaining:	349ms
1777:	learn:	3224.6466400	total:	2.78s	remaining:	347ms
1778:	learn:	3224.6271374	total:	2.78s	remaining:	346ms
1779:	learn:	3224.0563186	total:	2.79s	remaining:	344ms
1780:	learn:	3222.5400069	total:	2.79s	remaining:	343ms
1781:	learn:	3222.4027209	total:	2.79s	remaining:	341ms
1782:	learn:	3222.4027209	total:	2.79s	remaining:	340ms

1783:	learn:	3222.4027209	total:	2.79s	remaining:	338ms
1784:	learn:	3222.2928774	total:	2.79s	remaining:	336ms
1785:	learn:	3221.8128906	total:	2.79s	remaining:	335ms
1786:	learn:	3221.7618866	total:	2.8s	remaining:	333ms
1787:	learn:	3221.2949108	total:	2.8s	remaining:	332ms
1788:	learn:	3221.2949108	total:	2.8s	remaining:	330ms
1789:	learn:	3221.2240167	total:	2.8s	remaining:	329ms
1790:	learn:	3221.0322063	total:	2.8s	remaining:	327ms
1791:	learn:	3221.0322063	total:	2.8s	remaining:	325ms
1792:	learn:	3220.9381865	total:	2.81s	remaining:	324ms
1793:	learn:	3220.9381865	total:	2.81s	remaining:	322ms
1794:	learn:	3220.9381865	total:	2.81s	remaining:	321ms
1795:	learn:	3220.9377104	total:	2.81s	remaining:	319ms
1796:	learn:	3220.7727369	total:	2.81s	remaining:	317ms
1797:	learn:	3220.7356709	total:	2.81s	remaining:	316ms
1798:	learn:	3220.7356709	total:	2.81s	remaining:	314ms
1799:	learn:	3220.6184967	total:	2.81s	remaining:	313ms
1800:	learn:	3220.6175269	total:	2.81s	remaining:	311ms
1801:	learn:	3220.1059973	total:	2.81s	remaining:	309ms
1802:	learn:	3220.1059973	total:	2.82s	remaining:	308ms
1803:	learn:	3217.1888413	total:	2.82s	remaining:	306ms
1804:	learn:	3217.1172900	total:	2.82s	remaining:	305ms
1805:	learn:	3217.0688467	total:	2.82s	remaining:	303ms
1806:	learn:	3216.7132980	total:	2.82s	remaining:	301ms
1807:	learn:	3216.3568737	total:	2.82s	remaining:	300ms
1808:	learn:	3216.3157387	total:	2.83s	remaining:	298ms
1809:	learn:	3216.3157387	total:	2.83s	remaining:	297ms
1810:	learn:	3216.0763913	total:	2.83s	remaining:	295ms
1811:	learn:	3216.0763913	total:	2.83s	remaining:	294ms
1812:	learn:	3216.0763913	total:	2.83s	remaining:	292ms
1813:	learn:	3215.6931887	total:	2.83s	remaining:	290ms
1814:	learn:	3215.6931887	total:	2.83s	remaining:	289ms
1815:	learn:	3214.2313706	total:	2.83s	remaining:	287ms
1816:	learn:	3213.7688487	total:	2.83s	remaining:	286ms
1817:	learn:	3213.4543847	total:	2.84s	remaining:	284ms
1818:	learn:	3212.0359410	total:	2.84s	remaining:	282ms
1819:	learn:	3211.4011396	total:	2.84s	remaining:	281ms
1820:	learn:	3211.2998259	total:	2.84s	remaining:	279ms
1821:	learn:	3211.2998259	total:	2.84s	remaining:	278ms
1822:	learn:	3211.1857236	total:	2.85s	remaining:	276ms
1823:	learn:	3211.1852452	total:	2.85s	remaining:	275ms
1824:	learn:	3211.0107423	total:	2.85s	remaining:	273ms
1825:	learn:	3210.4542562	total:	2.85s	remaining:	272ms

1826:	learn:	3210.1349881	total:	2.85s	remaining:	270ms
1827:	learn:	3210.1349881	total:	2.85s	remaining:	268ms
1828:	learn:	3210.1349881	total:	2.85s	remaining:	267ms
1829:	learn:	3209.7725069	total:	2.85s	remaining:	265ms
1830:	learn:	3208.8106518	total:	2.85s	remaining:	264ms
1831:	learn:	3208.4329045	total:	2.86s	remaining:	262ms
1832:	learn:	3208.3958028	total:	2.86s	remaining:	261ms
1833:	learn:	3208.3958028	total:	2.86s	remaining:	259ms
1834:	learn:	3208.0052413	total:	2.86s	remaining:	257ms
1835:	learn:	3208.0052413	total:	2.86s	remaining:	256ms
1836:	learn:	3208.0006715	total:	2.86s	remaining:	254ms
1837:	learn:	3208.0006715	total:	2.86s	remaining:	252ms
1838:	learn:	3207.6299710	total:	2.87s	remaining:	251ms
1839:	learn:	3207.0709428	total:	2.87s	remaining:	249ms
1840:	learn:	3206.2722778	total:	2.87s	remaining:	248ms
1841:	learn:	3205.9844701	total:	2.87s	remaining:	246ms
1842:	learn:	3205.9844701	total:	2.87s	remaining:	245ms
1843:	learn:	3205.9844701	total:	2.87s	remaining:	243ms
1844:	learn:	3205.9051384	total:	2.87s	remaining:	241ms
1845:	learn:	3205.5338684	total:	2.88s	remaining:	240ms
1846:	learn:	3205.3602770	total:	2.88s	remaining:	238ms
1847:	learn:	3205.2578576	total:	2.88s	remaining:	237ms
1848:	learn:	3203.8365263	total:	2.88s	remaining:	235ms
1849:	learn:	3203.0163520	total:	2.88s	remaining:	234ms
1850:	learn:	3202.9417611	total:	2.88s	remaining:	232ms
1851:	learn:	3202.9417611	total:	2.88s	remaining:	231ms
1852:	learn:	3201.1659404	total:	2.89s	remaining:	229ms
1853:	learn:	3200.6824813	total:	2.89s	remaining:	227ms
1854:	learn:	3200.4047298	total:	2.89s	remaining:	226ms
1855:	learn:	3200.2798995	total:	2.89s	remaining:	224ms
1856:	learn:	3200.0748374	total:	2.89s	remaining:	223ms
1857:	learn:	3199.9563505	total:	2.9s	remaining:	221ms
1858:	learn:	3199.8089603	total:	2.9s	remaining:	220ms
1859:	learn:	3199.8089603	total:	2.9s	remaining:	218ms
1860:	learn:	3197.9298648	total:	2.9s	remaining:	217ms
1861:	learn:	3197.7025775	total:	2.9s	remaining:	215ms
1862:	learn:	3197.3721597	total:	2.9s	remaining:	214ms
1863:	learn:	3197.3140130	total:	2.9s	remaining:	212ms
1864:	learn:	3196.0015779	total:	2.91s	remaining:	210ms
1865:	learn:	3195.3910311	total:	2.91s	remaining:	209ms
1866:	learn:	3195.3308914	total:	2.91s	remaining:	207ms
1867:	learn:	3195.2076011	total:	2.91s	remaining:	206ms
1868:	learn:	3194.7759795	total:	2.91s	remaining:	204ms

1869:	learn: 3192.4044117	total: 2.92s	remaining: 203ms
1870:	learn: 3192.3708795	total: 2.92s	remaining: 201ms
1871:	learn: 3192.3708795	total: 2.92s	remaining: 199ms
1872:	learn: 3192.2939071	total: 2.92s	remaining: 198ms
1873:	learn: 3192.2895993	total: 2.92s	remaining: 196ms
1874:	learn: 3191.9587267	total: 2.92s	remaining: 195ms
1875:	learn: 3191.9567183	total: 2.92s	remaining: 193ms
1876:	learn: 3191.8971818	total: 2.92s	remaining: 192ms
1877:	learn: 3191.1792680	total: 2.93s	remaining: 190ms
1878:	learn: 3191.0838705	total: 2.93s	remaining: 189ms
1879:	learn: 3190.8872837	total: 2.93s	remaining: 187ms
1880:	learn: 3190.8872837	total: 2.93s	remaining: 185ms
1881:	learn: 3190.3398846	total: 2.93s	remaining: 184ms
1882:	learn: 3190.3178516	total: 2.93s	remaining: 182ms
1883:	learn: 3190.3178516	total: 2.94s	remaining: 181ms
1884:	learn: 3190.3178516	total: 2.94s	remaining: 179ms
1885:	learn: 3190.1615305	total: 2.94s	remaining: 178ms
1886:	learn: 3189.2103039	total: 2.94s	remaining: 176ms
1887:	learn: 3188.4273779	total: 2.94s	remaining: 174ms
1888:	learn: 3188.4238113	total: 2.94s	remaining: 173ms
1889:	learn: 3188.2809772	total: 2.94s	remaining: 171ms
1890:	learn: 3187.9026207	total: 2.94s	remaining: 170ms
1891:	learn: 3187.7516608	total: 2.95s	remaining: 168ms
1892:	learn: 3187.0001016	total: 2.95s	remaining: 167ms
1893:	learn: 3186.8764795	total: 2.95s	remaining: 165ms
1894:	learn: 3186.1777226	total: 2.95s	remaining: 164ms
1895:	learn: 3185.9146383	total: 2.95s	remaining: 162ms
1896:	learn: 3185.8595390	total: 2.96s	remaining: 160ms
1897:	learn: 3185.6498040	total: 2.96s	remaining: 159ms
1898:	learn: 3185.4838792	total: 2.96s	remaining: 157ms
1899:	learn: 3185.1089346	total: 2.96s	remaining: 156ms
1900:	learn: 3184.9103971	total: 2.96s	remaining: 154ms
1901:	learn: 3184.9103971	total: 2.96s	remaining: 153ms
1902:	learn: 3184.7112840	total: 2.96s	remaining: 151ms
1903:	learn: 3184.4933206	total: 2.97s	remaining: 150ms
1904:	learn: 3184.2238274	total: 2.97s	remaining: 148ms
1905:	learn: 3183.9800255	total: 2.97s	remaining: 147ms
1906:	learn: 3183.8295774	total: 2.97s	remaining: 145ms
1907:	learn: 3182.8877936	total: 2.97s	remaining: 143ms
1908:	learn: 3182.8877936	total: 2.97s	remaining: 142ms
1909:	learn: 3182.8605341	total: 2.98s	remaining: 140ms
1910:	learn: 3182.7561028	total: 2.98s	remaining: 139ms
1911:	learn: 3182.6976531	total: 2.98s	remaining: 137ms

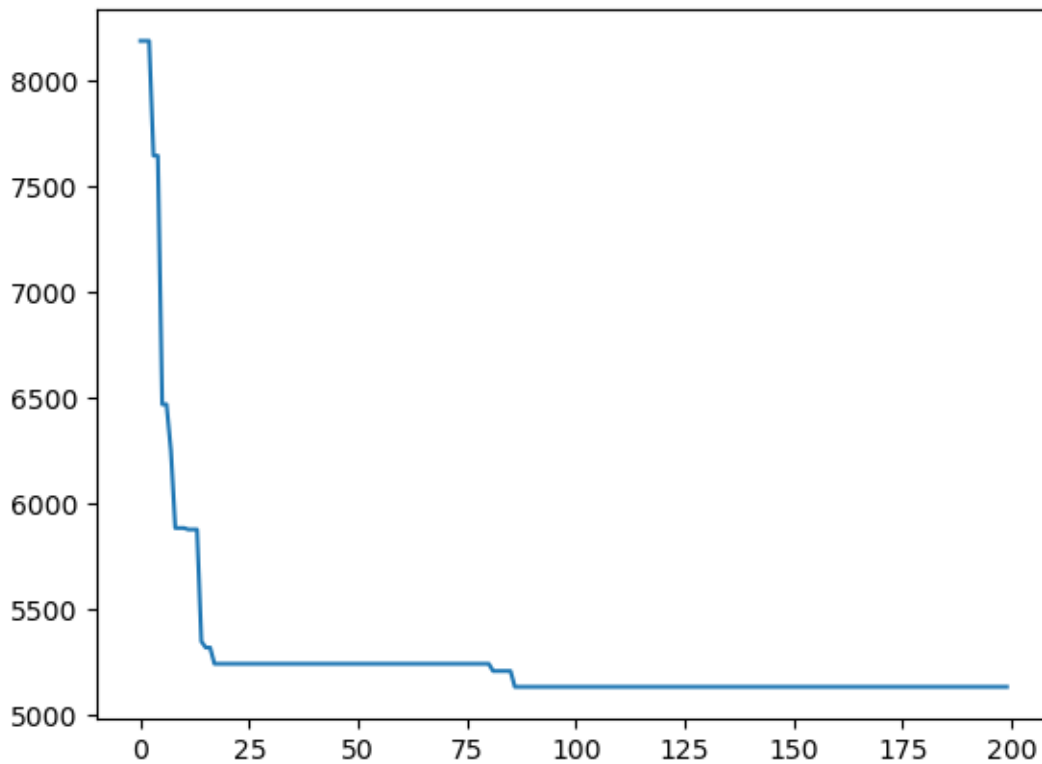
1912:	learn:	3182.4886802	total:	2.98s	remaining:	136ms
1913:	learn:	3182.4267129	total:	2.98s	remaining:	134ms
1914:	learn:	3181.8080179	total:	2.98s	remaining:	133ms
1915:	learn:	3181.8080179	total:	2.98s	remaining:	131ms
1916:	learn:	3181.5897020	total:	2.99s	remaining:	129ms
1917:	learn:	3181.3470077	total:	2.99s	remaining:	128ms
1918:	learn:	3180.6396235	total:	2.99s	remaining:	126ms
1919:	learn:	3180.4227108	total:	2.99s	remaining:	125ms
1920:	learn:	3179.2487757	total:	3s	remaining:	123ms
1921:	learn:	3178.8277430	total:	3s	remaining:	122ms
1922:	learn:	3178.8277430	total:	3s	remaining:	120ms
1923:	learn:	3178.8277430	total:	3s	remaining:	118ms
1924:	learn:	3178.8277430	total:	3s	remaining:	117ms
1925:	learn:	3178.6801247	total:	3s	remaining:	115ms
1926:	learn:	3177.4687686	total:	3s	remaining:	114ms
1927:	learn:	3176.8356898	total:	3s	remaining:	112ms
1928:	learn:	3176.7893483	total:	3s	remaining:	111ms
1929:	learn:	3176.6002622	total:	3.01s	remaining:	109ms
1930:	learn:	3175.5122001	total:	3.01s	remaining:	108ms
1931:	learn:	3175.5115561	total:	3.01s	remaining:	106ms
1932:	learn:	3175.3155671	total:	3.01s	remaining:	104ms
1933:	learn:	3175.0862539	total:	3.01s	remaining:	103ms
1934:	learn:	3173.7085725	total:	3.02s	remaining:	101ms
1935:	learn:	3173.6273355	total:	3.02s	remaining:	99.7ms
1936:	learn:	3173.6273355	total:	3.02s	remaining:	98.1ms
1937:	learn:	3172.2604329	total:	3.02s	remaining:	96.6ms
1938:	learn:	3170.7569996	total:	3.02s	remaining:	95ms
1939:	learn:	3170.7210008	total:	3.02s	remaining:	93.4ms
1940:	learn:	3170.6571722	total:	3.02s	remaining:	91.9ms
1941:	learn:	3170.4286382	total:	3.02s	remaining:	90.3ms
1942:	learn:	3170.4038996	total:	3.02s	remaining:	88.7ms
1943:	learn:	3167.9652011	total:	3.03s	remaining:	87.2ms
1944:	learn:	3167.3331960	total:	3.03s	remaining:	85.6ms
1945:	learn:	3167.0481107	total:	3.03s	remaining:	84.1ms
1946:	learn:	3165.3433385	total:	3.03s	remaining:	82.5ms
1947:	learn:	3163.1094795	total:	3.03s	remaining:	81ms
1948:	learn:	3163.0667467	total:	3.04s	remaining:	79.4ms
1949:	learn:	3163.0667467	total:	3.04s	remaining:	77.8ms
1950:	learn:	3162.4798653	total:	3.04s	remaining:	76.3ms
1951:	learn:	3161.3348713	total:	3.04s	remaining:	74.7ms
1952:	learn:	3161.3117989	total:	3.04s	remaining:	73.2ms
1953:	learn:	3160.8023680	total:	3.04s	remaining:	71.6ms
1954:	learn:	3160.1140905	total:	3.04s	remaining:	70.1ms

1955:	learn:	3158.9981598	total:	3.05s	remaining:	68.5ms
1956:	learn:	3156.8978382	total:	3.05s	remaining:	67ms
1957:	learn:	3156.7772601	total:	3.05s	remaining:	65.4ms
1958:	learn:	3156.5825227	total:	3.05s	remaining:	63.9ms
1959:	learn:	3156.1921972	total:	3.05s	remaining:	62.3ms
1960:	learn:	3155.5738299	total:	3.06s	remaining:	60.8ms
1961:	learn:	3154.9745268	total:	3.06s	remaining:	59.2ms
1962:	learn:	3154.9745268	total:	3.06s	remaining:	57.7ms
1963:	learn:	3154.9321185	total:	3.06s	remaining:	56.1ms
1964:	learn:	3154.9193510	total:	3.06s	remaining:	54.5ms
1965:	learn:	3153.3045270	total:	3.06s	remaining:	53ms
1966:	learn:	3153.1427141	total:	3.06s	remaining:	51.4ms
1967:	learn:	3152.9119379	total:	3.07s	remaining:	49.9ms
1968:	learn:	3152.9117927	total:	3.07s	remaining:	48.3ms
1969:	learn:	3152.9117927	total:	3.07s	remaining:	46.7ms
1970:	learn:	3152.8367126	total:	3.07s	remaining:	45.2ms
1971:	learn:	3152.8124488	total:	3.07s	remaining:	43.6ms
1972:	learn:	3152.5892578	total:	3.07s	remaining:	42.1ms
1973:	learn:	3152.4632281	total:	3.08s	remaining:	40.5ms
1974:	learn:	3152.4632281	total:	3.08s	remaining:	38.9ms
1975:	learn:	3152.4610389	total:	3.08s	remaining:	37.4ms
1976:	learn:	3152.4070619	total:	3.08s	remaining:	35.8ms
1977:	learn:	3151.5088242	total:	3.08s	remaining:	34.3ms
1978:	learn:	3151.3192003	total:	3.08s	remaining:	32.7ms
1979:	learn:	3151.0934751	total:	3.08s	remaining:	31.2ms
1980:	learn:	3151.0934751	total:	3.09s	remaining:	29.6ms
1981:	learn:	3150.9537433	total:	3.09s	remaining:	28ms
1982:	learn:	3150.9537433	total:	3.09s	remaining:	26.5ms
1983:	learn:	3150.8674274	total:	3.09s	remaining:	24.9ms
1984:	learn:	3150.8674274	total:	3.09s	remaining:	23.4ms
1985:	learn:	3149.2328055	total:	3.09s	remaining:	21.8ms
1986:	learn:	3149.0072684	total:	3.09s	remaining:	20.2ms
1987:	learn:	3148.3315876	total:	3.1s	remaining:	18.7ms
1988:	learn:	3147.7977344	total:	3.1s	remaining:	17.1ms
1989:	learn:	3147.6247163	total:	3.1s	remaining:	15.6ms
1990:	learn:	3146.5977276	total:	3.1s	remaining:	14ms
1991:	learn:	3146.1891474	total:	3.1s	remaining:	12.5ms
1992:	learn:	3146.1621749	total:	3.11s	remaining:	10.9ms
1993:	learn:	3144.2741570	total:	3.11s	remaining:	9.36ms
1994:	learn:	3144.2189615	total:	3.11s	remaining:	7.8ms
1995:	learn:	3143.8690645	total:	3.11s	remaining:	6.24ms
1996:	learn:	3143.3502296	total:	3.12s	remaining:	4.68ms
1997:	learn:	3142.8227286	total:	3.12s	remaining:	3.12ms

```

1998:  learn: 3142.8227286 total: 3.12s    remaining: 1.56ms
1999:  learn: 3142.6323020 total: 3.12s    remaining: 0us

```



```

BayesSearchCV(cv=KFold(n_splits=5, random_state=1, shuffle=True),
               estimator=<catboost.core.CatBoostRegressor object at 0x000001C05095EFD0>,
               n_iter=200, n_jobs=-1, random_state=1,
               scoring='neg_root_mean_squared_error',
               search_spaces={'colsample_bylevel': Real(low=0.1, high=1.0, prior='uniform', transform='log'),
                              'learning_rate': Real(low=0.0001, high=1.0, prior='uniform', transform='log'),
                              'n_estimators': Integer(low=2, high=2000, prior='uniform', transform='log'),
                              'num_leaves': Integer(low=4, high=64, prior='uniform', transform='log'),
                              'reg_lambda': Real(low=0, high=10000.0, prior='uniform', transform='log'),
                              'subsample': Real(low=0.1, high=1.0, prior='uniform', transform='log')})

```

13.2.4 Tuning Tips

Check the [documentation](#) for some tuning tips.

1. It is not recommended to use values greater than 64 for `num_leaves`, since it can significantly slow down the training process.
2. The maximum possible value of `max_depth` is 16.

14 Ensemble modeling

Ensembling models can help reduce error by leveraging the diversity and collective wisdom of multiple models. When ensembling, several individual models are trained independently and their predictions are combined to make the final prediction.

We have already seen examples of ensemble models in chapters 5 - 9. The ensembled models may reduce error by reducing the bias (*boosting*) and / or reducing the variance (*bagging* / *random forests* / *boosting*).

However, in this chapter we'll ensemble different types of models, instead of the same type of model. We may ensemble a linear regression model, a random forest, a gradient boosting model, and as many different types of models as we wish.

Below are a couple of reasons why ensembling models can be effective in reducing error:

1. **Bias reduction:** Different models may have different biases and the ensemble can help mitigate the individual biases, leading to a more generalized and accurate prediction. For example, consider that one model has a positive bias, and another model has a negative bias for the same instance. By averaging or combining the predictions of the two models, the biases may cancel out.
2. **Variance reduction:** As seen in the case of random forests and bagged trees, by averaging or combining the predictions of multiple models, the ensemble can reduce the overall variance and improve the accuracy of the final prediction. Note that for variance reduction, the models should have a low correlation (*recall the variance reduction formula of random forests*).

Mathematically also, we can show the effectiveness of an ensemble model. Let's consider the case of regression, and let the predictors be denoted as X , and the response as Y . Let f_1, \dots, f_m be the individual models. The expected MSE of an ensemble can be written as:

$$MSE_{Ensemble} = E \left[\left(\frac{1}{m} \sum_{i=1}^m f_i(X) - Y \right)^2 \right] = \frac{1}{m^2} E \left[(f_i(X) - Y)^2 \right] + \frac{1}{m^2} \sum_{i \neq j} E \left[(f_i(X) - Y)(f_j(X) - Y) \right]$$

Assuming the **models are uncorrelated** (*i.e., they have a zero correlation*), the second term (*covariance of $f_i(\cdot)$ and $f_j(\cdot)$*) reduces to zero, and the expected MSE of the ensemble reduces to:

$$MSE_{Ensemble} = \frac{1}{m} \left(\frac{1}{m} \sum_{i=1}^m MSE_{f_i} \right) \quad (14.1)$$

Thus, the expected MSE of an ensemble model with uncorrelated models is much smaller than the average MSE of all the models. Unless there is a model that is much better than the rest of the models, the MSE of the ensemble model is likely to be lower than the MSE of the individual models. However, there is no guarantee that the MSE of the ensemble model will be lower than the MSE of the individual models. Consider an extreme case where only one of the models have a zero MSE. The MSE of this model will be lower than the expected MSE of the ensemble model.

```
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, GridSearchCV, ParameterGrid
from sklearn.metrics import mean_squared_error, r2_score, roc_curve, auc, precision_recall_curve
from sklearn.model_selection import KFold
from sklearn.tree import DecisionTreeRegressor, DecisionTreeClassifier
from sklearn.ensemble import VotingRegressor, VotingClassifier, StackingRegressor, StackingClassifier
from sklearn.linear_model import LinearRegression, LogisticRegression, LassoCV, RidgeCV, ElasticNetCV
from sklearn.neighbors import KNeighborsRegressor
import itertools as it
import time as time
import xgboost as xgb
from pyearth import Earth
```

```
#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

	carID	brand	model	year	transmission	mileage	fuelType	tax	mpg	engineSize	price
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']
```

14.1 Ensembling regression models

14.1.1 Voting Regressor

Here, we will combine the predictions of different models. The function `VotingRegressor()` averages the predictions of all the models.

Below are the individual models tuned in the previous chapters.

```
# Tuned XGBoost model from Section 9.2.6
model_xgb = xgb.XGBRegressor(random_state=1,max_depth=8,n_estimators=1000, subsample = 0.75,
                             learning_rate = 0.01,reg_lambda=1, gamma = 100).fit(X, y)
print("RMSE for XGBoost = ", np.sqrt(mean_squared_error(model_xgb.predict(Xtest), ytest)))

#Tuned AdaBoost model from Section 7.2.4
model_ada = AdaBoostRegressor(base_estimator=DecisionTreeRegressor(max_depth=10),n_estimators=100,
                              random_state=1).fit(X, y)
print("RMSE for AdaBoost = ", 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("RMSE for Random forest = ", 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("RMSE for Gradient Boosting = ", np.sqrt(mean_squared_error(model_gb.predict(Xtest), ytest)))
```

```
RMSE for XGBoost = 5497.553788113875
RMSE for AdaBoost = 5693.165811600585
RMSE for Random forest = 5642.45839697972
RMSE for Gradient Boosting = 5405.787029062213
```

```
#Voting ensemble: Averaging the predictions of all models
en=VotingRegressor(estimators = [('xgb',model_xgb),('ada',model_ada),('rf',model_rf),('gb',model_gb)])
en.fit(X,y)
print("Ensemble model RMSE = ", np.sqrt(mean_squared_error(en.predict(Xtest),ytest)))
```

```
Ensemble model RMSE = 5361.7260763197
```

RMSE of the ensembled model is less than that of each of the individual models.

14.1.2 Stacking Regressor

Stacking is a more sophisticated method of ensembling models. The method is as follows:

1. The training data is split into K folds. Each of the K folds serves as a test data in one of the K iterations, and the rest of the folds serve as train data.
2. Each model is used to make predictions on each of the K folds, after being trained on the remaining $K-1$ folds. In this manner, each model predicts the response on each train data point - when that train data point was not used to train the model.
3. Predictions at each training data points are generated by each model in step 2 (the above step). These predictions are now used as predictors to train a meta-model (referred by the argument `final_estimator`), with the original response as the response. The meta-model (or `final_estimator`) learns to combine predictions of different models to make a better prediction.

```
#Stacking using LinearRegression as the metamodel
en = StackingRegressor(estimators = [('xgb', model_xgb),('ada', model_ada),('rf', model_rf),
                                   final_estimator=LinearRegression(),
                                   cv = KFold(n_splits = 5, shuffle = True, random_state=1))
en.fit(X,y)
print("Linear regression metamodel RMSE = ", np.sqrt(mean_squared_error(en.predict(Xtest),ytest)))
```

```
Linear regression metamodel RMSE = 5311.789386389769
```



```
#Co-efficients of the meta-model
en.final_estimator_.coef_
```

```
array([0.29641759, 0.25626987, 0.051808 , 0.41978153])
```

Note the above coefficients of the meta-model. The model gives the highest weight to the gradient boosting model, and the lowest weight to the random forest model. Also, note that the coefficients need not sum to one.

```
#Stacking using Lasso as the metamodel
en = StackingRegressor(estimators = [('xgb', model_xgb), ('ada', model_ada), ('rf', model_rf),
                                final_estimator=LassoCV(),
                                cv = KFold(n_splits = 5, shuffle = True, random_state=1))
en.fit(X,y)
print("Lasso metamodel RMSE = ", np.sqrt(mean_squared_error(en.predict(Xtest),ytest)))
```

```
Lasso metamodel RMSE = 5311.185592456483
```

```
#Coefficients of the lasso metamodel
en.final_estimator_.coef_
```

```
array([0.17639973, 0.28186944, 0.1152561 , 0.45119952])
```

```
#Stacking using MARS as the meta-model
en = StackingRegressor(estimators = [('xgb',m1), ('ada',m2), ('rf',m3), ('gb',m4)],
                        final_estimator=Earth(max_degree=1),
                        cv = KFold(n_splits = 5, shuffle = True, random_state=1))
en.fit(X,y)
print("MARS metamodel RMSE = ", np.sqrt(mean_squared_error(en.predict(Xtest),ytest)))
```

```
Ensemble model RMSE = 5303.308982301974
```

```
C:\Users\akl0407\Anaconda3\lib\site-packages\pyearth\earth.py:813: FutureWarning: `rcond` pa
To use the future default and silence this warning we advise to pass `rcond=None`, to keep us
pruning_passer.run()
C:\Users\akl0407\Anaconda3\lib\site-packages\pyearth\earth.py:1066: FutureWarning: `rcond` pa
To use the future default and silence this warning we advise to pass `rcond=None`, to keep us
coef, resid = np.linalg.lstsq(B, weighted_y[:, i])[0:2]
```

```
print(en.final_estimator_.summary())
```

Earth Model

Basis Function	Pruned	Coefficient

(Intercept)	No	59644
h(x3-75435)	No	0.402779
h(75435-x3)	No	-0.406517
h(x1-74988)	No	0.822699
h(74988-x1)	No	-0.119104
h(x2-72702.8)	No	-0.449716
h(72702.8-x2)	No	-0.280938
x0	No	0.211986

MSE: 25038308.7322, GCV: 25226136.6357, RSQ: 0.9070, GRSQ: 0.9063

14.2 Ensembling classification models

We'll ensemble models for predicting accuracy of identifying people having a heart disease.

```
data = pd.read_csv('./Datasets/Heart.csv')
data.dropna(inplace = True)
#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)

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

Let us tune the individual models first.

AdaBoost

```

# Tuning Adaboost for maximizing accuracy
model = AdaBoostClassifier(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['base_estimator'] = [DecisionTreeClassifier(max_depth=1), DecisionTreeClassifier(max_depth=2),
                          DecisionTreeClassifier(max_depth=3),DecisionTreeClassifier(max_depth=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, scoring='accuracy')
# execute the grid search
grid_result = grid_search.fit(Xtrain, ytrain)
# summarize the best score and configuration
print("Best: %f using %s" % (grid_result.best_score_, grid_result.best_params_))

```

Best: 0.871494 using {'base_estimator': DecisionTreeClassifier(max_depth=1), 'learning_rate': 0.0001}

Gradient Boosting

```

# Tuning gradient boosting for maximizing accuracy
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, scoring='accuracy')
# execute the grid search
grid_result = grid_search.fit(Xtrain, ytrain)
# summarize the best score and configuration
print("Best: %f using %s" % (grid_result.best_score_, grid_result.best_params_))

```

Best: 0.871954 using {'learning_rate': 1.0, 'max_depth': 4, 'n_estimators': 100, 'subsample': 0.5}

XGBoost

```
# Tuning XGBoost for maximizing accuracy
start_time = time.time()
param_grid = {'n_estimators': [25, 100, 250, 500],
              'max_depth': [4, 6, 8],
              'learning_rate': [0.01, 0.1, 0.2],
              'gamma': [0, 1, 10, 100],
              'reg_lambda': [0, 10, 100],
              'subsample': [0.5, 0.75, 1.0]
              'scale_pos_weight': [1.25, 1.5, 1.75] # Control the balance of positive and negative samples
            }

cv = StratifiedKFold(n_splits=5, shuffle=True, random_state=1)
optimal_params = GridSearchCV(estimator=xgb.XGBClassifier(random_state=1),
                             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 972 candidates, totalling 4860 fits

```
{'gamma': 0, 'learning_rate': 0.2, 'max_depth': 4, 'n_estimators': 25, 'reg_lambda': 0, 'scale_pos_weight': 1.25}
Time taken = 0.9524135629336039 minutes
```

```
# Tuned Adaboost model
model_ada = AdaBoostClassifier(base_estimator=DecisionTreeClassifier(max_depth=1), n_estimators=100,
                              random_state=1, learning_rate=0.01).fit(Xtrain, ytrain)
test_accuracy_ada = model_ada.score(Xtest, ytest) # Returns the classification accuracy of the model

# Tuned Random forest model from Section 6.3
model_rf = RandomForestClassifier(n_estimators=500, random_state=1, max_features=3,
                                 n_jobs=-1, oob_score=False).fit(Xtrain, ytrain)
test_accuracy_rf = model_rf.score(Xtest, ytest) # Returns the classification accuracy of the model

# Tuned gradient boosting model
model_gb = GradientBoostingClassifier(n_estimators=100, random_state=1, max_depth=4, learning_rate=0.1,
                                     subsample=1.0).fit(Xtrain, ytrain)
```

```

test_accuracy_gb = model_gb.score(Xtest,ytest) #Returns the classification accuracy of the model

#Tuned XGBoost model
model_xgb = xgb.XGBClassifier(random_state=1,gamma=0,learning_rate = 0.2,max_depth=4,
                              n_estimators = 25,reg_lambda = 0,scale_pos_weight=1.25).fit(Xtrain,ytrain)
test_accuracy_xgb = model_xgb.score(Xtest,ytest) #Returns the classification accuracy of the model

print("Adaboost accuracy = ",test_accuracy_ada)
print("Random forest accuracy = ",test_accuracy_rf)
print("Gradient boost accuracy = ",test_accuracy_gb)
print("XGBoost model accuracy = ",test_accuracy_xgb)

```

```

Adaboost accuracy = 0.7986577181208053
Random forest accuracy = 0.8120805369127517
Gradient boost accuracy = 0.7986577181208053
XGBoost model accuracy = 0.7785234899328859

```

14.2.1 Voting classifier - hard voting

In this type of ensembling, the predicted class is the one predicted by the majority of the classifiers.

```

ensemble_model = VotingClassifier(estimators=[('ada',model_ada),('rf',model_rf),('gb',model_gb)])
ensemble_model.fit(Xtrain,ytrain)
ensemble_model.score(Xtest, ytest)

```

```
0.825503355704698
```

Note that the prediction accuracy of the ensemble is higher than the prediction accuracy of each of the individual models on unseen data.

14.2.2 Voting classifier - soft voting

In this type of ensembling, the predicted class is the one based on the average predicted probabilities of all the classifiers. The threshold probability is 0.5.

```

ensemble_model = VotingClassifier(estimators=[('ada',model_ada),('rf',model_rf),('gb',model_gb)],
                                voting='soft')
ensemble_model.fit(Xtrain,ytrain)
ensemble_model.score(Xtest, ytest)

```

0.7919463087248322

Note that soft voting will be good only for well calibrated classifiers, i.e., all the classifiers must have probabilities at the same scale.

14.2.3 Stacking classifier

Conceptually, the idea is similar to that of Stacking regressor.

```
#Using Logistic regression as the meta model (final_estimator)
ensemble_model = StackingClassifier(estimators=[('ada',model_ada),('rf',model_rf),('gb',model_gb)],
                                   final_estimator=LogisticRegression(random_state=1,max_iter=1000),
                                   cv = StratifiedKFold(n_splits=5,shuffle=True,random_state=1))
ensemble_model.fit(Xtrain,ytrain)
ensemble_model.score(Xtest, ytest)
```

0.7986577181208053

```
#Coefficients of the logistic regression metamodel
ensemble_model.final_estimator_.coef_
```

array([[0.81748051, 1.28663164, 1.64593342, 1.50947087]])

```
#Using random forests as the meta model (final_estimator). Note that random forest will require tuning.
ensemble_model = StackingClassifier(estimators=[('ada',model_ada),('rf',model_rf),('gb',model_gb)],
                                   final_estimator=RandomForestClassifier(n_estimators=500, max_features='sqrt',
                                                                           random_state=1,oob_score=True),
                                   cv = StratifiedKFold(n_splits=5,shuffle=True,random_state=1))
ensemble_model.fit(Xtrain,ytrain)
ensemble_model.score(Xtest, ytest)
```

0.8322147651006712

Note that a complex `final_estimator` such as random forest will require tuning. In the above case, the `max_features` argument of random forests has been tuned to obtain the maximum OOB score. The tuning is shown below.

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

i=0
for pr in range(1,5):
    model = StackingClassifier(estimators=[('ada',model_ada),('rf',model_rf),('gb',model_gb)],
                              final_estimator=RandomForestClassifier(n_estimators=500,
                              random_state=1,oob_score=True),n_jobs=-1,
                              cv = StratifiedKFold(n_splits=5,shuffle=True,random_state=1))
    oob_score[pr] = model.final_estimator_.oob_score_

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 = 0.33713538646698 minutes
max accuracy = 0.8445945945945946
Best value of max_features= 1
```

```
#The final predictor (metamodel) - random forest obtains the maximum oob_score for max_features=1
oob_score
```

```
{1: 0.8445945945945946,
 2: 0.831081081081081,
 3: 0.8378378378378378,
 4: 0.831081081081081}
```

14.2.4 Tuning all models simultaneously

Individual model hyperparameters can be tuned simultaneously while ensembling them with a `VotingClassifier()`. However, this approach can be too expensive for even moderately-sized datasets.

```
# Create the param grid with the names of the models as prefixes

model_ada = AdaBoostClassifier(base_estimator = DecisionTreeClassifier())
model_rf = RandomForestClassifier()
model_gb = GradientBoostingClassifier()
```

```

model_xgb = xgb.XGBClassifier()

ensemble_model = VotingClassifier(estimators=[('ada',model_ada),('rf',model_rf),('gb',model_gb)])

hp_grid = dict()

# XGBoost
hp_grid['xgb__n_estimators'] = [25, 100,250,50]
hp_grid['xgb__max_depth'] = [4, 6 ,8]
hp_grid['xgb__learning_rate'] = [0.01, 0.1, 1.0]
hp_grid['xgb__gamma'] = [0, 1, 10, 100]
hp_grid['xgb__reg_lambda'] = [0, 1, 10, 100]
hp_grid['xgb__subsample'] = [0, 1, 10, 100]
hp_grid['xgb__scale_pos_weight'] = [1.0, 1.25, 1.5]
hp_grid['xgb__colsample_bytree'] = [0.5, 0.75, 1.0]

# AdaBoost
hp_grid['ada__n_estimators'] = [10, 50, 100,200,500]
hp_grid['ada__base_estimator__max_depth'] = [1, 3, 5]
hp_grid['ada__learning_rate'] = [0.01, 0.1, 0.2]

# Random Forest
hp_grid['rf__n_estimators'] = [100]
hp_grid['rf__max_features'] = [3, 6, 9, 12, 15]

# GradBoost
hp_grid['gb__n_estimators'] = [10, 50, 100,200,500]
hp_grid['gb__max_depth'] = [1, 3, 5]
hp_grid['gb__learning_rate'] = [0.01, 0.1, 0.2, 1.0]
hp_grid['gb__subsample'] = [0.5, 0.75, 1.0]

start_time = time.time()
grid = RandomizedSearchCV(ensemble_model, hp_grid, cv=5, scoring='accuracy', verbose = True,
                          n_iter = 100, n_jobs=-1).fit(Xtrain, ytrain)
print("Time taken = ", round((time.time()-start_time)/60), " minutes")

grid.best_estimator_.score(Xtest, ytest)

```

0.8120805369127517

Part III

Assignments

15 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**)

15.1 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.

15.1.1 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
```

15.1.2 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.

15.1.3 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)**

15.1.4 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.

15.1.5 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)**

15.1.6 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)**

15.2 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.

15.2.1 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)**

15.2.2 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)**

15.2.3 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 hyperparameter values in the range $[1, 100]$.

15.2.4 d)

Repeat part 1e with Ridge regularization, using the results from 2c. **(2 points)**

15.2.5 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)**

15.2.6 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)**

15.3 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>

15.3.1 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)

15.3.2 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.

15.3.3 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)

15.3.4 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)

15.3.5 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)

15.3.6 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')
```


16 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**)

16.1 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.

16.1.1 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)

16.1.2 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)*

16.1.3 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)*

16.1.4 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)*

16.1.5 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)*

16.1.6 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)*

16.1.7 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)*

16.1.8 1h)

Use the tuned classifier and threshold from part 1(f) to find the test accuracy. *(1 point)*

16.1.9 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)*

16.1.10 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)

16.2 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.

16.2.1 2a)

Find the optimal hyperparameter values and the corresponding 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 simple 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)

16.2.2 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)

16.2.3 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)

16.2.4 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)

16.2.5 2e)

How did you decide the range of hyperparameter values to consider in this question? Discuss for `p` and `n_neighbors`.

(4 points)

16.2.6 2f)

Is it possible to further improve the results if we also optimize the `metric` hyperparameter along with the hyperparameters specified in 2(a)? Why or why not?

(4 points)

16.2.7 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)

17 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)

17.1 1) Regression Problem - Miami housing

17.1.1 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)

17.1.2 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)

17.1.3 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 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)

17.1.4 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)

17.1.5 1e) Bagging without bootstrapping

Bag decision trees without bootstrapping, i.e., put `bootstrap = False` while bagging the trees, and compute the cross-validated 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)

17.1.6 1f) Bagging without bootstrapping samples, but bootstrapping features

Bag decision trees without bootstrapping samples, 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)

17.1.7 1g) Tuning bagged tree model

17.1.7.1 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)

17.1.7.2 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-validated MAE obtained 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)

17.1.8 1h) Random forest

17.1.8.1 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)

17.1.8.2 1h)(ii) Feature importance

Arrange and print the predictors in decreasing order of importance.

(4 points)

17.1.8.3 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)

17.1.8.4 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)

17.2 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.)

17.2.1 2a) Data preparation

Convert all the categorical predictors in the data to dummy variables. Note that **month** and **education** are categorical variables.

(2 points)

17.2.2 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.

17.3 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)

18 Assignment 4

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 **Friday, 24th 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 **(1 point)**. *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.*
 - No name can be written on the assignment, nor can there be any indicator of the student's identity—e.g. printouts of the working directory should not be included in the final submission. **(1 point)**
 - 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)**

18.1 1) AdaBoost vs Bagging (4 points)

Which model among AdaBoost and Random Forest is more sensitive to outliers? **(1 point)**
Explain your reasoning with the theory you learned on the training process of both models. **(3 points)**

18.2 2) Regression with Boosting (55 points)

For this question, you will use the `miami_housing.csv` file. You can find the description for the variables [here](#).

The `SALE_PRC` variable is the regression response and the rest of the variables, except `PARCELNO`, are the predictors.

18.2.1 a)

Read the dataset. Create the training and test sets with a 60%-40% split and `random_state = 1`. **(1 point)**

18.2.2 b)

Tune an AdaBoost model to get below a cross-validation MAE of \$48000. Keep **all** the `random_states` as 1. **Getting below the given cutoff with a different `random_state` in ANY object will not receive any credit. (5 points for a search that makes sense + 5 points for the cutoff = 10 points)**

Hints:

- Remember how you need to approach the tuning process with coarse and fine grids.
- Remember that you have different cross-validation settings available.

18.2.3 c)

Find the test MAE of the tuned AdaBoost model to see if it generalizes well. **(1 point)**

18.2.4 d)

Using the tuned AdaBoost model, print the predictor names with their importances in **decreasing order**. You need to print a DataFrame with the predictor names in the first column and the importances in the second. **(1 points)**

Note: Features importances can be taken with pretty much the same line of code for all the models in this assignment. It is asked only for AdaBoost and omitted for the remaining models to avoid repetition.

18.2.5 e)

Moving on to Gradient Boosting, in general, which is the most preferred loss function? **(1 point)** What are its advantages over other loss functions? **(3 points)**

18.2.6 f)

Tune a Gradient Boosting model to get below a cross-validation MAE of \$45000. Keep **all** the `random_states` as 1. **Getting below the given cutoff with a different `random_state` in ANY object will not receive any credit.** **(5 points for a search that makes sense + 5 points for the cutoff = 10 points)**

Hints:

- Remember how you need to approach the grid of Gradient Boosting.
- Remember that you have different cross-validation settings available.

18.2.7 g)

Find the test MAE of the tuned Gradient Boosting model to see if it generalizes well. **(1 point)**

18.2.8 h)

Explain how the tuned hyperparameters of AdaBoost and Gradient Boosting affect the bias and the variance of their model. Note that most hyperparameters are the same between the models, so give only one explanation for those. (You need to include four hyperparameters in total.) **(1x4 = 4 points)**

18.2.9 i)

Moving on to XGBoost:

- What are the additions that makes XGBoost superior to Gradient Boosting? You need to explain this in terms of runtime (**1 point**) with its reason (**1 point**) and the hyper-parameters (**1 point**) with their effect of model behavior. (**2 points**).
- What is missing in XGBoost that is well-implemented in Gradient Boosting? (**1 point**)

18.2.10 j)

Tune a XGBoost model to get below a cross-validation MAE of \$43500. Keep **all** the `random_states` as 1. **Getting below the given cutoff with a different `random_state` in ANY object will not receive any credit.** (5 points for a search that makes sense + 5 points for the cutoff = 10 points)

Hints:

- Remember how you need to approach the grid of XGBoost.
- Remember that you have different cross-validation settings available.

18.2.11 k)

Find the test MAE of the tuned XGBoost model to see if it generalizes well. (**1 point**)

18.3 2) Classification with Boosting (42 points)

For this question, you will use the **train.csv** and **test.csv** files. Each observation is a marketing call from a banking institution. `y` variable represents if the client subscribed for a term deposit (1) or not (0) and it is the classification response.

The predictors are **age**, **day**, **month**, and **education**. (As mentioned last quarter, **duration** cannot be used as a predictor - no credit will be given to models that use it.)

18.3.1 a)

Preprocess the data:

- Read the files.
- Create the predictor and response variables.
- Convert the response to 1s and 0s.
- One-hot-encode the categorical predictors (**Do not use drop_first.**)

(1 point)

18.3.2 b)

Moving on to LightGBM and CatBoost, what are their advantages compared to Gradient Boosting and XGBoost? (2 points) How are these advantages implemented into the models? (2 points) Does any of them have any disadvantages? Describe if there is any. (1 point)

18.3.3 c)

For all extensions of Gradient Boosting, (XGBoost/LightGBM/CatBoost) is there an additional input/hyperparameter you can use to handle a certain issue that is specific to classification? (1 point) If yes, describe what it stands for (1 point) and how its value should be handled most efficiently. (1 point)

18.3.4 d)

Tune a LightGBM model to get above a cross-validation accuracy of 70% and a cross-validation recall of 65%. Keep **all** the random_states as 1. **Getting above the given cutoffs with a different random_state in ANY object will not receive any credit.** (7.5 points for a search that makes sense + 7.5 points for the cutoff = 15 points)

Hints:

- Handling the grid efficiently can be useful again.
- Remember that there are cross-validation settings that are specific to classification.
- Remember that for classification, you need to tune the threshold as well.

18.3.5 e)

Find the test accuracy and the test recall of the tuned LightGBM model and threshold to see if they generalize well. (2 points)

18.3.6 f)

Tune a CatBoost model to get above a cross-validation accuracy of 70% and a cross-validation recall of 65%. Keep **all** the `random_states` as 1. **Getting above the given cutoffs with a different `random_state` in ANY object will not receive any credit.** (7.5 points for a search that makes sense + 7.5 points for the cutoff = 15 points)

Hints:

- Handling the grid efficiently can be useful again.
- Remember that there are cross-validation settings that are specific to classification.
- Remember that for classification, you need to tune the threshold as well. (Use a stepsize of 0.001)

18.3.7 g)

Find the test accuracy and the test recall of the tuned CatBoost model and threshold to see if they generalize well. (1 point)

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 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 test
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 x_1 , x_2 , 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 x_1 and x_2 , a continuous predictor x_3 , 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_CatPredictors_stratified'})

# 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

# 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 = i)
    model = LogisticRegression()
    model.fit(X_train, y_train)

    # Model accuracy on train and test data, with stratification only on response while splitting
    # 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 train and test data
    X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.2, random_state = i,
                                                        stratify=pd.concat([x1, x2, y], axis=1))
    model.fit(X_train, y_train)

    # Model accuracy on train and test data, with stratification on response and predictors while splitting
    # the complete data into train and test
    accuracy_iter.loc[(i-1), 'train_y_CatPredictors_stratified'] = model.score(X_train, y_train)
    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()
```

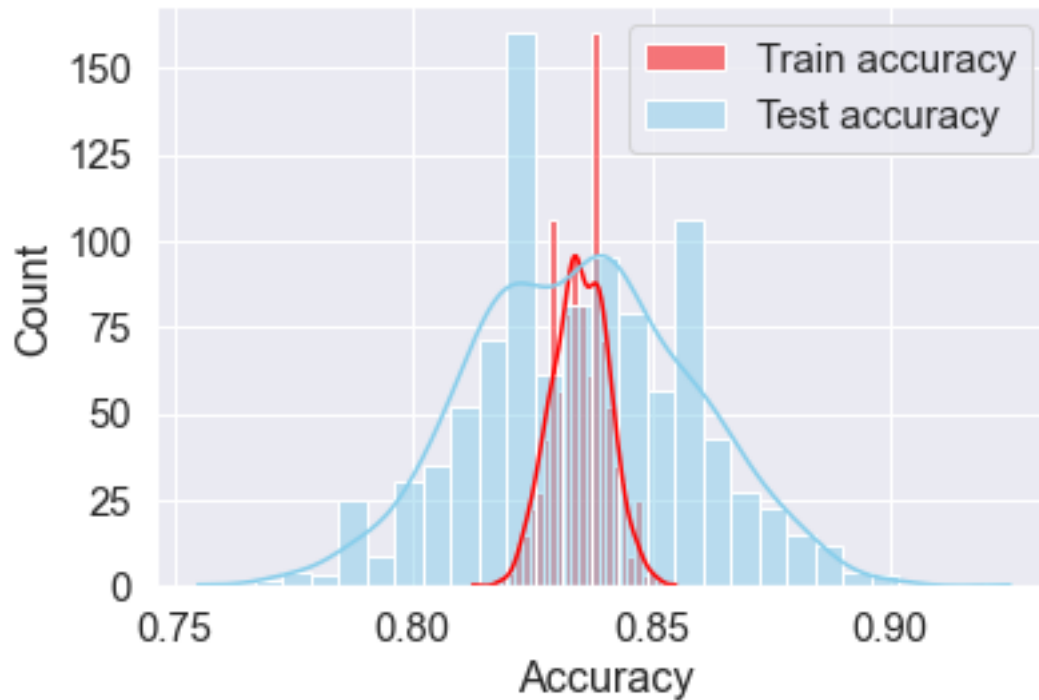
	train_y_stratified	test_y_stratified	train_y_CatPredictors_stratified	test_y_CatPredictors_stratified
count	999.000000	999.000000	9.990000e+02	9.990000e+02
mean	0.834962	0.835150	8.350000e-01	8.350000e-01
std	0.005833	0.023333	8.552999e-15	8.552999e-15
min	0.812500	0.755000	8.350000e-01	8.350000e-01
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 accuracy")
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="Train accuracy")
sns.histplot(data=accuracy_iter, x="test_y_CatPredictors_stratified", color="skyblue", label="Test accuracy")
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, Rep
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 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 template can be found [here](#)