Data Science III with python (Class notes)

STAT 303-3

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Preface

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

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

Part I

Sklearn; Bias & Variance; KNN

1 Introduction to scikit-learn

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

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

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

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

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

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

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

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

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

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

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

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

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

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

1.1 Splitting data into `train` and `test`

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

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

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

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

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

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

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

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

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

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

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

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

1.1.1 Stratified splitting

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

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

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

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

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

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

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

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

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

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

1.2 Scaling data

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

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

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\_logisti
STOP: TOTAL NO. of ITERATIONS REACHED LIMIT.

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

```
LogisticRegression()
```

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

Let us fit the model to the scaled data.

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

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

```
LogisticRegression()
```

The model converges to a solution with the scaled data!

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

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

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

1.4 Computing performance metrics

1.4.1 Accuracy

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

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

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

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

```
73.37662337662337
```

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

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

```
73.37662337662337
```

1.4.2 ROC-AUC

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

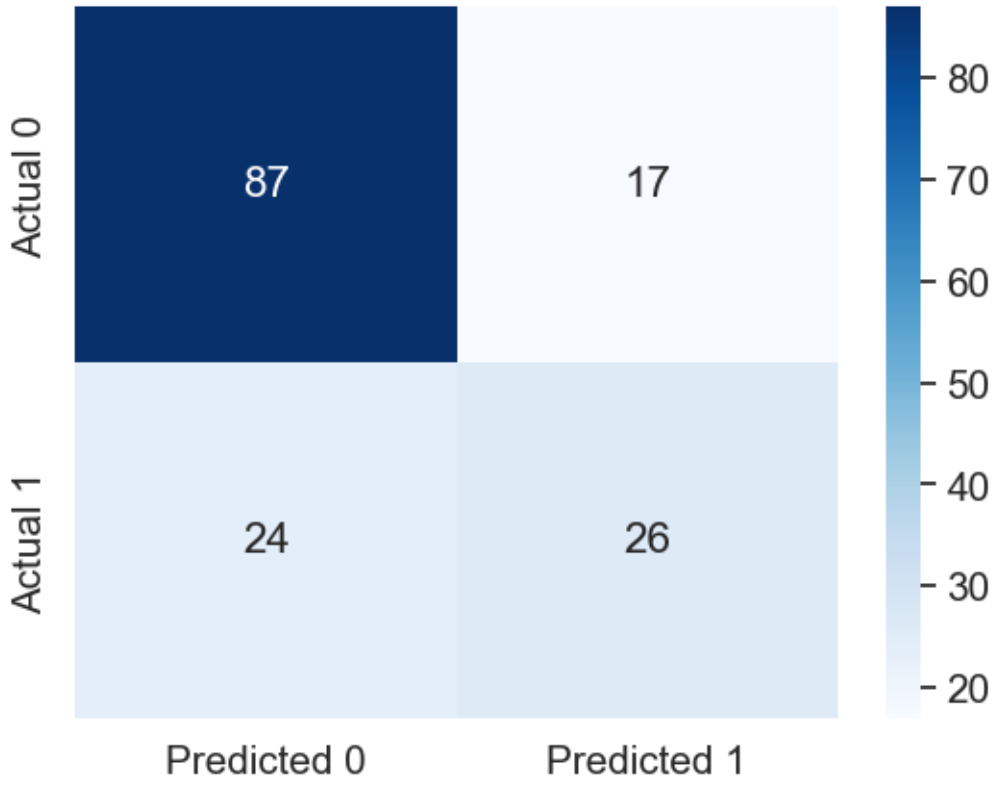
```
#Computing the predicted probability for the observation to belong to the positive class (y=
#The 2nd column in the output of predict_proba() consists of the probability of the observati
#belong to the positive class (y=1)
y_pred_prob = logreg.predict_proba(X_test_scaled)[:,1]

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

```
0.7923076923076922
```

1.4.3 Confusion matrix & precision-recall

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

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




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

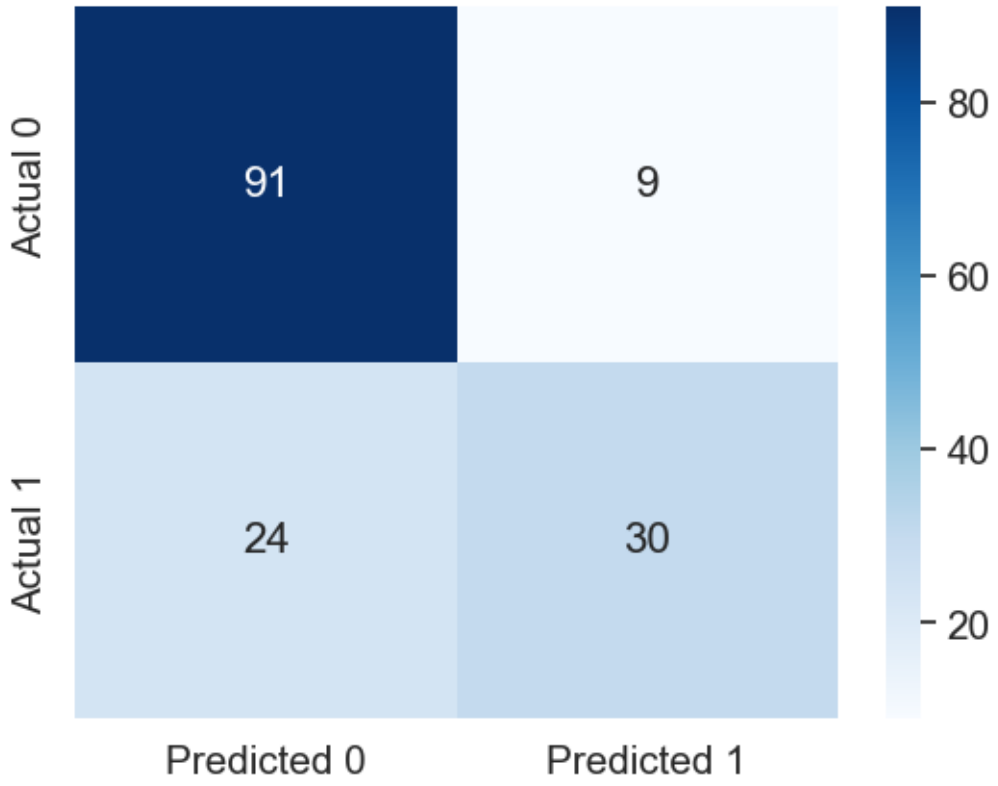
```
Precision:  0.6046511627906976
Recall:  0.52
```

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

```
# Developing the model with stratified splitting

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

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

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

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

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

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

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



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

1.5 Tuning the model hyperparameters

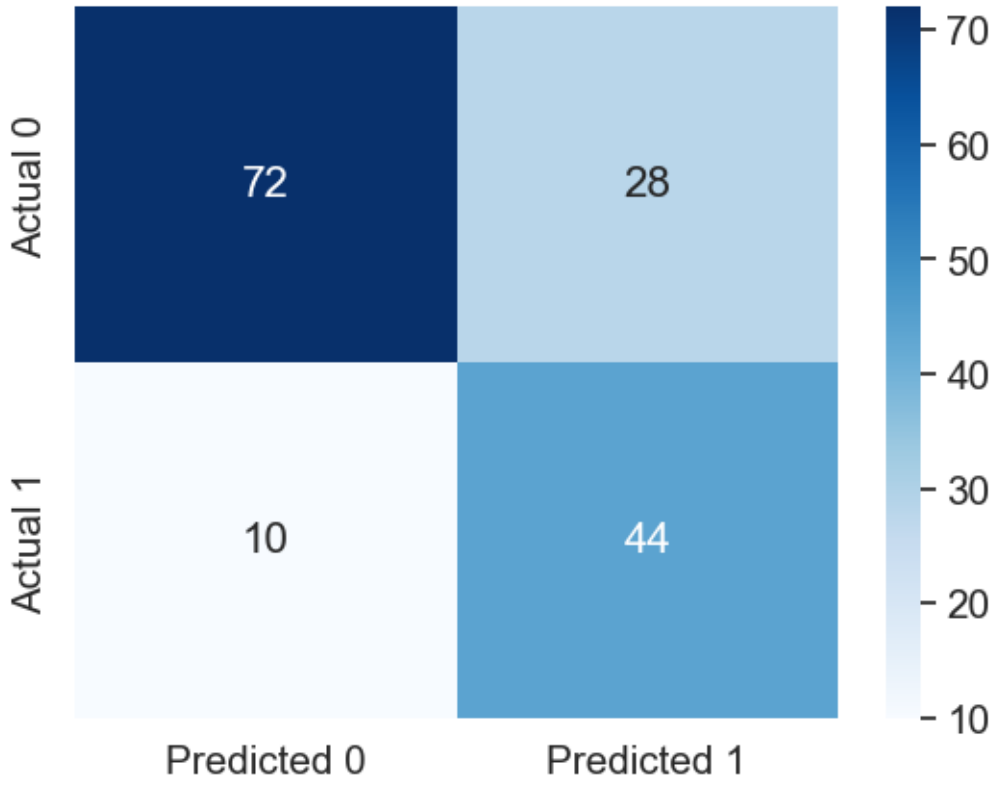
A hyperparameter (among others) that can be trained in a logistic regression model is the regularization parameter.

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

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

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

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

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

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

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

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

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



1.5.1 Tuning decision threshold probability

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

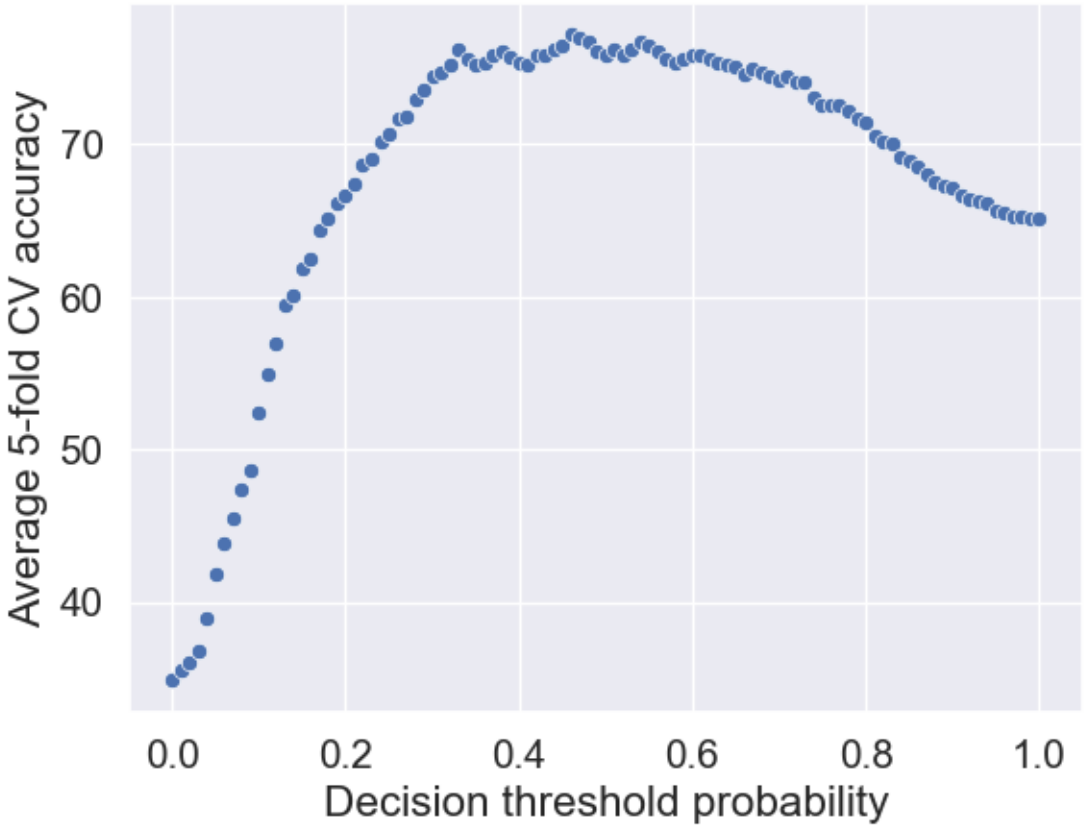
We'll use the `cross_val_predict()` function from the `model_selection` module of `sklearn` to compute the K-fold cross validated predicted probabilities. Note that this function simplifies the task of manually creating the K-folds, training the model K-times, and computing the predicted probabilities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

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

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

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

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

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

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



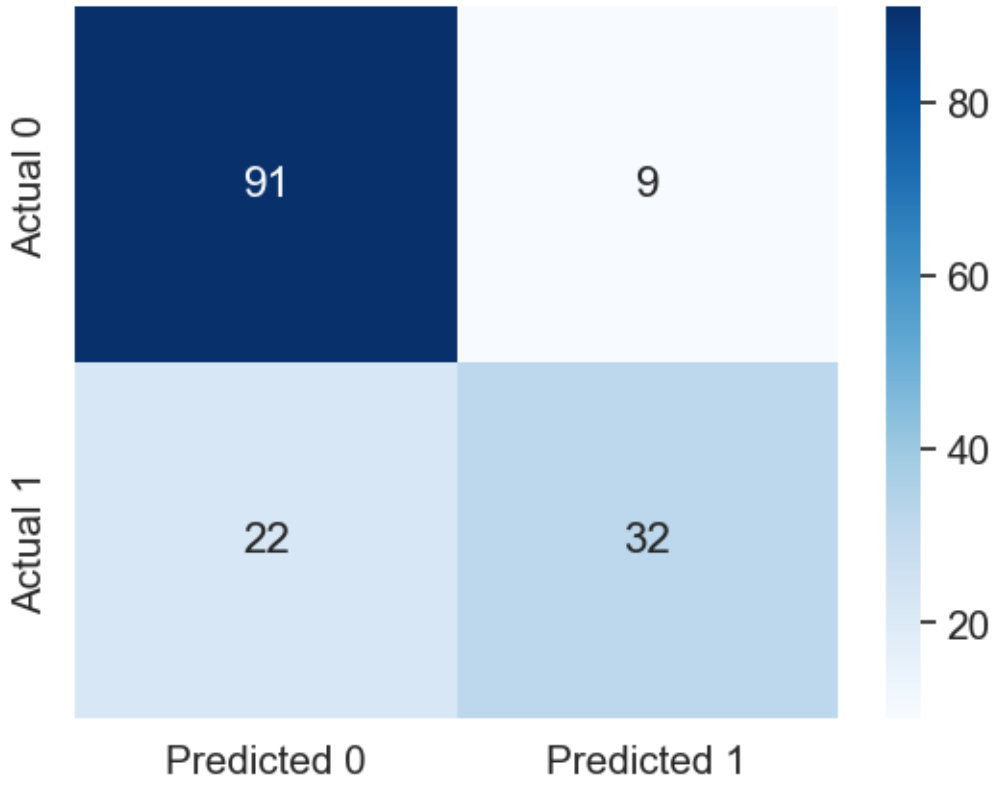
The optimal decision threshold probability is the one that maximizes the K-fold cross validation accuracy.

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

```
0.46
```

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

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

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

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

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

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

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



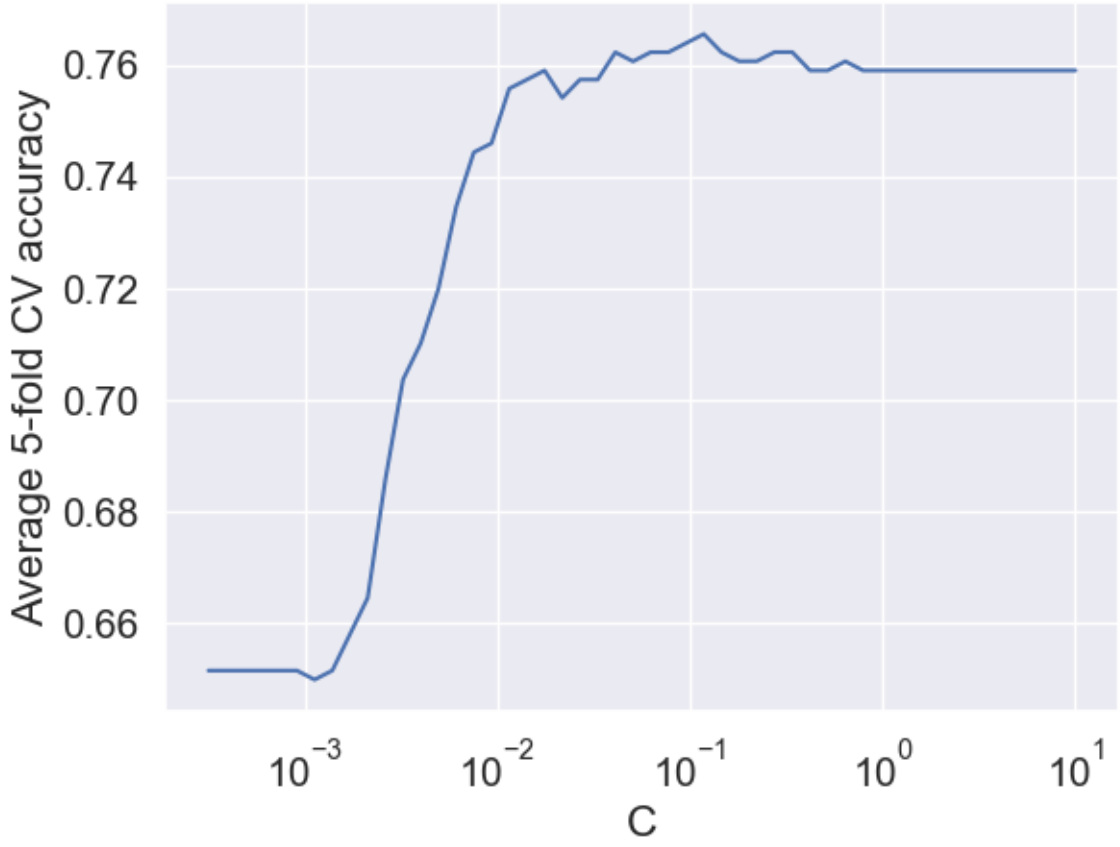
Model performance on test data has improved with the optimal decision threshold probability.

1.5.2 Tuning the regularization parameter

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

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

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

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

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



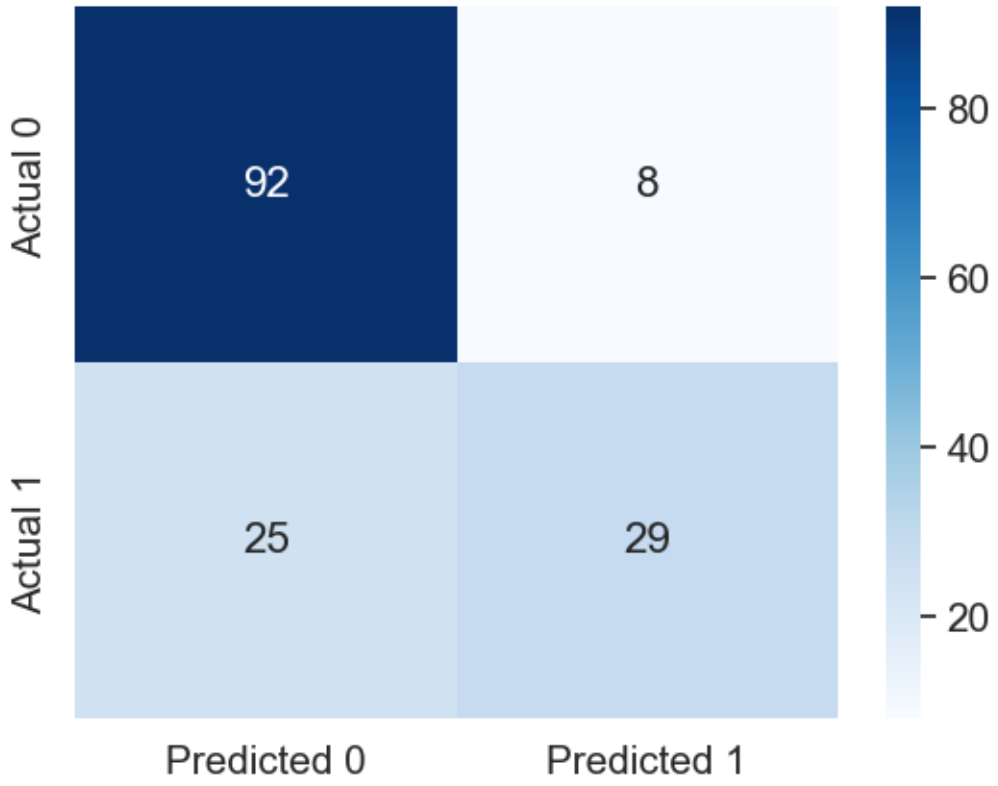

```
# Optimal value of the regularization parameter 'C'
optimal_C = hyperparam_vals[np.argmax(np.array(accuracy_iter).mean(axis=1))]
optimal_C
```

```
0.11787686347935879
```

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

#Scaling data
```

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

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

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

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

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

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

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



1.5.3 Tuning the decision threshold probability and the regularization parameter simultaneously

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

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

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

        #Computing the accuracy
```

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

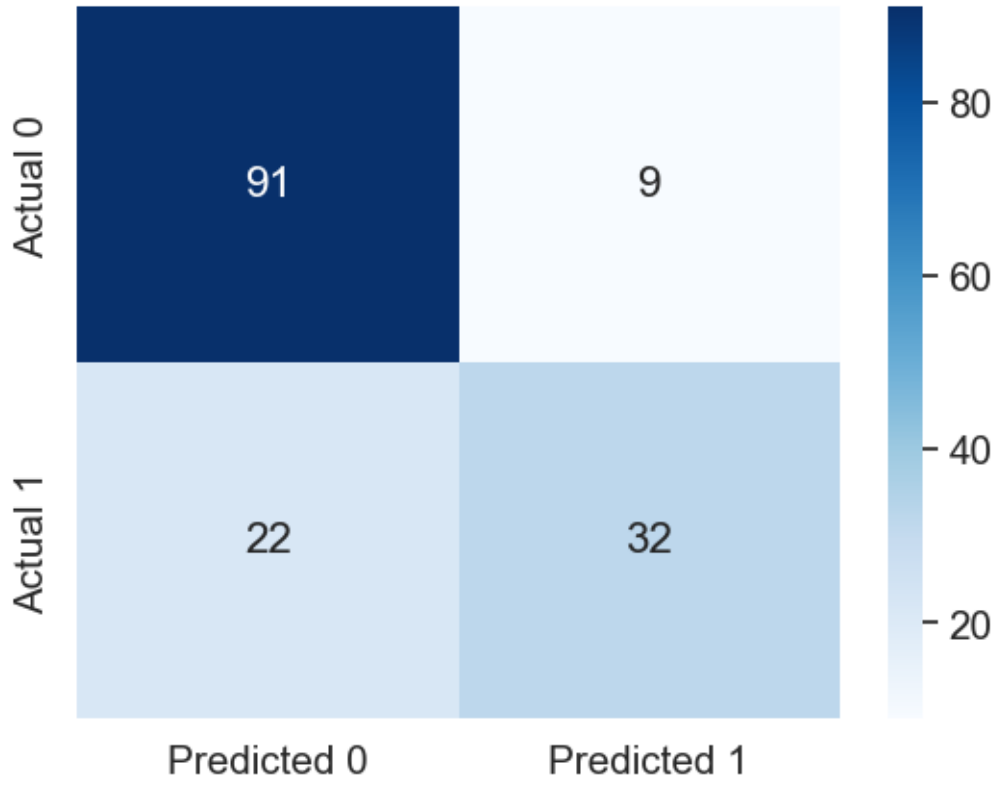
```
# Parameters for highest accuracy
optimal_C = accuracy_iter.sort_values(by = 'accuracy', ascending = False).iloc[0,:]['C']
optimal_threshold = accuracy_iter.sort_values(by = 'accuracy', ascending = False).iloc[0, :]

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

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

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

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

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

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

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

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

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

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

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

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

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



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

2 Bias-variance tradeoff

Read section 2.2.2 of the book before using these notes.

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

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

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

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

2.1 Simple model (Less flexible)

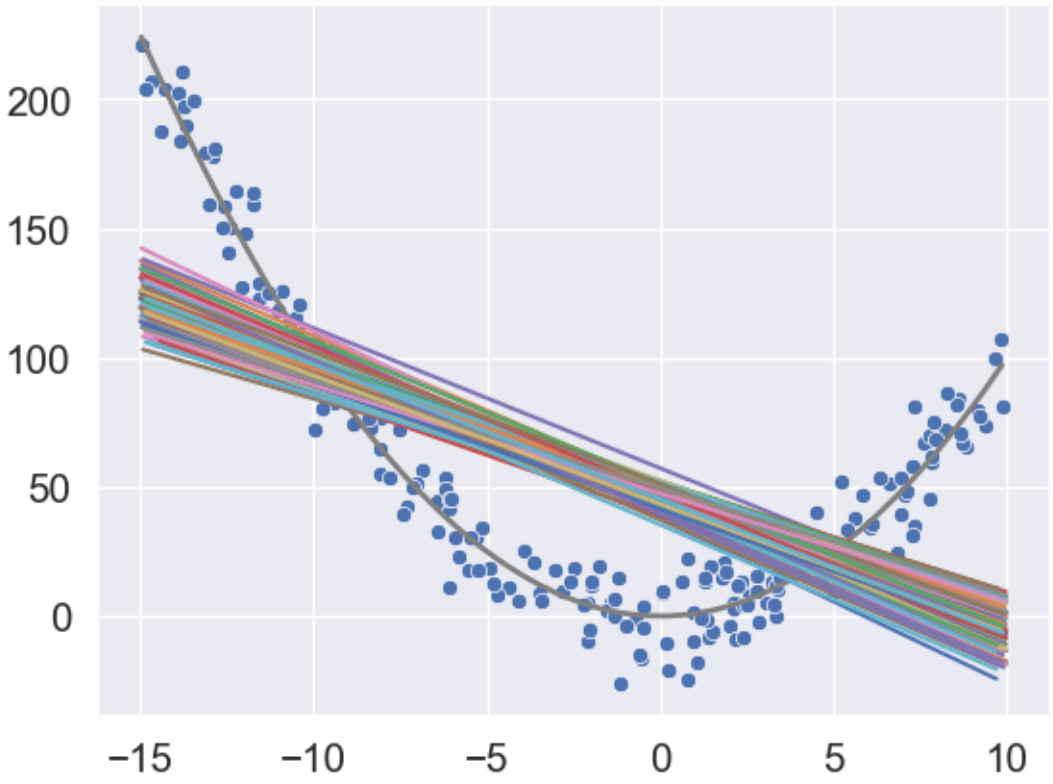
Let us consider a linear regression model as the less-flexible *(or relatively simple)* model.

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

```
np.random.seed(101)

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

```
2042.104126728109
```

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

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

```
28.37397844429763
```

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

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

```
2201.957555529835
```

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

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

```
sq_bias + mean_var + 100
```

```
2170.4781051724067
```

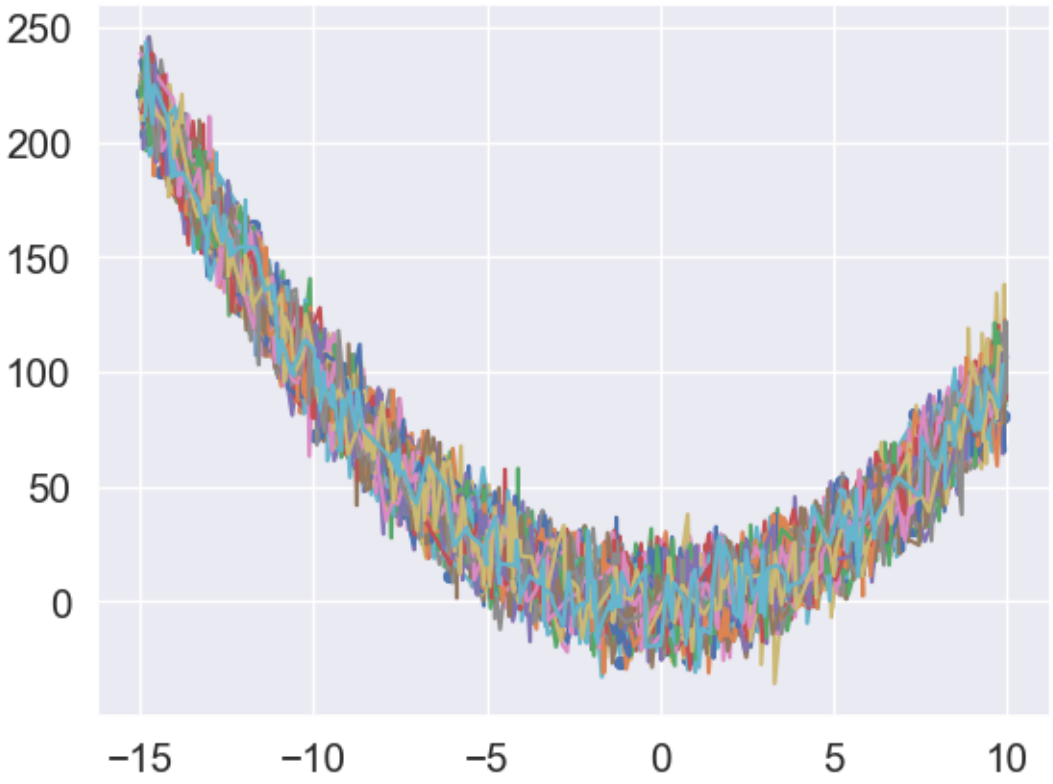
Note that this is approximately, but not exactly, the same as the mean squared error computed above as we are developing a finite number of models, and making predictions on a finite number of test data points.

2.2 Complex model (more flexible)

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

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

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



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

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

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

```
1.3117561629333938
```

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

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

```
102.5226748977198
```

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

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

```
225.92027460924726
```

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

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

3 KNN

Read section 4.7.6 of the book before using these notes.

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

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

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

3.1 KNN for regression

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

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

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

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

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

Let us scale data as we are using KNN.

3.1.1 Scaling data

```
# Scale
sc = StandardScaler()

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

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

3.1.2 Fitting and validating model

```
knn_model = KNeighborsRegressor()

knn_model.fit(X_train_scaled, (y_train))

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

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

```
6329.691192885354
```

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

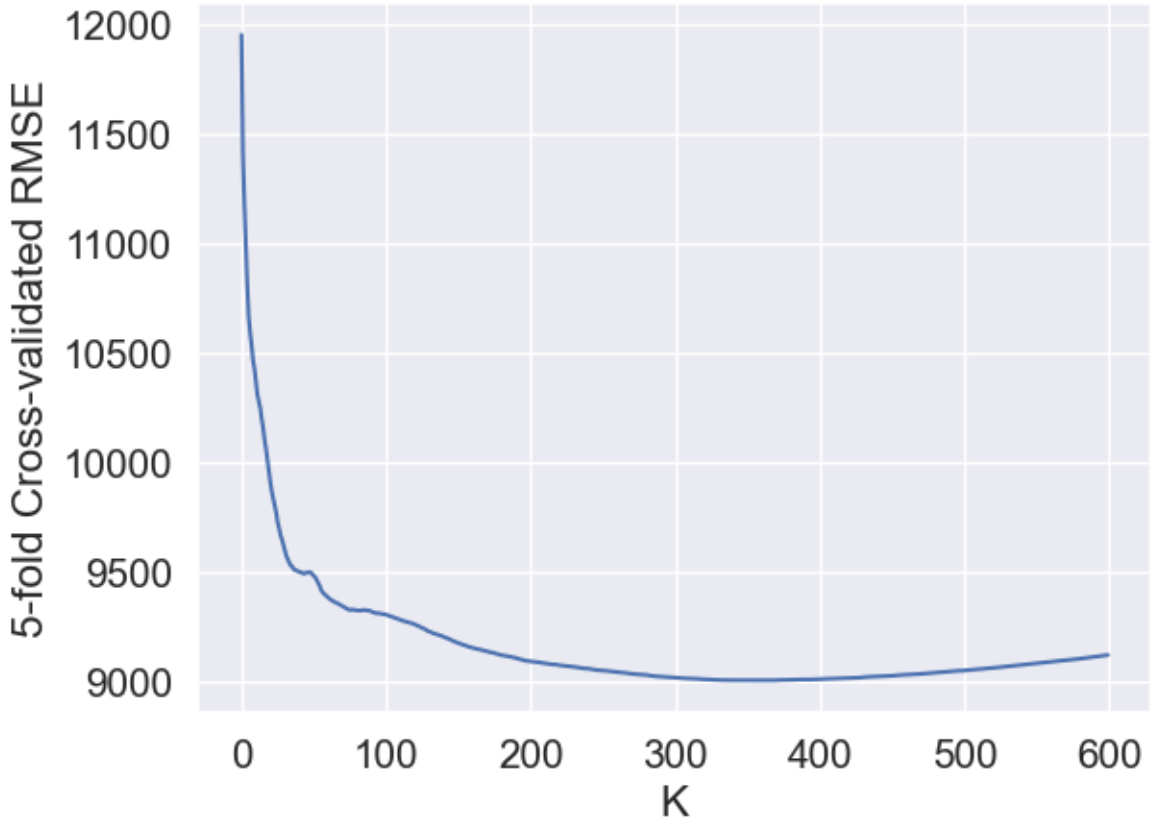
```
Ks = np.arange(1,601)

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.

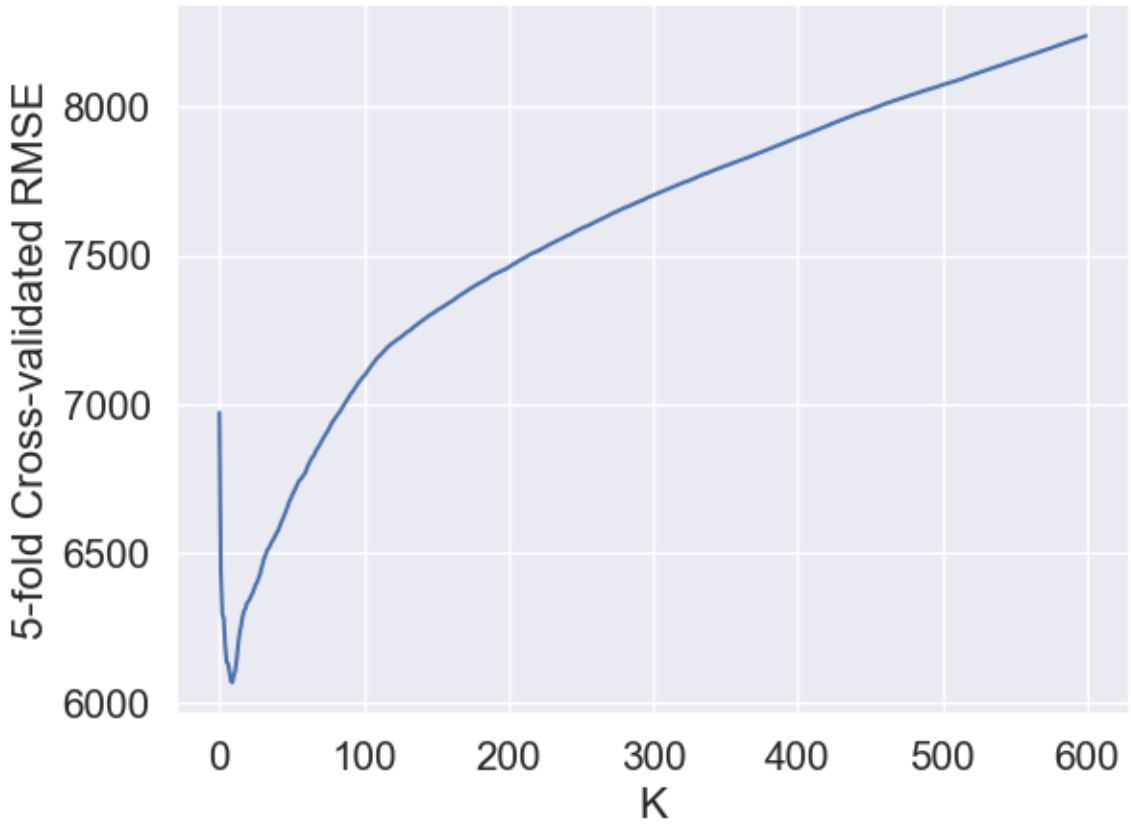
3.1.3.1 `KFold()`

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

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

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

cv_scores = []

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

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



The optimal K is:

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

```
10
```

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

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

```
6043.889393238132
```

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

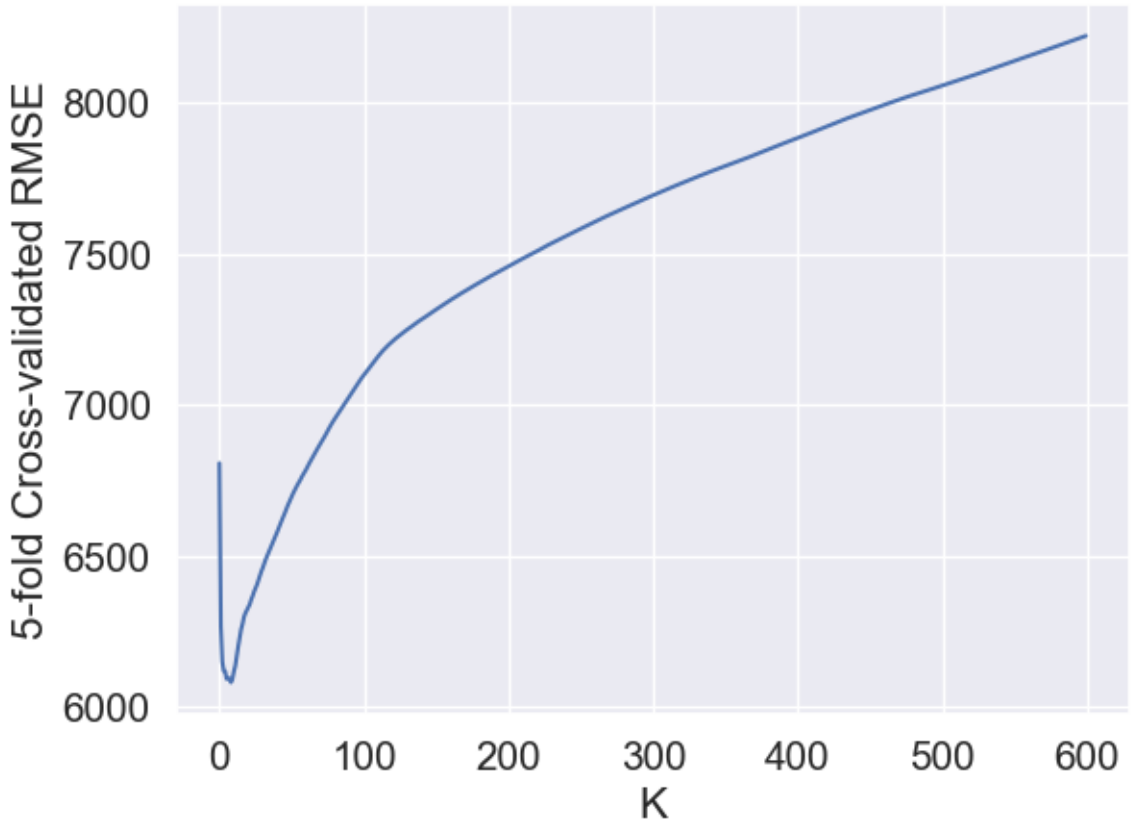
The function `RepeatedKFold()` repeats k-fold cross validation multiple times *(10 times by default)*. Let us use it to have a more robust optimal value of the number of neighbors K.

3.1.3.2 `RepeatedKFold()`

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

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

cv_scores = []

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

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



The optimal K is:

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

```
9
```

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

```
knn_model2 = KNeighborsRegressor(n_neighbors = 9, weights='distance') # Default weights is 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 gr
grid = {'n_neighbors': np.arange(5, 151, 5), 'weights':['uniform', 'distance'],
        'metric': ['manhattan', 'euclidean', 'chebyshev']}
# 3) Create the Kfold object (Using RepeatedKFold will be more robust, but more expensive, us
# have the budget)
```

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

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

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

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

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

The optimal estimator based on cross-validation is:

```
gcv.best_estimator_
```

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

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

```
gcv.best_params_
```

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

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

```
-gcv.best_score_
```

```
5740.928686723918
```

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

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

```
5747.466851437544
```

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

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

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

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

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

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

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

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

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

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

```
5800.418957612656
```

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

```
5722.4859230146685
```

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

4.2 RandomizedSearchCV()

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

```
# RandomizedSearchCV works in three steps:

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

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


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

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

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

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

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

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

```
gcv.best_params_
```

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

```
gcv.best_score_
```

```
-6239.171627183809
```

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

```
6176.533397589911
```

Note that in this example, `RandomizedSearchCV()` helps search for optimal values of the hyperparameter p over a continuous domain space. In this dataset, $p = 1$ seems to be the optimal value. However, if the optimal value was somewhere in the middle of a larger

continuous domain space *(instead of the boundary of the domain space)*, and there were several other hyperparameters, some of which were not influencing the response *(effect sparsity)*, `RandomizedSearchCV()` is likely to be more effective in estimating the optimal value of the continuous hyperparameter.

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

1. `RandomizedSearchCV()` fixes the computational cost in case of large number of hyperparameters / large number of levels of individual hyperparameters. If there are n hyper parameters, each with 3 levels, the number of all possible hyperparameter values will be 3^n. The computational cost increase exponentially with increase in number of hyperparameters.
2. In case of a hyperparameter having continuous values, the distribution of the hyperparameter can be specified in `RandomizedSearchCV()`.
3. In case of effect sparsity of hyperparameters, i.e., if only a few hyperparameters significantly effect prediction accuracy, `RandomizedSearchCV()` is likely to consider more unique values of the influential hyperparameters as compared to `GridSearchCV()`, and is thus likely to provide more optimal hyperparameter values as compared to `GridSearchCV()`. The figure below shows effect sparsity where there are 2 hyperparameters, but only one of them is associated with the cross-validated score, Here, it is more likely that the optimal cross-validated score will be obtained by `RandomizedSearchCV()`, as it is evaluating the model on 9 unique values of the relevant hyperparameter, instead of just 3.

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

4.3 BayesSearchCV()

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

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

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

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

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

```
# BayesSearchCV works in three steps:

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

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

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

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

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

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

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

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

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

```
gcv.best_params_
```

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

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

```
-gcv.best_score_
```

```
5756.172382596493
```

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

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

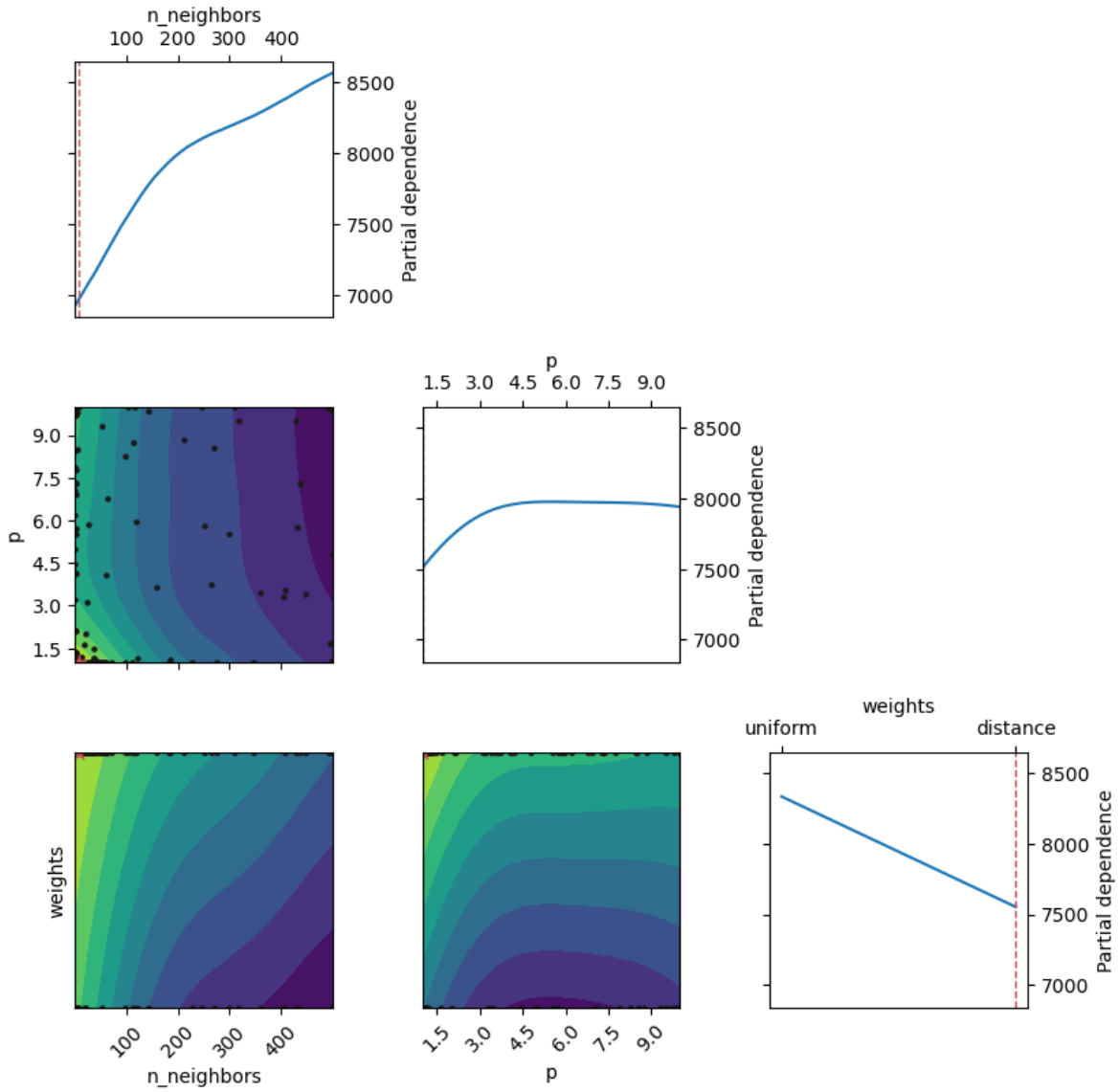
```
5740.432278861367
```

4.3.1 Diagonosis of cross-validated score optimization

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

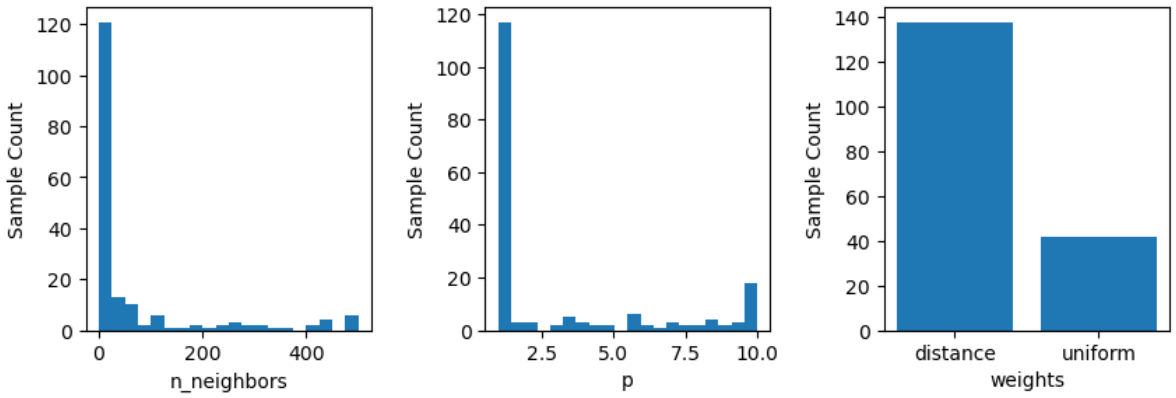
Check the `plot_objective()` documentation to interpret the plots.

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



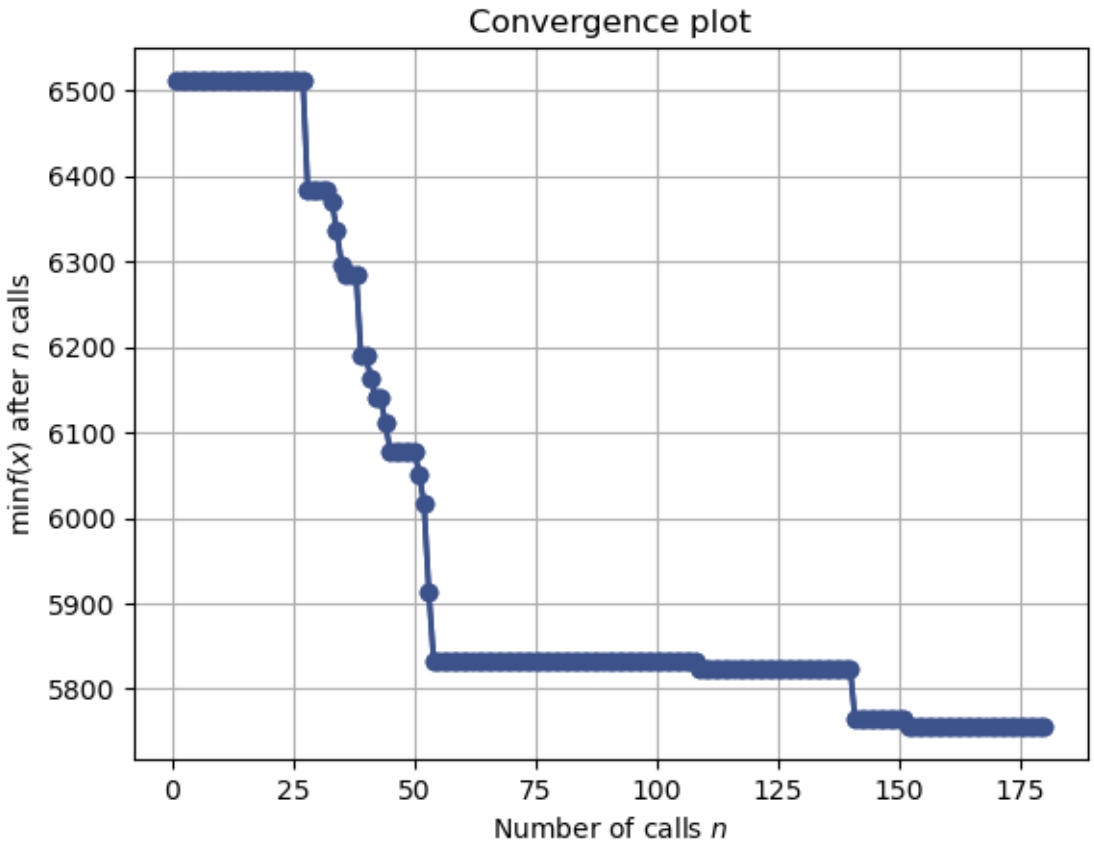
The frequence of individual hyperparameter values considered can also be visualized as below.

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



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

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



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

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

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

```
5831.87280274334
```

The hyperparameter values at the 53rd iterations are:

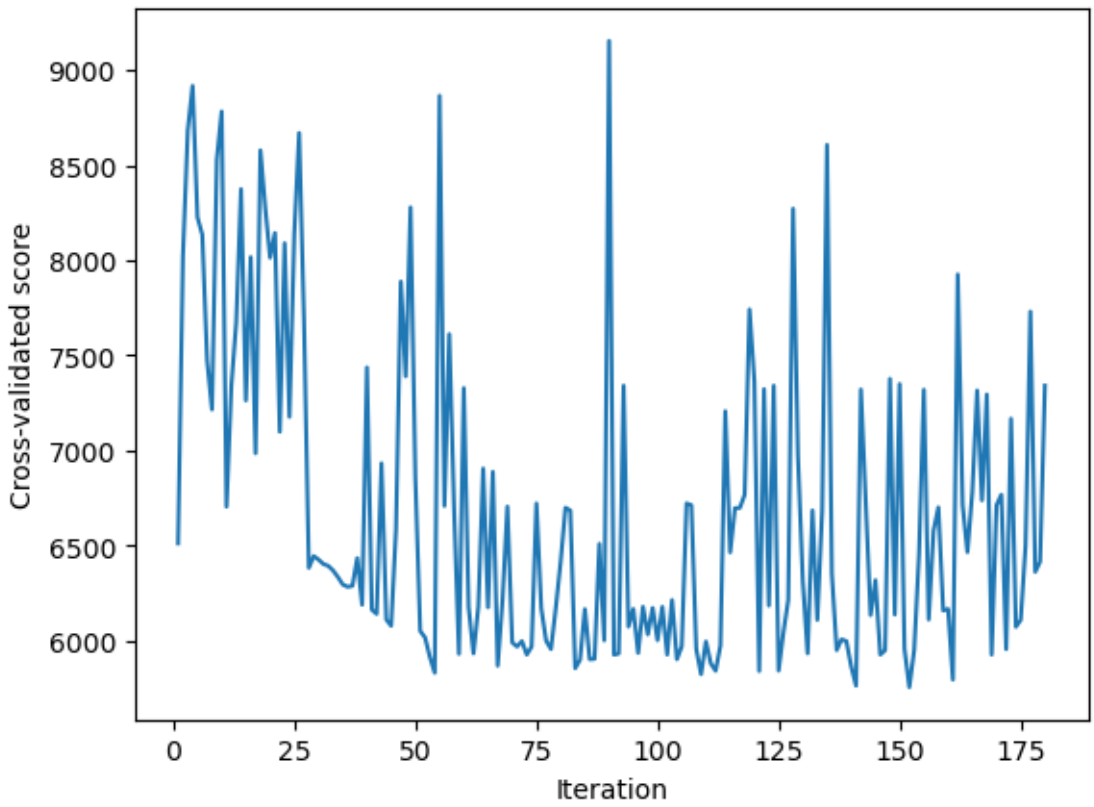
```
gcv.optimizer_results_[0]['x_iters'][53]
```

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

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

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

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



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

1. The Bayesian Optimization approach gives the benefit that we can give a much larger range of possible values, since over time we identify and exploit the most promising regions and discard the not so promising ones. Plain grid-search would burn computational resources to explore all regions of the domain space with the same granularity, even the not promising ones. Since we search much more effectively in Bayesian search, we can search over a larger domain space.
2. BayesSearch CV may help us identify the optimal hyperparameter value in fewer iterations if the Gaussian process model estimating the cross-validated score is relatively accurate. However, this is not certain. Grid and random search are completely uninformed by past evaluations, and as a result, often spend a significant amount of time evaluating "bad" hyperparameters.
3. BayesSearch CV is more reliable in cases of a large search space, where random selection may miss sampling values from optimal regions of the search space.

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

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

4.3.2 Live monitoring of cross-validated score

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

```
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(optim_result['x_iters'][min_ind], pd.Series(optim_result['func_vals']).min())
    sns.lineplot(cv_values)
    plt.show()
```

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

4.4 `cross_validate()`

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

When can we use one over the other?

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

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

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

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

Let us pre-process the data.

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

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

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

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

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

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

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

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

scores = []

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

```
scores

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

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

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

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


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

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

The optimal 'K' will be:

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

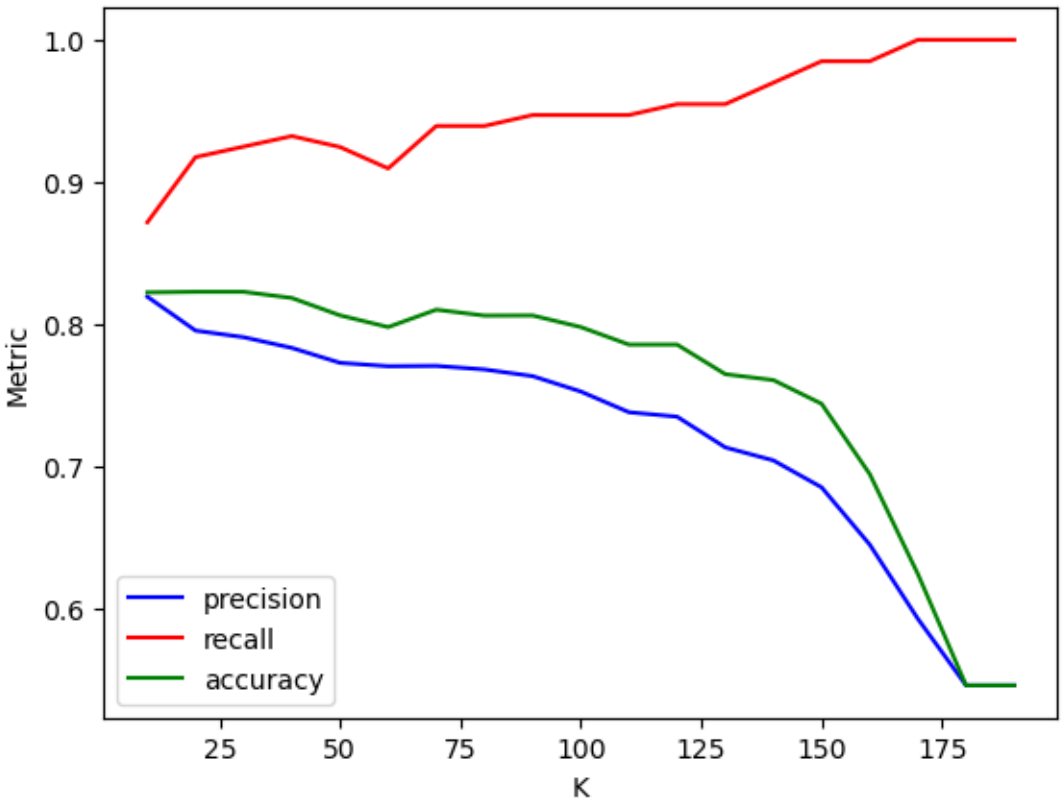
```
120
```

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

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

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

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



Part II

Tree based models

5 Regression trees

Read section 8.1.1 of the book before using these notes.

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

```
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.metrics import mean_squared_error
from sklearn.model_selection import cross_val_score,train_test_split
from sklearn.metrics import mean_squared_error,r2_score
from sklearn.model_selection import KFold
from sklearn.tree import DecisionTreeRegressor
from sklearn.model_selection import GridSearchCV, ParameterGrid

#Libraries for visualizing trees
from sklearn.tree import export_graphviz
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

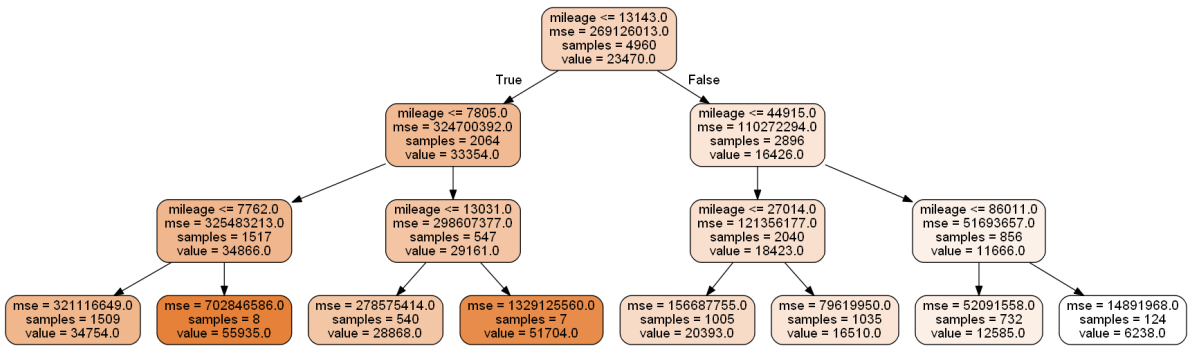
Develop a regression tree to predict car price based on mileage

```
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())
```

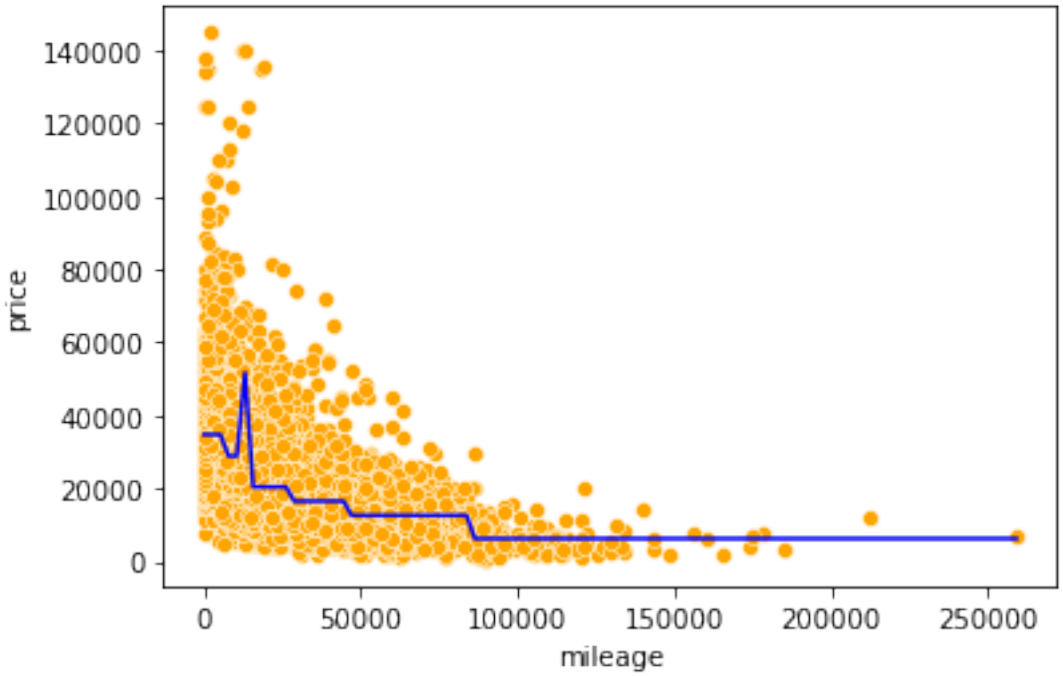


```
#prediction on test data
pred=model.predict(test[['mileage']])
```

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

```
13764.798425410803
```

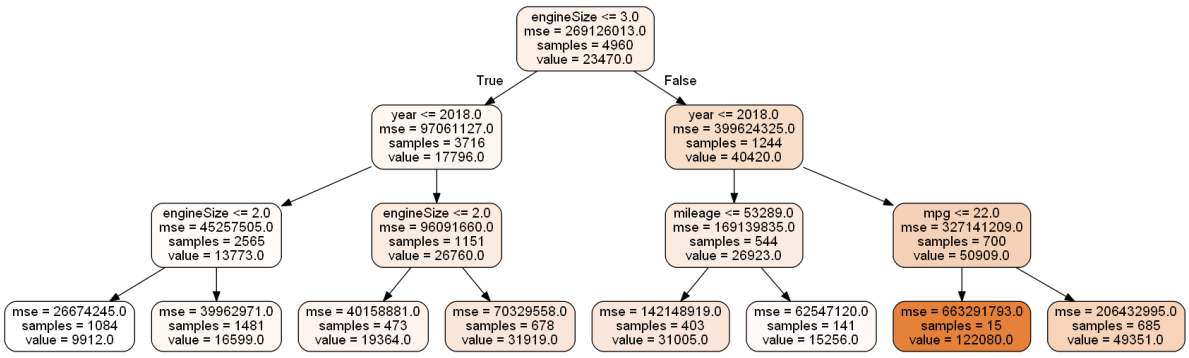
```
#Visualizing the model fit
Xtest = np.linspace(min(X), max(X), 100)
pred_test = model.predict(Xtest.reshape(-1,1))
sns.scatterplot(x = 'mileage', y = 'price', data = train, color = 'orange')
sns.lineplot(x = Xtest, y = pred_test, color = 'blue')
```



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())
```



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 the mean squared error, 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_mean_squared_error', 'r2'], refit = 'neg_mean_squared_erro
model.fit(X, y)
print (model.best_score_, model.best_params_)
```

```
Fitting 5 folds for each of 490 candidates, totalling 2450 fits
-42064467.15261547 {'max_depth': 11, 'max_leaf_nodes': 302}
```

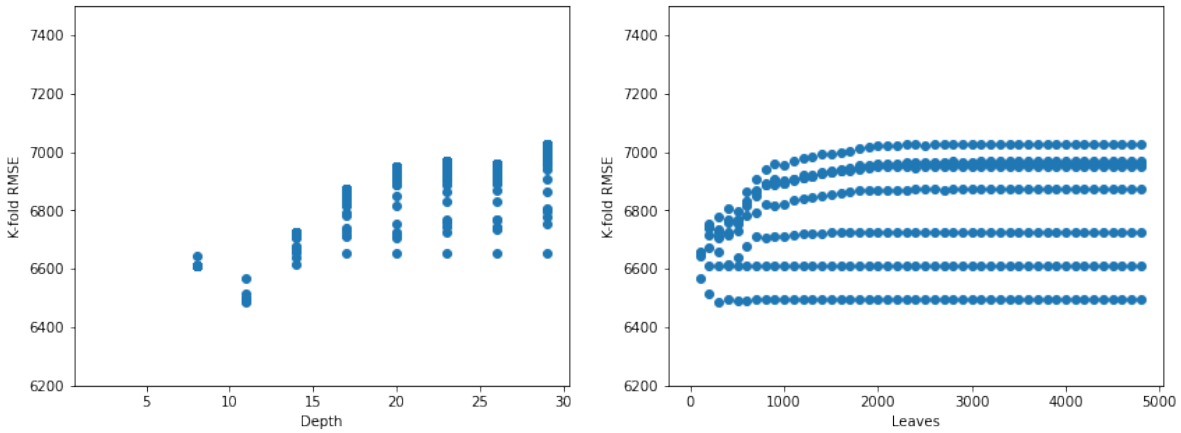
Note that as the `GridSearchCV` function maximizes the performance metric to find the optimal hyperparameters, we are maximizing the negative mean squared error

(`neg_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()
```

```
fig, axes = plt.subplots(1,2,figsize=(14,5))
plt.subplots_adjust(wspace=0.2)
axes[0].plot(cv_results.param_max_depth, np.sqrt(-cv_results.mean_test_neg_mean_squared_erro
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, np.sqrt(-cv_results.mean_test_neg_mean_squared_
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,
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
0.8465176078797111 {'max_depth': 10, 'max_leaf_nodes': 262}
Time taken = 1 minutes
```

From the above cross-validation, the optimal hyperparameter values are `max_depth = 10` and `max_leaf_nodes = 262`.

```
#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 and spline regression models (including MARS), with these four predictors. This may be probably due to car price having a highly non-linear association with the predictors.

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

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

Why?

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

```
model.feature_importances_
```

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

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

5.3 Cost complexity pruning

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

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

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

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

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

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

```
len(alphas)
```

```
4126
```

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

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

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

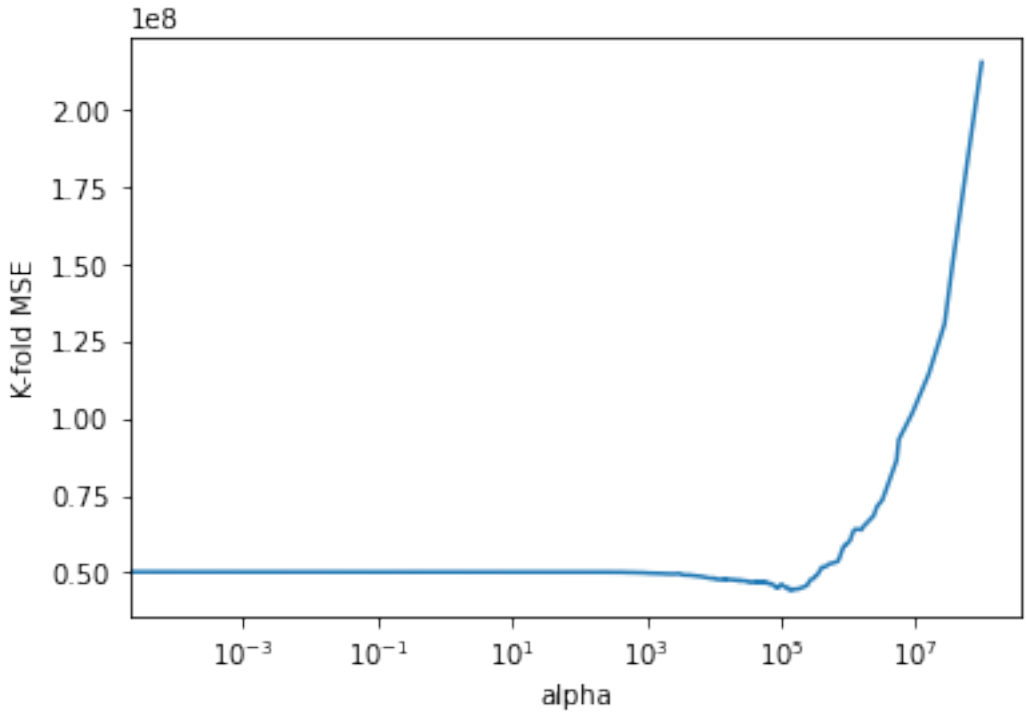
```
model = DecisionTreeRegressor(ccp_alpha=143722.94076639024,random_state=1)
model.fit(X, y)
pred = model.predict(Xtest)
np.sqrt(mean_squared_error(test.price, pred))
```

```
7306.592294294368
```

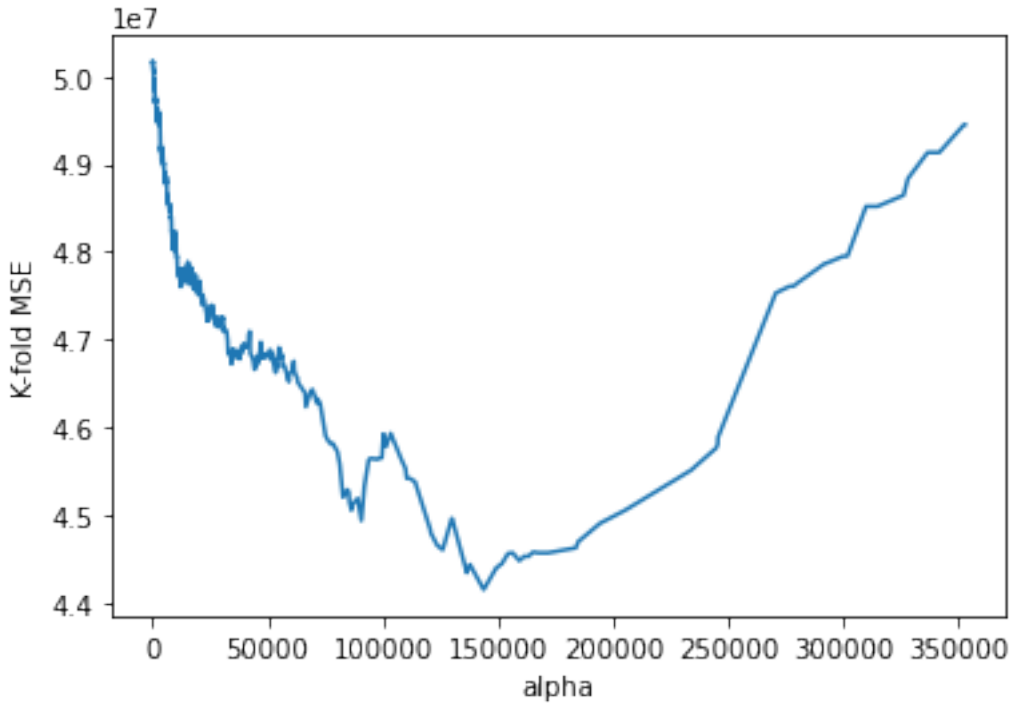
The RMSE for the decision tree with cost complexity pruning is lower than that of linear regression models and spline regression models (including MARS), with these four predictors. However, it is higher than the one obtained with tuning tree parameters using grid search (shown previously). Cost complexity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

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

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




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



5.3.1 Depth vs alpha; Node counts vs alpha

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

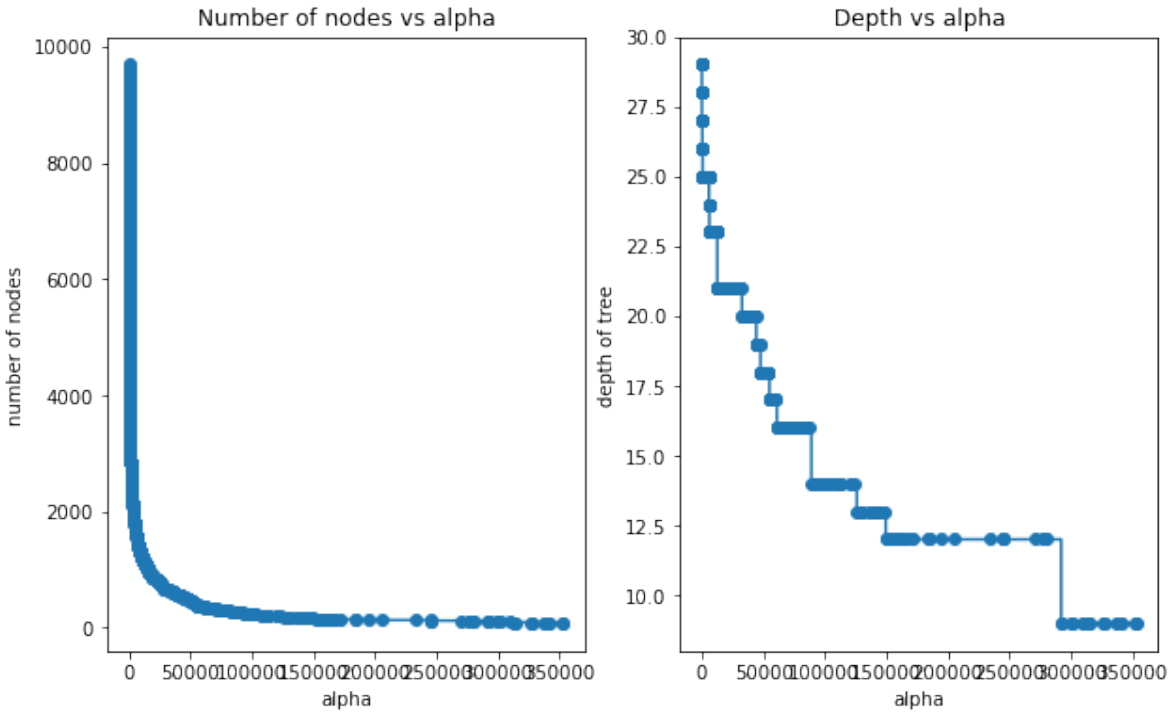
```
268.10325384140015
```

This code takes 4.5 minutes to run

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

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

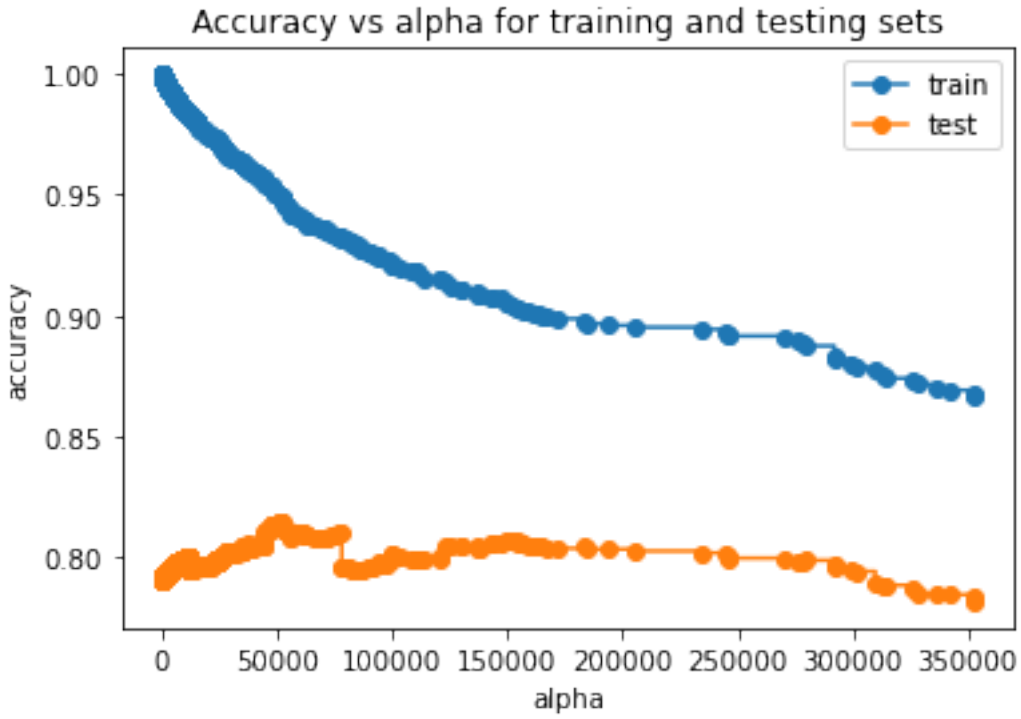
```
Text(0.5, 1.0, 'Depth vs alpha')
```



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-pos
ax.plot(alphas[0:4093], test_scores[0:4093], marker="o", label="test", drawstyle="steps-post"
ax.legend()
plt.show()
```



6 Classification trees

Read section 8.1.2 of the book before using these notes.

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

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

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

import time as time
```

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

```
test.head()
```

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

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

6.1 Building a classification tree

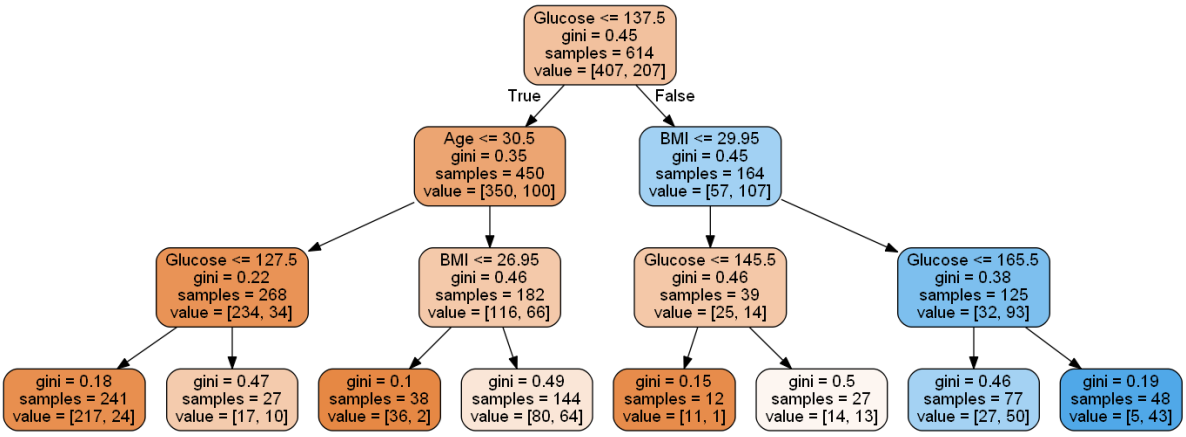
Develop a classification tree to predict if a person has diabetes.

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

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

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

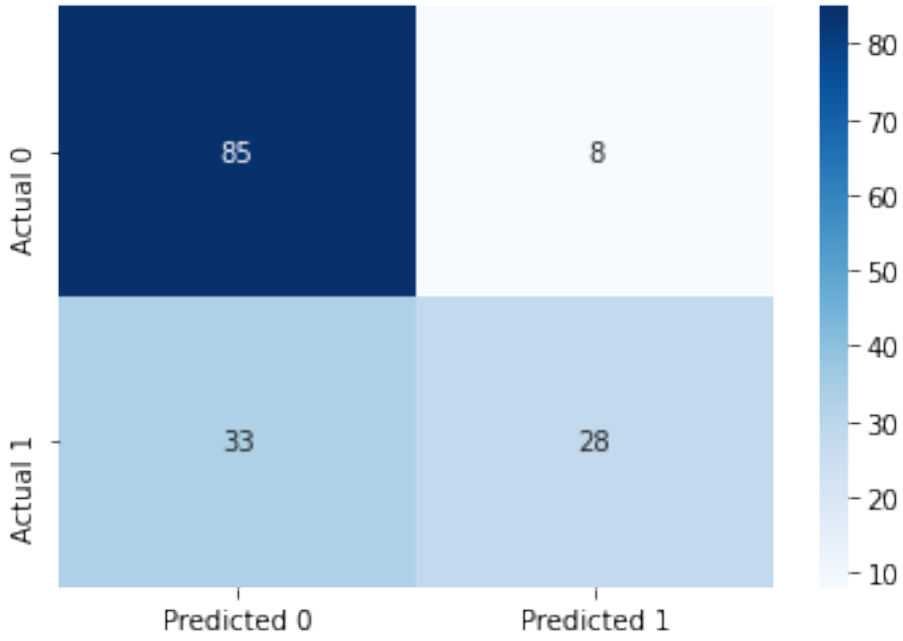
```
DecisionTreeClassifier(max_depth=3, random_state=1)
```

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




```
# Performance metrics computation

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

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

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

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

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



6.2 Optimizing hyperparameters to optimize performance

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

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

Find the maximum values of depth and number of leaves.

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

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

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

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

```
118
```

```
# 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.

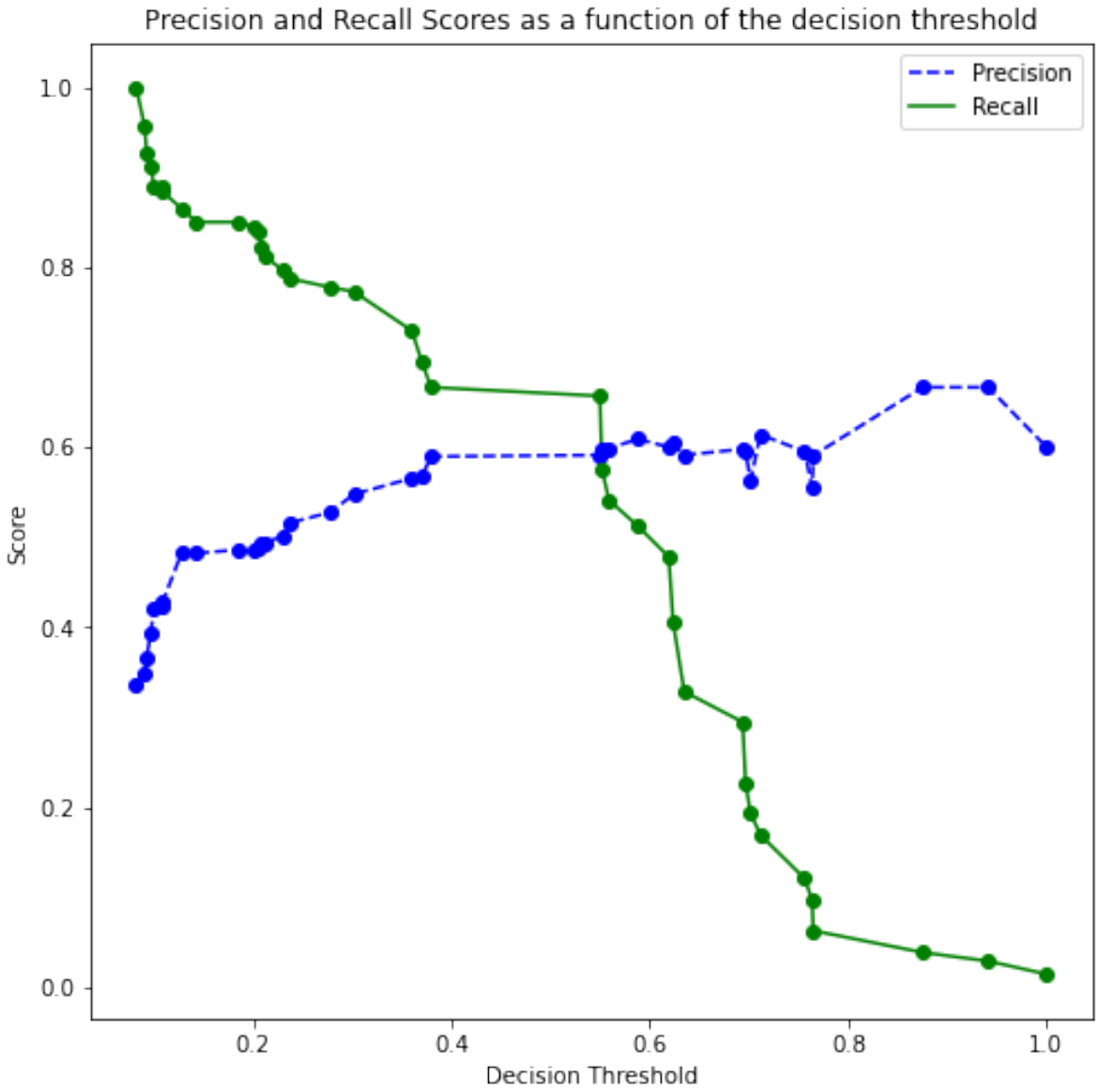
As the recall will always be 100% for a decision threshold probability of zero, we'll find a decision threshold probability that balances recall with another performance metric such as precision, false positive rate, accuracy, etc. Below are a couple of examples that show we can balance recall with (1) 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 usi
# predicted probabilities on train data, as the model may be overfitting on the train data, a
# may lead to misleading results
cross_val_ypred = cross_val_predict(DecisionTreeClassifier(random_state=1, max_depth = 4,
                                                           max_leaf_nodes=8, max_features=2), X
                                                    y, cv = 5, method = 'predict_proba')

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

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




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

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

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

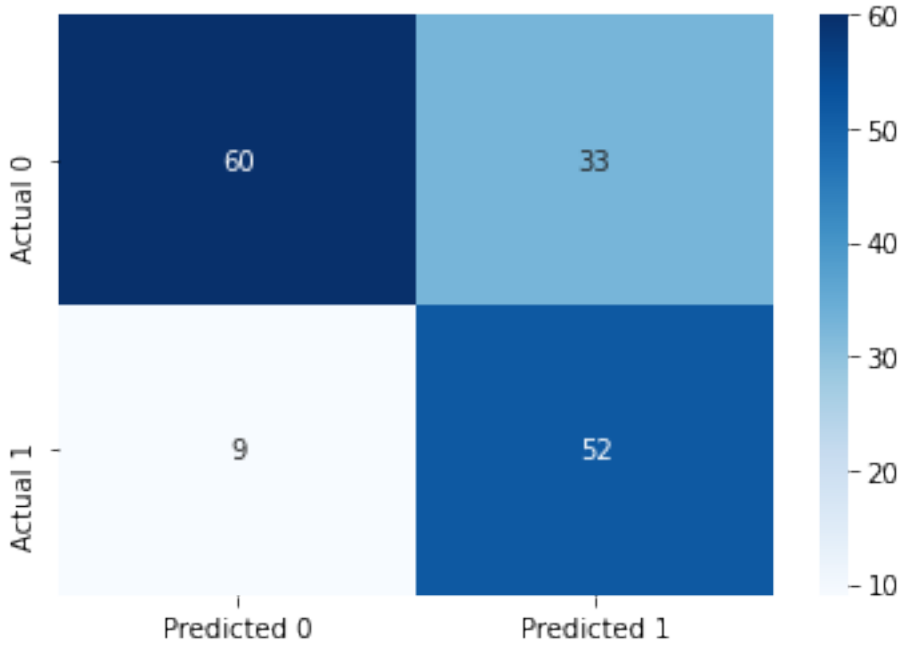
Suppose, we wish to have at least 80% recall, with the highest possible precision. Then, based on the precision-recall curve *(or the table above)*, we should have a decision threshold probability of 0.21.

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

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

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

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

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

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

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

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

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



6.3.2 Balancing recall with false positive rate

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

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

```
#Grid search to optimize parameter values

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

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

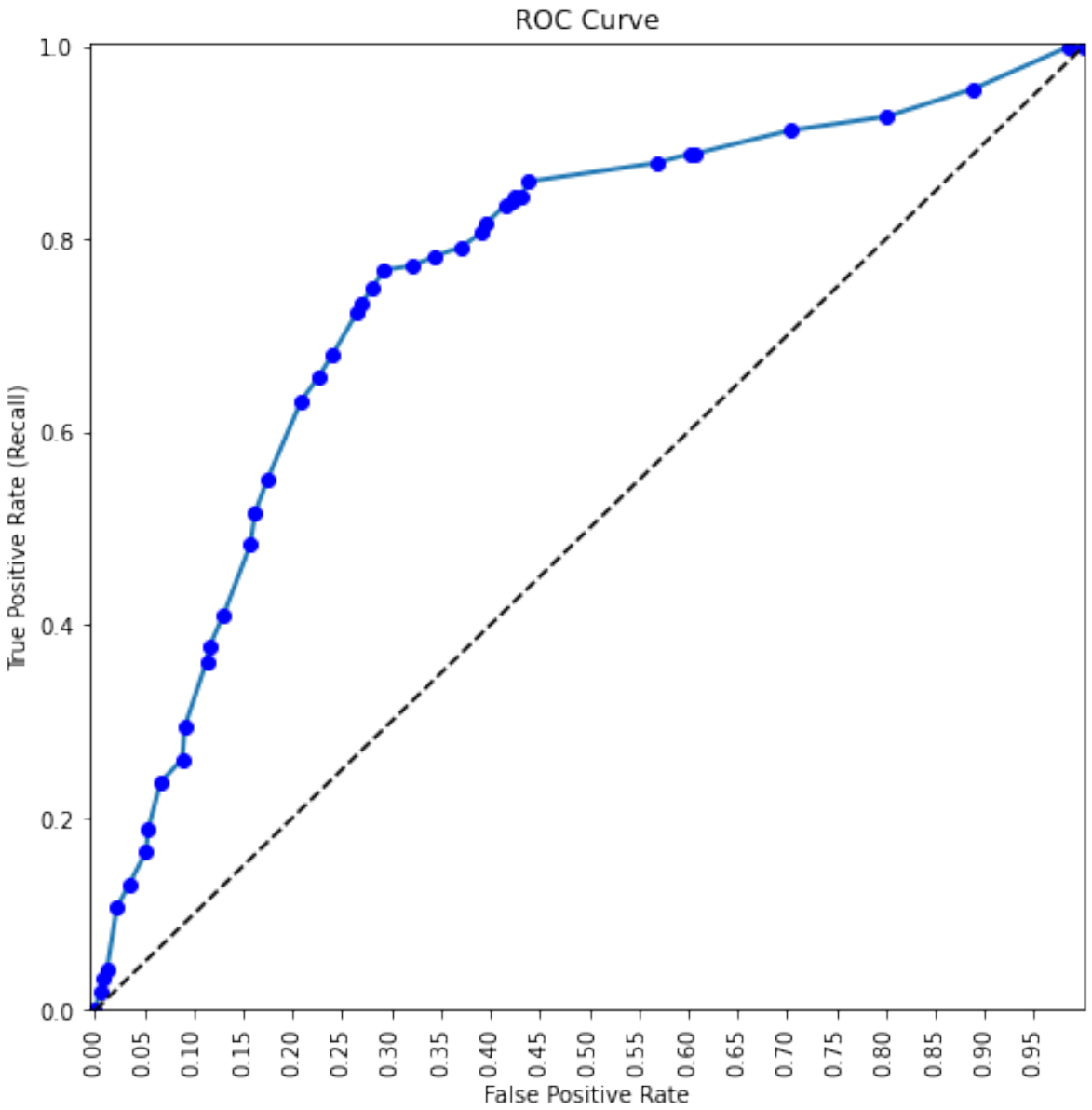
```
# make the predictions
y_pred = grid_search.predict(Xtest)

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

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

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

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

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

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

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

```
0.7605075431162388
```




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

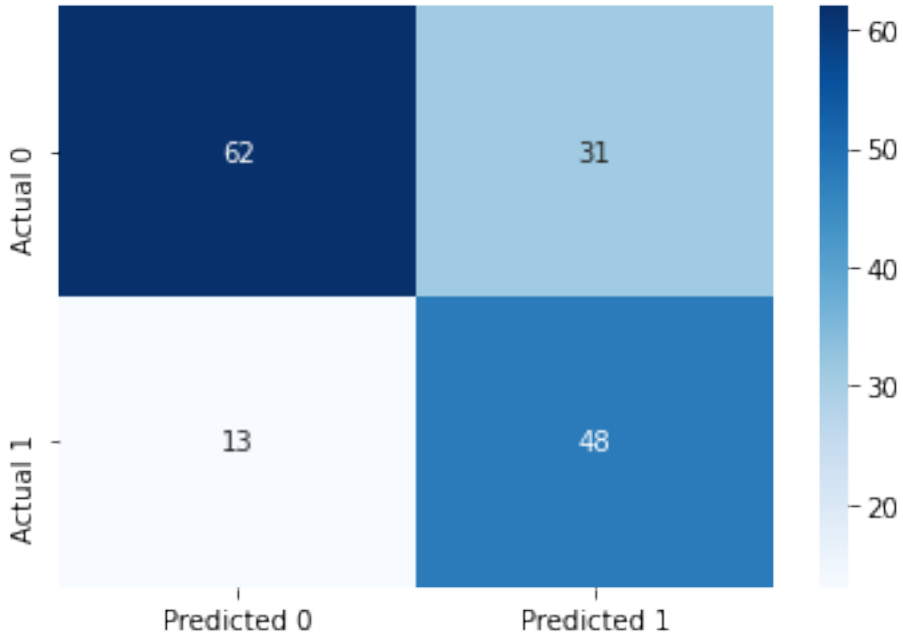
```
array([0.21276596, 0.80676329, 0.39066339])
```

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

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

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

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

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

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

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

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

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

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



6.4 Cost complexity pruning

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

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

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

58

```
#Grid search to optimize parameter values

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

```
# 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.

Part III

Assignments

7 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)**

7.1 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.

7.1.1 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
```

7.1.2 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.

7.1.3 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)**

7.1.4 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.

7.1.5 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)**

7.1.6 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)**

7.2 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.

7.2.1 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)**

7.2.2 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)**

7.2.3 c)

Repeat 1c and 1d with Ridge regularization. **Exclude the degrees you found in 2b and also degree 7**. Use Leave-One-Out (LOO) cross-validation (CV) to tune the model hyperparameter and use `neg_root_mean_squared_error` as the scoring metric. **(7 points)**

Consider hyperparamter values in the range [1, 100].

7.2.4 d)

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

7.2.5 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)**

7.2.6 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)**

7.3 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>
```

7.3.1 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)**

7.3.2 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.

7.3.3 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)**

7.3.4 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)**

7.3.5 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)**

7.3.6 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')
```

A Stratified splitting (classification problem)

A.1 Stratified splitting with respect to response

Q: When splitting data into train and test for developing and assessing a classification model, it is recommended to stratify the split with respect to the response. Why?

A: The main advantage of stratified splitting is that it can help ensure that the training and testing sets have similar distributions of the target variable, which can lead to more accurate and reliable model performance estimates.

In many real-world datasets, the target variable may be imbalanced, meaning that one class is more prevalent than the other(s). For example, in a medical dataset, the majority of patients may not have a particular disease, while only a small fraction may have the disease. If a random split is used to divide the dataset into training and testing sets, there is a risk that the testing set may not have enough samples from the minority class, which can lead to biased model performance estimates.

Stratified splitting addresses this issue by ensuring that both the training and testing sets have similar proportions of the target variable. This can lead to more accurate model performance estimates, especially for imbalanced datasets, by ensuring that the testing set contains enough samples from each class to make reliable predictions.

Another advantage of stratified splitting is that it can help ensure that the model is not overfitting to a particular class. If a random split is used and one class is overrepresented in the training set, the model may learn to predict that class well but perform poorly on the other class(es). Stratified splitting can help ensure that the model is exposed to a representative sample of all classes during training, which can improve its generalization performance on new, unseen data.

In summary, the advantages of stratified splitting are that it can lead to more accurate and reliable model performance estimates, especially for imbalanced datasets, and can help prevent overfitting to a particular class.

A.2 Stratified splitting with respect to response and categorical predictors

Q: Will it be better to stratify the split with respect to the response as well as categorical predictors, instead of only the response? In that case, the train and test datasets will be even more representative of the complete data.

A: It is not recommended to stratify with respect to both the response and categorical predictors simultaneously, while splitting a dataset into train and test, because doing so may result in the test data being very similar to train data, thereby defeating the purpose of assessing the model on unseen data. This kind of a stratified splitting will tend to make the relationships between the response and predictors in train data also appear in test data, which will result in the performance on test data being very similar to that in train data. Thus, in this case, the ability of the model to generalize to new, unseen data won't be assessed by test data.

Therefore, it is generally recommended to only stratify the response variable when splitting the data for model training, and to use random sampling for the predictor variables. This helps to ensure that the model is able to capture the underlying relationships between the predictor variables and the response variable, while still being able to generalize well to new, unseen data.

In the extreme scenario, when there are no continuous predictors, and there are enough observations for stratification with respect to the response and the categorical predictors, the train and test datasets may turn out to be exactly the same. Example 1 below illustrates this scenario.

A.3 Example 1

The example below shows that the train and test data can be exactly the same if we stratify the split with respect to response and the categorical predictors.

```
# Importing necessary libraries
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import train_test_split, cross_val_predict, cross_val_score
from sklearn.metrics import accuracy_score
from itertools import product
sns.set(font_scale=1.35)
```

Let us simulate a dataset with 8 observations, two categorical predictors `x1` and `x2` and the the binary response `y`.

```
#Setting a seed for reproducible results
np.random.seed(9)

# 8 observations
n = 8

#Simulating the categorical predictors
x1 = pd.Series(np.random.randint(0,2,n), name = 'x1')
x2 = pd.Series(np.random.randint(0,2,n), name = 'x2')

#Simulating the response
pr = (x1==1)*0.7+(x2==0)*0.3# + (x3*0.1>0.1)*0.1
y = pd.Series(1*(np.random.uniform(size = n) < pr), name = 'y')

#Defining the predictor object 'X'
X = pd.concat([x1, x2], axis = 1)

#Stratified splitting with respect to the response and predictors to create 50% train and tes
X_train_stratified, X_test_stratified, y_train_stratified,\
y_test_stratified = train_test_split(X, y, test_size = 0.5, random_state = 45, stratify=data

#Train and test data resulting from the above stratified splitting
data_train = pd.concat([X_train_stratified, y_train_stratified], axis = 1)
data_test = pd.concat([X_test_stratified, y_test_stratified], axis = 1)
```

Let us check the train and test datasets created with stratified splitting with respect to both the predictors and the response.

```
data_train
```

	x1	x2	y
2	0	0	1
7	0	1	0
3	1	0	1
1	0	1	0

```
data_test
```

	x1	x2	y
4	0	1	0
6	1	0	1
0	0	1	0
5	0	0	1

Note that the train and test datasets are exactly the same! Stratified splitting tends to have the same proportion of observations corresponding to each strata in both the train and test datasets, where each strata is a unique combination of values of `x1`, `x2`, and `y`. This will tend to make the train and test datasets quite similar!

A.4 Example 2: Simulation results

The example below shows that train and test set performance will tend to be quite similar if we stratify the datasets with respect to the predictors and the response.

We'll simulate a dataset consisting of 1000 observations, 2 categorical predictors `x1` and `x2`, a continuous predictor `x3`, and a binary response `y`.

```
#Setting a seed for reproducible results
np.random.seed(99)

# 1000 Observations
n = 1000

#Simulating categorical predictors x1 and x2
x1 = pd.Series(np.random.randint(0,2,n), name = 'x1')
x2 = pd.Series(np.random.randint(0,2,n), name = 'x2')

#Simulating continuous predictor x3
x3 = pd.Series(np.random.normal(0,1,n), name = 'x3')

#Simulating the response
pr = (x1==1)*0.7+(x2==0)*0.3 + (x3*0.1>0.1)*0.1
y = pd.Series(1*(np.random.uniform(size = n) < pr), name = 'y')

#Defining the predictor object 'X'
X = pd.concat([x1, x2, x3], axis = 1)
```

We'll comparing model performance metrics when the data is split into train and test by performing stratified splitting

1. Only with respect to the response
2. With respect to the response and categorical predictors

We'll perform 1000 simulations, where the data is split using a different seed in each simulation.

```
#Creating an empty dataframe to store simulation results of 1000 simulations
accuracy_iter = pd.DataFrame(columns = {'train_y_stratified','test_y_stratified',
                                        'train_y_CatPredictors_stratified','test_y_CatPredict
```

```
# Comparing model performance metrics when the data is split into train and test by performi
# (1) only with respect to the response
# (2) with respect to the response and categorical predictors

# Stratified splitting is performed 1000 times and the results are compared
for i in np.arange(1,1000):

    #--------Case 1-------------------#
    # Stratified splitting with respect to response only to create train and test data
    X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.2, random_state =
    model = LogisticRegression()
    model.fit(X_train, y_train)

    # Model accuracy on train and test data, with stratification only on response while split
    # the complete data into train and test
    accuracy_iter.loc[(i-1), 'train_y_stratified'] = model.score(X_train, y_train)
    accuracy_iter.loc[(i-1), 'test_y_stratified'] = model.score(X_test, y_test)

    #--------Case 2-------------------#
    # Stratified splitting with respect to response and categorical predictors to create trai
    # and test data
    X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.2, random_state =
                                                        stratify=pd.concat([x1, x2, y], axis
    model.fit(X_train, y_train)

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

```
# Converting accuracy to numeric
accuracy_iter = accuracy_iter.apply(lambda x:x.astype(float), axis = 1)
```

Distribution of train and test accuracies

The table below shows the distribution of train and test accuracies when the data is split into train and test by performing stratified splitting:

1. Only with respect to the response (see `train_y_stratified` and `test_y_stratified`)
2. With respect to the response and categorical predictors (see `train_y_CatPredictors_stratified` and `test_y_CatPredictors_stratified`)

```
accuracy_iter.describe()
```

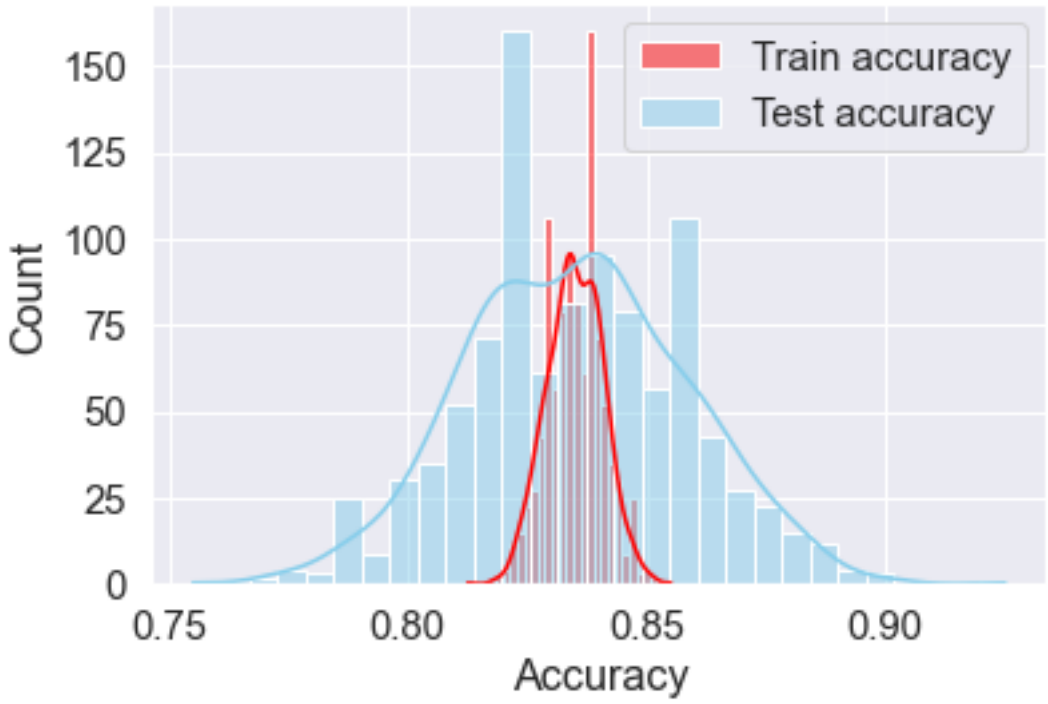
	train_y_stratified	test_y_stratified	train_y_CatPredictors_stratified	test_y_CatPredictors_st
count	999.000000	999.000000	9.990000e+02	9.990000e+02
mean	0.834962	0.835150	8.350000e-01	8.350000e-01
std	0.005833	0.023333	8.552999e-15	8.552999e-15
min	0.812500	0.755000	8.350000e-01	8.350000e-01
25%	0.831250	0.820000	8.350000e-01	8.350000e-01
50%	0.835000	0.835000	8.350000e-01	8.350000e-01
75%	0.838750	0.850000	8.350000e-01	8.350000e-01
max	0.855000	0.925000	8.350000e-01	8.350000e-01

Let us visualize the distribution of these accuracies.

A.4.1 Stratified splitting only with respect to the response

```
sns.histplot(data=accuracy_iter, x="train_y_stratified", color="red", label="Train accuracy"
sns.histplot(data=accuracy_iter, x="test_y_stratified", color="skyblue", label="Test accurac
plt.legend()
plt.xlabel('Accuracy')
```

```
Text(0.5, 0, 'Accuracy')
```

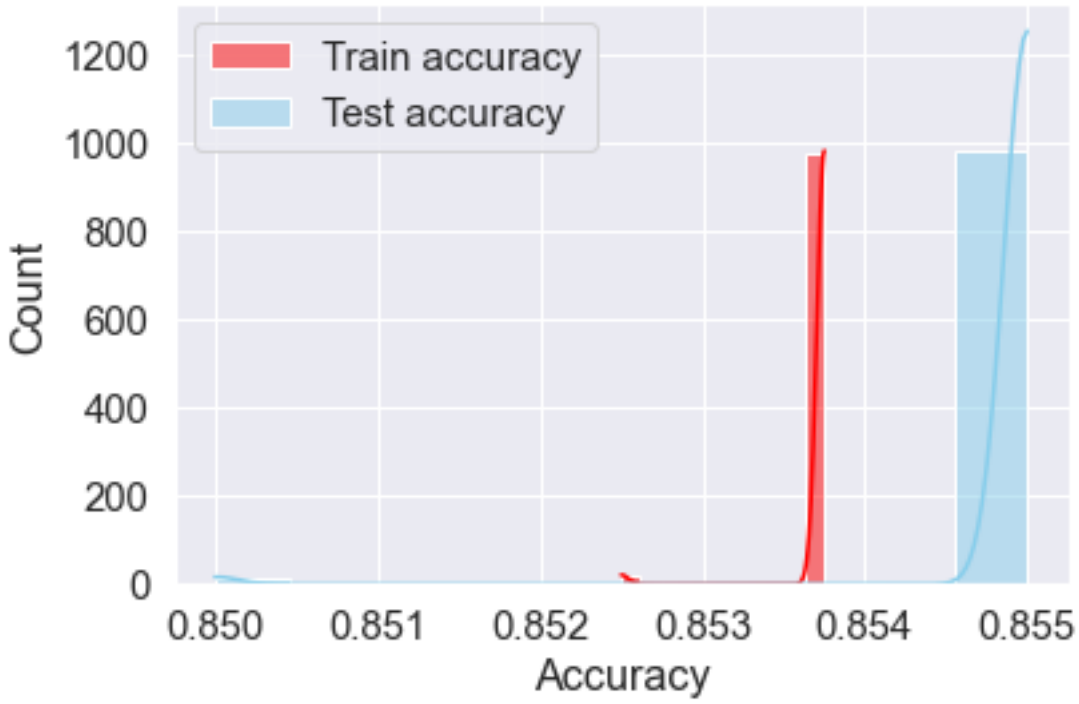


Note the variability in train and test accuracies when the data is stratified only with respect to the response. The train accuracy varies between 81.2% and 85.5%, while the test accuracy varies between 75.5% and 92.5%.

A.4.2 Stratified splitting with respect to the response and categorical predictors

```
sns.histplot(data=accuracy_iter, x="train_y_CatPredictors_stratified", color="red", label="Tr
sns.histplot(data=accuracy_iter, x="test_y_CatPredictors_stratified", color="skyblue", label=
plt.legend()
plt.xlabel('Accuracy')
```

```
Text(0.5, 0, 'Accuracy')
```



The train and test accuracies are between 85% and 85.5% for all the simulations. As a results of stratifying the splitting with respect to both the response and the categorical predictors, the train and test datasets are almost the same because the datasets are engineered to be quite similar, thereby making the test dataset inappropriate for assessing accuracy on unseen data. Thus, it is recommended to stratify the splitting only with respect to the response.

B Parallel processing bonus Q

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

```
#Using the same datasets as used for linear regression in STAT303-2,
#so that we can compare the non-linear models with linear regression
trainf = pd.read_csv('./Datasets/Car_features_train.csv')
trainp = pd.read_csv('./Datasets/Car_prices_train.csv')
testf = pd.read_csv('./Datasets/Car_features_test.csv')
testp = pd.read_csv('./Datasets/Car_prices_test.csv')
train = pd.merge(trainf,trainp)
test = pd.merge(testf,testp)
train.head()
predictors = ['mpg', 'engineSize', 'year', 'mileage']
X_train = train[predictors]
y_train = train['price']
X_test = test[predictors]
y_test = test['price']

# Scale
sc = StandardScaler()
```

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

C Case 1: No parallelization

```
time_taken_case1 = []
for i in range(50):
    start_time = tm.time()
    Ks = range(1, 20)
    kfold = KFold(n_splits=5, shuffle=True, random_state=1)
    cross_val_error = []
    for k in Ks:
        cross_val_error.append(-cross_val_score(KNeighborsRegressor(n_neighbors=k),
                           X_train_scaled, y_train, cv = kfold,
                            scoring="neg_root_mean_squared_error").mean())
    time_taken_case1.append(tm.time() - start_time)
```

D Case 2: Parallelization in `cross_val_score()`

```
time_taken_case2 = []
for i in range(50):
    start_time = tm.time()
    Ks = range(1, 20)
    kfold = KFold(n_splits=5, shuffle=True, random_state=1)
    cross_val_error = []
    for k in Ks:
        cross_val_error.append(-cross_val_score(KNeighborsRegressor(n_neighbors=k),
                        X_train_scaled, y_train, cv = kfold, n_jobs = -1,
                                scoring="neg_root_mean_squared_error").mean())
    time_taken_case2.append(tm.time() - start_time)
```

E Case 3: Parallelization in `KNeighborsRegressor()`

```
time_taken_case3 = []
for i in range(50):
    start_time = tm.time()
    Ks = range(1, 20)
    kfold = KFold(n_splits=5, shuffle=True, random_state=1)
    cross_val_error = []
    for k in Ks:
        cross_val_error.append(-cross_val_score(KNeighborsRegressor(n_neighbors=k,
                n_jobs= -1), X_train_scaled, y_train, cv = kfold,
                                    scoring="neg_root_mean_squared_error").mean())
    time_taken_case3.append(tm.time() - start_time)
```

F Case 4: Nested parallelization: Both `cross_val_score()` and `KNeighborsRegressor()`

```
time_taken_case4 = []
for i in range(50):
    start_time = tm.time()
    Ks = range(1, 20)
    kfold = KFold(n_splits=5, shuffle=True, random_state=1)
    cross_val_error = []
    for k in Ks:
        cross_val_error.append(-cross_val_score(KNeighborsRegressor(n_neighbors=k,
                n_jobs= -1), X_train_scaled, y_train, cv = kfold, n_jobs = -1,
                scoring="neg_root_mean_squared_error").mean())
    time_taken_case4.append(tm.time() - start_time)
```

```
sns.boxplot([time_taken_case1, time_taken_case2, time_taken_case3, time_taken_case4])
plt.xticks([0, 1, 2, 3], ['Case 1', 'Case 2', 'Case 3', 'Case 4']);
plt.ylabel('Time');
```

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

G Q1

Case 1 is without parallelization. Why is Case 3 with parallelization of `KNeighborsRegressor()` taking more time than case 1?

H Q2

If nested parallelization is worse than parallelization, why is case 4 with nested parallelization taking less time than case 3 with parallelization of KNeighborsRegressor()?

I Q3

If nested parallelization is worse than no parallelization, why is case 4 with nested parallelization taking less time than case 1 with no parallelization?

J Q4

If nested parallelization is the best scenario, why is case 4 with nested parallelization taking more time than case 2 with with parallelization in `cross_val_score()`?

K Datasets, assignment and project files

Datasets used in the book, assignment files, project files, and prediction problems report tempate can be found here