Data Science III with python (Class notes)

STAT 303-3

Arvind Krishna, Emre Besler, and Lizhen Shi

3/24/23

Table of contents

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

Moving towards non-linearity

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.

```
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 valid
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_sc
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 (di
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
    # 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 =
```

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 dif
# of magn., scaling is necessary. This is to enable the training algo. which we did not co
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, jus
```

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\Anaconda3\lib\site-packages\sklearn\linear_model\_logistic.py:763: Converge
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.

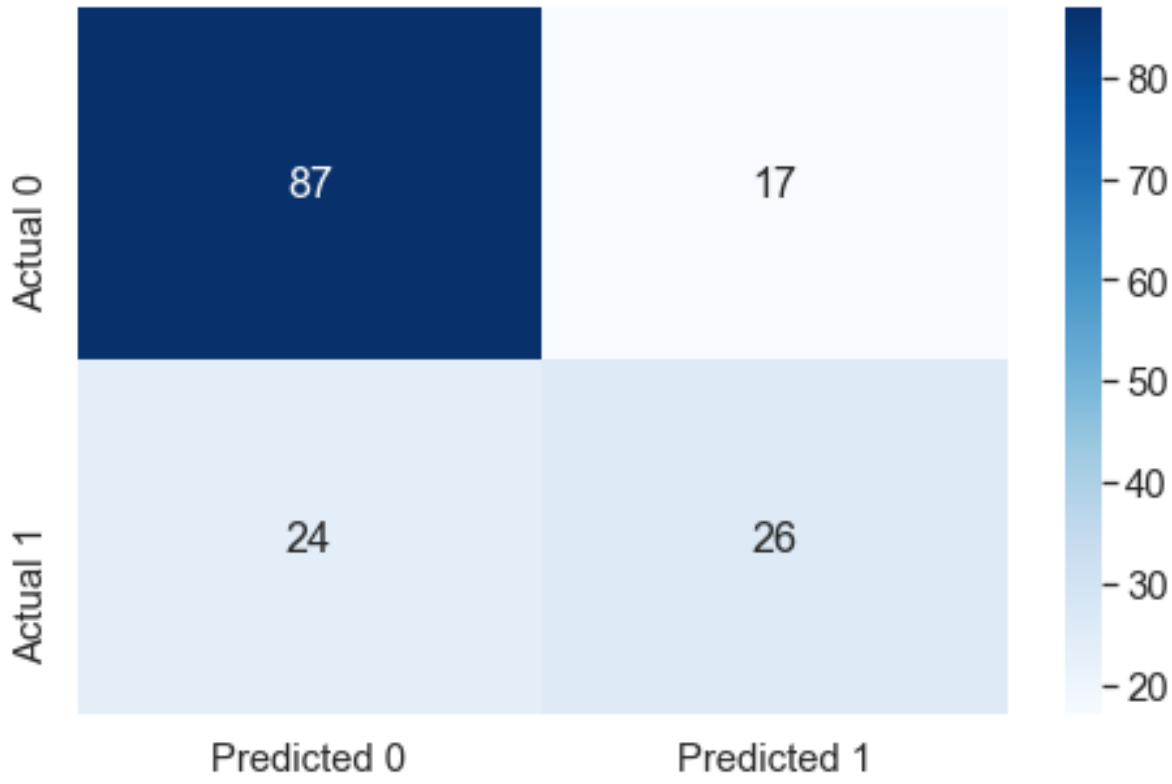
```
#Computing the predicted probability for the observation to belong to the positive class (
#The 2nd column in the output of predict_proba() consists of the probability of the observ
#belong to the positive class (y=1)
y_pred_prob = logreg.predict_proba(X_test_scaled)[:,1]

#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))
```

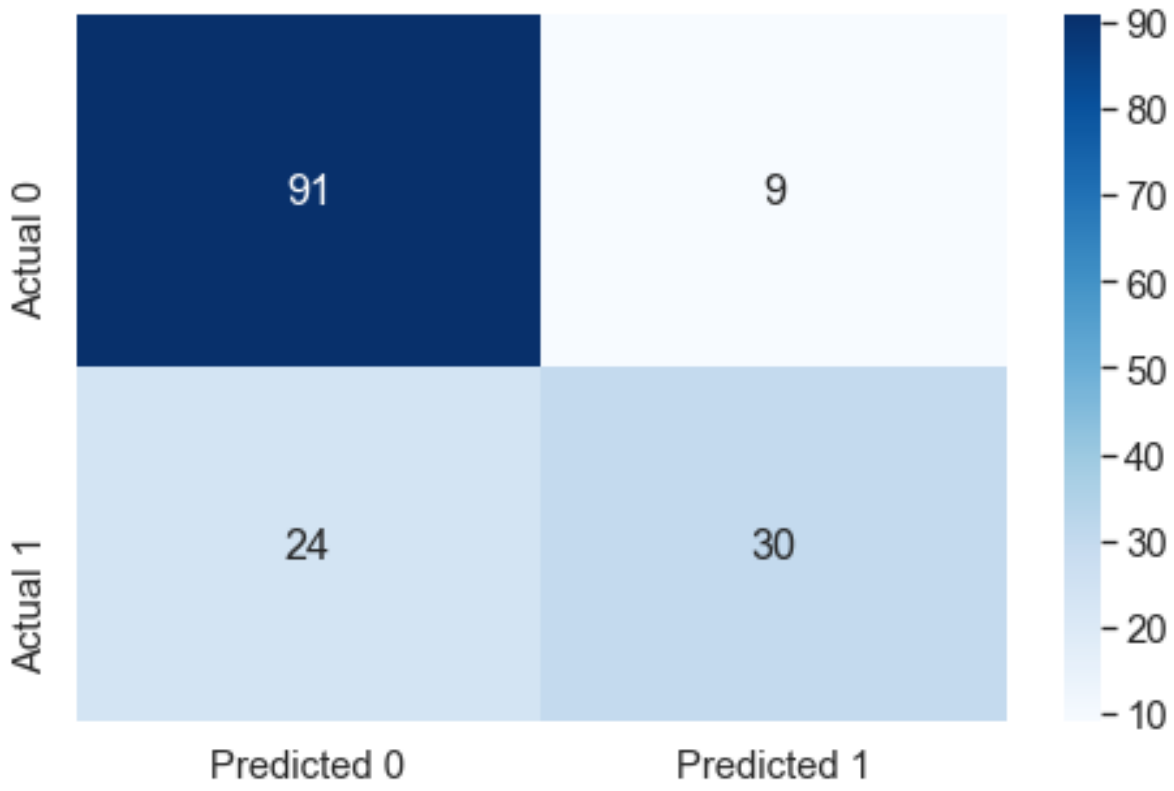
```
Precision:  0.6046511627906976
Recall:  0.52
```

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=['Predic
            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 couple of hyperparameters (among others) that can be trained in a logistic regression model are:

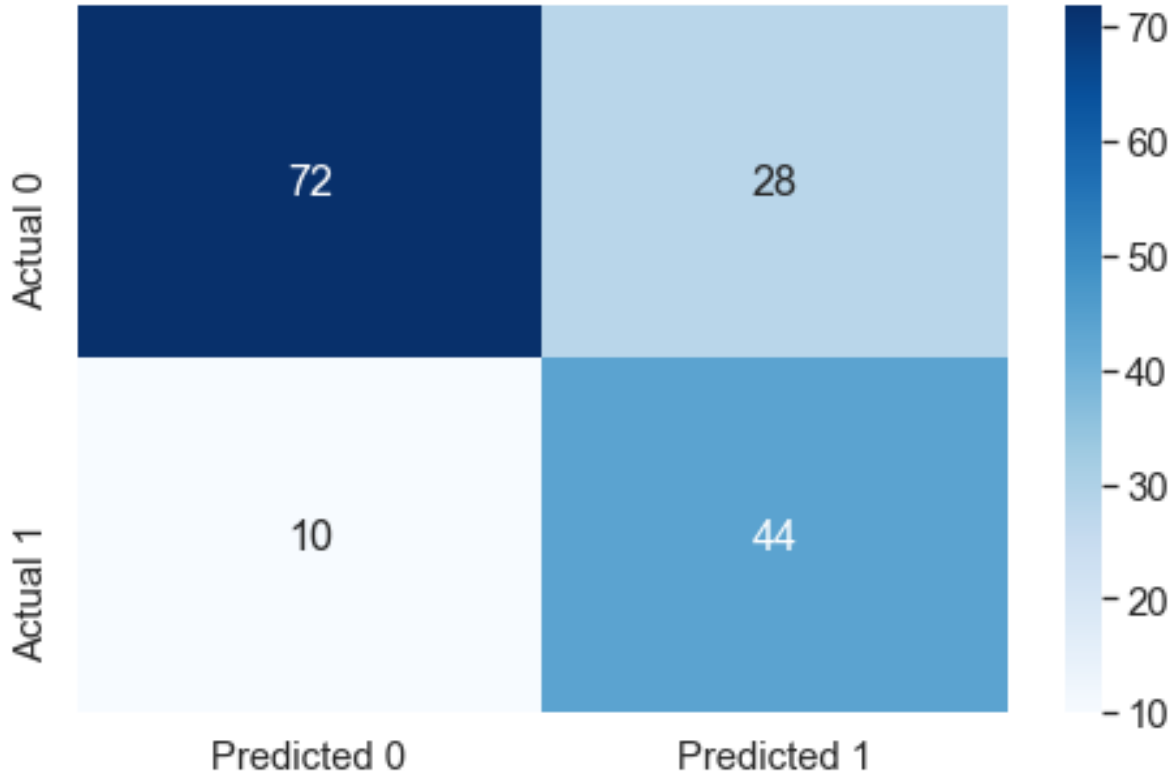
1. Decision threshold probability
2. Regularization parameter

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 g
# 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.

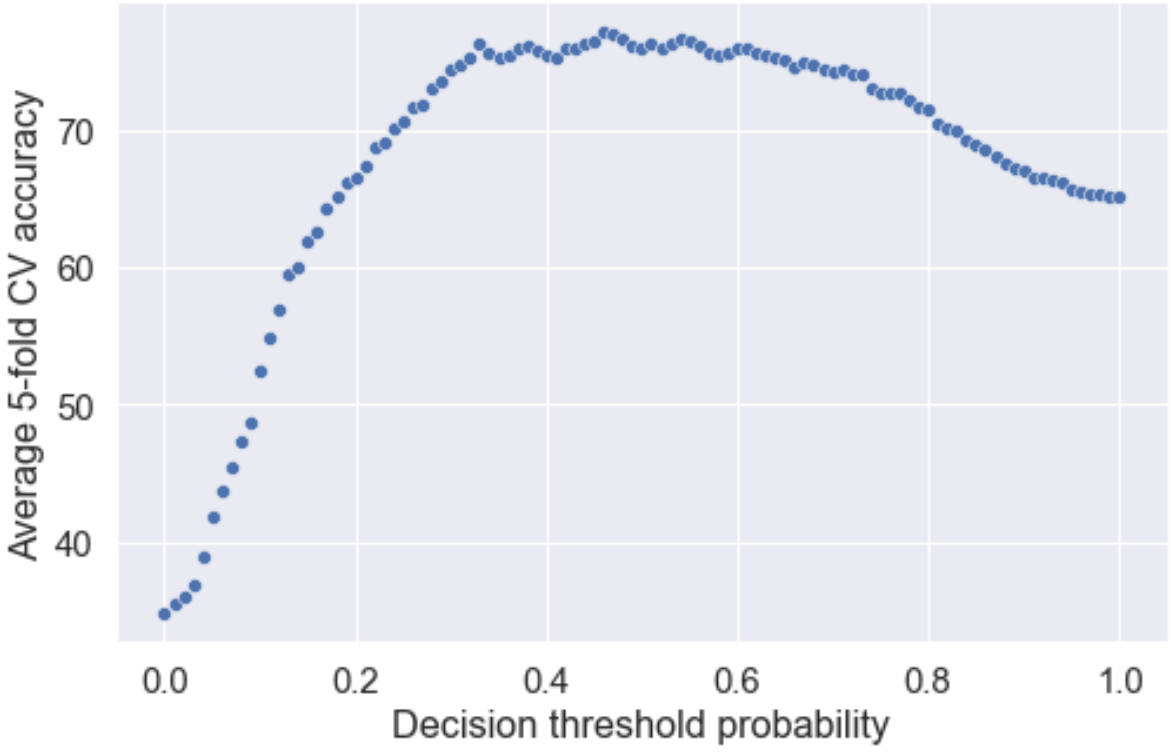
We'll use the `cross_val_predict()` function from the `model_selection` module of `sklearn` to compute the K-fold cross validated predicted probabilities. Note that this function simplifies the task of manually creating the K-folds, training the model K-times, and computing the predicted probabilities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

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');
```



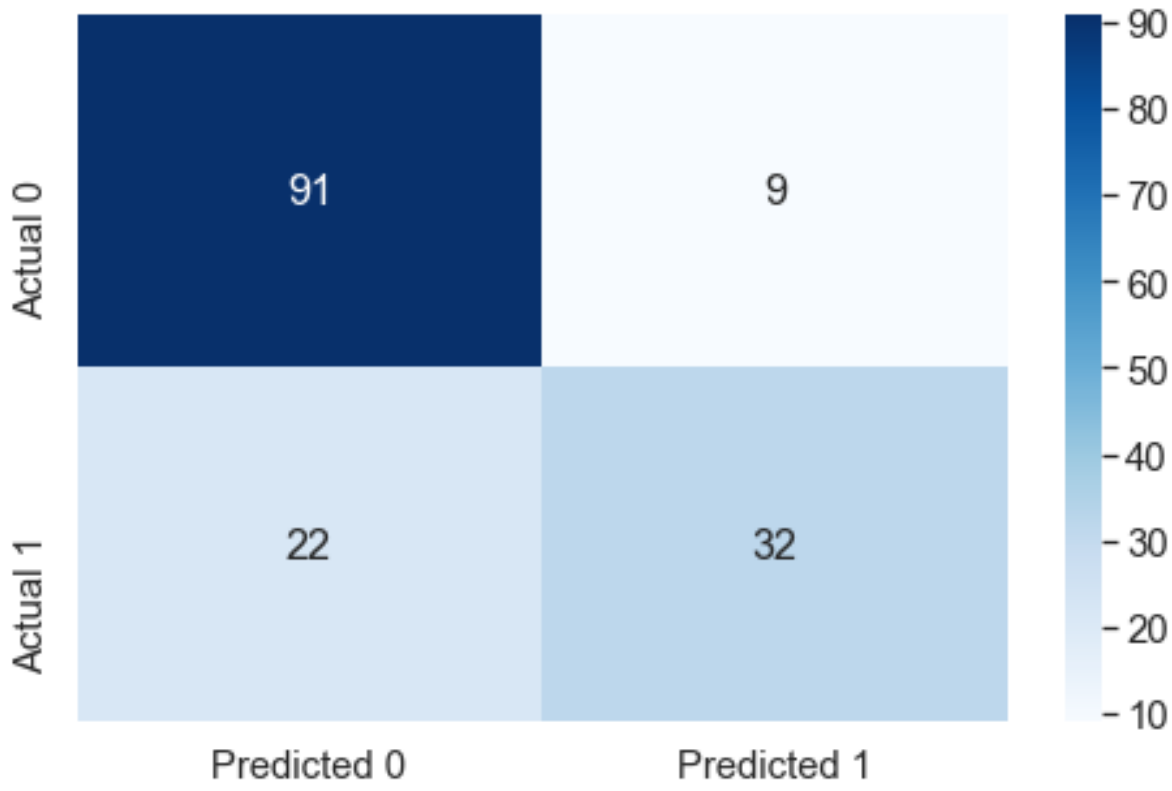
The optimal decision threshold probability is the one that maximizes the K-fold cross validation accuracy.

```
# 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 g
# 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
```



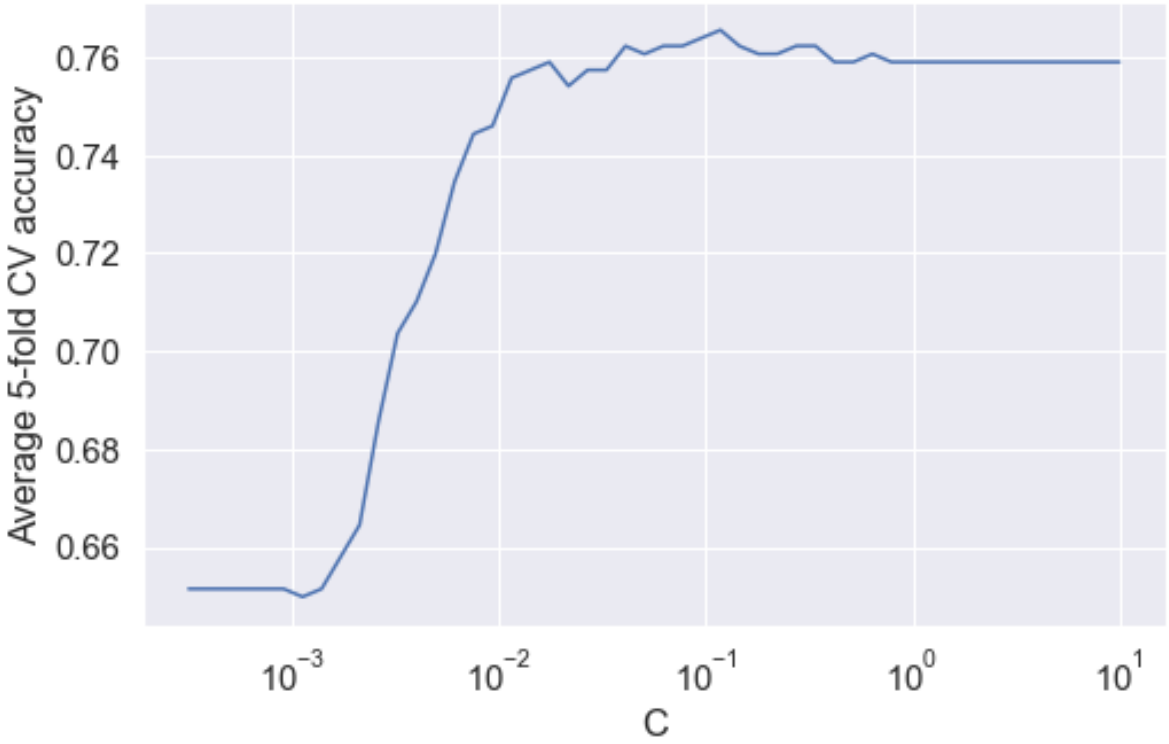
Model performance on test data has improved with the optimal decision threshold probability.

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_
                                         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()
```



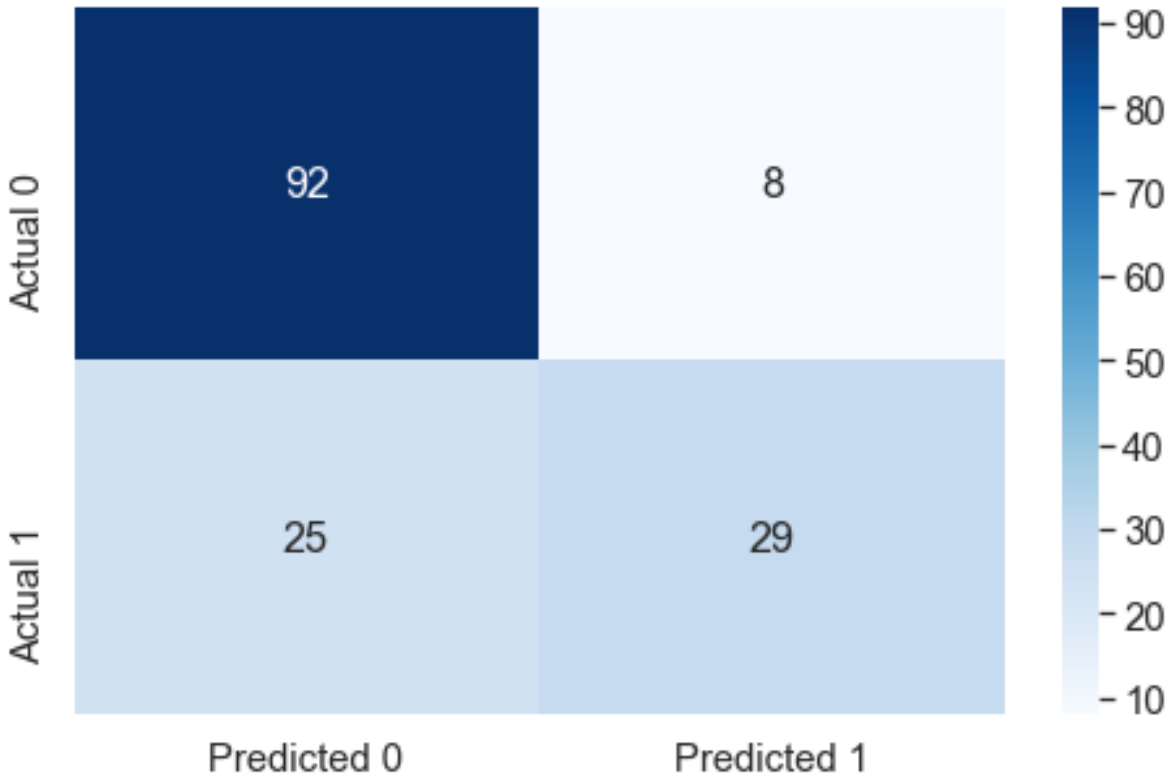

```
# Optimal value of the regularization parameter 'C'
optimal_C = hyperparam_vals[np.argmax(np.array(accuracy_iter).mean(axis=1))]
optimal_C
```

```
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=['Predic
            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 = []

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

    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.append(accuracy)
```

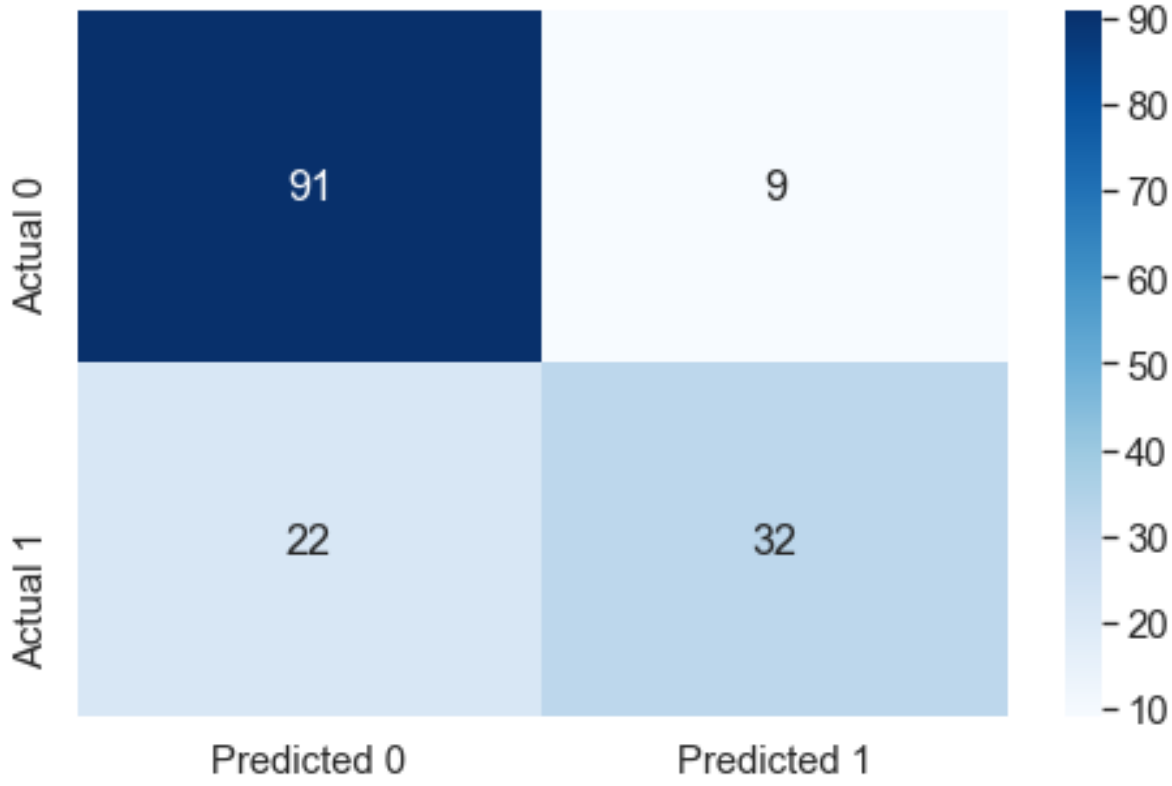
```
max_acc_iter = np.argmax(accuracy_iter)

#Optimal decision threshold probability
optimal_threshold = threshold_hyperparam_vals[max_acc_iter%len(threshold_hyperparam_vals)]
print("Optimal decision threshold = ", optimal_threshold)

#Optimal C
optimal_C = C_hyperparam_vals[int(max_acc_iter/len(threshold_hyperparam_vals))]
print("Optimal C = ", optimal_C)
```

```
Optimal decision threshold =  0.46
Optimal C =  2.2758459260747887
```

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

#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 g
# 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=[
            index = ['Actual 0', 'Actual 1'])
sns.heatmap(cm, annot=True, cmap='Blues', fmt='g');
```

```
Accuracy:  79.87012987012987
ROC-AUC:  0.8507407407407408
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 Regression splines

Read sections 7.1-7.4 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 statsmodels.formula.api as smf
import statsmodels.api as sm
import seaborn as sns
import matplotlib.pyplot as plt
from patsy import dmatrix
from sklearn.metrics import mean_squared_error
from pyearth import Earth
```

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

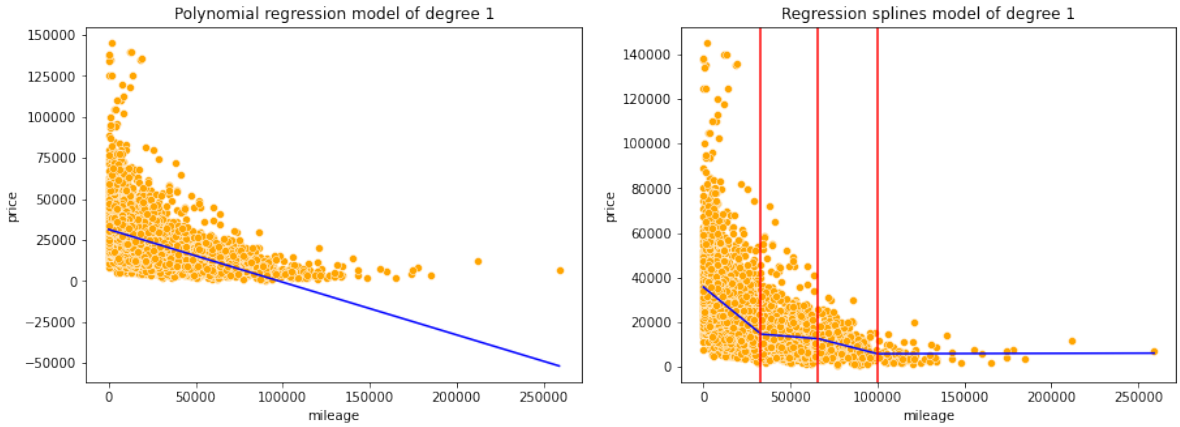
2.1 Polynomial regression vs Regression splines

2.1.1 Model of degree 1

```
ols_object = smf.ols(formula = 'price~mileage', data = train)
lr_model = ols_object.fit()
```

```
#Regression spline of degree 1

#Creating basis functions for splines of degree 1
transformed_x = dmatrix("bs(mileage , knots=(33000,66000,100000), degree = 1, include_inte
                        data = {'mileage':train['mileage']},return_type = 'dataframe')

#Developing a linear regression model on the spline basis functions - this is the regressi
reg_spline_model = sm.OLS(train['price'], transformed_x).fit()
```

```
#Visualizing polynomial model and the regression spline model of degree 1

knots = [33000,66000,100000] #Knots for the spline
d=1 #Degree of predictor in the model
#Writing a function to visualize polynomial model and the regression spline model of degre
def viz_models():
    fig, axes = plt.subplots(1,2,figsize = (15,5))
    plt.subplots_adjust(wspace=0.2)

    #Visualizing the linear regression model
    pred_price = lr_model.predict(train)
    sns.scatterplot(ax = axes[0],x = 'mileage', y = 'price', data = train, color = 'orange
    sns.lineplot(ax = axes[0],x = train.mileage, y = pred_price, color = 'blue')
    axes[0].set_title('Polynomial regression model of degree '+str(d))

    #Visualizing the regression splines model of degree 'd'
    axes[1].set_title('Regression splines model of degree '+ str(d))
    sns.scatterplot(ax=axes[1],x = 'mileage', y = 'price', data = train, color = 'orange')
    sns.lineplot(ax=axes[1],x = train.mileage, y = reg_spline_model.predict(), color = 'bl
    for i in range(3):
        plt.axvline(knots[i], 0,100,color='red')
viz_models()
```



We observe the regression splines model better fits the data as compared to the polynomial regression model. This is because regression splines of degree 1 fit piecewise polynomials, or linear models on sub-sections of the predictor, which helps better capture the trend. However, this added flexibility may also lead to overfitting. Hence, one must be careful to check for overfitting when using splines. Overfitting may be checked by k-fold cross validation or comparing test and train errors.

The red lines in the plot on the right denote the position of knots. Knots separate distinct splines.

```
#Creating basis functions for test data for prediction
test_x = dmatrix("bs(mileage , knots=(33000,66000,100000), degree = 1, include_intercept =
```

```
#Function to compute RMSE (root mean squared error on train and test datasets)
def rmse():
    #Error on train data for the linear regression model
    print("RMSE on train data:")
    print("Linear regression:", np.sqrt(mean_squared_error(lr_model.predict(),train.price)

    #Error on train data for the regression spline model
    print("Regression splines:", np.sqrt(mean_squared_error(reg_spline_model.predict(),tra

    #Error on test data for the linear regression model
    print("\nRMSE on test data:")
    print("Linear regression:",np.sqrt(mean_squared_error(lr_model.predict(test),test.pric

    #Error on test data for the regression spline model
```

```
    print("Regression splines:",np.sqrt(mean_squared_error(reg_spline_model.predict(test_x
rmse()
```

```
RMSE on train data:
Linear regression: 14403.250083261853
Regression splines: 13859.640716531134

RMSE on test data:
Linear regression: 14370.94086395544
Regression splines: 13770.133025694666
```

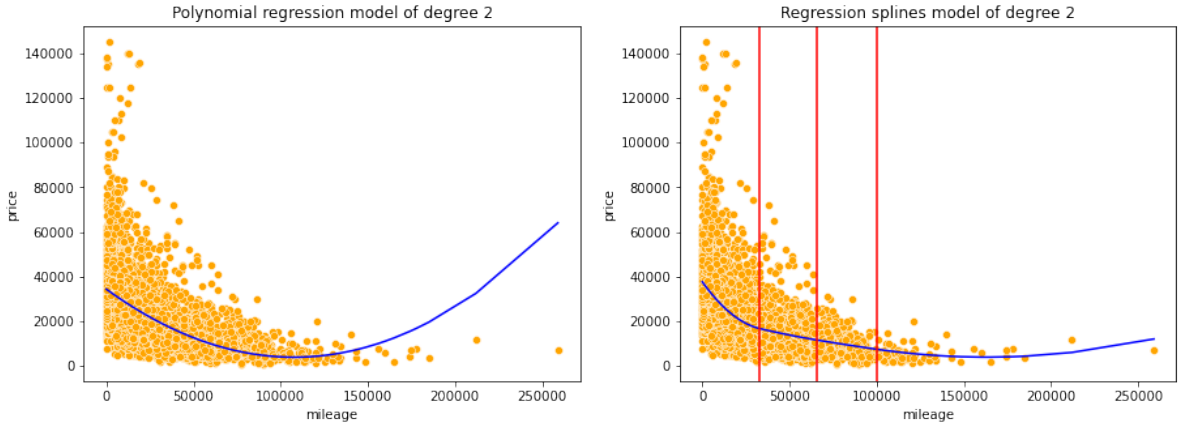
2.1.2 Model of degree 2

A higher degree model will lead to additional flexibility for both polynomial and regression splines models.

```
#Including mileage squared as a predictor and developing the model
ols_object = smf.ols(formula = 'price~mileage+I(mileage**2)', data = train)
lr_model = ols_object.fit()
```

```
#Regression spline of degree 2

#Creating basis functions for splines of degree 2
transformed_x = dmatrix("bs(mileage , knots=(33000,66000,100000), degree = 2, include_inte
                        data = {'mileage':train['mileage']},return_type = 'dataframe')

#Developing a linear regression model on the spline basis functions - this is the regressi
reg_spline_model = sm.OLS(train['price'], transformed_x).fit()
```

```
d=2
viz_models()
```



Unlike polynomial regression, splines functions avoid imposing a global structure on the non-linear function of X. This provides a better local fit to the data.

```
#Creating basis functions for test data for prediction
test_x = dmatrix("bs(mileage , knots=(33000,66000,100000), degree = 2, include_intercept =
```

```
rmse()
```

```
RMSE on train data:
Linear regression: 14403.250083261853
Regression splines: 13859.640716531134

RMSE on test data:
Linear regression: 14370.94086395544
Regression splines: 13770.133025694666
```

2.1.3 Model of degree 3

```
ols_object = smf.ols(formula = 'price~mileage+I(mileage**2)+I(mileage**3)', data = train)
lr_model = ols_object.fit()
```

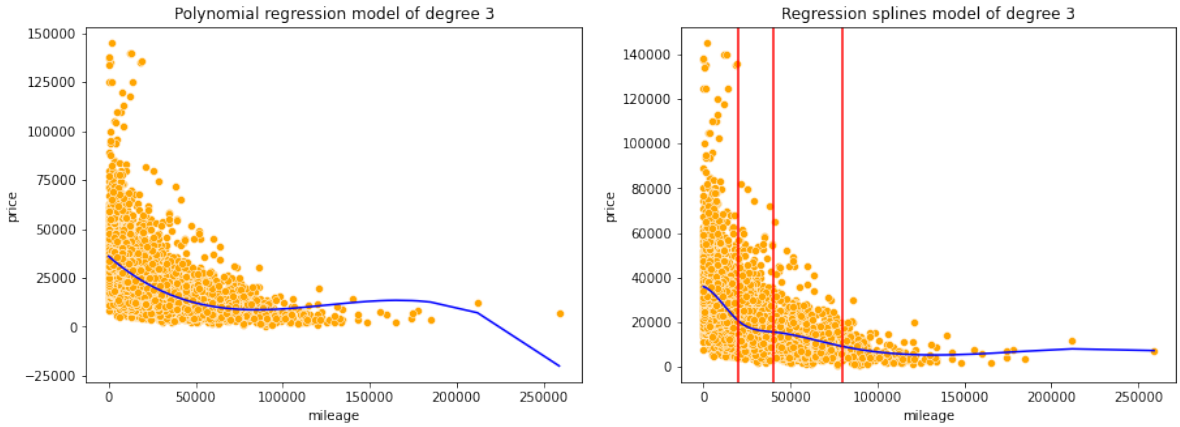
```
#Regression spline of degree 3

#Creating basis functions for splines of degree 3
transformed_x = dmatrix("bs(mileage , knots=(20000,40000,80000), degree = 3, include_inter
```

```
                        data = {'mileage':train['mileage']},return_type = 'dataframe')

#Developing a linear regression model on the spline basis functions - this is the regressi
reg_spline_model = sm.OLS(train['price'], transformed_x).fit()
```

```
transformed_x
```

	Intercept	bs(mileage, knots=(20000, 40000, 80000), degree=3, include_intercept=False)[0]	bs(mileag
0	1.0	0.001499	3.749187e
1	1.0	0.583162	3.001491e
2	1.0	0.000750	9.374336e
3	1.0	0.293446	6.009875e
4	1.0	0.000000	2.580169e
...	...	...	...
4955	1.0	0.005441	4.824519e
4956	1.0	0.206763	6.438755e
4957	1.0	0.000000	0.000000e
4958	1.0	0.198162	6.468919e
4959	1.0	0.000000	2.233101e

```
d=3
knots=[20000,40000,80000]
viz_models()
```



Unlike polynomial regression, splines functions avoid imposing a global structure on the non-linear function of X. This provides a better local fit to the data.

```
#Creating basis functions for test data for prediction
test_x = dmatrix("bs(mileage , knots=(20000,40000,80000), degree = 3, include_intercept =
```

```
rmse()
```

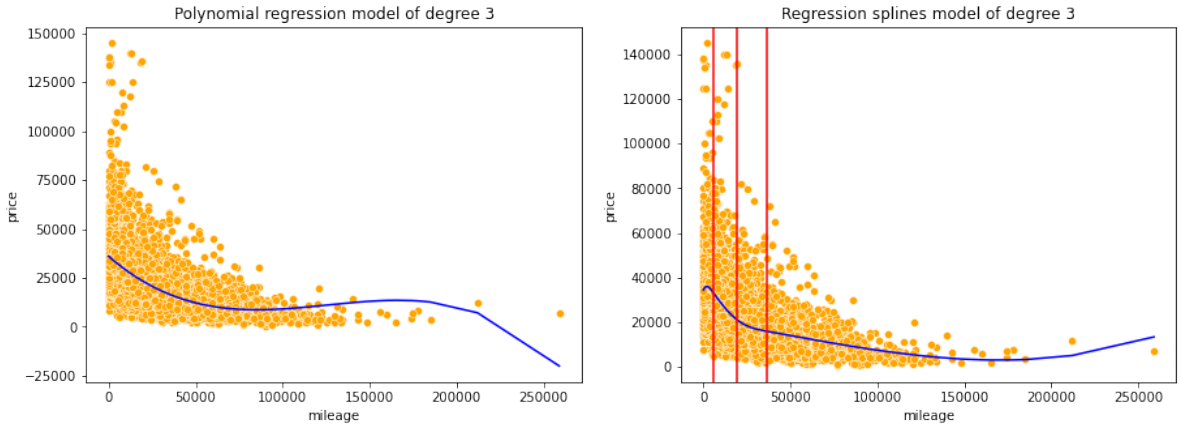
```
RMSE on train data:
Linear regression: 13891.962447594644
Regression splines: 13792.371446327243

RMSE on test data:
Linear regression: 13789.708418357186
Regression splines: 13651.288965905529
```

2.2 Regression splines with knots at uniform quantiles of data

If degrees of freedom are provided instead of knots, the knots are by default chosen at uniform quantiles of data. For example if there are 7 degrees of freedom (including the intercept), then there will be 7-4 = 3 knots. These knots will be chosen at the 255h, 50th and 75th quantiles of the data.

```
#Regression spline of degree 3

#Creating basis functions for splines of degree 3
transformed_x = dmatrix("bs(mileage , df=6, degree = 3, include_intercept = False)",
                        data = {'mileage':train['mileage']},return_type = 'dataframe')

#Developing a linear regression model on the spline basis functions - this is the regressi
reg_spline_model = sm.OLS(train['price'], transformed_x).fit()
```

```
d=3
unif_knots = pd.qcut(train.mileage,4,retbins=True)[1][1:4]
knots=unif_knots
viz_models()
```



Splines can be unstable at the outer range of predictors. In the figure (on the right), the left-most spline may be overfitting.

```
#Creating basis functions for test data for prediction
test_x = dmatrix("bs(mileage , knots=" +str(tuple(unif_knots)) + ", degree = 3, include_in
```

```
rmse()
```

```
RMSE on train data:
Linear regression: 13891.962447594644
Regression splines: 13781.79102252679

RMSE on test data:
Linear regression: 13789.708418357186
Regression splines: 13676.271829882426
```

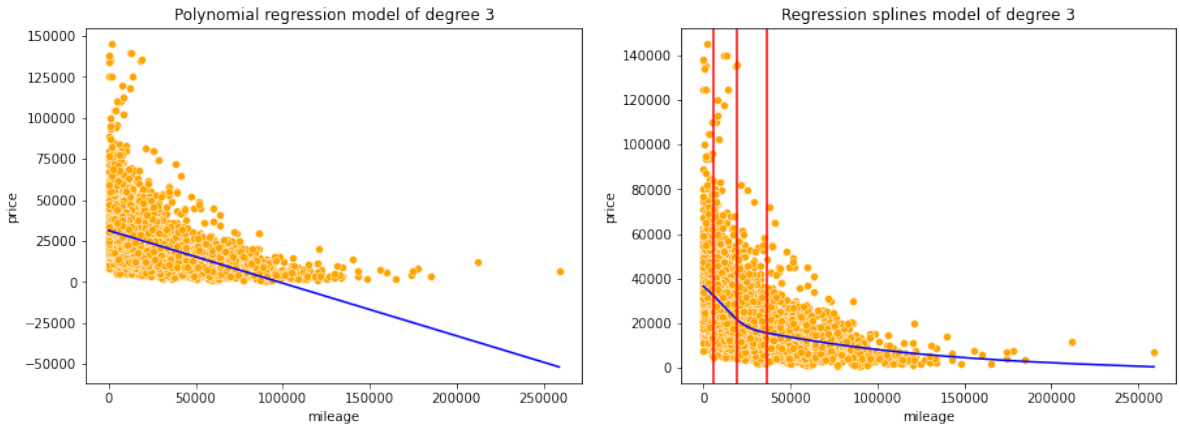
2.3 Natural cubic splines

Page 298: "A natural spline is a regression spline with additional boundary constraints: the function is required to be linear at the boundary (in the region where X is smaller than the smallest knot, or larger than the largest knot). This additional constraint means that natural splines generally produce more stable estimates at the boundaries."

```
#Natural cubic spline
```

```
#Creating basis functions for the natural cubic spline
transformed_x = dmatrix("cr(mileage , df=4,constraints='center')",
                        data = {'mileage':train['mileage']},return_type = 'dataframe')
reg_spline_model = sm.GLM(train['price'], transformed_x).fit()
```

```
d=3;
unif_knots = pd.qcut(train.mileage,4,retbins=True)[1][1:4]
knots=unif_knots
viz_models()
```



Note that the natural cubic spline is more stable than a cubic splines with knots at uniformly distributed quantiles.

```
#Creating basis functions for test data for prediction
test_x = dmatrix("cr(mileage , knots="+str(tuple(unif_knots))+",constraints='center')",dat
```

```
rmse()
```

```
RMSE on train data:
Linear regression: 13891.962447594644
Regression splines: 13805.022189679756

RMSE on test data:
Linear regression: 13789.708418357186
Regression splines: 13666.943224268975
```

2.4 Generalized additive model (GAM)

GAM allow for flexible nonlinearities in several variables, but retain the additive structure of linear models. In a GAM, non-linear basis functions of predictors can be used as predictors of a linear regression model. For example,

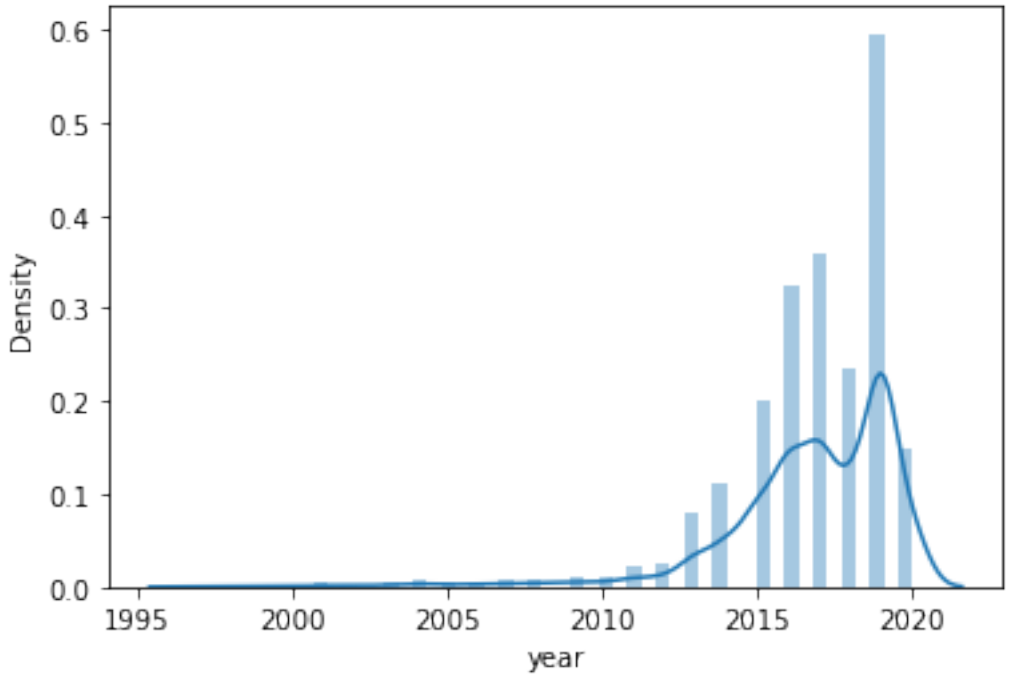
$$y = f_1(X_1) + f_2(X_2) + \epsilon$$

is a GAM, where $f_1(.)$ may be a cubic spline based on the predictor X_1, and $f_2(.)$ may be a step function based on the predictor X_2.

```
sns.distplot(train.year)
```

```
C:\Users\akl0407\Anaconda3\lib\site-packages\seaborn\distributions.py:2557: FutureWarning: `d
  warnings.warn(msg, FutureWarning)
```

```
<AxesSubplot:xlabel='year', ylabel='Density'>
```



```
#GAM
#GAM includes cubic splines for mileage. Other predictors are year, engineSize, mpg, milea
X_transformed = dmatrix('bs(mileage,df=6,degree = 3)+year*engineSize*mpg*mileage',
                data = {'year':train['year'],'engineSize':train['engineSize'],'mpg':train[
                                                                        return_type =
# fit the model
model_gam = sm.OLS(train['price'],X_transformed).fit()

#Creating basis functions for test data for prediction
X_test = dmatrix('bs(mileage,df=6,degree = 3, include_intercept = False)+year*engineSize*m
                data = {'year':test['year'],'engineSize':test['engineSize'],'mpg':test['mp
                                                                        return_type =

preds = model_gam.predict(X_test)
np.sqrt(mean_squared_error(preds,test.price))
```

8434.756663328963

```
#GAM
#GAM includes cubic splines for mileage, year, engineSize, mpg, and interactions of all pr
X_transformed = dmatrix('bs(mileage,df=6,degree = 3)+bs(mpg,df=6,degree = 3)+bs(engineSize
                data = {'year':train['year'],'engineSize':train['engineSize'],'mpg':train[
                                                                        return_type =
# fit the model
model_gam = sm.OLS(train['price'],X_transformed).fit()

#Creating basis functions for test data for prediction
X_test = dmatrix('bs(mileage,df=6,degree = 3, include_intercept = False)+bs(mpg,df=6,degre
                data = {'year':test['year'],'engineSize':test['engineSize'],'mpg':test['mp
                                                                        return_type =

preds = model_gam.predict(X_test)
np.sqrt(mean_squared_error(preds,test.price))
```

7997.325718841729

```
ols_object = smf.ols(formula = 'price~(year+engineSize+mileage+mpg)**2+I(mileage**2)+I(mil
model = ols_object.fit()
model.summary()
```

Table 2.3: OLS Regression Results

Dep. Variable:	price	R-squared:	0.704
Model:	OLS	Adj. R-squared:	0.703
Method:	Least Squares	F-statistic:	1308.
Date:	Sun, 27 Mar 2022	Prob (F-statistic):	0.00
Time:	01:08:50	Log-Likelihood:	-52157.
No. Observations:	4960	AIC:	1.043e+05
Df Residuals:	4950	BIC:	1.044e+05
Df Model:	9		
Covariance Type:	nonrobust		

	coef	std err	t	P>|t|	[0.025	0.975]
Intercept	-0.0009	0.000	-2.752	0.006	-0.002	-0.000
year	-1.1470	0.664	-1.728	0.084	-2.448	0.154
engineSize	0.0052	0.000	17.419	0.000	0.005	0.006
mileage	-31.4751	2.621	-12.010	0.000	-36.613	-26.337
mpg	-0.0201	0.002	-13.019	0.000	-0.023	-0.017
year:engineSize	9.5957	0.254	37.790	0.000	9.098	10.094
year:mileage	0.0154	0.001	11.816	0.000	0.013	0.018
year:mpg	0.0572	0.013	4.348	0.000	0.031	0.083
engineSize:mileage	-0.1453	0.008	-18.070	0.000	-0.161	-0.130
engineSize:mpg	-98.9062	11.832	-8.359	0.000	-122.102	-75.710
mileage:mpg	0.0011	0.000	2.432	0.015	0.000	0.002
I(mileage ** 2)	7.713e-06	3.75e-07	20.586	0.000	6.98e-06	8.45e-06
I(mileage ** 3)	-1.867e-11	1.43e-12	-13.077	0.000	-2.15e-11	-1.59e-11

Omnibus:	1830.457	Durbin-Watson:	0.634
Prob(Omnibus):	0.000	Jarque-Bera (JB):	34927.811
Skew:	1.276	Prob(JB):	0.00
Kurtosis:	15.747	Cond. No.	2.50e+18

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

```
9026.775740000594
```

Note the RMSE with GAM that includes regression splines for mileage is lesser than that of the linear regression model, indicating a better fit.

2.5 MARS (Multivariate Adaptive Regression Splines)

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

2.5.1 MARS of degree 1

```
model = Earth(max_terms=500, max_degree=1) # note, terms in brackets are the hyperparamete
model.fit(X,y)
```

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

```
Earth(max_degree=1, max_terms=500)
```

```
print(model.summary())
```

```
Earth Model
--------------------------------------
Basis Function  Pruned  Coefficient
--------------------------------------
(Intercept)     No      -553155
h(x0-22141)     Yes     None
h(22141-x0)     Yes     None
h(x0-3354)      No      -6.23571
h(3354-x0)      Yes     None
h(x0-15413)     No      -36.9613
h(15413-x0)     No      38.167
h(x0-106800)    Yes     None
h(106800-x0)    No      0.221844
h(x0-500)       No      170.039
h(500-x0)       Yes     None
h(x0-741)       Yes     None
```

```
h(741-x0)       No      -54.5265
h(x0-375)       No      -126.804
h(375-x0)       Yes     None
h(x0-2456)      Yes     None
h(2456-x0)      No      7.04609
---------------------------------------
MSE: 188429705.7549, GCV: 190035470.5664, RSQ: 0.2998, GRSQ: 0.2942
```

Model equation:

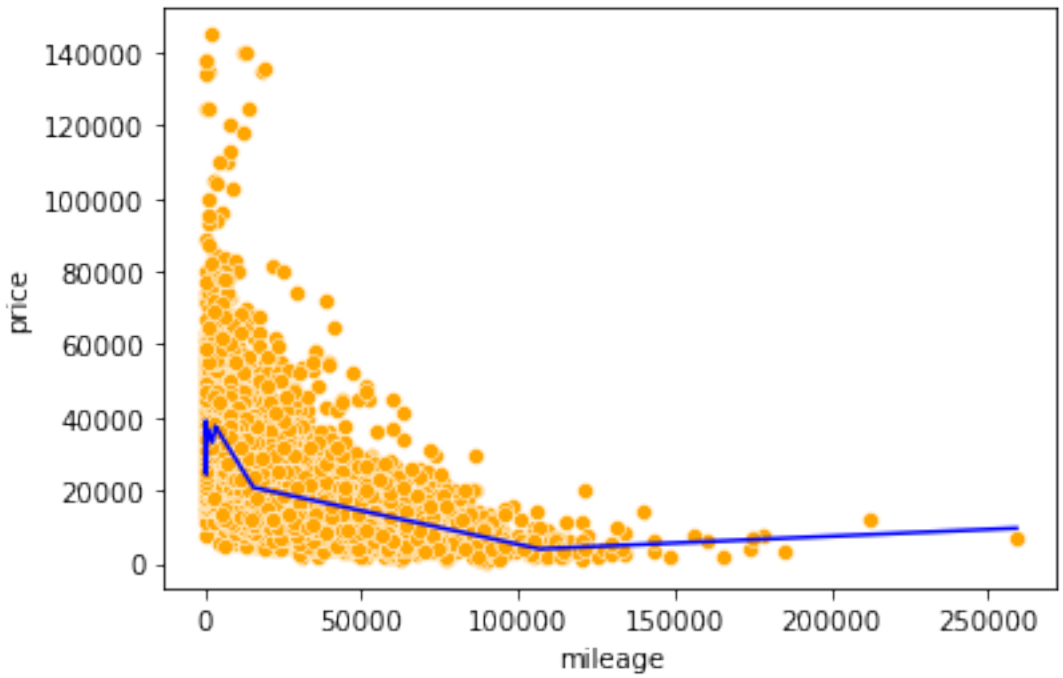
$$-553155 - 6.23(h(x0 - 3354)) - 36.96(h(x0 - 15413) + ... - 7.04(h(2456 - x0)$$

```
pred = model.predict(test.mileage)
np.sqrt(mean_squared_error(pred,test.price))
```

```
13650.2113154515
```

```
sns.scatterplot(x = 'mileage', y = 'price', data = train, color = 'orange')
sns.lineplot(x = train.mileage, y = model.predict(train.mileage), color = 'blue')
```

```
<AxesSubplot:xlabel='mileage', ylabel='price'>
```



2.5.2 MARS of degree 2

```
model = Earth(max_terms=500, max_degree=2) # note, terms in brackets are the hyperparamete
model.fit(X,y)
print(model.summary())
```

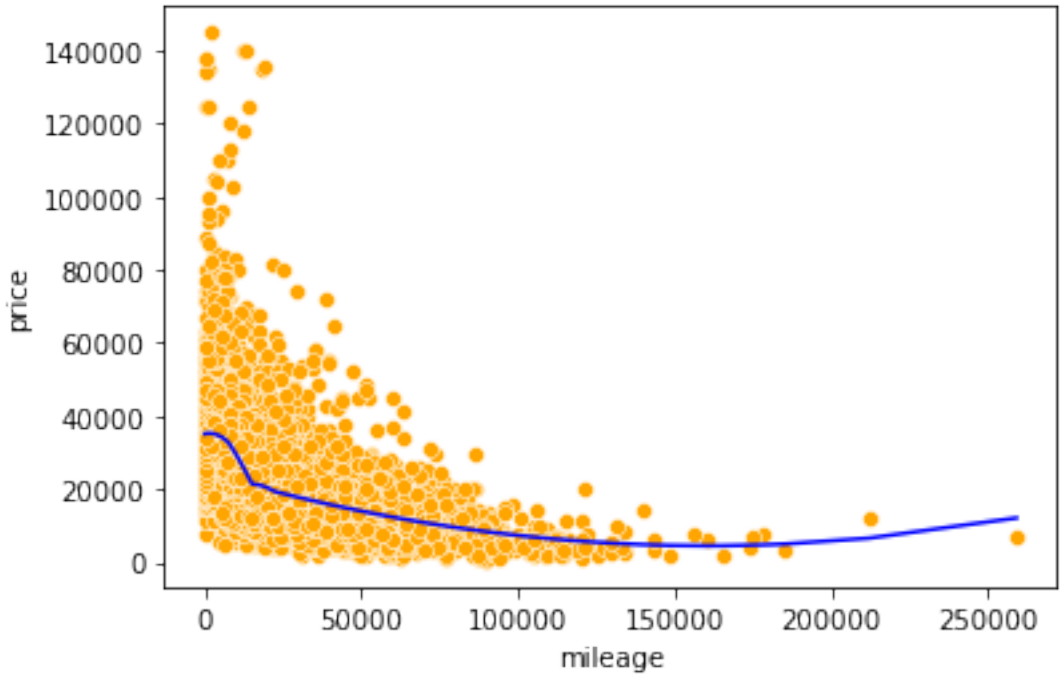
```
Earth Model
----------------------------------------------
Basis Function           Pruned  Coefficient
----------------------------------------------
(Intercept)              No      19369.7
h(x0-22141)              Yes     None
h(22141-x0)              Yes     None
h(x0-7531)*h(22141-x0)   No      3.74934e-05
h(7531-x0)*h(22141-x0)   No      -6.74252e-05
x0*h(x0-22141)           No      -8.0703e-06
h(x0-15012)              Yes     None
h(15012-x0)              No      1.79813
h(x0-26311)*h(x0-22141)  No      8.85097e-06
h(26311-x0)*h(x0-22141)  Yes     None
----------------------------------------------
MSE: 189264421.5682, GCV: 190298913.1652, RSQ: 0.2967, GRSQ: 0.2932

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

```
pred = model.predict(test.mileage)
np.sqrt(mean_squared_error(pred,test.price))
```

```
13590.995419204985
```

```
sns.scatterplot(x = 'mileage', y = 'price', data = train, color = 'orange')
sns.lineplot(x = train.mileage, y = model.predict(train.mileage), color = 'blue')
```

```
<AxesSubplot:xlabel='mileage', ylabel='price'>
```



MARS provides a better fit than the splines that we used above. This is because MARS tunes the positions of the knots and considers interactions (also with tuned knots) to improve the model fit. Tuning of knots may improve the fit of splines as well.

2.5.3 MARS including categorical variables

```
#A categorical variable can be turned to dummy variables to use the Earth package for fitt
train_cat = pd.concat([train,pd.get_dummies(train.fuelType)],axis=1)
test_cat = pd.concat([test,pd.get_dummies(test.fuelType)],axis=1)
```

```
train_cat.head()
```

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

```
X = train_cat[['mileage','mpg','engineSize','year','Diesel','Electric','Hybrid','Petrol']]
Xtest = test_cat[['mileage','mpg','engineSize','year','Diesel','Electric','Hybrid','Petrol
```

```
model = Earth(max_terms=500, max_degree=2) # note, terms in brackets are the hyperparamete
model.fit(X,y)
print(model.summary())
```

```
C:\Users\akl0407\Anaconda3\lib\site-packages\pyearth\earth.py:813: FutureWarning: `rcond` pa
To use the future default and silence this warning we advise to pass `rcond=None`, to keep us
  pruning_passer.run()

Earth Model
------------------------------------------------------------
Basis Function                        Pruned  Coefficient
------------------------------------------------------------
(Intercept)                           No      2.17604e+06
h(engineSize-5.5)                     No      9.80752e+06
h(5.5-engineSize)                     No      1.92817e+06
h(mileage-21050)                      No      18.687
h(21050-mileage)                      No      -177.871
h(mileage-21050)*h(5.5-engineSize)    Yes     None
h(21050-mileage)*h(5.5-engineSize)    No      -0.224909
year                                  No      4126.41
h(mpg-53.3495)                        No      344595
h(53.3495-mpg)                        Yes     None
Hybrid*h(5.5-engineSize)              No      6124.34
h(mileage-21050)*year                 No      -0.00930239
h(21050-mileage)*year                 No      0.0886455
h(engineSize-5.5)*year                No      -4864.84
h(5.5-engineSize)*year                No      -952.92
h(mileage-1422)*h(53.3495-mpg)        No      -16.62
h(1422-mileage)*h(53.3495-mpg)        No      16.4306
Hybrid                                No      -89090.6
h(mpg-21.1063)*h(53.3495-mpg)         Yes     None
h(21.1063-mpg)*h(53.3495-mpg)         No      -8815.99
h(mpg-23.4808)*h(5.5-engineSize)      No      -3649.97
h(23.4808-mpg)*h(5.5-engineSize)      Yes     None
h(mpg-20.5188)*year                   No      31.7341
h(20.5188-mpg)*year                   Yes     None
h(mpg-22.2566)*h(53.3495-mpg)         No      -52.2531
h(22.2566-mpg)*h(53.3495-mpg)         No      7916.19
```

```
h(mpg-22.6767)                      No      7.56432e+06
h(22.6767-mpg)                      Yes     None
h(mpg-23.9595)*h(mpg-22.6767)       Yes     None
h(23.9595-mpg)*h(mpg-22.6767)       No      -63225.4
h(mpg-21.4904)*h(22.6767-mpg)       No      -149055
h(21.4904-mpg)*h(22.6767-mpg)       Yes     None
h(mpg-21.1063)                      No      -887098
h(21.1063-mpg)                      Yes     None
h(mpg-29.5303)*h(mpg-22.6767)       No      -3028.87
h(29.5303-mpg)*h(mpg-22.6767)       Yes     None
h(mpg-28.0681)*h(5.5-engineSize)    No      3572.89
h(28.0681-mpg)*h(5.5-engineSize)    Yes     None
engineSize*h(5.5-engineSize)        No      -2952.65
h(mpg-25.3175)*h(mpg-21.1063)       No      -332551
h(25.3175-mpg)*h(mpg-21.1063)       No      324298
Petrol*year                         No      -1.37031
h(mpg-68.9279)*Hybrid               No      -4087.9
h(68.9279-mpg)*Hybrid               Yes     None
h(mpg-31.5043)*h(5.5-engineSize)    Yes     None
h(31.5043-mpg)*h(5.5-engineSize)    No      3691.82
h(mpg-32.7011)*h(5.5-engineSize)    Yes     None
h(32.7011-mpg)*h(5.5-engineSize)    No      -2262.78
h(mpg-44.9122)*h(mpg-22.6767)       No      335577
h(44.9122-mpg)*h(mpg-22.6767)       No      -335623
h(engineSize-5.5)*h(mpg-21.1063)    No      27815
h(5.5-engineSize)*h(mpg-21.1063)    Yes     None
h(mpg-78.1907)*Hybrid               Yes     None
h(78.1907-mpg)*Hybrid               No      2221.49
h(mpg-63.1632)*h(mpg-22.6767)       Yes     None
h(63.1632-mpg)*h(mpg-22.6767)       No      21.0093
Hybrid*h(mpg-53.3495)               No      4121.91
h(mileage-22058)*h(53.3495-mpg)     No      16.6177
h(22058-mileage)*h(53.3495-mpg)     No      -16.6044
h(mpg-21.8985)                      Yes     None
h(21.8985-mpg)                      No      371659
---------------------------------------------------------
MSE: 45859836.5623, GCV: 47884649.3622, RSQ: 0.8296, GRSQ: 0.8221

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

```
pred = model.predict(Xtest)
np.sqrt(mean_squared_error(pred,test2.price))
```

```
7499.709075454322
```

Let us compare the RMSE of a MARS model with *mileage, mpg, engineSize* and *year* with a linear regression model having the same predictors.

```
X = train[['mileage','mpg','engineSize','year']]
```

```
model = Earth(max_terms=500, max_degree=2) # note, terms in brackets are the hyperparamete
model.fit(X,y)
print(model.summary())
```

```
C:\Users\akl0407\Anaconda3\lib\site-packages\pyearth\earth.py:813: FutureWarning: `rcond` pa
To use the future default and silence this warning we advise to pass `rcond=None`, to keep us
  pruning_passer.run()

Earth Model
------------------------------------------------------------
Basis Function                      Pruned  Coefficient
------------------------------------------------------------
(Intercept)                         No      -8.13682e+06
h(engineSize-5.5)                   No      9.53908e+06
h(5.5-engineSize)                   Yes     None
h(mileage-21050)                    No      23.4448
h(21050-mileage)                    No      -215.861
h(mileage-21050)*h(5.5-engineSize)  Yes     None
h(21050-mileage)*h(5.5-engineSize)  No      -0.278562
year                                No      4125.85
h(mpg-53.3495)                      Yes     None
h(53.3495-mpg)                      Yes     None
h(mileage-21050)*year               No      -0.0116601
h(21050-mileage)*year               No      0.107624
h(mpg-53.2957)*h(5.5-engineSize)    No      -59801.3
h(53.2957-mpg)*h(5.5-engineSize)    No      59950.5
h(engineSize-5.5)*year              No      -4713.74
h(5.5-engineSize)*year              No      -755.742
h(mileage-1766)*h(53.3495-mpg)      No      -0.00337072
h(1766-mileage)*h(53.3495-mpg)      No      -0.144905
```

```
h(mpg-19.1277)*h(53.3495-mpg)       No      161.153
h(19.1277-mpg)*h(53.3495-mpg)       Yes     None
h(mpg-23.4808)*h(5.5-engineSize)    Yes     None
h(23.4808-mpg)*h(5.5-engineSize)    Yes     None
h(mpg-21.4971)*h(5.5-engineSize)    Yes     None
h(21.4971-mpg)*h(5.5-engineSize)    Yes     None
h(mpg-40.224)*h(5.5-engineSize)     Yes     None
h(40.224-mpg)*h(5.5-engineSize)     No      298.139
engineSize*h(5.5-engineSize)        No      -2553.17
h(mpg-22.2566)                      Yes     None
h(22.2566-mpg)                      No      29257.3
h(mpg-20.7712)*h(22.2566-mpg)       No      143796
h(20.7712-mpg)*h(22.2566-mpg)       No      -1249.17
h(mpg-21.4971)*h(22.2566-mpg)       No      -315486
h(21.4971-mpg)*h(22.2566-mpg)       Yes     None
h(mpg-27.0995)*h(mpg-22.2566)       No      3855.71
h(27.0995-mpg)*h(mpg-22.2566)       Yes     None
h(mpg-29.3902)*year                 No      6.05449
h(29.3902-mpg)*year                 No      -20.176
h(mpg-28.0681)*h(5.5-engineSize)    No      59901.6
h(28.0681-mpg)*h(5.5-engineSize)    No      -55502.2
h(mpg-23.2962)*h(mpg-22.2566)       No      -56126
h(23.2962-mpg)*h(mpg-22.2566)       No      73153.9
h(mpg-69.0719)*h(mpg-53.3495)       Yes     None
h(69.0719-mpg)*h(mpg-53.3495)       No      -124.847
h(engineSize-5.5)*h(22.2566-mpg)    No      -20955.8
h(5.5-engineSize)*h(22.2566-mpg)    No      -8336.23
h(mpg-23.9595)*h(mpg-22.2566)       No      -62983
h(23.9595-mpg)*h(mpg-22.2566)       Yes     None
h(mpg-23.6406)*h(mpg-22.2566)       No      115253
h(23.6406-mpg)*h(mpg-22.2566)       Yes     None
h(mpg-56.1908)                      Yes     None
h(56.1908-mpg)                      No      -2239.85
h(mpg-29.7993)*h(53.3495-mpg)       No      -139.61
h(29.7993-mpg)*h(53.3495-mpg)       No      788.756
------------------------------------------------------------
MSE: 49704412.0771, GCV: 51526765.3943, RSQ: 0.8153, GRSQ: 0.8086

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

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

```
7614.158359050244
```

```
ols_object = smf.ols(formula = 'price~(year+engineSize+mileage+mpg)**2', data = train)
model = ols_object.fit()
pred = model.predict(test)
np.sqrt(mean_squared_error(pred,test.price))
```

```
8729.912066822455
```

The RMSE for the MARS model is lesser than that of the linear regression model, as expected.

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 reponse 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 respone 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)

#Statfied splitting with respect to the response and predictors to create 50% train and te
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=da

#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 repect 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_CatPred
```

```
# Comparing model performance metrics when the data is split into train and test by perfor
# (1) only with repect 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_stat
    model = LogisticRegression()
    model.fit(X_train, y_train)

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

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

# 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 repect 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()
```

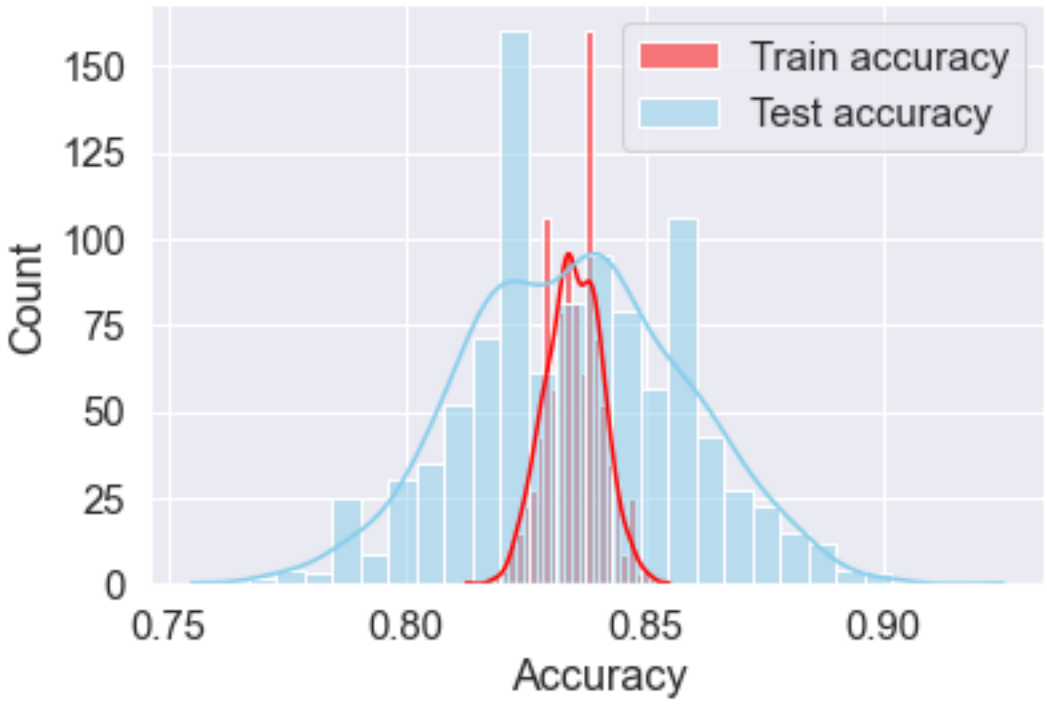
	train_y_stratified	test_y_stratified	train_y_CatPredictors_stratified	test_y_CatPredictors_st
count	999.000000	999.000000	9.990000e+02	9.990000e+02
mean	0.834962	0.835150	8.350000e-01	8.350000e-01
std	0.005833	0.023333	8.552999e-15	8.552999e-15
min	0.812500	0.755000	8.350000e-01	8.350000e-01
25%	0.831250	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 accurac
sns.histplot(data=accuracy_iter, x="test_y_stratified", color="skyblue", label="Test accur
plt.legend()
plt.xlabel('Accuracy')
```

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

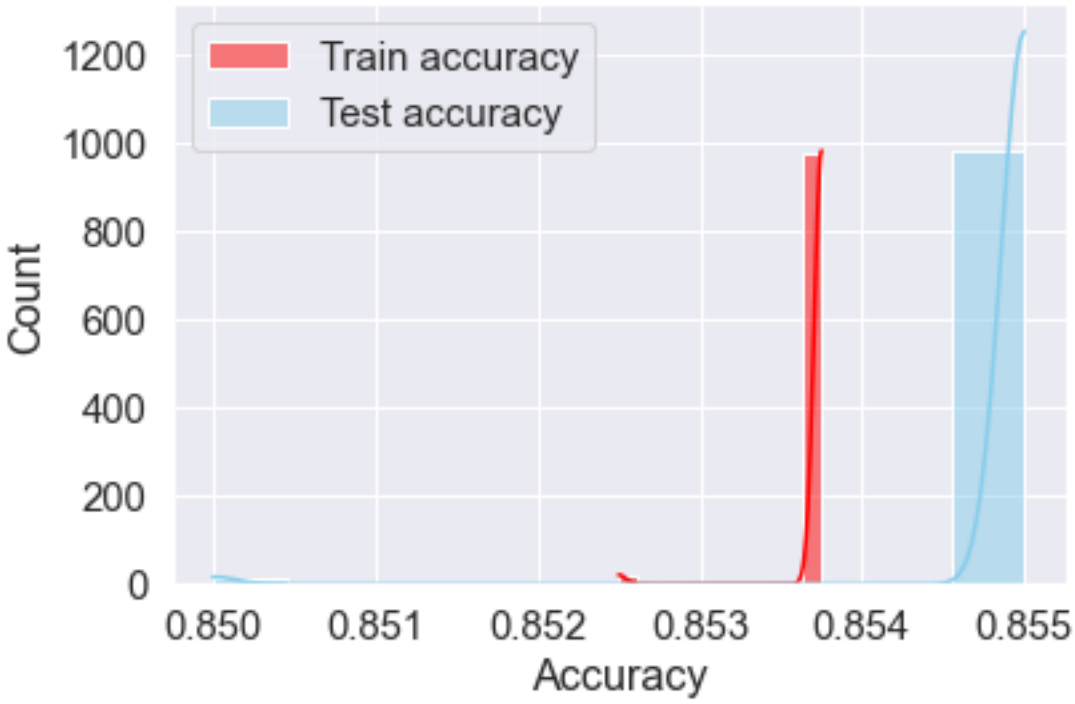


Note the variability in train and test accuracies when the data is stratified only with respect to the response. The train accuracy varies betweem 81.2% and 85.5%, while the test accuracy varies between 75.5% and 92.5%.

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=
sns.histplot(data=accuracy_iter, x="test_y_CatPredictors_stratified", color="skyblue", lab
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 startifying 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 Datasets, assignment and project files

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

References