Model Evaluation and Refinement Lab

January 10, 2024

1 Model Evaluation and Refinement

Estimated time needed: 30 minutes

1.1 Objectives

After completing this lab you will be able to:

• Evaluate and refine prediction models

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Grid Search

If you are running the lab in your browser in Skills Network lab, so need to install the libraries using piplite.

```
#you are running the lab in your browser, so we will install the libraries

using `piplite`

'''import piplite
await piplite.install(['pandas'])
await piplite.install(['matplotlib'])
await piplite.install(['scipy'])
await piplite.install(['scikit-learn'])
await piplite.install(['seaborn'])'''
```

[1]: "import piplite\nawait piplite.install(['pandas'])\nawait piplite.install(['matplotlib'])\nawait piplite.install(['scipy'])\nawait piplite.install(['scikit-learn'])\nawait piplite.install(['seaborn'])"

If you run the lab locally using Anaconda, you can load the correct library and versions by uncommenting the following:

```
[2]: #If you run the lab locally using Anaconda, you can load the correct library and versions by uncommenting the following:
#install specific version of libraries used in lab
```

```
#! mamba install pandas==1.3.3-y
#! mamba install numpy=1.21.2-y
#! mamba install sklearn=0.20.1-y
```

Import libraries:

```
[3]: import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import warnings
warnings.filterwarnings('ignore')
```

This function will download the dataset into your browser

```
[4]: #This function will download the dataset into your browser

'''from pyodide.http import pyfetch

async def download(url, filename):
    response = await pyfetch(url)
    if response.status == 200:
        with open(filename, "wb") as f:
        f.write(await response.bytes())'''
```

[4]: 'from pyodide.http import pyfetch\n\nasync def download(url, filename):\n
response = await pyfetch(url)\n if response.status == 200:\n with
open(filename, "wb") as f:\n f.write(await response.bytes())'

This dataset was hosted on IBM Cloud object. Click HERE for free storage.

you will need to download the dataset; using the 'download()' function.

```
[5]: #you will need to download the dataset;

#await download('https://cf-courses-data.s3.us.cloud-object-storage.appdomain.

-cloud/IBMDeveloperSkillsNetwork-DA0101EN-SkillsNetwork/labs/Data%20files/

-module_5_auto.csv', 'module_5_auto.csv')
```

Load the data and store it in dataframe df:

```
[6]: df = pd.read_csv("usedCars.csv", header=0)
```

```
[7]: df.head()
```

```
[7]:
        symboling normalized-losses
                                               make aspiration num-of-doors
     0
                3
                                  122 alfa-romero
                                                            std
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                3
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                                  122 alfa-romero
                                                            std
                                                                         two
     3
                2
                                  164
                                                            std
                                                                        four
                                               audi
     4
                2
                                  164
                                                                        four
                                               audi
                                                            std
```

```
body-style drive-wheels engine-location wheel-base
                                                             length ...
  convertible
                                                    88.6 0.811148
                                       front
0
                        rwd
1
  convertible
                        rwd
                                       front
                                                    88.6 0.811148
                                                    94.5 0.822681
2
     hatchback
                        rwd
                                       front
3
         sedan
                        fwd
                                                    99.8 0.848630
                                       front
         sedan
                        4wd
                                       front
                                                    99.4 0.848630
   compression-ratio horsepower
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                                                               27 16500.0
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                           102.0
                                     5500.0
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                                                               30 13950.0
                 8.0
                           115.0
                                     5500.0
                                                  18
                                                               22 17450.0
  city-L/100km horsepower-binned
                                    diesel
                                            gas
     11.190476
0
                           Medium
                                         0
                                              1
     11.190476
                                         0
                                              1
1
                           Medium
2
     12.368421
                           Medium
                                         0
                                              1
3
     9.791667
                           Medium
                                         0
                                              1
     13.055556
                           Medium
```

[5 rows x 29 columns]

First, let's only use numeric data:

Let's remove the columns 'Unnamed:0.1' and 'Unnamed:0' since they do not provide any value to the models.

```
[9]: #df.drop(['Unnamed: 0.1', 'Unnamed: 0'], axis=1, inplace=True)

# Let's take a look at the updated DataFrame
#df.head()
```

Libraries for plotting:

```
[10]: from ipywidgets import interact, interactive, fixed, interact_manual
```

Functions for Plotting

```
[11]: def DistributionPlot(RedFunction, BlueFunction, RedName, BlueName, Title):
    width = 12
    height = 10
    plt.figure(figsize=(width, height))

ax1 = sns.kdeplot(RedFunction, color="r", label=RedName)
    ax2 = sns.kdeplot(BlueFunction, color="b", label=BlueName, ax=ax1)
```

```
plt.title(Title)
plt.xlabel('Price (in dollars)')
plt.ylabel('Proportion of Cars')
plt.show()
plt.close()
```

```
[12]: def PollyPlot(xtrain, xtest, y_train, y_test, lr,poly_transform):
          width = 12
          height = 10
          plt.figure(figsize=(width, height))
          #training data
          #testing data
          # lr: linear regression object
          #poly_transform: polynomial transformation object
          xmax=max([xtrain.values.max(), xtest.values.max()])
          xmin=min([xtrain.values.min(), xtest.values.min()])
          x=np.arange(xmin, xmax, 0.1)
          plt.plot(xtrain, y_train, 'ro', label='Training Data')
          plt.plot(xtest, y_test, 'go', label='Test Data')
          plt.plot(x, lr.predict(poly_transform.fit_transform(x.reshape(-1, 1))),__
       ⇔label='Predicted Function')
          plt.ylim([-10000, 60000])
          plt.ylabel('Price')
          plt.legend()
```

Part 1: Training and Testing

An important step in testing your model is to split your data into training and testing data. We will place the target data price in a separate dataframe y_data:

```
[13]: y_data = df['price']
```

Drop price data in dataframe **x** data:

```
[14]: x_data=df.drop('price',axis=1)
```

Now, we randomly split our data into training and testing data using the function train_test_split.

```
[15]: from sklearn.model_selection import train_test_split
```

```
number of test samples: 21 number of training samples: 180
```

The test_size parameter sets the proportion of data that is split into the testing set. In the above, the testing set is 10% of the total dataset.

Question #1):

Use the function "train_test_split" to split up the dataset such that 40% of the data samples will be utilized for testing. Set the parameter "random_state" equal to zero. The output of the function should be the following: "x_train1", "x_test1", "y_train1" and "y_test1".

```
number of test samples : 81
number of training samples: 120
```

Let's import LinearRegression from the module linear model.

```
[17]: from sklearn.linear_model import LinearRegression
```

We create a Linear Regression object:

```
[18]: lre=LinearRegression()
```

We fit the model using the feature "horsepower":

```
[19]: | lre.fit(x_train[['horsepower']], y_train)
```

[19]: LinearRegression()

Let's calculate the R² on the test data:

```
[20]: | lre.score(x_test[['horsepower']], y_test)
```

[20]: 0.36358755750788263

We can see the R² is much smaller using the test data compared to the training data.

```
[21]: lre.score(x_train[['horsepower']], y_train)
```

[21]: 0.6619724197515104

Question #2):

Find the R² on the test data using 40% of the dataset for testing.

[22]: 0.7139364665406973

Sometimes you do not have sufficient testing data; as a result, you may want to perform cross-validation. Let's go over several methods that you can use for cross-validation.

Cross-Validation Score

Let's import cross val score from the module model selection.

```
[23]: from sklearn.model_selection import cross_val_score
```

We input the object, the feature ("horsepower"), and the target data (y_data). The parameter 'cv' determines the number of folds. In this case, it is 4.

```
[24]: Rcross = cross_val_score(lre, x_data[['horsepower']], y_data, cv=4)
```

The default scoring is R². Each element in the array has the average R² value for the fold:

```
[25]: Rcross
```

```
[25]: array([0.7746232, 0.51716687, 0.74785353, 0.04839605])
```

We can calculate the average and standard deviation of our estimate:

```
[26]: print("The mean of the folds are", Rcross.mean(), "and the standard deviation

→is" , Rcross.std())
```

The mean of the folds are 0.522009915042119 and the standard deviation is 0.29118394447560286

We can use negative squared error as a score by setting the parameter 'scoring' metric to 'neg mean squared error'.

```
[27]: -1 * cross_val_score(lre,x_data[['horsepower']],__

y_data,cv=4,scoring='neg_mean_squared_error')
```

```
[27]: array([20254142.84026704, 43745493.26505169, 12539630.34014931, 17561927.7224759])
```

Question #3):

Calculate the average R^2 using two folds, then find the average R^2 for the second fold utilizing the "horsepower" feature:

```
[28]: Rc=cross_val_score(lre,x_data[['horsepower']], y_data,cv=2)
Rc.mean()
```

[28]: 0.5166761697127429

You can also use the function 'cross_val_predict' to predict the output. The function splits up the data into the specified number of folds, with one fold for testing and the other folds are used for training. First, import the function:

```
[29]: from sklearn.model_selection import cross_val_predict
```

We input the object, the feature "horsepower", and the target data y_data. The parameter 'cv' determines the number of folds. In this case, it is 4. We can produce an output:

```
[30]: yhat = cross_val_predict(lre,x_data[['horsepower']], y_data,cv=4) yhat[0:5]
```

```
[30]: array([14141.63807508, 14141.63807508, 20814.29423473, 12745.03562306, 14762.35027598])
```

Part 2: Overfitting, Underfitting and Model Selection

It turns out that the test data, sometimes referred to as the "out of sample data", is a much better measure of how well your model performs in the real world. One reason for this is overfitting.

Let's go over some examples. It turns out these differences are more apparent in Multiple Linear Regression and Polynomial Regression so we will explore overfitting in that context.

Let's create Multiple Linear Regression objects and train the model using 'horsepower', 'curb-weight', 'engine-size' and 'highway-mpg' as features.

```
[31]: lr = LinearRegression()
lr.fit(x_train[['horsepower', 'curb-weight', 'engine-size', 'highway-mpg']],

→y_train)
```

[31]: LinearRegression()

Prediction using training data:

```
[32]: array([7426.6731551, 28323.75090803, 14213.38819709, 4052.34146983, 34500.19124244])
```

Prediction using test data:

```
[33]: array([11349.35089149, 5884.11059106, 11208.6928275, 6641.07786278, 15565.79920282])
```

Let's perform some model evaluation using our training and testing data separately. First, we import the seaborn and matplotlib library for plotting.

```
[34]: import matplotlib.pyplot as plt
%matplotlib inline
import seaborn as sns
```

Let's examine the distribution of the predicted values of the training data.

```
[35]: Title = 'Distribution Plot of Predicted Value Using Training Data vs Training

⇔Data Distribution'

DistributionPlot(y_train, yhat_train, "Actual Values (Train)", "Predicted

⇔Values (Train)", Title)
```

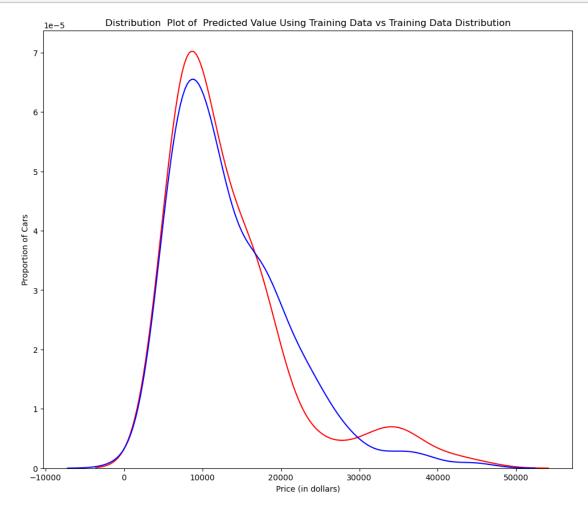


Figure 1: Plot of predicted values using the training data compared to the actual values of the training data.

So far, the model seems to be doing well in learning from the training dataset. But what happens when the model encounters new data from the testing dataset? When the model generates new values from the test data, we see the distribution of the predicted values is much different from the actual target values.

```
[36]: Title='Distribution Plot of Predicted Value Using Test Data vs Data

⇔Distribution of Test Data'

DistributionPlot(y_test,yhat_test,"Actual Values (Test)","Predicted Values

⇔(Test)",Title)
```

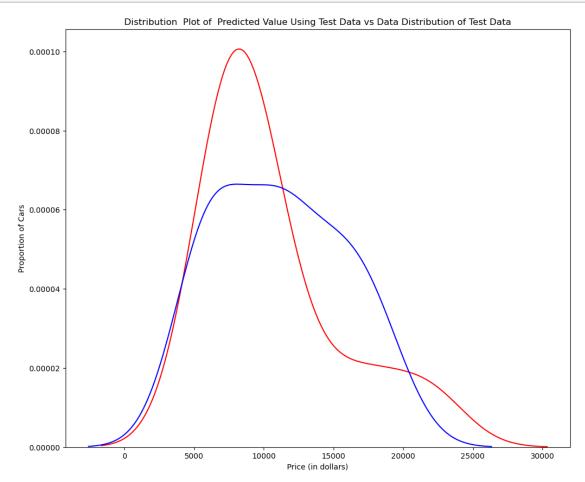


Figure 2: Plot of predicted value using the test data compared to the actual values of the test data.

Comparing Figure 1 and Figure 2, it is evident that the distribution of the test data in Figure 1 is much better at fitting the data. This difference in Figure 2 is apparent in the range of 5000 to 15,000. This is where the shape of the distribution is extremely different. Let's see if polynomial regression also exhibits a drop in the prediction accuracy when analysing the test dataset.

```
[37]: from sklearn.preprocessing import PolynomialFeatures
```

Overfitting

Overfitting occurs when the model fits the noise, but not the underlying process. Therefore, when testing your model using the test set, your model does not perform as well since it is modelling noise, not the underlying process that generated the relationship. Let's create a degree 5 polynomial model.

Let's use 55 percent of the data for training and the rest for testing:

```
[38]: x_train, x_test, y_train, y_test = train_test_split(x_data, y_data, test_size=0. 45, random_state=0)
```

We will perform a degree 5 polynomial transformation on the feature 'horsepower'.

```
[39]: pr = PolynomialFeatures(degree=5)
    x_train_pr = pr.fit_transform(x_train[['horsepower']])
    x_test_pr = pr.fit_transform(x_test[['horsepower']])
    pr
```

[39]: PolynomialFeatures(degree=5)

Now, let's create a Linear Regression model "poly" and train it.

```
[40]: poly = LinearRegression()
poly.fit(x_train_pr, y_train)
```

[40]: LinearRegression()

We can see the output of our model using the method "predict." We assign the values to "yhat".

```
[41]: yhat = poly.predict(x_test_pr)
yhat[0:5]
```

[41]: array([6728.58615619, 7307.91973653, 12213.73734432, 18893.37966315, 19996.10669225])

Let's take the first five predicted values and compare it to the actual targets.

```
[42]: print("Predicted values:", yhat[0:4])
print("True values:", y_test[0:4].values)
```

```
Predicted values: [ 6728.58615619 7307.91973653 12213.73734432 18893.37966315]
True values: [ 6295. 10698. 13860. 13499.]
```

We will use the function "PollyPlot" that we defined at the beginning of the lab to display the training data, testing data, and the predicted function.

```
[43]: PollyPlot(x_train['horsepower'], x_test['horsepower'], y_train, y_test, poly,pr)
```

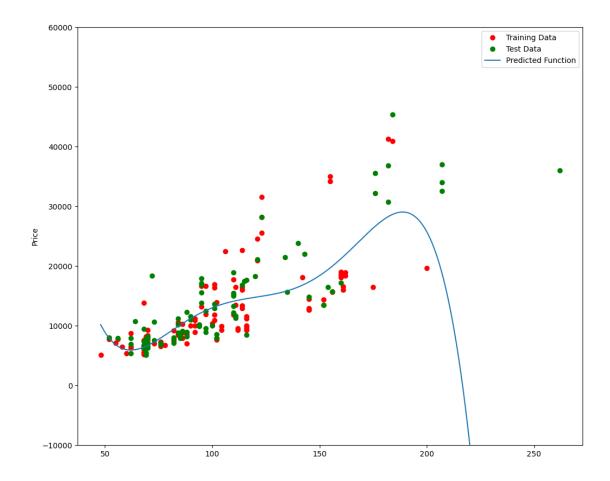


Figure 3: A polynomial regression model where red dots represent training data, green dots represent test data, and the blue line represents the model prediction.

We see that the estimated function appears to track the data but around 200 horsepower, the function begins to diverge from the data points.

R² of the training data:

```
[44]: poly.score(x_train_pr, y_train)
```

[44]: 0.5567716897727109

R^2 of the test data:

```
[45]: poly.score(x_test_pr, y_test)
```

[45]: -29.870994900857237

We see the R² for the training data is 0.5567 while the R² on the test data was -29.87. The lower the R², the worse the model. A negative R² is a sign of overfitting.

Let's see how the R^2 changes on the test data for different order polynomials and then plot the results:

```
[46]: Rsqu_test = []

order = [1, 2, 3, 4]
for n in order:
    pr = PolynomialFeatures(degree=n)

    x_train_pr = pr.fit_transform(x_train[['horsepower']])

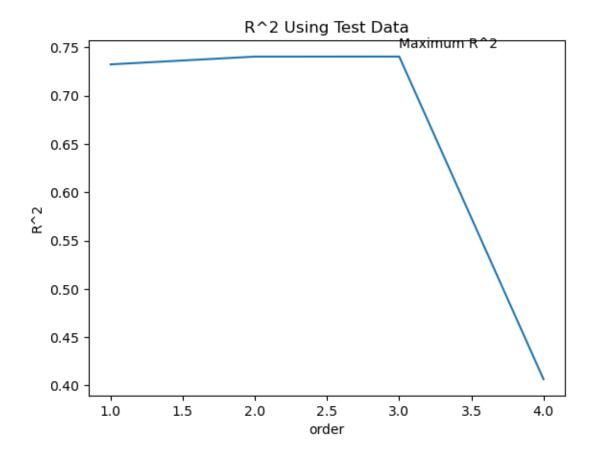
    x_test_pr = pr.fit_transform(x_test[['horsepower']])

    lr.fit(x_train_pr, y_train)

    Rsqu_test.append(lr.score(x_test_pr, y_test))

plt.plot(order, Rsqu_test)
plt.xlabel('order')
plt.ylabel('R^2')
plt.title('R^2 Using Test Data')
plt.text(3, 0.75, 'Maximum R^2 ')
```

[46]: Text(3, 0.75, 'Maximum R^2')



We see the R² gradually increases until an order three polynomial is used. Then, the R² dramatically decreases at an order four polynomial.

The following function will be used in the next section. Please run the cell below.

The following interface allows you to experiment with different polynomial orders and different amounts of data.

```
[48]: interact(f, order=(0, 6, 1), test_data=(0.05, 0.95, 0.05))
```

interactive(children=(IntSlider(value=3, description='order', max=6), \$\infty\$FloatSlider(value=0.45, description='tes...)

[48]: <function __main__.f(order, test_data)>

Question #4a):

We can perform polynomial transformations with more than one feature. Create a "PolynomialFeatures" object "pr1" of degree two.

```
[49]: pr1=PolynomialFeatures(degree=2)
```

Question #4b):

Transform the training and testing samples for the features 'horsepower', 'curb-weight', 'engine-size' and 'highway-mpg'. Hint: use the method "fit_transform".

Question #4c):

How many dimensions does the new feature have? Hint: use the attribute "shape".

```
[51]: x_train_pr1.shape #there are now 15 features
```

[51]: (110, 15)

Question #4d):

Create a linear regression model "poly1". Train the object using the method "fit" using the polynomial features.

[52]: poly1=LinearRegression().fit(x_train_pr1,y_train)

Question #4e):

Use the method "predict" to predict an output on the polynomial features, then use the function "DistributionPlot" to display the distribution of the predicted test output vs. the actual test data.

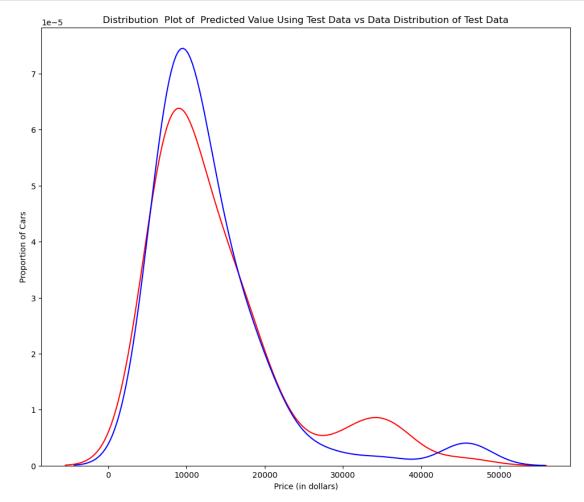
```
[53]: yhat_test1=poly1.predict(x_test_pr1)

Title='Distribution Plot of Predicted Value Using Test Data vs Data

→Distribution of Test Data'

DistributionPlot(y_test, yhat_test1, "Actual Values (Test)", "Predicted Values

→(Test)", Title)
```



Question #4f):

Using the distribution plot above, describe (in words) the two regions where the predicted prices are less accurate than the actual prices.

Part 3: Ridge Regression

In this section, we will review Ridge Regression and see how the parameter alpha changes the model. Just a note, here our test data will be used as validation data.

Let's perform a degree two polynomial transformation on our data.

Let's import Ridge from the module linear models.

```
[56]: from sklearn.linear_model import Ridge
```

Let's create a Ridge regression object, setting the regularization parameter (alpha) to 0.1

```
[57]: RigeModel=Ridge(alpha=1)
```

Like regular regression, you can fit the model using the method fit.

```
[58]: RigeModel.fit(x_train_pr, y_train)
```

[58]: Ridge(alpha=1)

Similarly, you can obtain a prediction:

```
[59]: yhat = RigeModel.predict(x_test_pr)
```

Let's compare the first five predicted samples to our test set:

```
[60]: print('predicted:', yhat[0:4]) print('test set :', y_test[0:4].values)
```

```
predicted: [ 6570.82441941 9636.24891471 20949.92322737 19403.60313255]
test set : [ 6295. 10698. 13860. 13499.]
```

We select the value of alpha that minimizes the test error. To do so, we can use a for loop. We have also created a progress bar to see how many iterations we have completed so far.

```
[61]: from tqdm import tqdm
      Rsqu_test = []
      Rsqu_train = []
      dummy1 = []
      Alpha = 10 * np.array(range(0,1000))
      pbar = tqdm(Alpha)
      for alpha in pbar:
          RigeModel = Ridge(alpha=alpha)
          RigeModel.fit(x_train_pr, y_train)
          test_score, train_score = RigeModel.score(x_test_pr, y_test), RigeModel.
       score(x_train_pr, y_train)
          pbar.set_postfix({"Test Score": test_score, "Train Score": train_score})
          Rsqu_test.append(test_score)
          Rsqu_train.append(train_score)
     100%|
                                 | 1000/1000 [00:05<00:00,
     176.89it/s, Test Score=0.564, Train Score=0.859]
     We can plot out the value of R<sup>2</sup> for different alphas:
[62]: width = 12
      height = 10
      plt.figure(figsize=(width, height))
      plt.plot(Alpha,Rsqu_test, label='validation data ')
      plt.plot(Alpha,Rsqu_train, 'r', label='training Data ')
      plt.xlabel('alpha')
      plt.ylabel('R^2')
      plt.legend()
```

[62]: <matplotlib.legend.Legend at 0x13bac6c5d50>

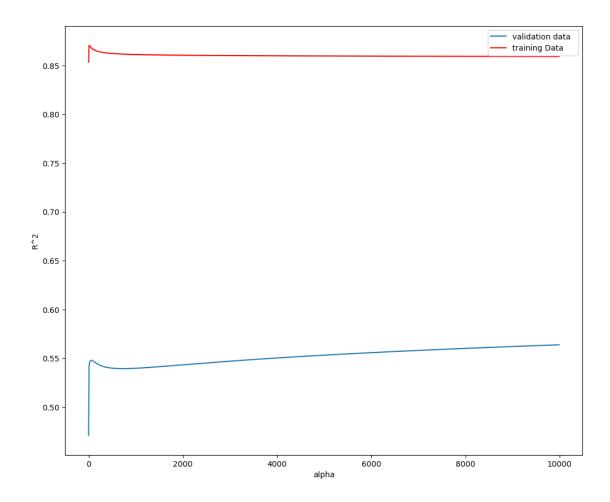


Figure 4: The blue line represents the R² of the validation data, and the red line represents the R² of the training data. The x-axis represents the different values of Alpha.

Here the model is built and tested on the same data, so the training and test data are the same.

The red line in Figure 4 represents the R^2 of the training data. As alpha increases the R^2 decreases. Therefore, as alpha increases, the model performs worse on the training data

The blue line represents the R² on the validation data. As the value for alpha increases, the R² increases and converges at a point.

Question #5):

Perform Ridge regression. Calculate the R^2 using the polynomial features, use the training data to train the model and use the test data to test the model. The parameter alpha should be set to 10.

```
[63]: RigeModel = Ridge(alpha=10)
RigeModel.fit(x_train_pr, y_train)
RigeModel.score(x_test_pr, y_test)
```

[63]: 0.5418576440206405

Part 4: Grid Search

The term alpha is a hyperparameter. Sklearn has the class GridSearchCV to make the process of finding the best hyperparameter simpler.

Let's import GridSearchCV from the module model_selection.

```
[64]: from sklearn.model_selection import GridSearchCV
```

We create a dictionary of parameter values:

```
[65]: parameters1= [{'alpha': [0.001,0.1,1, 10, 100, 1000, 10000, 100000]}] parameters1
```

```
[65]: [{'alpha': [0.001, 0.1, 1, 10, 100, 1000, 10000, 100000, 100000]}]
```

Create a Ridge regression object:

```
[66]: RR=Ridge()
RR
```

[66]: Ridge()

Create a ridge grid search object:

```
[67]: Grid1 = GridSearchCV(RR, parameters1,cv=4)
```

Fit the model:

```
[68]: Grid1.fit(x_data[['horsepower', 'curb-weight', 'engine-size', 'highway-mpg']], ⊔  
□y_data)
```

```
[68]: GridSearchCV(cv=4, estimator=Ridge(),
param_grid=[{'alpha': [0.001, 0.1, 1, 10, 100, 10000, 100000, 100000]}])
```

The object finds the best parameter values on the validation data. We can obtain the estimator with the best parameters and assign it to the variable BestRR as follows:

```
[69]: BestRR=Grid1.best_estimator_
BestRR
```

[69]: Ridge(alpha=10000)

We now test our model on the test data:

[70]: 0.841164983103615

Question #6):

Perform a grid search for the alpha parameter and the normalization parameter, then find the best values of the parameters:

[71]: Ridge(alpha=10000)

[]: