Model Evaluation and Refinement

January 23, 2024

1 Model Evaluation and Refinement

Estimated time needed: 30 minutes

Lab Component by Dhesika

1.1 Objectives

• Evaluate and refine prediction models

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Over-fitting, Under-fitting and Model Selection

Ridge Regression

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(['scaborn'])'''
```

[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())'
```

```
[5]: #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]:
        Unnamed: O symboling normalized-losses
                                                           make num-of-doors \
     0
                 0
                             3
                                              122 alfa-romero
                                                                         two
                             3
     1
                 1
                                              122 alfa-romero
                                                                         two
                 2
     2
                             1
                                              122 alfa-romero
                                                                         two
     3
                 3
                             2
                                              164
                                                           audi
                                                                        four
     4
                             2
                                              164
                                                           audi
                                                                        four
```

```
body-style drive-wheels engine-location wheel-base length ... \ 0 convertible rwd front 88.6 0.811148 ... 1 convertible rwd front 88.6 0.811148 ...
```

```
2
     hatchback
                        rwd
                                       front
                                                     94.5 0.822681
3
         sedan
                         fwd
                                       front
                                                     99.8 0.848630
4
         sedan
                        4wd
                                       front
                                                     99.4 0.848630
   peak-rpm
            city-mpg
                       highway-mpg
                                       price city-L/100km horsepower-binned
0
     5000.0
                                    13495.0
                                                 11.190476
                   21
                           8.703704
                                                                           Low
     5000.0
1
                   21
                           8.703704
                                     16500.0
                                                 11.190476
                                                                           Low
2
     5000.0
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                   19
                           9.038462
                                     16500.0
                                                 12.368421
3
     5500.0
                   24
                           7.833333
                                     13950.0
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                                                 9.791667
4
     5500.0
                   18
                          10.681818
                                     17450.0
                                                 13.055556
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  fuel-type-diesel
                   fuel-type-gas
                                    aspiration-std aspiration-turbo
0
             False
                              True
                                              True
                                                                False
                                              True
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1
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2
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                                                                False
3
                              True
             False
                                              True
                                                                False
4
             False
                              True
                                              True
                                                                False
```

[5 rows x 31 columns]

First, let's only use numeric data:

```
[8]: df=df._get_numeric_data() df.head(20)
```

[8]:	IInnomod. O	symboling	normalized-losses	rrhool-bogo	longth	i d+h	\
	Unnamed: 0	·			length	width	\
0	0	3	122	88.6	0.811148	0.890278	
1	1	3	122	88.6	0.811148	0.890278	
2	2	1	122	94.5	0.822681	0.909722	
3	3	2	164	99.8	0.848630	0.919444	
4	4	2	164	99.4	0.848630	0.922222	
5	5	2	122	99.8	0.851994	0.920833	
6	6	1	158	105.8	0.925997	0.991667	
7	7	1	122	105.8	0.925997	0.991667	
8	8	1	158	105.8	0.925997	0.991667	
9	9	2	192	101.2	0.849592	0.900000	
10	10	0	192	101.2	0.849592	0.900000	
11	11	0	188	101.2	0.849592	0.900000	
12	12	0	188	101.2	0.849592	0.900000	
13	13	1	122	103.5	0.908217	0.929167	
14	14	0	122	103.5	0.908217	0.929167	
15	15	0	122	103.5	0.931283	0.943056	
16	16	0	122	110.0	0.946660	0.984722	
17	17	2	121	88.4	0.678039	0.837500	
18	18	1	98	94.5	0.749159	0.883333	
19	19	0	81	94.5	0.763095	0.883333	

height curb-weight engine-size bore ... horsepower peak-rpm \

^	0.046054	0540		400	0 47		444	F000	_
0	0.816054	2548		130	3.47	•••	111	5000	
1	0.816054	2548		130	3.47	•••	111	5000	.0
2	0.876254	2823		152	2.68	•••	154	5000	.0
3	0.908027	2337		109	3.19	•••	102	5500	.0
4	0.908027	2824		136	3.19	•••	115	5500	.0
5	0.887960	2507		136	3.19	•••	110	5500	
6	0.931438	2844		136	3.19		110	5500	
						•••			
7	0.931438	2954		136	3.19	•••	110	5500	
8	0.934783	3086		131	3.13	•••	140	5500	
9	0.908027	2395		108	3.50	•••	101	5800	
10	0.908027	2395		108	3.50	•••	101	5800	.0
11	0.908027	2710		164	3.31	•••	121	4250	.0
12	0.908027	2765		164	3.31	•••	121	4250	.0
13	0.931438	3055		164	3.31	•••	121	4250	.0
14	0.931438	3230		209	3.62	•••	182	5400	
15	0.897993	3380		209	3.62		182	5400	
16				209	3.62			5400	
	0.941472	3505				•••	182		
17	0.889632	1488		61	2.91	•••	48	5100	
18	0.869565	1874		90	3.03	•••	70	5400	
19	0.869565	1909		90	3.03	•••	70	5400	.0
	city-mpg	highway-mpg	price	cit	y-L/10	Okm :	fuel-type-	-diesel	\
0	21	8.703704	13495.0		11.190	476		False	
1	21	8.703704	16500.0		11.190			False	
2	19	9.038462	16500.0		12.368			False	
3	24	7.833333	13950.0		9.791			False	
4	18	10.681818	17450.0		13.055			False	
5	19	9.400000	15250.0		12.368			False	
6	19	9.400000	17710.0		12.368			False	
7	19	9.400000	18920.0		12.368	421		False	
8	17	11.750000	23875.0		13.823	529		False	
9	23	8.103448	16430.0		10.217	391		False	
10	23	8.103448	16925.0		10.217	391		False	
11	21	8.392857	20970.0		11.190	476		False	
12	21	8.392857	21105.0		11.190			False	
13	20	9.400000	24565.0		11.750			False	
14	16	10.681818	30760.0		14.687			False	
15	16	10.681818	41315.0		14.687			False	
16	15	11.750000	36880.0		15.666	667		False	
17	47	4.433962	5151.0		5.000	000		False	
18	38	5.465116	6295.0		6.184	211		False	
19	38	5.465116	6575.0		6.184	211		False	
	fuel-type	-gas aspirat	ion-std	asni	ration	-turb	0		
^									
()		True	True			Falc	e		
0		True True	True			Fals			
1 2		True True True	True True True			False False	е		

3	True	True	False
4	True	True	False
5	True	True	False
6	True	True	False
7	True	True	False
8	True	False	True
9	True	True	False
10	True	True	False
11	True	True	False
12	True	True	False
13	True	True	False
14	True	True	False
15	True	True	False
16	True	True	False
17	True	True	False
18	True	True	False
19	True	True	False

[20 rows x 22 columns]

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.

```
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.

```
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]: 0.3635480624962414

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]: 0.662028747521533

[22]: 0.7139737368233015

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 R^2. Each element in the array has the average R^2 value for the fold:

```
[25]: Rcross
```

[25]: array([0.77465419, 0.51718424, 0.74814454, 0.04825398])

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 0.5220592359225413 and the standard deviation is 0.29130480666118463

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([20251357.7835463 , 43743920.05390439, 12525158.34507633, 17564549.69976654])

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

[28]: 0.516835099979672

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([14142.23793549, 14142.23793549, 20815.3029844 , 12745.549902 , 14762.9881726])
```

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]: yhat_train = lr.predict(x_train[['horsepower', 'curb-weight', 'engine-size',

→'highway-mpg']])

yhat_train[0:5]
```

[32]: array([7625.80349764, 28447.913572 , 14843.22185221, 3855.72028472, 34567.84349196])

Prediction using test data:

[33]: array([11043.92953392, 5844.12954446, 11258.50532848, 6886.86402714, 15325.73021747])

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)
```

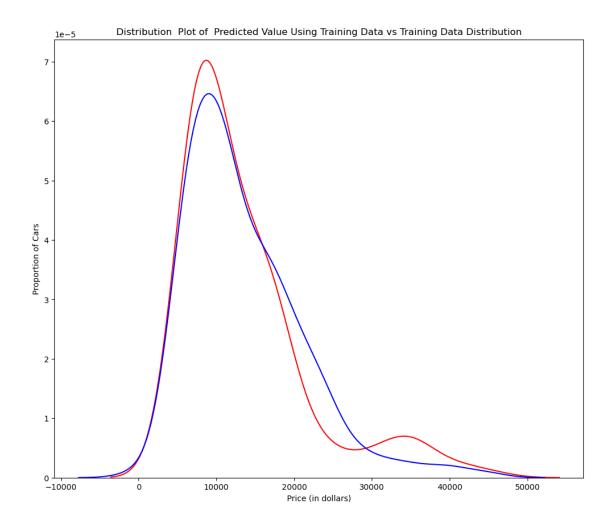


Figure 1: Plot of predicted values using the training data compared to the actual values of the training data.

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)
```

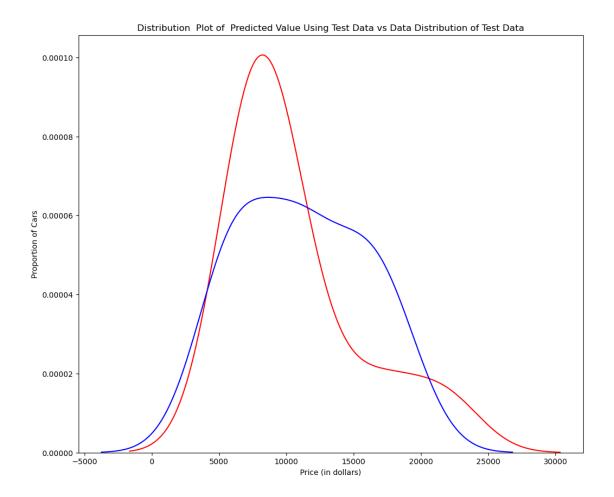


Figure 2: Plot of predicted value using the test data compared to the actual values of the test data.

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([6727.50134739, 7306.62980155, 12213.64942948, 18895.18190498, 19997.01014697])

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: [6727.50134739 7306.62980155 12213.64942948 18895.18190498] 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)
```

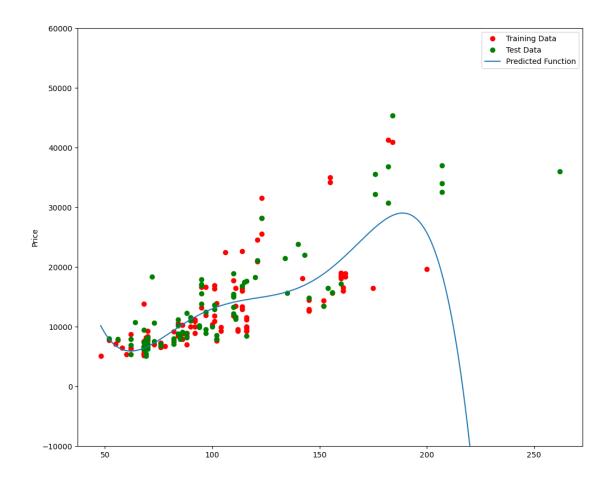


Figure 3: A polynomial regression model where red dots represent training data, green dots represent test data, and the blue line represents the model prediction.

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]: 0.5568527852117562

R^2 of the test data:

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

[45]: -29.815108072386607

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']])

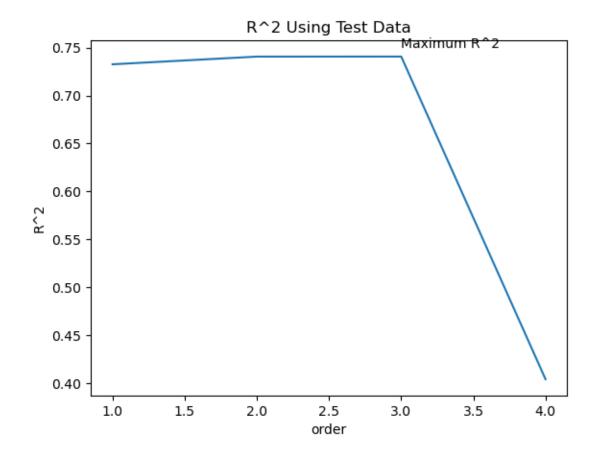
    x_test_pr = pr.fit_transform(x_test[['horsepower']])

    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 ')
```

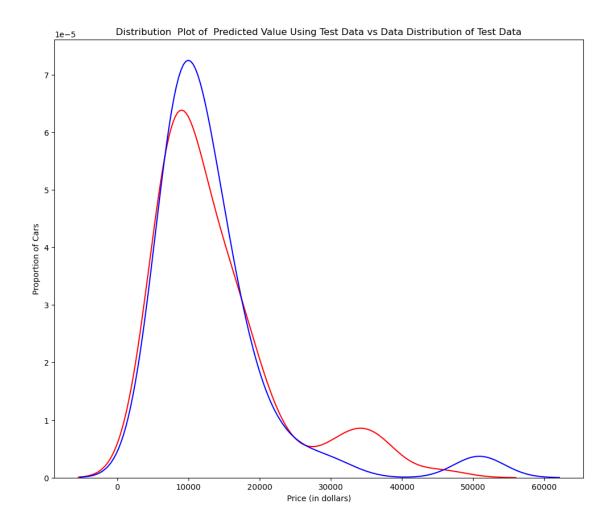
[46]: Text(3, 0.75, 'Maximum R^2')



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), ___
      ⇒FloatSlider(value=0.45, description='tes...
[48]: <function __main__.f(order, test_data)>
[49]: pr1=PolynomialFeatures(degree=2)
[50]: x_train_pr1=pr1.fit_transform(x_train[['horsepower', 'curb-weight',_
       x_test_pr1=pr1.fit_transform(x_test[['horsepower', 'curb-weight',_
       ⇔'engine-size', 'highway-mpg']])
[51]: x_train_pr1.shape #there are now 15 features
[51]: (110, 15)
[52]: poly1=LinearRegression().fit(x_train_pr1,y_train)
[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_
```



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: [ 5501.44956318 10293.7232663 21646.09716839 19329.3421769 ]
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.

```
100%| | 1000/1000 [00:10<00:00, 94.76it/s, Test Score=0.673, Train Score=0.86]
```

We can plot out the value of R² 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 0x17512f53410>

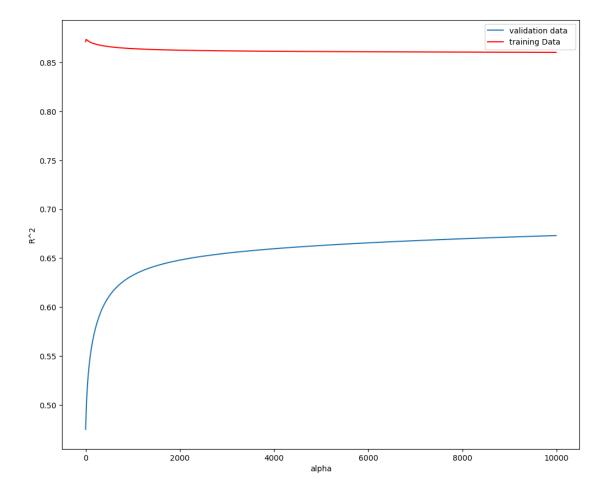


Figure 4: The blue line represents the R² of the validation data, and the red line represents the R² of the training data. The x-axis represents the different values of Alpha.

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 R² of the training data. As alpha increases the R² 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.

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

[63]: 0.4905348461839951

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, 1000, 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: