model-development

January 31, 2019

Data Analysis with Python

Module 4: Model Development

In this section, we will develop several models that will predict the price of the car using the variables or features. This is just an estimate but should give us an objective idea of how much the car should cost.

Some questions we want to ask in this module

```
do I know if the dealer is offering fair value for my trade-in?do I know if I put a fair value on my car?
```

Data Analytics, we often use Model Development to help us predict future observations from the data we have.

A Model will help us understand the exact relationship between different variables and how these variables are used to predict the result.

Setup

Import libraries

```
In [3]: import pandas as pd
     import numpy as np
     import matplotlib.pyplot as plt
```

load data and store in dataframe df:

```
0
                            122 alfa-romero
                                                     std
                                                                   two
1
           3
                            122 alfa-romero
                                                     std
                                                                   two
2
           1
                            122 alfa-romero
                                                     std
                                                                  two
3
           2
                            164
                                         audi
                                                     std
                                                                 four
4
           2
                            164
                                         audi
                                                     std
                                                                  four
```

```
body-style drive-wheels engine-location wheel-base
                                                             length ...
  convertible
                                                     88.6 0.811148 ...
0
                        rwd
                                       front
1
  convertible
                                                          0.811148 ...
                        rwd
                                       front
                                                     88.6
2
    hatchback
                        rwd
                                       front
                                                     94.5 0.822681 ...
3
         sedan
                        fwd
                                       front
                                                     99.8
                                                          0.848630 ...
4
         sedan
                         4wd
                                       front
                                                     99.4
                                                          0.848630 ...
   compression-ratio horsepower
                                   peak-rpm city-mpg highway-mpg
                                                                     price
                                     5000.0
0
                 9.0
                            111.0
                                                  21
                                                                   13495.0
                                                               27 16500.0
1
                 9.0
                            111.0
                                     5000.0
                                                  21
2
                           154.0
                                                   19
                                                               26 16500.0
                 9.0
                                     5000.0
3
                10.0
                            102.0
                                     5500.0
                                                   24
                                                               30 13950.0
4
                 8.0
                            115.0
                                     5500.0
                                                   18
                                                               22 17450.0
  city-L/100km horsepower-binned diesel
0
     11.190476
                           Medium
                                              1
1
     11.190476
                           Medium
                                         0
                                              1
2
     12.368421
                           Medium
                                         0
                                              1
3
      9.791667
                           Medium
                                         0
                                              1
4
     13.055556
                           Medium
                                              1
```

[5 rows x 29 columns]

1. Linear Regression and Multiple Linear Regression

Linear Regression

One example of a Data Model that we will be using is

Simple Linear Regression.

Simple Linear Regression is a method to help us understand the relationship between two variables:

```
The predictor/independent variable (X)
The response/dependent variable (that we want to predict)(Y)
```

The result of Linear Regression is a linear function that predicts the response (dependent) variable as a function of the predictor (independent) variable.

Y: Response VariableX: Predictor Variables

Linear function:

$$Yhat = a + bX$$

a refers to the intercept of the regression lineO, in other words: the value of Y whe
b refers to the slope of the regression line, in other words: the value with which Y

Lets load the modules for linear regression

In [6]: from sklearn.linear_model import LinearRegression

Create the linear regression object

How could Highway-mpg help us predict car price?

normalize=False)

For this example, we want to look at how highway-mpg can help us predict car price. Using simple linear regression, we will create a linear function with "highway-mpg" as the predictor variable and the "price" as the response variable.

Fit the linear model using highway-mpg.

```
In [9]: lm.fit(X,Y)
Out[9]: LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
```

We can output a prediction

What is the value of the intercept (a)?

```
In [11]: lm.intercept_
Out[11]: 38423.305858157386
```

What is the value of the Slope (b)?

```
In [12]: lm.coef_
Out[12]: array([-821.73337832])
```

What is the final estimated linear model we get?

As we saw above, we should get a final linear model with the structure:

$$Yhat = a + bX$$

Plugging in the actual values we get: price = 38423.31 - 821.73 x highway-mpg Question #1 a): Create a linear regression object?

```
In [13]: # Write your code below and press Shift+Enter to execute
         lm2 = LinearRegression()
         1m2
Out[13]: LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
                   normalize=False)
   Double-click here for the solution.
   Question #1 b):
   Train the model using 'engine-size' as the independent variable and 'price' as the dependent
variable?
In [14]: # Write your code below and press Shift+Enter to execute
         X2 = df[['engine-size']]
         Y = df['price']
         lm2.fit(X2,Y)
         Yhat2=1m2.predict(X)
         Yhat2[0:5]
Out[14]: array([-3458.11848261, -3458.11848261, -3624.9784983 , -2957.53843554,
                 -4292.41856107])
   Double-click here for the solution.
   Question #1 c):
   Find the slope and intercept of the model?
   Slope
In [15]: # Write your code below and press Shift+Enter to execute
         lm2.coef
Out[15]: array([166.86001569])
   Intercept
In [16]: # Write your code below and press Shift+Enter to execute
         lm2.intercept_
Out[16]: -7963.338906281049
   Double-click here for the solution.
   Ouestion #1 d):
   What is the equation of the predicted line. You can use x and yhat or 'engine-size' or 'price'?
```

1 You can type you answer here

```
price = -7963.338906281049 + 166.86001569 x engine-size
```

Double-click here for the solution.

Multiple Linear Regression

What if we want to predict car price using more than one variable?

If we want to use more variables in our model to predict car price, we can use Multiple Linear Regression. Multiple Linear Regression is very similar to Simple Linear Regression, but this method is used to explain the relationship between one continuous response (dependent) variable and two or more predictor (independent) variables. Most of the real-world regression models involve multiple predictors. We will illustrate the structure by using four predictor variables, but these results can generalize to any integer:

 $Y: Response\ Variable\ X_1: Predictor\ Variable\ 1X_2: Predictor\ Variable\ 2X_3: Predictor\ Variable\ 3X_4: Predictor\ Variable\ 3X_6: Predictor\ Variabl$

 $a:intercept b_1:coefficients\ of\ Variable\ 1b_2:coefficients\ of\ Variable\ 2b_3:coefficients\ of\ Variable\ 3b_4:coefficients$ The equation is given by

$$Yhat = a + b_1X_1 + b_2X_2 + b_3X_3 + b_4X_4$$

From the previous section we know that other good predictors of price could be:

```
Horsepower
Curb-weight
Engine-size
Highway-mpg
```

Let's develop a model using these variables as the predictor variables.

```
In [17]: Z = df[['horsepower', 'curb-weight', 'engine-size', 'highway-mpg']]
```

Fit the linear model using the four above-mentioned variables.

What is the value of the intercept(a)?

```
In [19]: lm.intercept_
Out[19]: -15806.624626329198
```

What are the values of the coefficients (b1, b2, b3, b4)?

```
In [20]: lm.coef_
Out[20]: array([53.49574423, 4.70770099, 81.53026382, 36.05748882])
```

What is the final estimated linear model that we get?

As we saw above, we should get a final linear function with the structure:

$$Yhat = a + b_1X_1 + b_2X_2 + b_3X_3 + b_4X_4$$

What is the linear function we get in this example?

 $Price = -15678.742628061467 + 52.65851272 \ x \ horsepower + 4.69878948 \ x \ curb-weight + 81.95906216 \ x \ engine-size + 33.58258185 \ x \ highway-mpg$

Question #2 a):

Create and train a Multiple Linear Regression model "lm2" where the response variable is price, and the predictor variable is 'normalized-losses' and 'highway-mpg'.

0	122	27
1	122	27
2	122	26
3	164	30
4	164	22
5	122	25
6	158	25
7	122	25
8	158	20
9	192	29
10	192	29
11	188	28
12	188	28
13	122	25
14	122	22
15	122	22
16	122	20
17	121	53
18	98	43
19	81	43
20	118	41
21	118	38
22	118	30
23	148	38
24	148	38
25	148	38
26	148	30
27	110	30
28	145	24

29	137	54
171	65	32
172	65	32
173	65	32
174	197	24
175	197	24
176	90	24
177	122	24
178	122	46
179	122	34
180	94	46
181	94	34
182	94	34
183	94	42
184	94	32
185	122	29
186	256	29
187	122	24
188	122	38
189	122	31
190	103	28
191	74	28
192	103	28
193	74	28
194	103	22
195	74	22
196	95	28
197	95	25
198	95	23
199	95	27
200	95	25

[201 rows x 2 columns]

Double-click here for the solution.

Question #2 b):

Find the coefficient of the model?

Double-click here for the solution.

2) Model Evaluation using Visualization

Now that we've developed some models, how do we evaluate our models and how do we choose the best one? One way to do this is by using visualization.

import the visualization package: seaborn

Regression Plot

Out [24]: (0, 48296.78157483029)

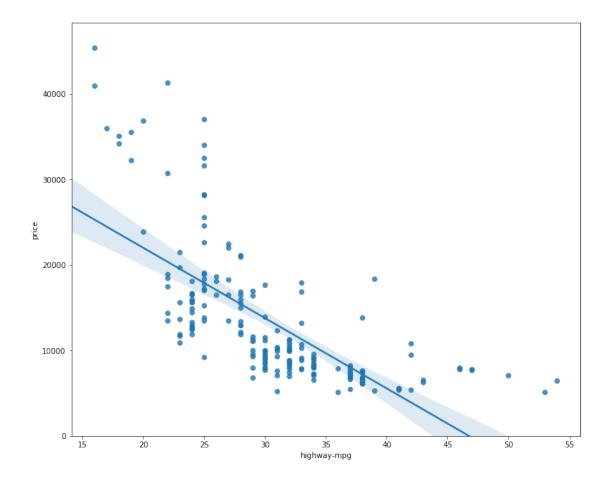
When it comes to simple linear regression, an excellent way to visualize the fit of our model is by using regression plots.

This plot will show a combination of a scattered data points (a scatter plot), as well as the fitted linear regression line going through the data. This will give us a reasonable estimate of the relationship between the two variables, the strength of the correlation, as well as the direction (positive or negative correlation).

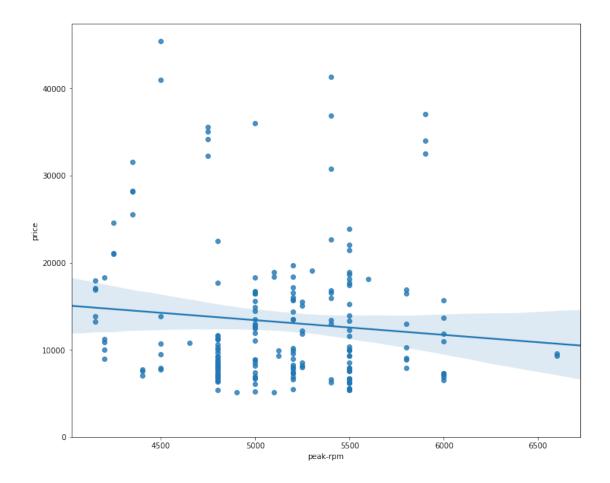
Let's visualize Horsepower as potential predictor variable of price:

```
In [24]: width = 12
          height = 10
          plt.figure(figsize=(width, height))
          sns.regplot(x="highway-mpg", y="price", data=df)
          plt.ylim(0,)

/home/jupyterlab/conda/lib/python3.6/site-packages/scipy/stats/stats.py:1713: FutureWarning: Usi
    return np.add.reduce(sorted[indexer] * weights, axis=axis) / sumval
```



We can see from this plot that price is negatively correlated to highway-mpg, since the regression slope is negative. One thing to keep in mind when looking at a regression plot is to pay attention to how scattered the data points are around the regression line. This will give you a good indication of the variance of the data, and whether a linear model would be the best fit or not. If the data is too far off from the line, this linear model might not be the best model for this data. Let's compare this plot to the regression plot of "peak-rpm".



Comparing the regression plot of "peak-rpm" and "highway-mpg" we see that the points for "highway-mpg" are much closer to the generated line and on the average decrease. The points for "peak-rpm" have more spread around the predicted line, and it is much harder to determine if the points are decreasing or increasing as the "highway-mpg" increases.

Question #3:

Given the regression plots above is "peak-rpm" or "highway-mpg" more strongly correlated with "price". Use the method ".corr()" to verify your answer.

Double-click here for the solution.

Residual Plot

A good way to visualize the variance of the data is to use a residual plot. What is a residual?

The difference between the observed value (y) and the predicted value (Yhat) is called the residual (e). When we look at a regression plot, the residual is the distance from the data point to the fitted regression line.

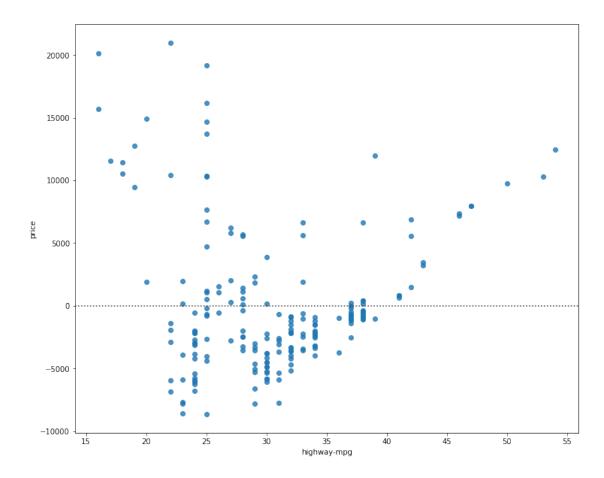
So what is a residual plot?

A residual plot is a graph that shows the residuals on the vertical y-axis and the independent variable on the horizontal x-axis.

What do we pay attention to when looking at a residual plot? We look at the spread of the residuals:

• If the points in a residual plot are randomly spread out around the x-axis, then a linear model is appropriate for the data. Why is that? Randomly spread out residuals means that the variance is constant, and thus the linear model is a good fit for this data.

```
In [32]: width = 12
    height = 10
    plt.figure(figsize=(width, height))
    sns.residplot(df['highway-mpg'], df['price'])
    plt.show()
```



What is this plot telling us?

We can see from this residual plot that the residuals are not randomly spread around the x-axis, which leads us to believe that maybe a non-linear model is more appropriate for this data.

Multiple Linear Regression

How do we visualize a model for Multiple Linear Regression? This gets a bit more complicated because you can't visualize it with regression or residual plot.

One way to look at the fit of the model is by looking at the distribution plot: We can look at the distribution of the fitted values that result from the model and compare it to the distribution of the actual values.

First lets make a prediction

In [35]: Y_hat = lm.predict(Z)

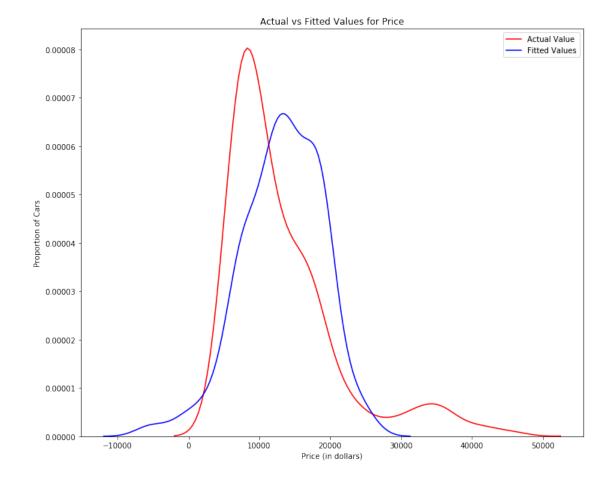
```
In [36]: plt.figure(figsize=(width, height))

ax1 = sns.distplot(df['price'], hist=False, color="r", label="Actual Value")
    sns.distplot(Yhat, hist=False, color="b", label="Fitted Values", ax=ax1)

plt.title('Actual vs Fitted Values for Price')
    plt.xlabel('Price (in dollars)')
    plt.ylabel('Proportion of Cars')

plt.show()
    plt.close()
```

/home/jupyterlab/conda/lib/python3.6/site-packages/scipy/stats/stats.py:1713: FutureWarning: Usi return np.add.reduce(sorted[indexer] * weights, axis=axis) / sumval



We can see that the fitted values are reasonably close to the actual values, since the two distributions overlap a bit. However, there is definitely some room for improvement.

Part 3: Polynomial Regression and Pipelines

Polynomial regression is a particular case of the general linear regression model or multiple linear regression models.

We get non-linear relationships by squaring or setting higher-order terms of the predictor variables.

There are different orders of polynomial regression:

Quadratic - 2nd order

$$Yhat = a + b_1 X^2 + b_2 X^2$$

Cubic - 3rd order

$$Yhat = a + b_1 X^2 + b_2 X^2 + b_3 X^3$$

Higher order:

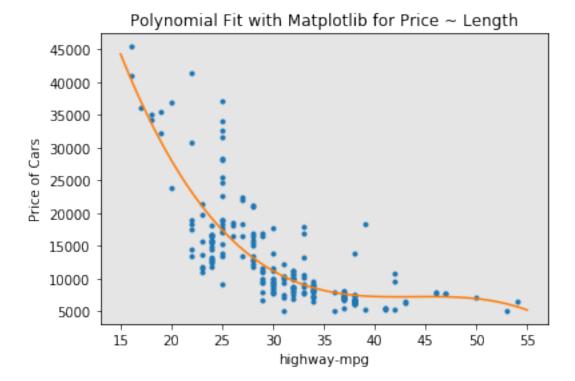
$$Y = a + b_1 X^2 + b_2 X^2 + b_3 X^3 \dots$$

We saw earlier that a linear model did not provide the best fit while using highway-mpg as the predictor variable. Let's see if we can try fitting a polynomial model to the data instead. We will use the following function to plot the data:

Let's fit the polynomial using the function polyfit, then use the function poly1d to display the polynomial function.

```
In [41]: PlotPolly(p, x, y, 'highway-mpg')
```

y = df['price']



```
In [42]: np.polyfit(x, y, 3)
Out[42]: array([-1.55663829e+00, 2.04754306e+02, -8.96543312e+03, 1.37923594e+05])
```

We can already see from plotting that this polynomial model performs better than the linear model. This is because the generated polynomial function "hits" more of the data points.

Question #4:

Create 11 order polynomial model with the variables x and y from above?

Double-click here for the solution.

The analytical expression for Multivariate Polynomial function gets complicated. For example, the expression for a second-order (degree=2)polynomial with two variables is given by:

$$Yhat = a + b_1X_1 + b_2X_2 + b_3X_1X_2 + b_4X_1^2 + b_5X_2^2$$

We can perform a polynomial transform on multiple features. First, we import the module:

```
In [46]: from sklearn.preprocessing import PolynomialFeatures
```

We create a PolynomialFeatures object of degree 2:

Out[47]: PolynomialFeatures(degree=2, include_bias=True, interaction_only=False)

```
In [48]: Z_pr=pr.fit_transform(Z)
```

The original data is of 201 samples and 4 features

```
In [49]: Z.shape
Out[49]: (201, 4)
```

after the transformation, there 201 samples and 15 features

```
In [50]: Z_pr.shape
Out[50]: (201, 15)
```

Pipeline

Data Pipelines simplify the steps of processing the data. We use the module Pipeline to create a pipeline. We also use StandardScaler as a step in our pipeline.

We create the pipeline, by creating a list of tuples including the name of the model or estimator and its corresponding constructor.

```
In [54]: Input=[('scale',StandardScaler()), ('polynomial', PolynomialFeatures(include_bias=False
we input the list as an argument to the pipeline constructor
```

We can normalize the data, perform a transform and fit the model simultaneously.

```
In [60]: pipe.fit(Z,y)
```

```
return self.partial_fit(X, y)
/home/jupyterlab/conda/lib/python3.6/site-packages/sklearn/base.py:465: DataConversionWarning: I
  return self.fit(X, y, **fit_params).transform(X)
Out[60]: Pipeline(memory=None,
              steps=[('scale', StandardScaler(copy=True, with_mean=True, with_std=True)), ('poly
                  normalize=False))])
   Similarly, we can normalize the data, perform a transform and produce a prediction simulta-
neously
In [61]: ypipe=pipe.predict(Z)
         ypipe[0:4]
/home/jupyterlab/conda/lib/python3.6/site-packages/sklearn/pipeline.py:331: DataConversionWarnir
 Xt = transform.transform(Xt)
Out[61]: array([13102.74784201, 13102.74784201, 18225.54572197, 10390.29636555])
   Question #5:
   Create a pipeline that Standardizes the data, then perform prediction using a linear regression
model using the features Z and targets y
In [67]: # Write your code below and press Shift+Enter to execute
         pipe2=Pipeline(Input)
         pipe2
         pipe.fit(Z,y)
         yhat3=pipe.predict(Z)
         yhat3[0:8]
/home/jupyterlab/conda/lib/python3.6/site-packages/sklearn/preprocessing/data.py:625: DataConver
  return self.partial_fit(X, y)
/home/jupyterlab/conda/lib/python3.6/site-packages/sklearn/base.py:465: DataConversionWarning: I
  return self.fit(X, y, **fit_params).transform(X)
/home/jupyterlab/conda/lib/python3.6/site-packages/sklearn/pipeline.py:331: DataConversionWarnir
 Xt = transform.transform(Xt)
Out[67]: array([13102.74784201, 13102.74784201, 18225.54572197, 10390.29636555,
```

/home/jupyterlab/conda/lib/python3.6/site-packages/sklearn/preprocessing/data.py:625: DataConver

Double-click here for the solution.

Part 4: Measures for In-Sample Evaluation

When evaluating our models, not only do we want to visualize the results, but we also want a quantitative measure to determine how accurate the model is.

16136.29619164, 13880.09787302, 15041.58694037, 15457.93465485])

Two very important measures that are often used in Statistics to determine the accuracy of a model are:

```
<b>R^2 / R-squared</b><b>Mean Squared Error (MSE)</b>
```

R-squared

R squared, also known as the coefficient of determination, is a measure to indicate how close the data is to the fitted regression line.

The value of the R-squared is the percentage of variation of the response variable (y) that is explained by a linear model.

Mean Squared Error (MSE)

The Mean Squared Error measures the average of the squares of errors, that is, the difference between actual value (y) and the estimated value ().

Model 1: Simple Linear Regression

Let's calculate the R²

We can say that \sim 49.659% of the variation of the price is explained by this simple linear model "horsepower_fit".

Let's calculate the MSE

We can predict the output i.e., "yhat" using the predict method, where X is the input variable:

Model 2: Multiple Linear Regression Let's calculate the R^2

The mean square error of price and predicted value is: 31635042.944639895

```
The R-square is: 0.8093562806577458
```

We can say that ~ 80.896 % of the variation of price is explained by this multiple linear regression "multi_fit".

Let's calculate the MSE we produce a prediction

```
In [108]: Y_predict_multifit = lm.predict(Z)
```

we compare the predicted results with the actual results

The mean square error of price and predicted value using multifit is: 11980366.870726489

Model 3: Polynomial Fit

Let's calculate the R²

let's import the function r2_score from the module metrics as we are using a different function

```
In [110]: from sklearn.metrics import r2_score
```

We apply the function to get the value of r²

The R-square value is: 0.7023769094721823

We can say that \sim 67.419 % of the variation of price is explained by this polynomial fit MSE

We can also calculate the MSE:

```
In [112]: mean_squared_error(df['price'], p(x))
Out[112]: 18703127.624789312
```

Part 5: Prediction and Decision Making

Prediction

In the previous section, we trained the model using the method fit. Now we will use the method predict to produce a prediction. Lets import pyplot for plotting; we will also be using some functions from numpy.

```
In [113]: import matplotlib.pyplot as plt
    import numpy as np
    %matplotlib inline
```

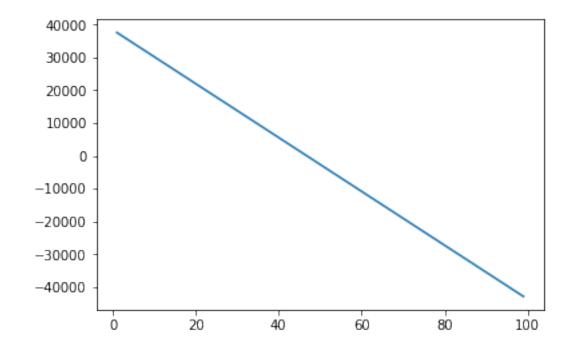
Create a new input

```
In [114]: new_input=np.arange(1, 100, 1).reshape(-1, 1)
```

Fit the model

Produce a prediction

we can plot the data



Decision Making: Determining a Good Model Fit

Now that we have visualized the different models, and generated the R-squared and MSE values for the fits, how do we determine a good model fit?

```
<i>What is a good R-squared value?</i>
```

When comparing models, the model with the higher R-squared value is a better fit for the data.

```
<i>What is a good MSE?</i>
```

When comparing models, the model with the smallest MSE value is a better fit for the data. Let's take a look at the values for the different models.

Simple Linear Regression: Using Highway-mpg as a Predictor Variable of Price.

```
R-squared: 0.49659118843391759MSE: 3.16 x10^7
```

Multiple Linear Regression: Using Horsepower, Curb-weight, Engine-size, and Highway-mpg as Predictor Variables of Price.

```
R-squared: 0.80896354913783497MSE: 1.2 x10^7
```

Polynomial Fit: Using Highway-mpg as a Predictor Variable of Price.

```
R-squared: 0.6741946663906514MSE: 2.05 x 10^7
```

Simple Linear Regression model (SLR) vs Multiple Linear Regression model (MLR)

Usually, the more variables you have, the better your model is at predicting, but this is not always true. Sometimes you may not have enough data, you may run into numerical problems, or many of the variables may not be useful and or even act as noise. As a result, you should always check the MSE and R^2.

So to be able to compare the results of the MLR vs SLR models, we look at a combination of both the R-squared and MSE to make the best conclusion about the fit of the model.

```
<b>MSE</b>The MSE of SLR is 3.16x10^7 while MLR has an MSE of 1.2 x10^7. The MSE of MLR i
<b>R-squared</b>: In this case, we can also see that there is a big difference between the F
```

This R-squared in combination with the MSE show that MLR seems like the better model fit in this case, compared to SLR.

Simple Linear Model (SLR) vs Polynomial Fit

```
<b>MSE</b>: We can see that Polynomial Fit brought down the MSE, since this MSE is smaller t
<b>R-squared</b>: The R-squared for the Polyfit is larger than the R-squared for the SLR, so
```

Since the Polynomial Fit resulted in a lower MSE and a higher R-squared, we can conclude that this was a better fit model than the simple linear regression for predicting Price with Highway-mpg as a predictor variable.

Multiple Linear Regression (MLR) vs Polynomial Fit

```
<1i><b>MSE</b>: The MSE for the MLR is smaller than the MSE for the Polynomial Fit.<b>R-squared</b>: The R-squared for the MLR is also much larger than for the Polynomial Fit.
```

Conclusion:

Comparing these three models, we conclude that the MLR model is the best model to be able to predict price from our dataset. This result makes sense, since we have 27 variables in total, and we know that more than one of those variables are potential predictors of the final car price.

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About the Authors:

This notebook was written by Mahdi Noorian PhD, Joseph Santarcangelo, Bahare Talayian, Eric Xiao, Steven Dong, Parizad, Hima Vsudevan and Fiorella Wenver.

Joseph Santarcangelo is a Data Scientist at IBM, and holds a PhD in Electrical Engineering. His research focused on using Machine Learning, Signal Processing, and Computer Vision to determine how videos impact human cognition. Joseph has been working for IBM since he completed his PhD.

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