# Data Science II with python (Class notes)

**STAT 303-2**

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2023-01-03

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# Preface

These are class notes for the course STAT303-2. 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 course textbook last quarter). Please report any typos / mistakes / inconsistencies / issues with the class notes / class presentations in your comments here. Thank you!

# 1 Simple Linear Regression

*Read section 3.1 of the book before using these notes.*

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

## 1.1 Simple Linear Regression

```
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 matplotlib.patches import Patch
from matplotlib.lines import Line2D
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_squared_error, mean_absolute_error, r2_score
```

**Develop a simple linear regression model that predicts car price based on engine size.** Datasets to be used: *Car_features_train.csv, Car_prices_train.csv*

```
# We are reading training data ONLY at this point.
# Test data is already separated in another file
trainf = pd.read_csv('./Datasets/Car_features_train.csv') # Predictors
trainp = pd.read_csv('./Datasets/Car_prices_train.csv') # Response
train = pd.merge(trainf,trainp)
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 |

| | carID | brand | model | year | transmission | mileage | fuelType | tax | mpg | engineSize | price |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 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 |

### 1.1.1 Training with `statsmodels`

Here, we will use the `statsmodels.formula.api` module of the `statsmodels` library. The use of "API" here doesn't refer to a traditional external web API but rather an interface within the library for users to interact with and perform specific tasks. The `statsmodels.formula.api` module provides a formulaic interface to the `statsmodels` library. A formula is a compact way to specify statistical models using a formula language. This module allows users to define statistical models using formulas similar to those used in R.

So, in summary, the `statsmodels.formula.api` module provides a formulaic interface as part of the `statsmodels` library, allowing users to specify statistical models using a convenient and concise formula syntax.

```
# Let's create the model

# ols stands for Ordinary Least Squares - the name of the algorithm that optimizes Linear Reg

# data input needs the dataframe that has the predictor and the response
# formula input needs to:
    # be a string
    # have the following syntax: "response~predictor"

# Using engineSize to predict price
ols_object = smf.ols(formula = 'price~engineSize', data = train)
```

```
#Using the fit() function of the 'ols' class to fit the model, i.e., train the model
model = ols_object.fit()
```

```
#Printing model summary which contains among other things, the model coefficients
model.summary()
```

| | | | |
|---|---|---|---|
| **Dep. Variable:** | price | **R-squared:** | 0.390 |
| **Model:** | OLS | **Adj. R-squared:** | 0.390 |
| **Method:** | Least Squares | **F-statistic:** | 3177. |
| **Date:** | Tue, 16 Jan 2024 | **Prob (F-statistic):** | 0.00 |
| **Time:** | 16:46:33 | **Log-Likelihood:** | -53949. |
| **No. Observations:** | 4960 | **AIC:** | 1.079e+05 |
| **Df Residuals:** | 4958 | **BIC:** | 1.079e+05 |
| **Df Model:** | 1 | | |
| **Covariance Type:** | nonrobust | | |

| | **coef** | **std err** | **t** | **P> \|t\|** | **[0.025** | **0.975]** |
|---|---|---|---|---|---|---|
| **Intercept** | -4122.0357 | 522.260 | -7.893 | 0.000 | -5145.896 | -3098.176 |
| **engineSize** | 1.299e+04 | 230.450 | 56.361 | 0.000 | 1.25e+04 | 1.34e+04 |

| | | | |
|---|---|---|---|
| **Omnibus:** | 1271.986 | **Durbin-Watson:** | 0.517 |
| **Prob(Omnibus):** | 0.000 | **Jarque-Bera (JB):** | 6490.719 |
| **Skew:** | 1.137 | **Prob(JB):** | 0.00 |
| **Kurtosis:** | 8.122 | **Cond. No.** | 7.64 |

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.

The model equation is: $\hat{price}$ = -4122.0357 + 12990 * `engineSize`

- R-squared is 39%. This is the proportion of variance in car price explained by `engineSize`.
- The coef of `engineSize` ($\hat{\beta}_1$) is statistically significant ($p$-value = 0). There is a linear relationship between X and Y.
- The 95% CI of $\hat{\beta}_1$ is [1.25e+04, 1.34e+04].
- PI is not shown here.

The coefficient of `engineSize` is 1.299e+04. - Unit change in `engineSize` increases the expected price by $ 12,990. - An increase of 3 increases the price by $ (3*1.299e+04) = $ 38,970.

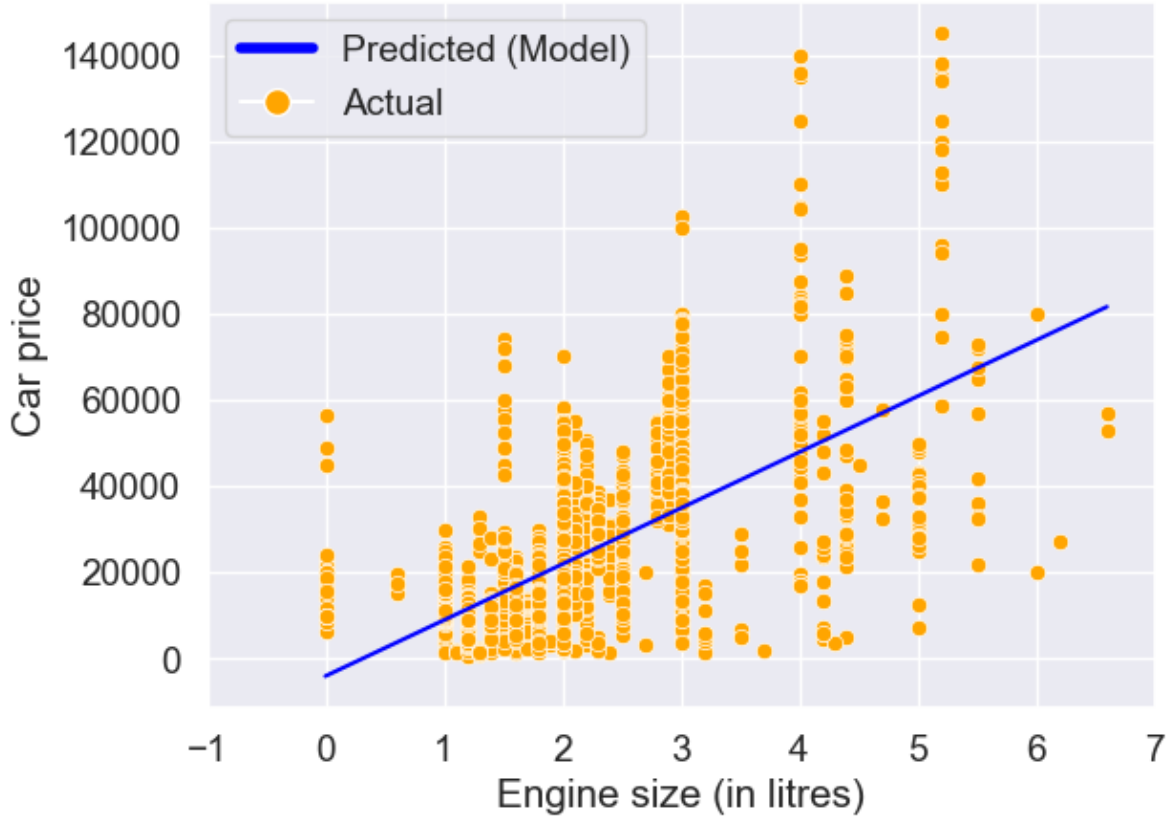
The coefficients can also be returned directly usign the `params` attribute of the `model` object returned by the `fit()` method of the `ols` class:

```
model.params
```

```
Intercept     -4122.035744
engineSize    12988.281021
dtype: float64
```

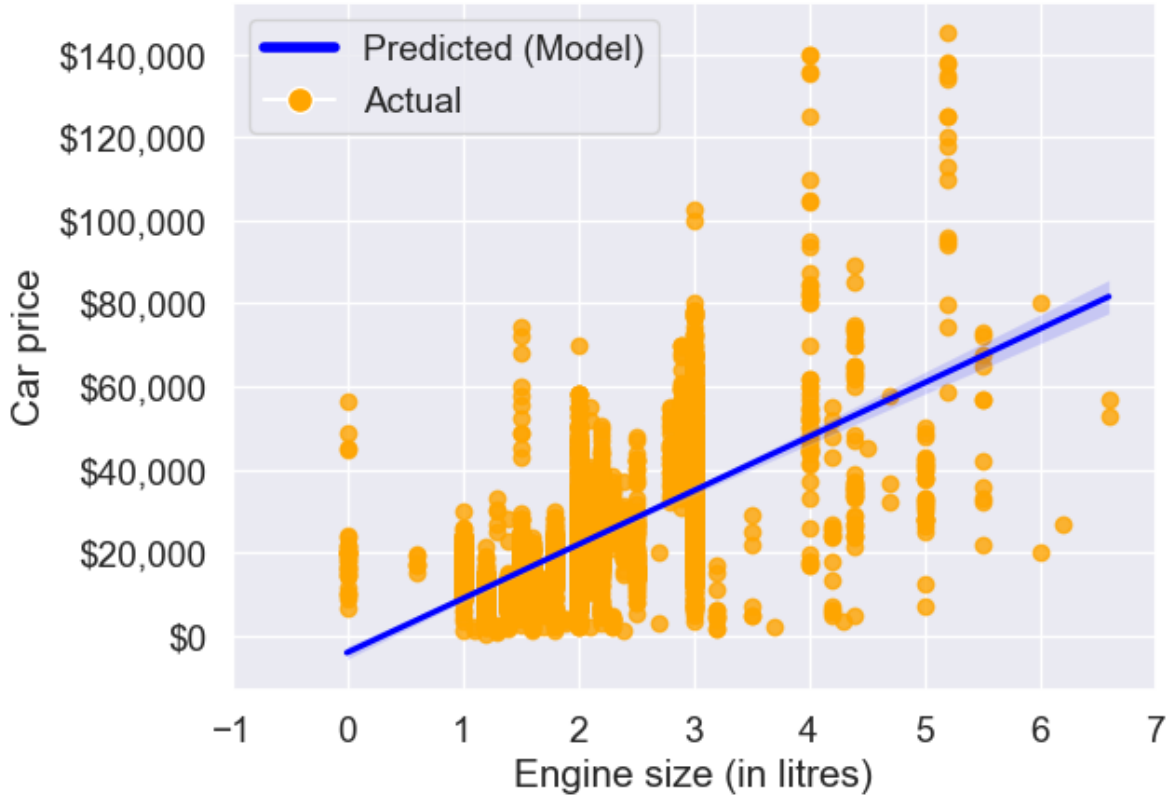
**Visualize the regression line**

```
sns.set(font_scale=1.25)
ax = sns.scatterplot(x = train.engineSize, y = train.price,color = 'orange')
sns.lineplot(x = train.engineSize, y = model.fittedvalues,color = 'blue')
plt.xlim(-1,7)
plt.xlabel('Engine size (in litres)')
plt.ylabel('Car price')
legend_elements = [Line2D([0], [0], color='blue', lw=4, label='Predicted (Model)'),
                   Line2D([0], [0], marker='o', color='w', label='Actual',
                          markerfacecolor='orange', markersize=10)]
ax.legend(handles=legend_elements, loc='upper left');
```




Note that the above plot can be made directly using the seaborn function `regplot()`. The function `regplot()` fits a simple linear regression model with `y` as the response, and `x` as the predictor, and then plots the model over a scatteplot of the data.

```
ax = sns.regplot(x = 'engineSize', y = 'price', data = train, color = 'orange',line_kws={"co
plt.xlim(-1,7)
plt.xlabel('Engine size (in litres)')
plt.ylabel('Car price')
ax.yaxis.set_major_formatter('${x:,.0f}')
ax.legend(handles=legend_elements, loc='upper left');
#Note that some of the engineSize values are 0. They are incorrect, and should ideally be im
```




The light shaded region around the blue line in the above plot is the confidence interval.

**Predict the car price for the cars in the test dataset**. Datasets to be used: *Car_features_test.csv, Car_prices_test.csv*

Now that the model has been trained, let us evaluate it on unseen data. Make sure that the columns names of the predictors are the same in train and test datasets.

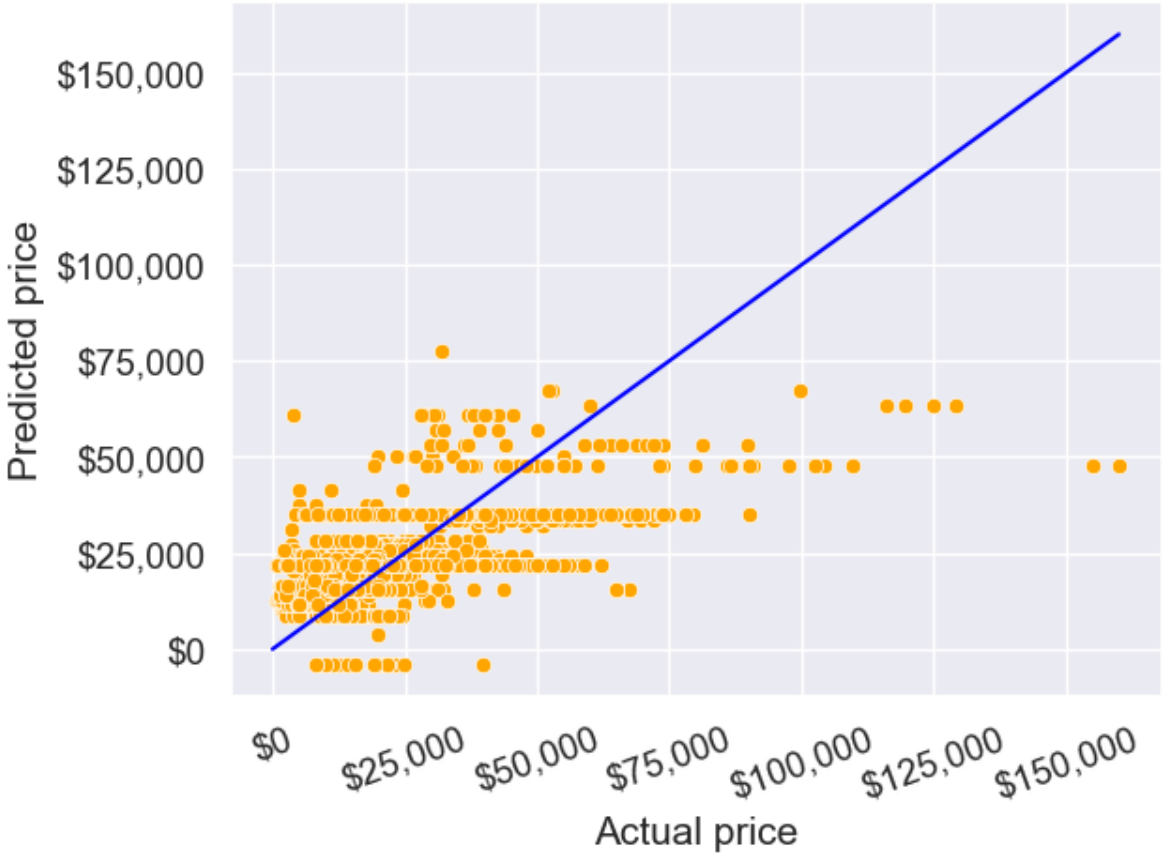
```
# Read the test data
testf = pd.read_csv('./Datasets/Car_features_test.csv') # Predictors
```

```
testp = pd.read_csv('./Datasets/Car_prices_test.csv') # Response
test = pd.merge(testf, testp)
```

```
#Using the predict() function associated with the 'model' object to make predictions of car p
pred_price = model.predict(testf)#Note that the predict() function finds the predictor 'engi
```

**Make a visualization that compares the predicted car prices with the actual car prices**

```
sns.scatterplot(x = testp.price, y = pred_price, color = 'orange')
#In case of a perfect prediction, all the points must lie on the line x = y.
ax = sns.lineplot(x = [0,testp.price.max()], y = [0,testp.price.max()],color='blue') #Plottin
plt.xlabel('Actual price')
plt.ylabel('Predicted price')
ax.yaxis.set_major_formatter('${x:,.0f}')
ax.xaxis.set_major_formatter('${x:,.0f}')
plt.xticks(rotation=20);
```



The prediction doesn't look too good. This is because we are just using one predictor - engine size. We can probably improve the model by adding more predictors when we learn multiple linear regression.

**What is the RMSE of the predicted car price on unseen data?**

```
np.sqrt(((testp.price - pred_price)**2).mean())
```

```
12995.106451548696
```

The root mean squared error in predicting car price is around $13k.

**What is the residual standard error based on the training data?**

```
np.sqrt(model.mse_resid)
```

```
12810.109175214138
```

The residual standard error on the training data is close to the RMSE on the test data. This shows that the performance of the model on unknown data is comparable to its performance on known data. This implies that the model is not overfitting, which is good! In case we overfit a model on the training data, its performance on unknown data is likely to be worse than that on the training data.

**Find the confidence and prediction intervals of the predicted car price**

```
#Using the get_prediction() function associated with the 'model' object to get the intervals
intervals = model.get_prediction(testf)
```

```
#The function requires specifying alpha (probability of Type 1 error) instead of the confide
intervals.summary_frame(alpha=0.05)
```

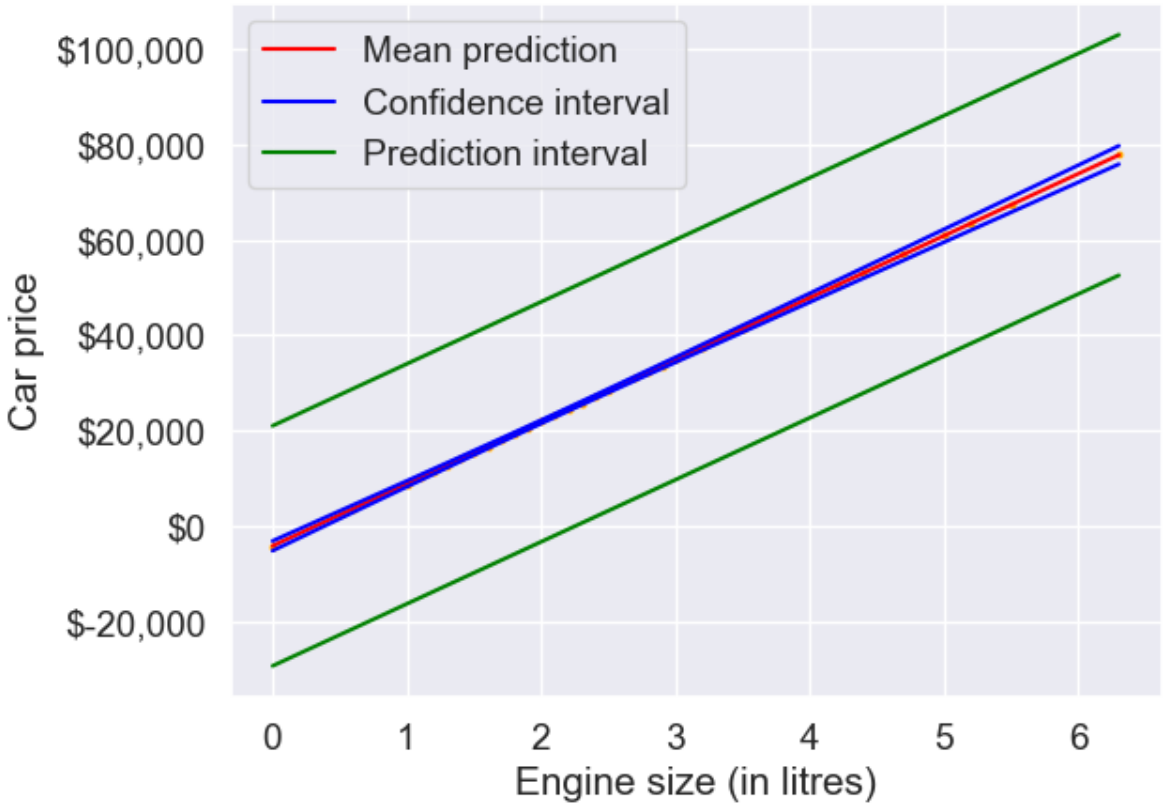
| | mean | mean_se | mean_ci_lower | mean_ci_upper | obs_ci_lower | obs_ci_upper |
|---|---|---|---|---|---|---|
| 0 | 34842.807319 | 271.666459 | 34310.220826 | 35375.393812 | 9723.677232 | 59961.937406 |
| 1 | 34842.807319 | 271.666459 | 34310.220826 | 35375.393812 | 9723.677232 | 59961.937406 |
| 2 | 34842.807319 | 271.666459 | 34310.220826 | 35375.393812 | 9723.677232 | 59961.937406 |
| 3 | 8866.245277 | 316.580850 | 8245.606701 | 9486.883853 | -16254.905974 | 33987.396528 |
| 4 | 47831.088340 | 468.949360 | 46911.740050 | 48750.436631 | 22700.782946 | 72961.393735 |
| ... | ... | ... | ... | ... | ... | ... |
| 2667 | 47831.088340 | 468.949360 | 46911.740050 | 48750.436631 | 22700.782946 | 72961.393735 |

| | mean | mean_se | mean_ci_lower | mean_ci_upper | obs_ci_lower | obs_ci_upper |
|---|---|---|---|---|---|---|
| 2668 | 34842.807319 | 271.666459 | 34310.220826 | 35375.393812 | 9723.677232 | 59961.937406 |
| 2669 | 8866.245277 | 316.580850 | 8245.606701 | 9486.883853 | -16254.905974 | 33987.396528 |
| 2670 | 21854.526298 | 184.135754 | 21493.538727 | 22215.513869 | -3261.551421 | 46970.604017 |
| 2671 | 21854.526298 | 184.135754 | 21493.538727 | 22215.513869 | -3261.551421 | 46970.604017 |

**Show the regression line predicting car price based on engine size for test data. Also show the confidence and prediction intervals for the car price.**

```
interval_table = intervals.summary_frame(alpha=0.05)
```

```
ax = sns.scatterplot(x = testf.engineSize, y = pred_price,color = 'orange', s = 10)
sns.lineplot(x = testf.engineSize, y = pred_price, color = 'red')
sns.lineplot(x = testf.engineSize, y = interval_table.mean_ci_lower, color = 'blue')
sns.lineplot(x = testf.engineSize, y = interval_table.mean_ci_upper, color = 'blue')
sns.lineplot(x = testf.engineSize, y = interval_table.obs_ci_lower, color = 'green')
sns.lineplot(x = testf.engineSize, y = interval_table.obs_ci_upper, color = 'green')

legend_elements = [Line2D([0], [0], color='red', label='Mean prediction'),
                   Line2D([0], [0], color='blue', label='Confidence interval'),
                  Line2D([0], [0], color='green', label='Prediction interval')]
ax.legend(handles=legend_elements, loc='upper left')
plt.xlabel('Engine size (in litres)')
plt.ylabel('Car price')
ax.yaxis.set_major_formatter('${x:,.0f}');
```




### 1.1.2 Training with `sklearn`

```
# Create the model as an object

model = LinearRegression() # No inputs, this will change for other models

# Train the model - separate the predictor(s) and the response for this!
X_train = train[['engineSize']]
y_train = train[['price']]

# Note that both are dfs, NOT series - necessary to avoid errors

model.fit(X_train, y_train)

# Check the slight syntax differences
    # predictors and response separate
    # We need to manually slice the predictor column(s) we want to include
```

```
    # No need to assign to an output

# Return the parameters
print("Coefficient of engine size = ", model.coef_) # slope
print("Intercept = ", model.intercept_) # intercept

# No .summary() here! - impossible to do much inference; this is a shortcoming of sklearn
```

```
Coefficient of engine size =  [[12988.28102112]]
Intercept =  [-4122.03574424]
```

```
# Prediction

# Again, separate the predictor(s) and the response of interest
X_test = test[['engineSize']]
y_test = test[['price']].to_numpy() # Easier to handle with calculations as np array

y_pred = model.predict(X_test)

# Evaluate
model_rmse = np.sqrt(np.mean((y_pred - y_test)**2)) # RMSE
model_mae = np.mean(np.abs(y_pred - y_test)) # MAE

print('Test RMSE: ', model_rmse)
```

```
Test RMSE:  12995.106451548696
```

```
# Easier way to calculate metrics with sklearn tools

# Note that we have imported the functions 'mean_squared_error' and 'mean_absolute_error'
# from the sklearn.metrics module (check top of the code)

model_rmse = np.sqrt(mean_squared_error(y_test,y_pred))
model_mae = mean_absolute_error(y_test,y_pred)
print('Test RMSE: ', model_rmse)
print('Test MAE: ', model_mae)
```

```
Test RMSE:  12995.106451548696
Test MAE:  9411.325912951994
```

```
y_pred_train = model.predict(X_train)
print('Train R-squared:', r2_score(y_train, y_pred_train))
print('Test R-squared:', r2_score(y_test, y_pred))
```

```
Train R-squared: 0.39049842625794573
Test R-squared: 0.3869900378620146
```

**Note:** Why did we repeat the same task in two different libraries?

- `statsmodels` and `sklearn` have different advantages - we will use both for our purposes
  - `statsmodels` returns a lot of statistical output, which is very helpful for inference (coming up next) but it has a limited variety of models.
  - With `statsmodels`, you may have columns in your DataFrame in addition to predictors and response, while with `sklearn` you need to make separate objects consisting of only the predictors and the response.
  - `sklearn` includes many models (`Lasso` and `Ridge` this quarter, many others next quarter) and helpful tools/functions (like metrics) that statsmodels does not but it does not have any inference tools.

### 1.1.3 Training with `statsmodels.api`

Earlier we had used the `statsmodels.formula.api` module, where we had to put the regression model as a formula. We can also use the `statsmodels.api` module to develop a regression model. The syntax of training a model with the `OLS()` function in this module is similar to that of `sklearn`'s `LinearRegression()` function. However, the order in which the predictors and response are specified is different. The formula-style syntax of the `statsmodels.formula.api` module is generally preferred. However, depending on the situation, the `OLS()` syntax of `statsmodels.api` may be preferred.

Note that you will manually need to add the predictor *(a column of ones)* corresponding to the intercept to train the model with this method.

```
# Create the model as an object

# Train the model - separate the predictor(s) and the response for this!
X_train = train[['engineSize']]
y_train = train[['price']]

X_train_with_intercept = np.concatenate((np.ones(X_train.shape[0]).reshape(-1,1), X_train), a

model = sm.OLS(y_train, X_train_with_intercept).fit()
```

```
# Return the parameters
print(model.params)
```

```
const    -4122.035744
x1       12988.281021
dtype: float64
```

The model summary and all other attributes and methods of the `model` object are the same as that with the object created using the `statsmodels.formula.api` module.

```
model.summary()
```

| | | | |
|---|---|---|---|
| **Dep. Variable:** | price | **R-squared:** | 0.390 |
| **Model:** | OLS | **Adj. R-squared:** | 0.390 |
| **Method:** | Least Squares | **F-statistic:** | 3177. |
| **Date:** | Mon, 08 Jan 2024 | **Prob (F-statistic):** | 0.00 |
| **Time:** | 11:17:55 | **Log-Likelihood:** | -53949. |
| **No. Observations:** | 4960 | **AIC:** | 1.079e+05 |
| **Df Residuals:** | 4958 | **BIC:** | 1.079e+05 |
| **Df Model:** | 1 | | |
| **Covariance Type:** | nonrobust | | |

| | **coef** | **std err** | **t** | **P> \|t\|** | **[0.025** | **0.975]** |
|---|---|---|---|---|---|---|
| **const** | -4122.0357 | 522.260 | -7.893 | 0.000 | -5145.896 | -3098.176 |
| **x1** | 1.299e+04 | 230.450 | 56.361 | 0.000 | 1.25e+04 | 1.34e+04 |

| | | | |
|---|---|---|---|
| **Omnibus:** | 1271.986 | **Durbin-Watson:** | 0.517 |
| **Prob(Omnibus):** | 0.000 | **Jarque-Bera (JB):** | 6490.719 |
| **Skew:** | 1.137 | **Prob(JB):** | 0.00 |
| **Kurtosis:** | 8.122 | **Cond. No.** | 7.64 |

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.

# 2 Multiple Linear Regression

*Read section 3.2 of the book before using these notes.*

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

## 2.1 Multiple Linear Regression

```
# importing libraries
import pandas as pd
import numpy as np
import statsmodels.formula.api as smf
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.linear_model import LinearRegression
```

**Develop a multiple linear regression model that predicts car price based on engine size, year, mileage, and mpg.** Datasets to be used: *Car_features_train.csv, Car_prices_train.csv*

```
# Reading datasets
trainf = pd.read_csv('./Datasets/Car_features_train.csv')
trainp = pd.read_csv('./Datasets/Car_prices_train.csv')
train = pd.merge(trainf,trainp)
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 |

| | carID | brand | model | year | transmission | mileage | fuelType | tax | mpg | engineSize | price |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 4 | 18492 | bmw | 6 Series | 2015 | Automatic | 62953 | Diesel | 160 | 51.4903 | 3.0 | 18990 |

### 2.1.1 Training the model

```
#Using the ols function to create an ols object. 'ols' stands for 'Ordinary least squares'
ols_object = smf.ols(formula = 'price~year+mileage+mpg+engineSize', data = train)
model = ols_object.fit()
model.summary()
```

| | | | |
|---|---|---|---|
| **Dep. Variable:** | price | **R-squared:** | 0.660 |
| **Model:** | OLS | **Adj. R-squared:** | 0.660 |
| **Method:** | Least Squares | **F-statistic:** | 2410. |
| **Date:** | Mon, 29 Jan 2024 | **Prob (F-statistic):** | 0.00 |
| **Time:** | 03:10:20 | **Log-Likelihood:** | -52497. |
| **No. Observations:** | 4960 | **AIC:** | 1.050e+05 |
| **Df Residuals:** | 4955 | **BIC:** | 1.050e+05 |
| **Df Model:** | 4 | | |
| **Covariance Type:** | nonrobust | | |

| | **coef** | **std err** | **t** | **P> \|t\|** | **[0.025** | **0.975]** |
|---|---|---|---|---|---|---|
| **Intercept** | -3.661e+06 | 1.49e+05 | -24.593 | 0.000 | -3.95e+06 | -3.37e+06 |
| **year** | 1817.7366 | 73.751 | 24.647 | 0.000 | 1673.151 | 1962.322 |
| **mileage** | -0.1474 | 0.009 | -16.817 | 0.000 | -0.165 | -0.130 |
| **mpg** | -79.3126 | 9.338 | -8.493 | 0.000 | -97.620 | -61.006 |
| **engineSize** | 1.218e+04 | 189.969 | 64.107 | 0.000 | 1.18e+04 | 1.26e+04 |

| | | | |
|---|---|---|---|
| **Omnibus:** | 2450.973 | **Durbin-Watson:** | 0.541 |
| **Prob(Omnibus):** | 0.000 | **Jarque-Bera (JB):** | 31060.548 |
| **Skew:** | 2.045 | **Prob(JB):** | 0.00 |
| **Kurtosis:** | 14.557 | **Cond. No.** | 3.83e+07 |

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
[2] The condition number is large, 3.83e+07. This might indicate that there are strong multicollinearity or other numerical problems.

The model equation is: estimated car `price` = -3.661e6 + 1818 * `year` -0.15 * `mileage` - 79.31 * `mpg` + 12180 * `engineSize`

The procedure to fit the model using `sklearn` will be similar to that in simple linear regression.

```
model = LinearRegression()

X_train = train[['year','engineSize','mpg','mileage']] # Slice out the predictors
y_train = train[['price']]

model.fit(X_train,y_train)
```

### 2.1.2 Hypothesis test for a relationship between the response and a subset of predictors

Let us test the hypothesis if there is relationship between car price and the set of predictors: `mpg` and `year`.

```
hypothesis = '(mpg = 0, year = 0)'

model.f_test(hypothesis) # the F test of these two predictors is stat. sig.
```

```
<class 'statsmodels.stats.contrast.ContrastResults'>
<F test: F=325.9206432972666, p=1.0499509223096256e-133, df_denom=4.96e+03, df_num=2>
```

As the $p$-value is low, we reject the null hypothesis, i.e., at least one of the predictors among `mpg` and `year` has a statistically significant relationship with car price.

**Predict the car price for the cars in the test dataset**. Datasets to be used: *Car_features_test.csv, Car_prices_test.csv*

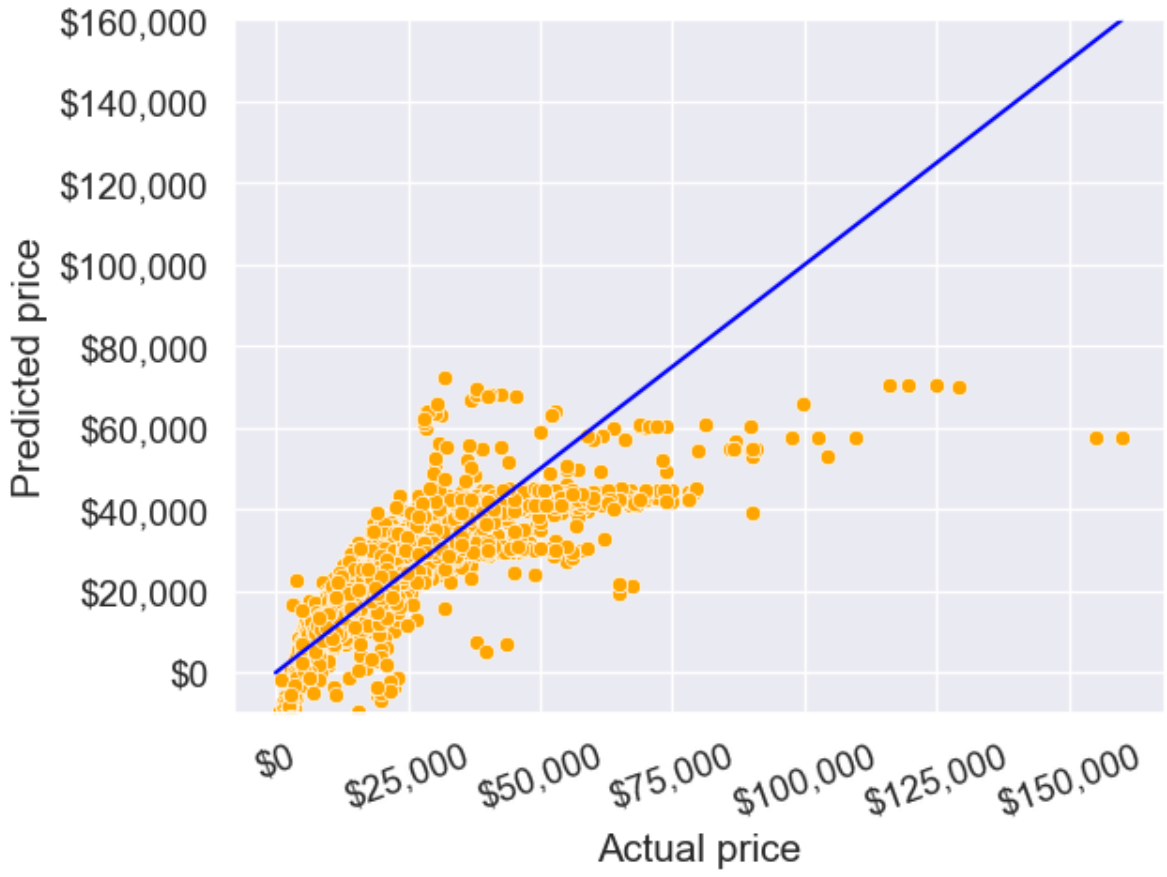
```
testf = pd.read_csv('./Datasets/Car_features_test.csv')
testp = pd.read_csv('./Datasets/Car_prices_test.csv')
```

### 2.1.3 Prediction

```
pred_price = model.predict(testf)
```

**Make a visualization that compares the predicted car prices with the actual car prices**

```
sns.set(font_scale=1.25)
sns.scatterplot(x = testp.price, y = pred_price, color = 'orange')
#In case of a perfect prediction, all the points must lie on the line x = y.
ax = sns.lineplot(x = [0,testp.price.max()], y = [0,testp.price.max()],color='blue') #Plotti
plt.xlabel('Actual price')
plt.ylabel('Predicted price')
plt.ylim([-10000, 160000])
ax.yaxis.set_major_formatter('${x:,.0f}')
ax.xaxis.set_major_formatter('${x:,.0f}')
plt.xticks(rotation=20);
```




The prediction looks better as compared to the one with simple linear regression. This is because we have four predictors to help explain the variation in car price, instead of just one in the case of simple linear regression. Also, all the predictors have a significant relationship with price as evident from their p-values. Thus, all four of them are contributing in explaining the variation. Note the higher values of $R^2$ as compared to the one in the case of simple linear regression.

**What is the RMSE of the predicted car price?**

```
np.sqrt(((testp.price - pred_price)**2).mean())
```

```
9956.82497993548
```

**What is the residual standard error based on the training data?**

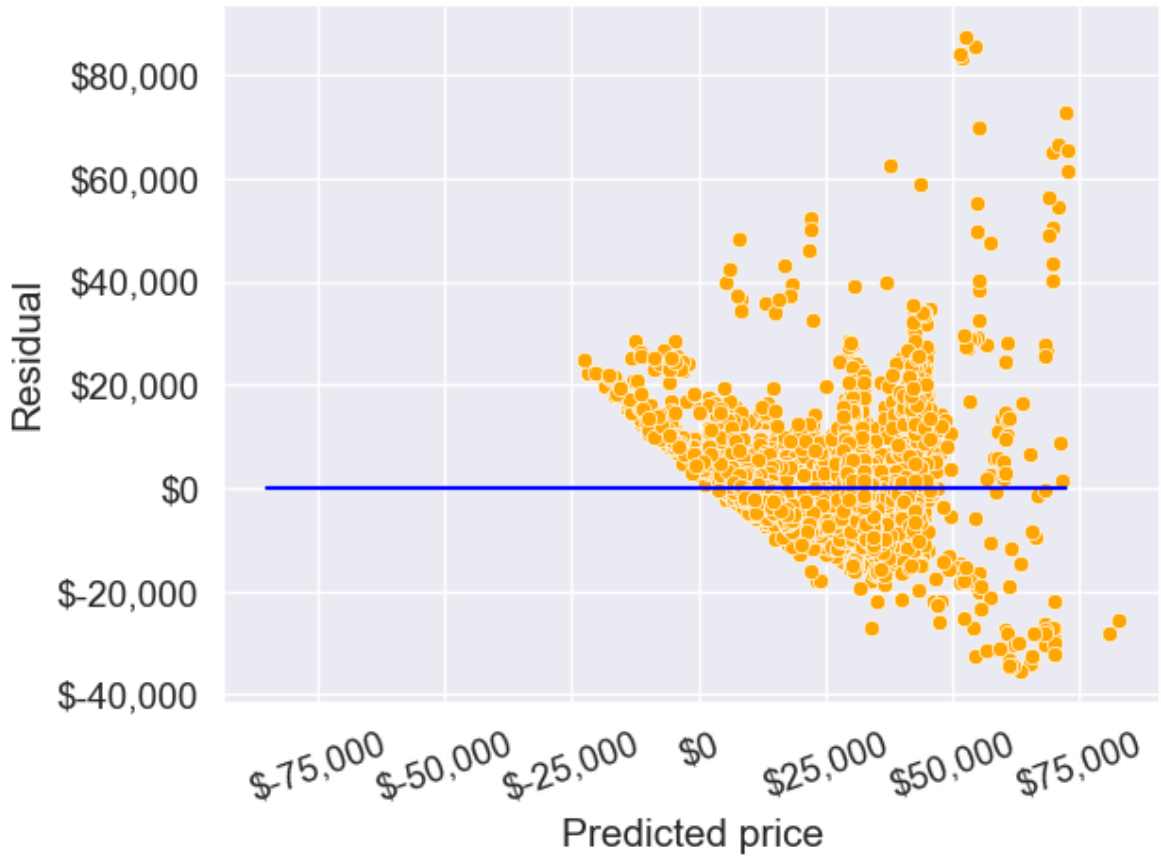
```
np.sqrt(model.mse_resid)
```

```
9563.74782917604
```

```
trainp.describe()
```

| | carID | price |
|---|---|---|
| count | 4960.000000 | 4960.000000 |
| mean | 15832.446169 | 23469.943750 |
| std | 2206.717006 | 16406.714563 |
| min | 12002.000000 | 450.000000 |
| 25% | 13929.250000 | 12000.000000 |
| 50% | 15840.000000 | 18999.000000 |
| 75% | 17765.750000 | 30335.750000 |
| max | 19629.000000 | 145000.000000 |

```
sns.scatterplot(x = model.fittedvalues, y=model.resid,color = 'orange')
ax = sns.lineplot(x = [pred_price.min(),pred_price.max()],y = [0,0],color = 'blue')
plt.xlabel('Predicted price')
plt.ylabel('Residual')
ax.yaxis.set_major_formatter('${x:,.0f}')
ax.xaxis.set_major_formatter('${x:,.0f}')
plt.xticks(rotation=20);
```




### 2.1.4 Effect of adding noisy predictors on $R^2$

**Will the explained variation (R-squared) in car price always increase if we add a variable?**

**Should we keep on adding variables as long as the explained variation (R-squared) is increasing?**

```
#Using the ols function to create an ols object. 'ols' stands for 'Ordinary least squares'
np.random.seed(1)
train['rand_col'] = np.random.rand(train.shape[0])
ols_object = smf.ols(formula = 'price~year+mileage+mpg+engineSize+rand_col', data = train)
model = ols_object.fit()
model.summary()
```

Table 2.3: OLS Regression Results

| | | | |
|---|---|---|---|
| Dep. Variable: | price | R-squared: | 0.661 |
| Model: | OLS | Adj. R-squared: | 0.660 |
| Method: | Least Squares | F-statistic: | 1928. |
| Date: | Tue, 27 Dec 2022 | Prob (F-statistic): | 0.00 |
| Time: | 01:07:38 | Log-Likelihood: | -52497. |
| No. Observations: | 4960 | AIC: | 1.050e+05 |
| Df Residuals: | 4954 | BIC: | 1.050e+05 |
| Df Model: | 5 | | |
| Covariance Type: | nonrobust | | |

| | coef | std err | t | P>\|t\| | [0.025 | 0.975] |
|---|---|---|---|---|---|---|
| Intercept | -3.662e+06 | 1.49e+05 | -24.600 | 0.000 | -3.95e+06 | -3.37e+06 |
| year | 1818.1672 | 73.753 | 24.652 | 0.000 | 1673.578 | 1962.756 |
| mileage | -0.1474 | 0.009 | -16.809 | 0.000 | -0.165 | -0.130 |
| mpg | -79.2837 | 9.338 | -8.490 | 0.000 | -97.591 | -60.976 |
| engineSize | 1.218e+04 | 189.972 | 64.109 | 0.000 | 1.18e+04 | 1.26e+04 |
| rand_col | 451.1226 | 471.897 | 0.956 | 0.339 | -474.004 | 1376.249 |

| | | | |
|---|---|---|---|
| Omnibus: | 2451.728 | Durbin-Watson: | 0.541 |
| Prob(Omnibus): | 0.000 | Jarque-Bera (JB): | 31040.331 |
| Skew: | 2.046 | Prob(JB): | 0.00 |
| Kurtosis: | 14.552 | Cond. No. | 3.83e+07 |

Adding a variable with random values to the model (`rand_col`) increased the explained variation ($R^2$). This is because the model has one more parameter to tune to reduce the residual squared error ($RSS$). However, the $p$-value of `rand_col` suggests that its coefficient is zero. Thus, using the model with `rand_col` may give poorer performance on unknown data, as compared to the model without `rand_col`. This implies that it is not a good idea to blindly add variables in the model to increase $R^2$.

# 3 Variable interactions and transformations

*Read sections 3.3.1 and 3.3.2 of the book before using these notes.*

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

## 3.1 Variable interactions

```
import pandas as pd
import numpy as np
import statsmodels.formula.api as smf
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.preprocessing import PolynomialFeatures
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_squared_error
```

```
trainf = pd.read_csv('./Datasets/Car_features_train.csv')
trainp = pd.read_csv('./Datasets/Car_prices_train.csv')
testf = pd.read_csv('./Datasets/Car_features_test.csv')
testp = pd.read_csv('./Datasets/Car_prices_test.csv')
train = pd.merge(trainf,trainp)
test = pd.merge(testf,testp)
train.head()
```

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

Until now, we have assumed that the association between a predictor $X_j$ and response $Y$ does not depend on the value of other predictors. For example, the multiple linear regression model that we developed in Chapter 2 assumes that the average increase in price associated with a unit increase in engineSize is always $12,180, regardless of the value of other predictors. However, this assumption may be incorrect.

### 3.1.1 Variable interaction between continuous predictors

We can relax this assumption by considering another predictor, called an interaction term. Let us assume that the average increase in `price` associated with a one-unit increase in `engineSize` depends on the model `year` of the car. In other words, there is an interaction between `engineSize` and `year`. This interaction can be included as a predictor, which is the product of `engineSize` and `year`. *Note that there are several possible interactions that we can consider. Here the interaction between* ***`engineSize`*** *and* ***`year`*** *is just an example.*

```
#Considering interaction between engineSize and year
ols_object = smf.ols(formula = 'price~year*engineSize+mileage+mpg', data = train)
model = ols_object.fit()
model.summary()
```

Table 3.2: OLS Regression Results

| | | | |
|---|---|---|---|
| Dep. Variable: | price | R-squared: | 0.682 |
| Model: | OLS | Adj. R-squared: | 0.681 |
| Method: | Least Squares | F-statistic: | 2121. |
| Date: | Tue, 24 Jan 2023 | Prob (F-statistic): | 0.00 |
| Time: | 15:28:11 | Log-Likelihood: | -52338. |
| No. Observations: | 4960 | AIC: | 1.047e+05 |
| Df Residuals: | 4954 | BIC: | 1.047e+05 |
| Df Model: | 5 | | |
| Covariance Type: | nonrobust | | |

| | coef | std err | t | P>\|t\| | [0.025 | 0.975] |
|---|---|---|---|---|---|---|
| Intercept | 5.606e+05 | 2.74e+05 | 2.048 | 0.041 | 2.4e+04 | 1.1e+06 |
| year | -275.3833 | 135.695 | -2.029 | 0.042 | -541.405 | -9.361 |
| engineSize | -1.796e+06 | 9.97e+04 | -18.019 | 0.000 | -1.99e+06 | -1.6e+06 |
| year:engineSize | 896.7687 | 49.431 | 18.142 | 0.000 | 799.861 | 993.676 |
| mileage | -0.1525 | 0.008 | -17.954 | 0.000 | -0.169 | -0.136 |
| mpg | -84.3417 | 9.048 | -9.322 | 0.000 | -102.079 | -66.604 |

| | | | |
|---|---|---|---|
| Omnibus: | 2330.413 | Durbin-Watson: | 0.524 |
| Prob(Omnibus): | 0.000 | Jarque-Bera (JB): | 29977.437 |
| Skew: | 1.908 | Prob(JB): | 0.00 |
| Kurtosis: | 14.423 | Cond. No. | 7.66e+07 |

Note that the R-squared has increased as compared to the model in Chapter 2 since we added a predictor.

The model equation is:

$$price = \beta_0 + \beta_1 * year + \beta_2 * engineSize + \beta_3 * (year * engineSize) + \beta 4 * mileage + \beta_5 * mpg, \quad (3.1)$$

or

$$price = \beta_0 + \beta_1 * year + (\beta_2 + \beta_3 * year) * engineSize + \beta 4 * mileage + \beta_5 * mpg, \quad (3.2)$$

or

$$price = \beta_0 + \beta_1 * year + \tilde{\beta} * engineSize + \beta 4 * mileage + \beta_5 * mpg, \quad (3.3)$$

Since $\tilde{\beta}$ is a function of `year`, the association between `engineSize` and `price` is no longer a constant. A change in the value of `year` will change the association between `price` and `engineSize`.

Substituting the values of the coefficients:

`price` = 5.606e5 - 275.3833*`year` + (-1.796e6+896.7687`year`)`engineSize` -0.1525*`mileage`* - *84.3417*`mpg`

Thus, for cars launched in the year 2010, the average increase in price for one liter increase in engine size is -1.796e6 + 896.7687 * 2010 ≈ \$6,500, assuming all the other predictors are constant. However, for cars launched in the year 2020, the average increase in price for one liter increase in engine size is -1.796e6 + 896.7687*2020 ≈ \$15,500 , assuming all the other predictors are constant.

Similarly, the equation can be re-arranged as:

`price` = 5.606e5 +(-275.3833+896.7687*`engineSize`)`year` -1.796e6*`engineSize`* -*0.1525*`mileage` -84.3417*`mpg`

Thus, for cars with an engine size of 2 litres, the average increase in price for a one year newer model is -275.3833+896.7687 * 2 ≈ \$1500, assuming all the other predictors are constant.

However, for cars with an engine size of 3 litres, the average increase in price for a one year newer model is -275.3833+896.7687 * 3 ≈ \$2400, assuming all the other predictors are constant.

```
#Computing the RMSE of the model with the interaction term
pred_price = model.predict(testf)
np.sqrt(((testp.price - pred_price)**2).mean())
```

```
9423.598872501092
```

Note that the RMSE is lower than that of the model in Chapter 2. This is because the interaction term between `engineSize` and `year` is significant and relaxes the assumption of constant association between price and engine size, and between price and year. This added flexibility makes the model better fit the data. Caution: Too much flexibility may lead to overfitting!

Note that interaction terms corresponding to other variable pairs, and higher order interaction terms (such as those containing 3 or 4 variables) may also be significant and improve the model fit & thereby the prediction accuracy of the model.

### 3.1.2 Including qualitative predictors in the model

Let us develop a model for predicting `price` based on `engineSize` and the qualitative predictor `transmission`.

```
#checking the distribution of values of transmission
train.transmission.value_counts()
```

```
Manual       1948
Automatic    1660
Semi-Auto    1351
Other           1
Name: transmission, dtype: int64
```

Note that the *Other* category of the variable *transmission* contains only a single observation, which is likely to be insufficient to train the model. We'll remove that observation from the training data. Another option may be to combine the observation in the *Other* category with the nearest category, and keep it in the data.

```
train_updated = train[train.transmission!='Other']
```

```
ols_object = smf.ols(formula = 'price ~ engineSize + transmission', data = train_updated)
model = ols_object.fit()
model.summary()
```

Table 3.5: OLS Regression Results

| | | | |
|---|---|---|---|
| Dep. Variable: | price | R-squared: | 0.459 |
| Model: | OLS | Adj. R-squared: | 0.458 |
| Method: | Least Squares | F-statistic: | 1400. |
| Date: | Tue, 24 Jan 2023 | Prob (F-statistic): | 0.00 |
| Time: | 15:28:21 | Log-Likelihood: | -53644. |
| No. Observations: | 4959 | AIC: | 1.073e+05 |
| Df Residuals: | 4955 | BIC: | 1.073e+05 |
| Df Model: | 3 | | |
| Covariance Type: | nonrobust | | |

| | coef | std err | t | P>\|t\| | [0.025 | 0.975] |
|---|---|---|---|---|---|---|
| Intercept | 3042.6765 | 661.190 | 4.602 | 0.000 | 1746.451 | 4338.902 |
| transmission[T.Manual] | -6770.6165 | 442.116 | -15.314 | 0.000 | -7637.360 | -5903.873 |
| transmission[T.Semi-Auto] | 4994.3112 | 442.989 | 11.274 | 0.000 | 4125.857 | 5862.765 |
| engineSize | 1.023e+04 | 247.485 | 41.323 | 0.000 | 9741.581 | 1.07e+04 |

| | | | |
|---|---|---|---|
| Omnibus: | 1575.518 | Durbin-Watson: | 0.579 |
| Prob(Omnibus): | 0.000 | Jarque-Bera (JB): | 11006.609 |
| Skew: | 1.334 | Prob(JB): | 0.00 |
| Kurtosis: | 9.793 | Cond. No. | 11.4 |

Note that there is no coefficient for the *Automatic* level of the variable `Transmission`. If a car doesn't have *Manual* or *Semi-Automatic* transmission, then it has an *Automatic* transmission. Thus, the coefficient of *Automatic* will be redundant, and the dummy variable corresponding to *Automatic* transmission is dropped from the model.

The level of the categorical variable that is dropped from the model is called the baseline level. Here *Automatic* transmission is the baseline level. The coefficients of other levels of `transmission` should be interpreted with respect to the baseline level.

**Q:** Interpret the intercept term

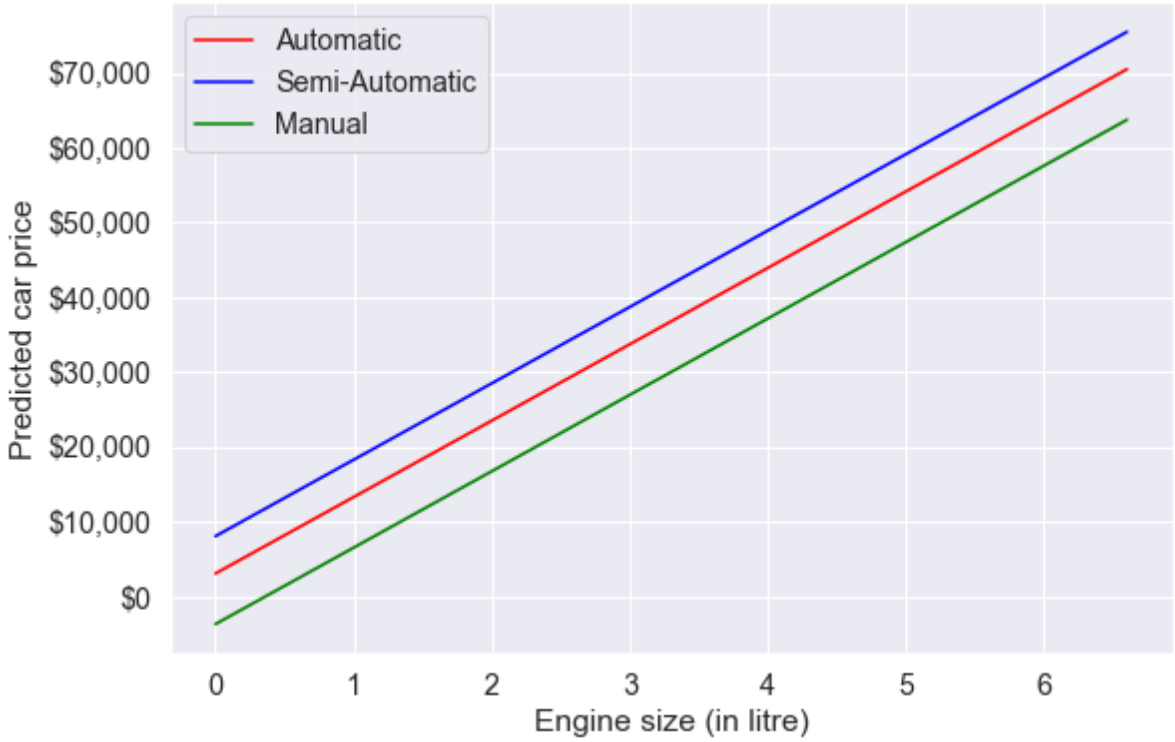
**Ans:** For the hypothetical scenario of a car with zero engine size and *Automatic* transmission, the estimated mean car price is ≈ \$3042.

**Q:** Interpret the coefficient of `transmission[T.Manual]`

**Ans:** The estimated mean price of a car with manual transmission is ≈ \$6770 less than that of a car with *Automatic* transmission.

Let us visualize the developed model.

```
#Visualizing the developed model
plt.rcParams["figure.figsize"] = (9,6)
sns.set(font_scale = 1.3)
x = np.linspace(train_updated.engineSize.min(),train_updated.engineSize.max(),100)
ax = sns.lineplot(x = x, y = model.params['engineSize']*x+model.params['Intercept'], color =
sns.lineplot(x = x, y = model.params['engineSize']*x+model.params['Intercept']+model.params[
sns.lineplot(x = x, y = model.params['engineSize']*x+model.params['Intercept']+model.params[
plt.legend(labels=["Automatic","Semi-Automatic", "Manual"])
plt.xlabel('Engine size (in litre)')
plt.ylabel('Predicted car price')
ax.yaxis.set_major_formatter('${x:,.0f}')
```



Based on the developed model, for a given engine size, the car with a semi-automatic transmission is estimated to be the most expensive on average, while the car with a manual transmission is estimated to be the least expensive on average.

**Changing the baseline level:** By default, the baseline level is chosen as the one that comes first if the levels are arranged in alphabetical order. However, you can change the baseline level by specifying one explicitly.

Internally, statsmodels uses the patsy package to convert formulas and data to the matrices that are used in model fitting. You may refer to this section in the patsy documentation to specify a particular level of the categorical variable as the baseline.

For example, suppose we wish to change the baseline level to *Manual* transmission. We can specify this in the formula as follows:

```
ols_object = smf.ols(formula = 'price~engineSize+C(transmission, Treatment("Manual"))', data
model = ols_object.fit()
model.summary()
```

Table 3.8: OLS Regression Results

| | | | |
|---|---|---|---|
| Dep. Variable: | price | R-squared: | 0.459 |
| Model: | OLS | Adj. R-squared: | 0.458 |
| Method: | Least Squares | F-statistic: | 1400. |
| Date: | Tue, 24 Jan 2023 | Prob (F-statistic): | 0.00 |
| Time: | 15:28:39 | Log-Likelihood: | -53644. |
| No. Observations: | 4959 | AIC: | 1.073e+05 |
| Df Residuals: | 4955 | BIC: | 1.073e+05 |
| Df Model: | 3 | | |
| Covariance Type: | nonrobust | | |

| | coef | std err | t | P>\|t\| | [0.025 | 0.9 |
|---|---|---|---|---|---|---|
| Intercept | -3727.9400 | 492.917 | -7.563 | 0.000 | -4694.275 | -27 |
| C(transmission, Treatment("Manual"))[T.Automatic] | 6770.6165 | 442.116 | 15.314 | 0.000 | 5903.873 | 763 |
| C(transmission, Treatment("Manual"))[T.Semi-Auto] | 1.176e+04 | 473.110 | 24.867 | 0.000 | 1.08e+04 | 1.2 |
| engineSize | 1.023e+04 | 247.485 | 41.323 | 0.000 | 9741.581 | 1.0 |

| | | | |
|---|---|---|---|
| Omnibus: | 1575.518 | Durbin-Watson: | 0.579 |
| Prob(Omnibus): | 0.000 | Jarque-Bera (JB): | 11006.609 |
| Skew: | 1.334 | Prob(JB): | 0.00 |
| Kurtosis: | 9.793 | Cond. No. | 8.62 |

### 3.1.3 Including qualitative predictors and their interaction with continuous predictors in the model

Note that the qualitative predictor leads to fitting 3 parallel lines to the data, as there are 3 categories.

However, note that we have made the constant association assumption. The fact that the lines are parallel means that the average increase in car price for one litre increase in engine size does not depend on the type of transmission. This represents a potentially serious limitation of the model, since in fact a change in engine size may have a very different association on the price of an automatic car versus a semi-automatic or manual car.

This limitation can be addressed by adding an interaction variable, which is the product of `engineSize` and the dummy variables for semi-automatic and manual transmissions.

```
#Using the ols function to create an ols object. 'ols' stands for 'Ordinary least squares'
ols_object = smf.ols(formula = 'price~engineSize*transmission', data = train_updated)
model = ols_object.fit()
model.summary()
```

Table 3.11: OLS Regression Results

| | | | |
|---|---|---|---|
| Dep. Variable: | price | R-squared: | 0.479 |
| Model: | OLS | Adj. R-squared: | 0.478 |
| Method: | Least Squares | F-statistic: | 909.9 |
| Date: | Sun, 22 Jan 2023 | Prob (F-statistic): | 0.00 |
| Time: | 22:55:55 | Log-Likelihood: | -53550. |
| No. Observations: | 4959 | AIC: | 1.071e+05 |
| Df Residuals: | 4953 | BIC: | 1.072e+05 |
| Df Model: | 5 | | |
| Covariance Type: | nonrobust | | |

| | coef | std err | t | P>\|t\| | [0.025 | 0.975] |
|---|---|---|---|---|---|---|
| Intercept | 3754.7238 | 895.221 | 4.194 | 0.000 | 1999.695 | 5509.753 |
| transmission[T.Manual] | 1768.5856 | 1294.071 | 1.367 | 0.172 | -768.366 | 4305.538 |
| transmission[T.Semi-Auto] | -5282.7164 | 1416.472 | -3.729 | 0.000 | -8059.628 | -2505.805 |
| engineSize | 9928.6082 | 354.511 | 28.006 | 0.000 | 9233.610 | 1.06e+04 |
| engineSize:transmission[T.Manual] | -5285.9059 | 646.175 | -8.180 | 0.000 | -6552.695 | -4019.117 |
| engineSize:transmission[T.Semi-Auto] | 4162.2428 | 552.597 | 7.532 | 0.000 | 3078.908 | 5245.578 |

| | | | |
|---|---|---|---|
| Omnibus: | 1379.846 | Durbin-Watson: | 0.622 |
| Prob(Omnibus): | 0.000 | Jarque-Bera (JB): | 9799.471 |
| Skew: | 1.139 | Prob(JB): | 0.00 |
| Kurtosis: | 9.499 | Cond. No. | 30.8 |

The model equation for the model with interactions is:

Automatic transmission: `price` = 3754.7238 + 9928.6082 * `engineSize`,

Semi-Automatic transmission: `price` = 3754.7238 + 9928.6082 * `engineSize` + (-5282.7164+4162.2428*`engineSize`),

Manual transmission: `price` = 3754.7238 + 9928.6082 * `engineSize` +(1768.5856-5285.9059 * `engineSize`),

or

Automatic transmission: `price` = 3754.7238 + 9928.6082 * `engineSize`,

Semi-Automatic transmission: `price` = -1527 + 7046 * `engineSize`,

Manual transmission: `price` = 5523 + 4642 * `engineSize`

**Q:** Interpret the coefficient of manual tranmission, i.e., the coefficient of `transmission[T.Manual]`.

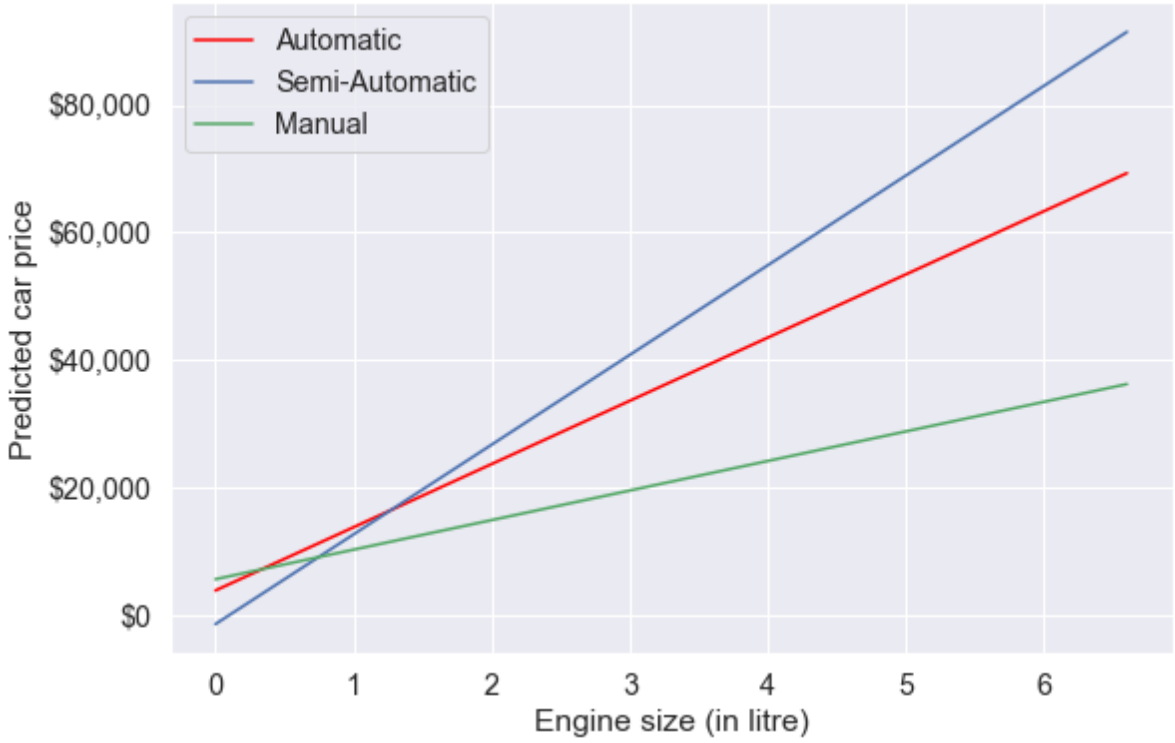
**A:** For a hypothetical scenario of zero engine size, the estimated mean `price` of a car with *Manual* `transmission` is ≈ \$1768 more than the estimated mean `price` of a car with *Automatic* `transmission`.

**Q:** Interpret the coefficient of the interaction between engine size and manual transmission, i.e., the coefficient of `engineSize:transmission[T.Manual]`.

**A:** For a unit (or a litre) increase in `engineSize` , the increase in estimated mean `price` of a car with *Manual* transmission is ≈ \$5285 less than the increase in estimated mean `price` of a car with *Automatic* transmission.

```
#Visualizing the developed model with interaction terms
plt.rcParams["figure.figsize"] = (9,6)
sns.set(font_scale = 1.3)
x = np.linspace(train_updated.engineSize.min(),train_updated.engineSize.max(),100)
ax = sns.lineplot(x = x, y = model.params['engineSize']*x+model.params['Intercept'], label='A
plt.plot(x, (model.params['engineSize']+model.params['engineSize:transmission[T.Semi-Auto]'])
plt.plot(x, (model.params['engineSize']+model.params['engineSize:transmission[T.Manual]'])*x+
plt.legend(loc='upper left')
plt.xlabel('Engine size (in litre)')
```

```
plt.ylabel('Predicted car price')
ax.yaxis.set_major_formatter('${x:,.0f}')
```




Note the interaction term adds flexibility to the model.

The slope of the regression line for semi-automatic cars is the largest. This suggests that increase in engine size is associated with a higher increase in car price for semi-automatic cars, as compared to other cars.

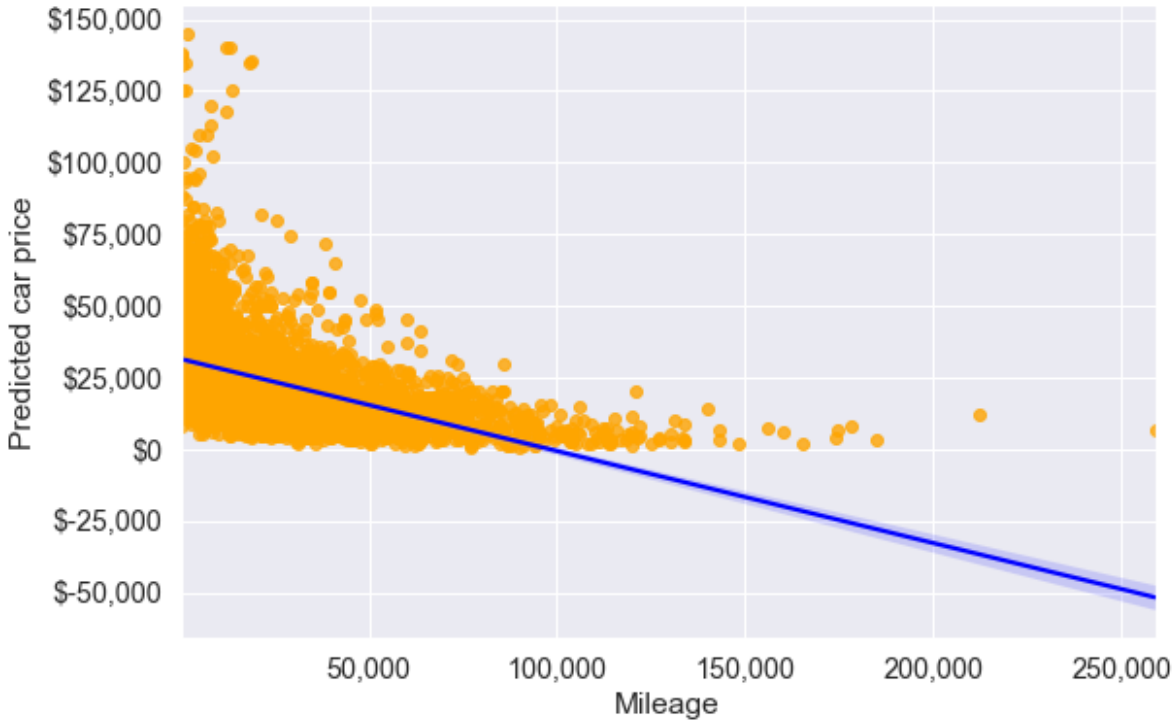
## 3.2 Variable transformations

So far we have considered only a linear relationship between the predictors and the response. However, the relationship may be non-linear.

Consider the regression plot of `price` on `mileage`.

```
ax = sns.regplot(x = train_updated.mileage, y =train_updated.price,color = 'orange', line_kws
plt.xlabel('Mileage')
plt.ylabel('Predicted car price')
```

```
ax.yaxis.set_major_formatter('${x:,.0f}')
ax.xaxis.set_major_formatter('{x:,.0f}')
```




```
#R-squared of the model with just mileage
model = smf.ols('price~mileage', data = train_updated).fit()
model.rsquared
```

```
0.22928048993376182
```

From the first scatterplot, we see that the relationship between `price` and `mileage` doesn't seem to be linear, as the points do not lie on a straight line. Also, we see the regression line (or the curve), which is the best fit line doesn't seem to fit the points well. However, `price` on average seems to decrease with `mileage`, albeit in a non-linear manner.

### 3.2.1 Quadratic transformation

So, we guess that if we model price as a quadratic function of `mileage`, the model may better fit the points (or the curve may better fit the points). Let us transform the predictor `mileage` to include $mileage^2$ (i.e., perform a quadratic transformation on the predictor).

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

Table 3.14: OLS Regression Results

| | | | |
|---|---|---|---|
| Dep. Variable: | price | R-squared: | 0.271 |
| Model: | OLS | Adj. R-squared: | 0.271 |
| Method: | Least Squares | F-statistic: | 920.6 |
| Date: | Sun, 22 Jan 2023 | Prob (F-statistic): | 0.00 |
| Time: | 23:26:05 | Log-Likelihood: | -54382. |
| No. Observations: | 4959 | AIC: | 1.088e+05 |
| Df Residuals: | 4956 | BIC: | 1.088e+05 |
| Df Model: | 2 | | |
| Covariance Type: | nonrobust | | |

| | coef | std err | t | P>\|t\| | [0.025 | 0.975] |
|---|---|---|---|---|---|---|
| Intercept | 3.44e+04 | 332.710 | 103.382 | 0.000 | 3.37e+04 | 3.5e+04 |
| mileage | -0.5662 | 0.017 | -33.940 | 0.000 | -0.599 | -0.534 |
| I(mileage ** 2) | 2.629e-06 | 1.56e-07 | 16.813 | 0.000 | 2.32e-06 | 2.94e-06 |

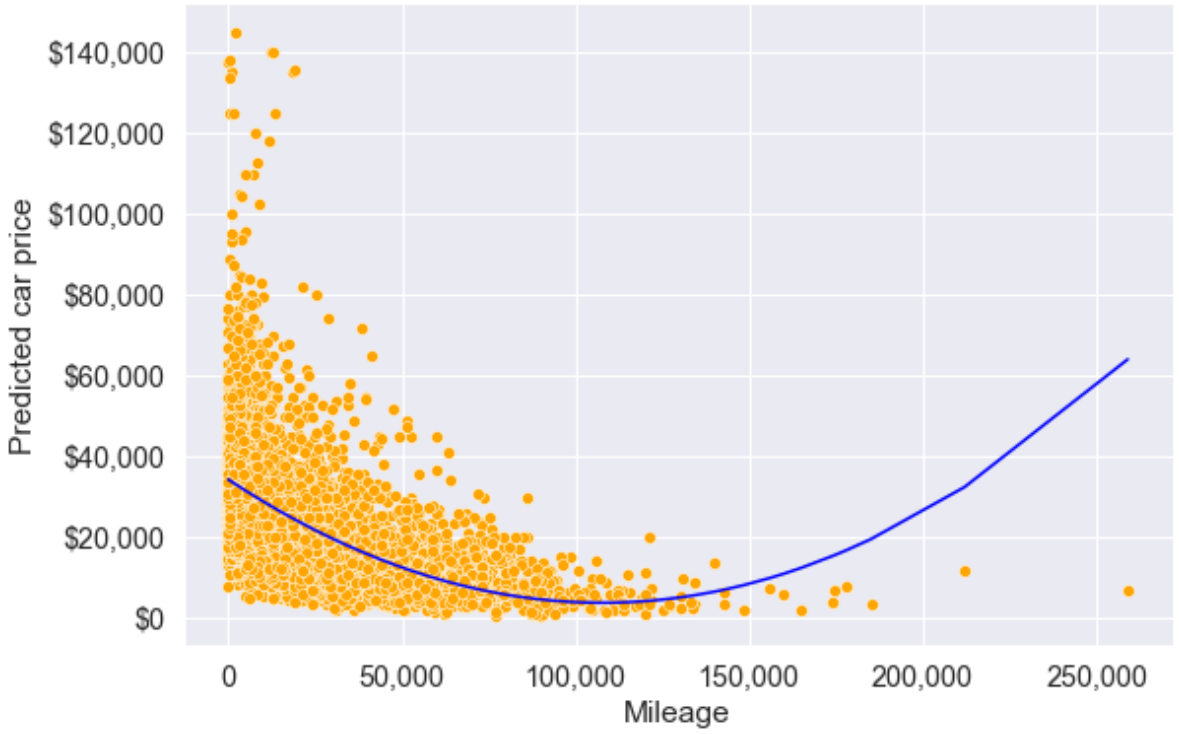
| | | | |
|---|---|---|---|
| Omnibus: | 2362.973 | Durbin-Watson: | 0.325 |
| Prob(Omnibus): | 0.000 | Jarque-Bera (JB): | 22427.952 |
| Skew: | 2.052 | Prob(JB): | 0.00 |
| Kurtosis: | 12.576 | Cond. No. | 4.81e+09 |

Note that in the formula specified within the `ols()` function, the `I()` operator isolates or insulates the contents within I(…) from the regular formula operators. Without the `I()` operator, `mileage**2` will be treated as the interaction of `mileage` with itself, which is `mileage`. Thus, to add the square of `mileage` as a separate predictor, we need to use the `I()` operator.

Let us visualize the model fit with the quadratic transformation of the predictor - `mileage`.

```
#Visualizing the regression line with the model consisting of the quadratic transformation o
pred_price = model.predict(train_updated)
ax = sns.scatterplot(x = 'mileage', y = 'price', data = train_updated, color = 'orange')
sns.lineplot(x = train_updated.mileage, y = pred_price, color = 'blue')
plt.xlabel('Mileage')
```

```
plt.ylabel('Predicted car price')
ax.yaxis.set_major_formatter('${x:,.0f}')
ax.xaxis.set_major_formatter('{x:,.0f}')
```




The above model seems to better fit the data (as compared to the model without transformation) at least upto mileage around 125,000. The $R^2$ of the model with the quadratic transformation of `mileage` is also higher than that of the model without transformation indicating a better fit.

### 3.2.2 Cubic transformation

Let us see if a cubic transformation of `mileage` can further improve the model fit.

```
#Including mileage squared and mileage cube as predictors and developing the model
ols_object = smf.ols(formula = 'price~mileage+I(mileage**2)+I(mileage**3)', data = train_upda
model = ols_object.fit()
model.summary()
```

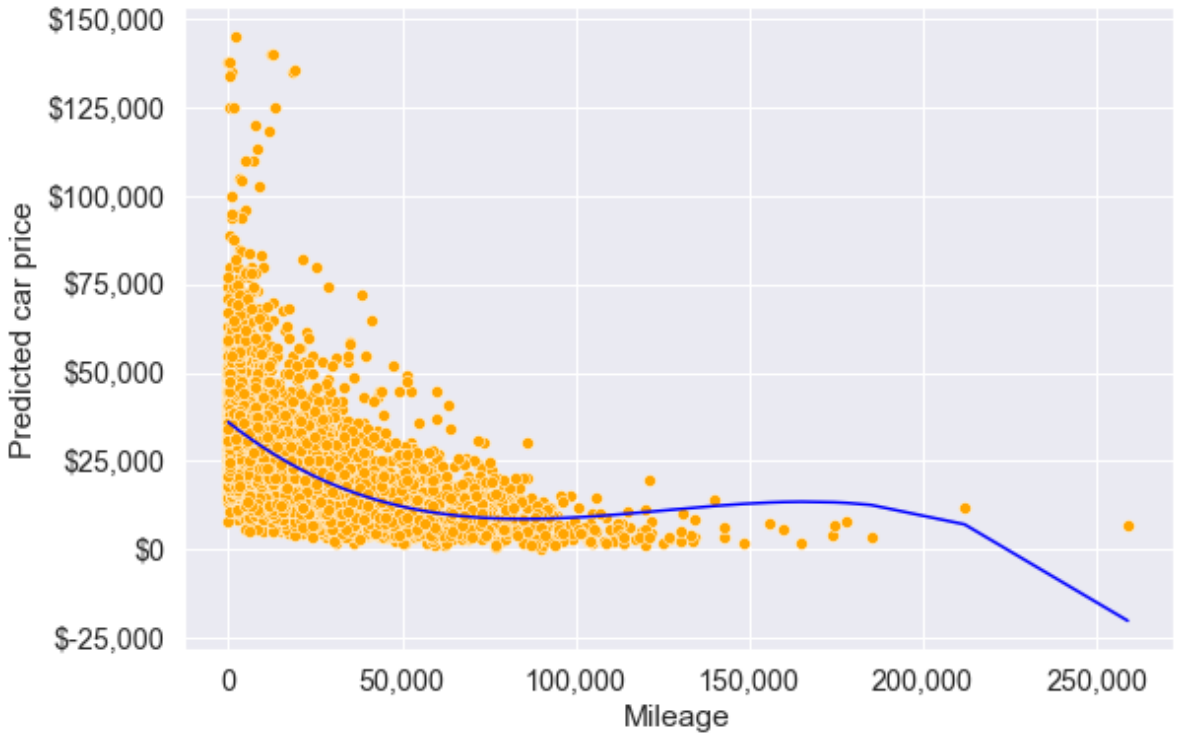
Table 3.17: OLS Regression Results

| | | | |
|---|---|---|---|
| Dep. Variable: | price | R-squared: | 0.283 |
| Model: | OLS | Adj. R-squared: | 0.283 |
| Method: | Least Squares | F-statistic: | 652.3 |
| Date: | Sun, 22 Jan 2023 | Prob (F-statistic): | 0.00 |
| Time: | 23:33:27 | Log-Likelihood: | -54340. |
| No. Observations: | 4959 | AIC: | 1.087e+05 |
| Df Residuals: | 4955 | BIC: | 1.087e+05 |
| Df Model: | 3 | | |
| Covariance Type: | nonrobust | | |

| | coef | std err | t | P>\|t\| | [0.025 | 0.975] |
|---|---|---|---|---|---|---|
| Intercept | 3.598e+04 | 371.926 | 96.727 | 0.000 | 3.52e+04 | 3.67e+04 |
| mileage | -0.7742 | 0.028 | -27.634 | 0.000 | -0.829 | -0.719 |
| I(mileage ** 2) | 6.875e-06 | 4.87e-07 | 14.119 | 0.000 | 5.92e-06 | 7.83e-06 |
| I(mileage ** 3) | -1.823e-11 | 1.98e-12 | -9.199 | 0.000 | -2.21e-11 | -1.43e-11 |

| | | | |
|---|---|---|---|
| Omnibus: | 2380.788 | Durbin-Watson: | 0.321 |
| Prob(Omnibus): | 0.000 | Jarque-Bera (JB): | 23039.307 |
| Skew: | 2.065 | Prob(JB): | 0.00 |
| Kurtosis: | 12.719 | Cond. No. | 7.73e+14 |

```
#Visualizing the model with the cubic transformation of mileage
pred_price = model.predict(train_updated)
ax = sns.scatterplot(x = 'mileage', y = 'price', data = train_updated, color = 'orange')
sns.lineplot(x = train_updated.mileage, y = pred_price, color = 'blue')
plt.xlabel('Mileage')
plt.ylabel('Predicted car price')
ax.yaxis.set_major_formatter('${x:,.0f}')
ax.xaxis.set_major_formatter('{x:,.0f}')
```




Note that the model fit with the cubic transformation of `mileage` seems slightly better as compared to the models with the quadratic transformation, and no transformation of mileage, for mileage up to 180k. However, the model should not be used to predict car prices of cars with a mileage higher than 180k.

Let's update the model created earlier (in the beginning of this chapter) to include the transformed predictor.

```
#Model with an interaction term and a variable transformation term
ols_object = smf.ols(formula = 'price~year*engineSize+mileage+mpg+I(mileage**2)', data = tra
model = ols_object.fit()
model.summary()
```

Table 3.20: OLS Regression Results

| | | | |
|---|---|---|---|
| Dep. Variable: | price | R-squared: | 0.702 |
| Model: | OLS | Adj. R-squared: | 0.702 |
| Method: | Least Squares | F-statistic: | 1947. |
| Date: | Sun, 22 Jan 2023 | Prob (F-statistic): | 0.00 |
| Time: | 23:42:13 | Log-Likelihood: | -52162. |
| No. Observations: | 4959 | AIC: | 1.043e+05 |

| | | | |
|---|---|---|---|
| Df Residuals: | 4952 | BIC: | 1.044e+05 |
| Df Model: | 6 | | |
| Covariance Type: | nonrobust | | |

| | coef | std err | t | P>\|t\| | [0.025 | 0.975] |
|---|---|---|---|---|---|---|
| Intercept | 1.53e+06 | 2.7e+05 | 5.671 | 0.000 | 1e+06 | 2.06e+06 |
| year | -755.7419 | 133.791 | -5.649 | 0.000 | -1018.031 | -493.453 |
| engineSize | -2.022e+06 | 9.72e+04 | -20.803 | 0.000 | -2.21e+06 | -1.83e+06 |
| year:engineSize | 1008.6993 | 48.196 | 20.929 | 0.000 | 914.215 | 1103.184 |
| mileage | -0.3548 | 0.014 | -25.973 | 0.000 | -0.382 | -0.328 |
| mpg | -54.7450 | 8.896 | -6.154 | 0.000 | -72.185 | -37.305 |
| I(mileage ** 2) | 1.926e-06 | 1.04e-07 | 18.536 | 0.000 | 1.72e-06 | 2.13e-06 |

| | | | |
|---|---|---|---|
| Omnibus: | 2355.448 | Durbin-Watson: | 0.562 |
| Prob(Omnibus): | 0.000 | Jarque-Bera (JB): | 38317.404 |
| Skew: | 1.857 | Prob(JB): | 0.00 |
| Kurtosis: | 16.101 | Cond. No. | 6.40e+12 |

Note that the R-squared has increased as compared to the model with just the interaction term.

```
#Computing RMSE on test data
pred_price = model.predict(testf)
np.sqrt(((testp.price - pred_price)**2).mean())
```

```
9074.494088619422
```

Note that the prediction accuracy of the model has further increased, as the RMSE has reduced. The transformed predictor is statistically significant and provides additional flexibility to better capture the trend in the data, leading to an increase in prediction accuracy.

## 3.3 `PolynomialFeatures()`

The function `PolynomialFeatures()` from the `sklearn` library can be used to generate a predictor matrix that includes all interactions and transformations upto a degree `d`.

```
X_train = train[['mileage', 'engineSize', 'year', 'mpg']]
y_train = train[['price']]
X_test = test[['mileage', 'engineSize', 'year', 'mpg']]
y_test = test[['price']]
```

### 3.3.1 Generating polynomial features

Let us generate polynomial features upto degree 2. This will include all the two-factor interactions, and all squared terms of degree 2.

```
poly = PolynomialFeatures(2, include_bias = False) # Create the object - degree is 2

# Generate the polynomial features
X_train_poly = poly.fit_transform(X_train)
```

Note that the `LinearRegression()` function adds the intercept by default *(check the `fit_intercept` argument)*. Thus, we have put `include_bias = False` while generating the polynomial features, as we don't need the intercept. The term `bias` here refers to the intercept *(you will learn about `bias` in detail in STAT303-3)*. Another option is to include the intercept while generating the polynomial features, and put `fit_intercept = False` in the `LinearRegression()` function.

Below are the polynomial features generated by the `PolynomialFeatures()` functions.

```
poly.get_feature_names_out()
```

```
array(['mileage', 'engineSize', 'year', 'mpg', 'mileage^2',
       'mileage engineSize', 'mileage year', 'mileage mpg',
       'engineSize^2', 'engineSize year', 'engineSize mpg', 'year^2',
       'year mpg', 'mpg^2'], dtype=object)
```

### 3.3.2 Fitting the model

```
model = LinearRegression()
model.fit(X_train_poly, y_train)
```

```
LinearRegression()
```

### 3.3.3 Testing the model

```
X_test_poly = poly.fit_transform(X_test)
```

```
#RMSE
np.sqrt(mean_squared_error(y_test, model.predict(X_test_poly)))
```

```
8896.175508213777
```

Note that the polynomial features have helped reduced the RMSE further.

# 4 Logistic regression

*Read sections 4.1 - 4.3 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.*

## 4.1 Theory Behind Logistic Regression

Logistic regression is the go-to linear classification algorithm for two-class problems. It is easy to implement, easy to understand and gets great results on a wide variety of problems, even when the expectations the method has for your data are violated.

### 4.1.1 Description

Logistic regression is named for the function used at the core of the method, the logistic function.

The logistic function, also called the **`Sigmoid function`** was developed by statisticians to describe properties of population growth in ecology, rising quickly and maxing out at the carrying capacity of the environment. It's an S-shaped curve that can take any real-valued number and map it into a value between 0 and 1, but never exactly at those limits.

$$\frac{1}{1+e^{-x}}$$

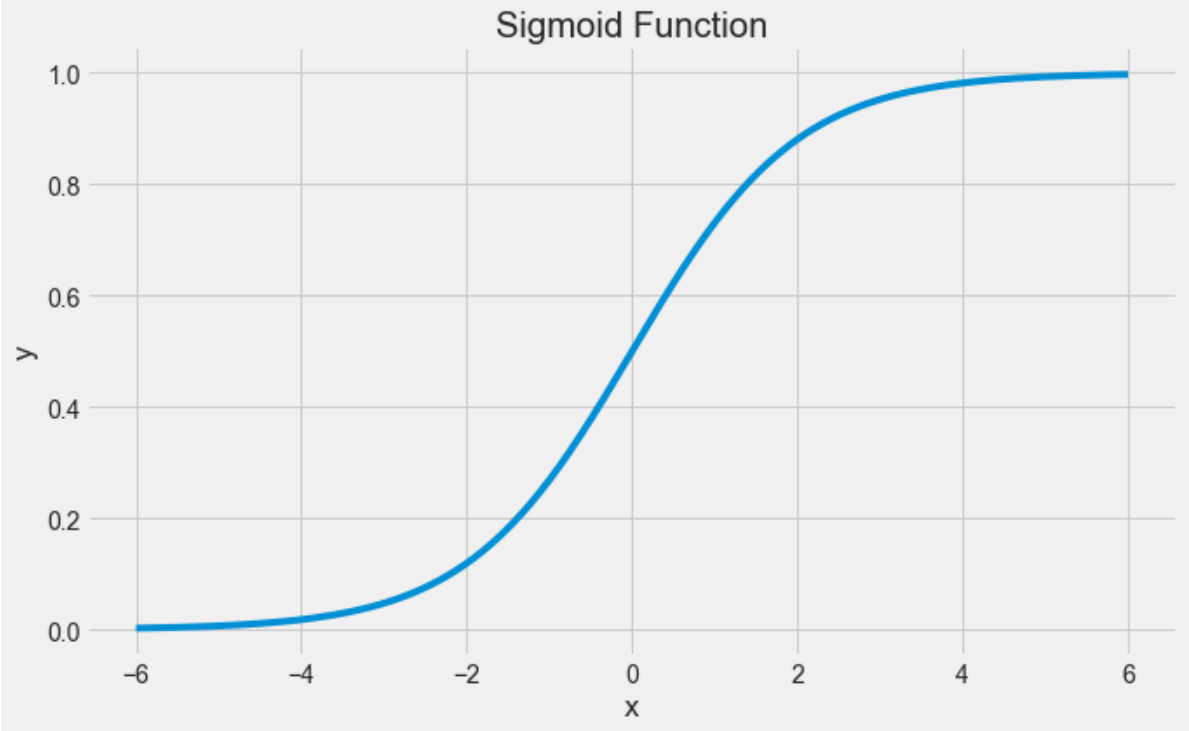
$e$ is the base of the natural logarithms and $x$ is value that you want to transform via the logistic function.

```
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
import statsmodels.formula.api as sm
```

```
from sklearn.metrics import precision_recall_curve, roc_curve, auc, accuracy_score
from sklearn.linear_model import LogisticRegression
```

```
%matplotlib inline
sns.set_style('whitegrid')
plt.style.use("fivethirtyeight")
x = np.linspace(-6, 6, num=1000)
plt.figure(figsize=(10, 6))
plt.plot(x, (1 / (1 + np.exp(-x))))
plt.xlabel("x")
plt.ylabel("y")
plt.title("Sigmoid Function")
```

```
Text(0.5, 1.0, 'Sigmoid Function')
```




The logistic regression equation has a very similar representation like linear regression. The difference is that the output value being modelled is binary in nature.

$$\hat{p} = \frac{e^{\hat{\beta}_0 + \hat{\beta}_1 x_1}}{1 + e^{\hat{\beta}_0 + \hat{\beta}_1 x_1}}$$

or

$$\hat{p} = \frac{1.0}{1.0 + e^{-(\hat{\beta}_0 + \hat{\beta}_1 x_1)}}$$

$\hat{\beta}_0$ is the estimated intercept term

$\hat{\beta}_1$ is the estimated coefficient for $x_1$

$\hat{p}$ is the predicted output with real value between 0 and 1. To convert this to binary output of 0 or 1, this would either need to be rounded to an integer value or a cutoff point be provided to specify the class segregation point.

### 4.1.2 Learning the Logistic Regression Model

The coefficients (Beta values b) of the logistic regression algorithm must be estimated from your training data. This is done using maximum-likelihood estimation.

Maximum-likelihood estimation is a common learning algorithm used by a variety of machine learning algorithms, although it does make assumptions about the distribution of your data (more on this when we talk about preparing your data).

The best coefficients should result in a model that would predict a value very close to 1 (e.g. male) for the default class and a value very close to 0 (e.g. female) for the other class. The intuition for maximum-likelihood for logistic regression is that a search procedure seeks values for the coefficients (Beta values) that maximize the likelihood of the observed data. In other words, in MLE, we estimate the parameter values (Beta values) which are the most likely to produce that data at hand.

Here is an analogy to understand the idea behind Maximum Likelihood Estimation (MLE). Let us say, you are listening to a song (data). You are not aware of the singer (parameter) of the song. With just the musical piece at hand, you try to guess the singer (parameter) who you feel is the most likely (MLE) to have sung that song. Your are making a maximum likelihood estimate! Out of all the singers (parameter space) you have chosen them as the one who is the most likely to have sung that song (data).

We are not going to go into the math of maximum likelihood. It is enough to say that a minimization algorithm is used to optimize the best values for the coefficients for your training data. This is often implemented in practice using efficient numerical optimization algorithm (like the Quasi-newton method).

When you are learning logistic, you can implement it yourself from scratch using the much simpler gradient descent algorithm.

### 4.1.3 Preparing Data for Logistic Regression

The assumptions made by logistic regression about the distribution and relationships in your data are much the same as the assumptions made in linear regression.

Much study has gone into defining these assumptions and precise probabilistic and statistical language is used. My advice is to use these as guidelines or rules of thumb and experiment with different data preparation schemes.

Ultimately in predictive modeling machine learning projects you are laser focused on making accurate predictions rather than interpreting the results. As such, you can break some assumptions as long as the model is robust and performs well.

- **Binary Output Variable:** This might be obvious as we have already mentioned it, but logistic regression is intended for binary (two-class) classification problems. It will predict the probability of an instance belonging to the default class, which can be snapped into a 0 or 1 classification.
- **Remove Noise:** Logistic regression assumes no error in the output variable (y), consider removing outliers and possibly misclassified instances from your training data.
- **Gaussian Distribution:** Logistic regression is a linear algorithm (with a non-linear transform on output). It does assume a linear relationship between the input variables with the output. Data transforms of your input variables that better expose this linear relationship can result in a more accurate model. For example, you can use log, root, Box-Cox and other univariate transforms to better expose this relationship.
- **Remove Correlated Inputs:** Like linear regression, the model can overfit if you have multiple highly-correlated inputs. Consider calculating the pairwise correlations between all inputs and removing highly correlated inputs.
- **Fail to Converge:** It is possible for the expected likelihood estimation process that learns the coefficients to fail to converge. This can happen if there are many highly correlated inputs in your data or the data is very sparse (e.g. lots of zeros in your input data).

## 4.2 Logistic Regression: Scikit-learn vs Statsmodels

Python gives us two ways to do logistic regression. Statsmodels offers modeling from the perspective of statistics. Scikit-learn offers some of the same models from the perspective of machine learning.

So we need to understand the difference between statistics and machine learning! Statistics makes mathematically valid inferences about a population based on sample data. Statistics answers the question, “What is the evidence that X is related to Y?” Machine learning has the goal of optimizing predictive accuracy rather than inference. Machine learning answers the question, “Given X, what prediction should we make for Y?”

Let us see the use of `statsmodels` for logistic regression. We'll see scikit-learn later in the course, when we learn methods that focus on prediction.

## 4.3 Training a logistic regression model

Read the data on social network ads. The data shows if the person purchased a product when targeted with an ad on social media. Fit a logistic regression model to predict if a user will purchase the product based on their characteristics such as age, gender and estimated salary.

```
train = pd.read_csv('./Datasets/Social_Network_Ads_train.csv') #Develop the model on train da
test = pd.read_csv('./Datasets/Social_Network_Ads_test.csv') #Test the model on test data
```

```
train.head()
```

| | User ID | Gender | Age | EstimatedSalary | Purchased |
|---|---|---|---|---|---|
| 0 | 15755018 | Male | 36 | 33000 | 0 |
| 1 | 15697020 | Female | 39 | 61000 | 0 |
| 2 | 15796351 | Male | 36 | 118000 | 1 |
| 3 | 15665760 | Male | 39 | 122000 | 1 |
| 4 | 15794661 | Female | 26 | 118000 | 0 |

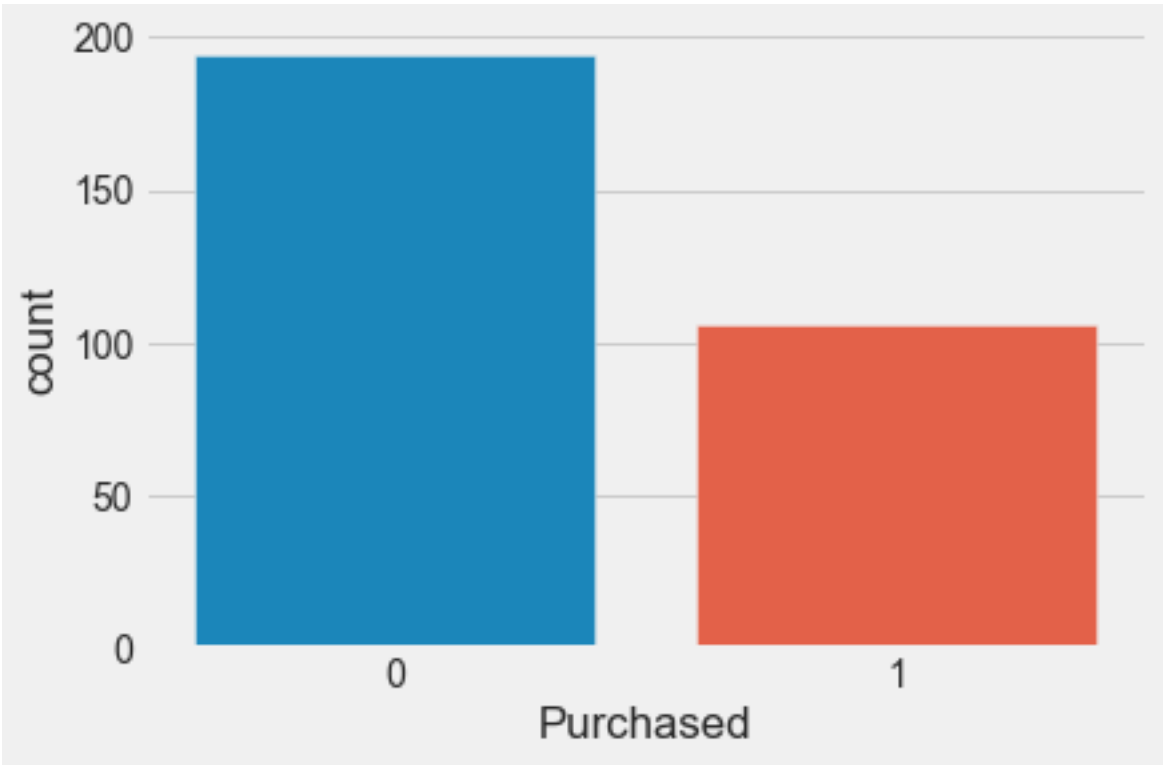
### 4.3.1 Examining the Distribution of the Target Column

Make sure our target is not severely imbalanced.

```
train.Purchased.value_counts()
```

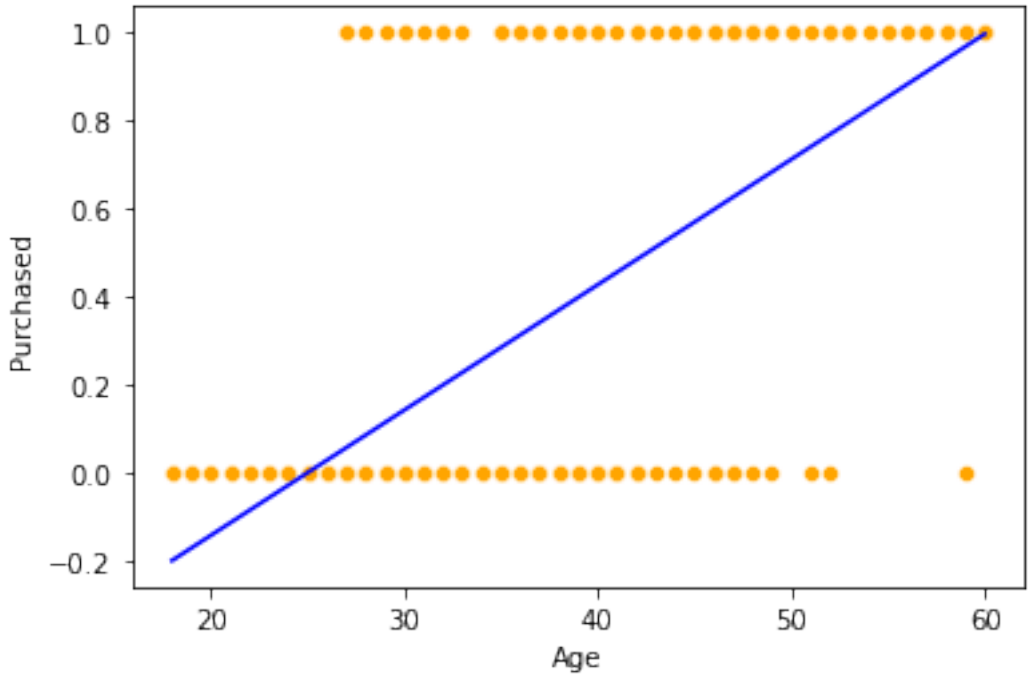
```
0    194
1    106
Name: Purchased, dtype: int64
```

```
sns.countplot(x = 'Purchased',data = train);
```




Let us try to fit a linear regression model, instead of logistic regression. We fit a linear regression model to predict probability of purchase based on age.

```
sns.scatterplot(x = 'Age', y = 'Purchased', data = train, color = 'orange') #Visualizing data
lm = sm.ols(formula = 'Purchased~Age', data = train).fit() #Developing linear regression mode
sns.lineplot(x = 'Age', y= lm.predict(train), data = train, color = 'blue') #Visualizing mode
```




Note the issues with the linear regression model:

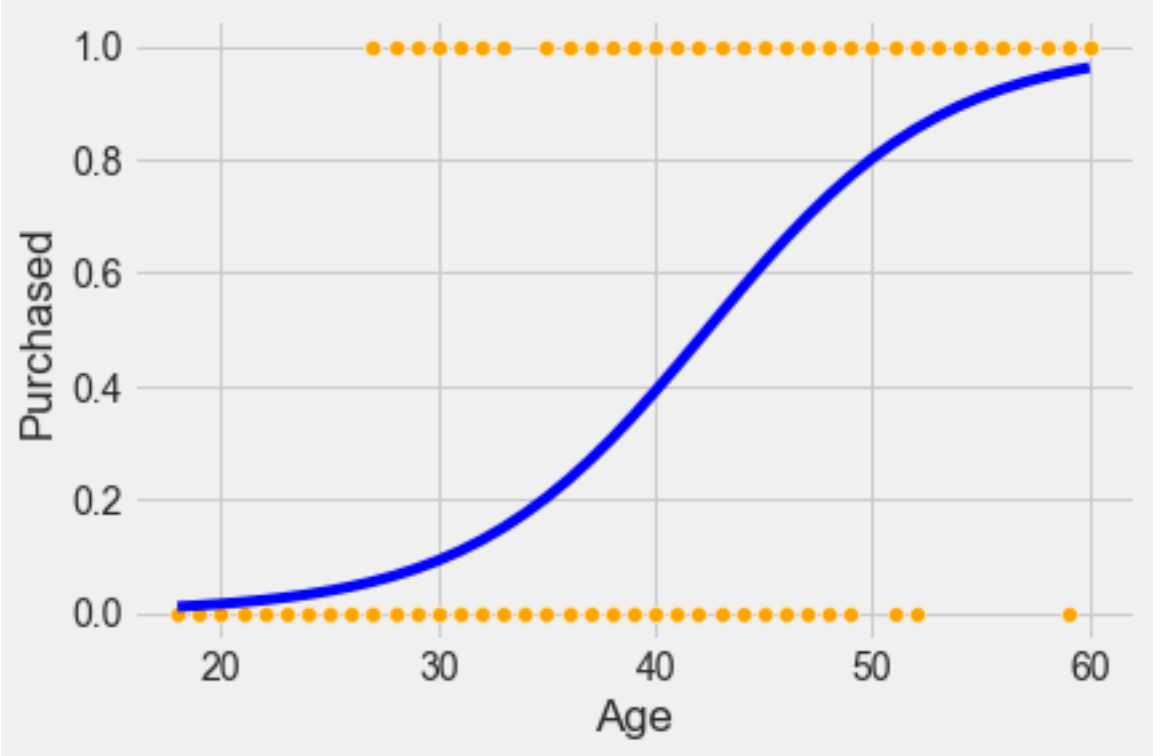
1. The regression line goes below 0 and over 1. However, probability of purchase must be in [0,1].
2. The linear regression model does not seem to fit the data well.

### 4.3.2 Fitting the logistic regression model

Now, let us fit a logistic regression model to predict probability of purchase based on `Age`.

```
sns.scatterplot(x = 'Age', y = 'Purchased', data = train, color = 'orange') #Visualizing data
logit_model = sm.logit(formula = 'Purchased~Age', data = train).fit() #Developing logistic re
sns.lineplot(x = 'Age', y= logit_model.predict(train), data = train, color = 'blue') #Visuali
```

```
Optimization terminated successfully.
         Current function value: 0.430107
         Iterations 7
```




As logistic regression uses the sigmoid function, the probability stays in [0,1]. Also, it seems to better fit the points as compared to linear regression.

```
logit_model.summary()
```

Table 4.2: Logit Regression Results

| | | | |
|---|---|---|---|
| Dep. Variable: | Purchased | No. Observations: | 300 |
| Model: | Logit | Df Residuals: | 298 |
| Method: | MLE | Df Model: | 1 |
| Date: | Tue, 19 Apr 2022 | Pseudo R-squ.: | 0.3378 |
| Time: | 16:46:02 | Log-Likelihood: | -129.03 |
| converged: | True | LL-Null: | -194.85 |
| Covariance Type: | nonrobust | LLR p-value: | 1.805e-30 |

| | coef | std err | z | P>\|z\| | [0.025 | 0.975] |
|---|---|---|---|---|---|---|
| Intercept | -7.8102 | 0.885 | -8.825 | 0.000 | -9.545 | -6.076 |
| Age | 0.1842 | 0.022 | 8.449 | 0.000 | 0.141 | 0.227 |

**Interpret the coefficient of age**

For a unit increase in age, the log odds of purchase increase by 0.18, or the odds of purchase get multiplied by exp(0.18) = 1.2

**Is the increase in probability of purchase constant with a unit increase in age?**

No, it depends on age.

**Is gender associated with probability of purchase?**

```
logit_model_gender = sm.logit(formula = 'Purchased~Gender', data = train).fit()
logit_model_gender.summary()
```

```
Optimization terminated successfully.
         Current function value: 0.648804
         Iterations 4
```

Table 4.4: Logit Regression Results

| | | | |
|---|---|---|---|
| Dep. Variable: | Purchased | No. Observations: | 300 |
| Model: | Logit | Df Residuals: | 298 |
| Method: | MLE | Df Model: | 1 |
| Date: | Tue, 19 Apr 2022 | Pseudo R-squ.: | 0.001049 |
| Time: | 16:46:04 | Log-Likelihood: | -194.64 |
| converged: | True | LL-Null: | -194.85 |
| Covariance Type: | nonrobust | LLR p-value: | 0.5225 |

| | coef | std err | z | P>\|z\| | [0.025 | 0.975] |
|---|---|---|---|---|---|---|
| Intercept | -0.5285 | 0.168 | -3.137 | 0.002 | -0.859 | -0.198 |
| Gender[T.Male] | -0.1546 | 0.242 | -0.639 | 0.523 | -0.629 | 0.319 |

No, assuming a significance level of $\alpha = 5\%$, `Gender` is not associated with probability of default, as the $p$-value for `Male` is greater than 0.05.

## 4.4 Confusion matrix and classification accuracy

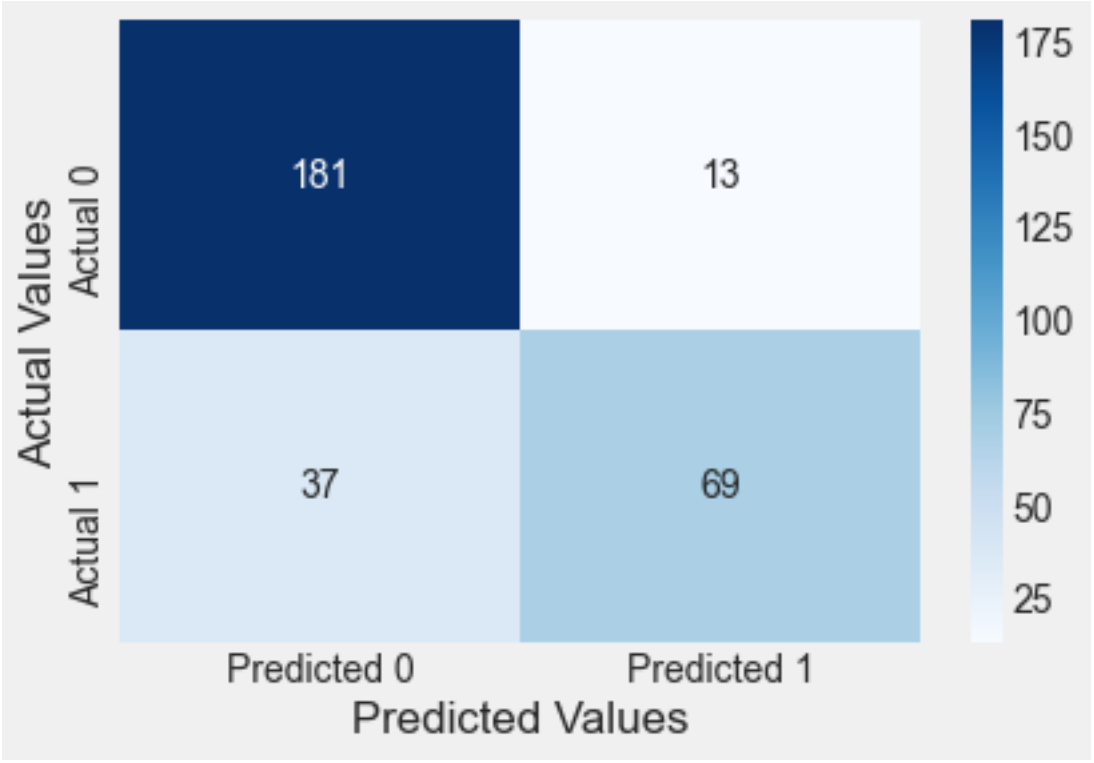
A confusion matrix is a summary of prediction results on a classification problem. The number of correct and incorrect predictions are summarized with count values and broken down by each class.

```
#Function to compute confusion matrix and prediction accuracy on training data
def confusion_matrix_train(model,cutoff=0.5):
    # Confusion matrix
    cm_df = pd.DataFrame(model.pred_table(threshold = cutoff))
    #Formatting the confusion matrix
    cm_df.columns = ['Predicted 0', 'Predicted 1']
    cm_df = cm_df.rename(index={0: 'Actual 0',1: 'Actual 1'})
    cm = np.array(cm_df)
    # Calculate the accuracy
    accuracy = (cm[0,0]+cm[1,1])/cm.sum()
    sns.heatmap(cm_df, annot=True, cmap='Blues', fmt='g')
    plt.ylabel("Actual Values")
    plt.xlabel("Predicted Values")
    print("Classification accuracy = {:.1%}".format(accuracy))
```

Find the confusion matrix and classification accuracy of the model with `Age` as the predictor on training data.

```
cm = confusion_matrix_train(logit_model)
```

```
Classification accuracy = 83.3%
```




**Confusion matrix:**

- Each row: actual class
- Each column: predicted class

First row: Non-purchasers, the negative class:

- 181 were correctly classified as Non-purchasers. **True negatives**.
- Remaining 13 were wrongly classified as Non-purchasers. **False positive**

Second row: Purchasers, the positive class:

- 37 were incorrectly classified as Non-purchasers. **False negatives**
- 69 were correctly classified Purchasers. **True positives**

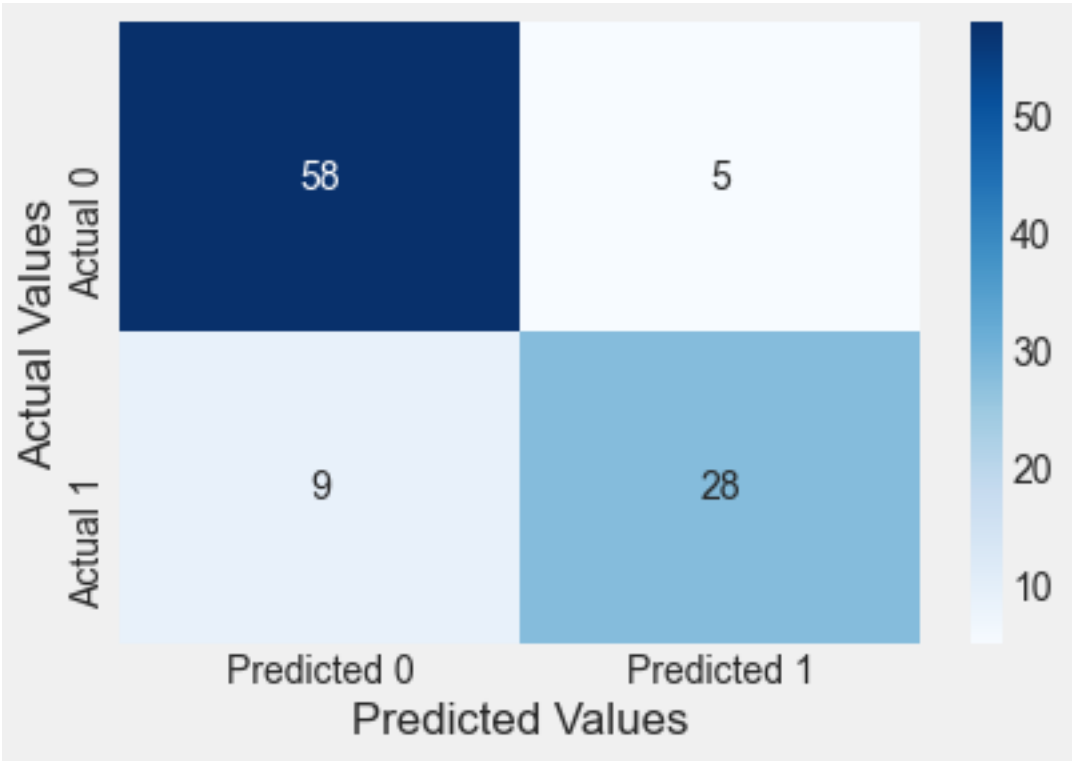
```
#Function to compute confusion matrix and prediction accuracy on test data
def confusion_matrix_test(data,actual_values,model,cutoff=0.5):
#Predict the values using the Logit model
    pred_values = model.predict(data)
# Specify the bins
    bins=np.array([0,cutoff,1])
#Confusion matrix
```

```
    cm = np.histogram2d(actual_values, pred_values, bins=bins)[0]
    cm_df = pd.DataFrame(cm)
    cm_df.columns = ['Predicted 0','Predicted 1']
    cm_df = cm_df.rename(index={0: 'Actual 0',1:'Actual 1'})
    accuracy = (cm[0,0]+cm[1,1])/cm.sum()
    sns.heatmap(cm_df, annot=True, cmap='Blues', fmt='g')
    plt.ylabel("Actual Values")
    plt.xlabel("Predicted Values")
    print("Classification accuracy = {:.1%}".format(accuracy))
```

Find the confusion matrix and classification accuracy of the model with `Age` as the predictor on test data.

```
confusion_matrix_test(test,test.Purchased,logit_model)
```

```
Classification accuracy = 86.0%
```




The model classifies a bit more accurately on test data as compared to the training data, which is a bit unusual. However, it shows that the model did not overfit on training data.

**Include `EstimatedSalary` as a predictor in the above model**

```
logit_model2 = sm.logit(formula = 'Purchased~Age+EstimatedSalary', data = train).fit()
logit_model2.summary()
```

```
Optimization terminated successfully.
         Current function value: 0.358910
         Iterations 7
```

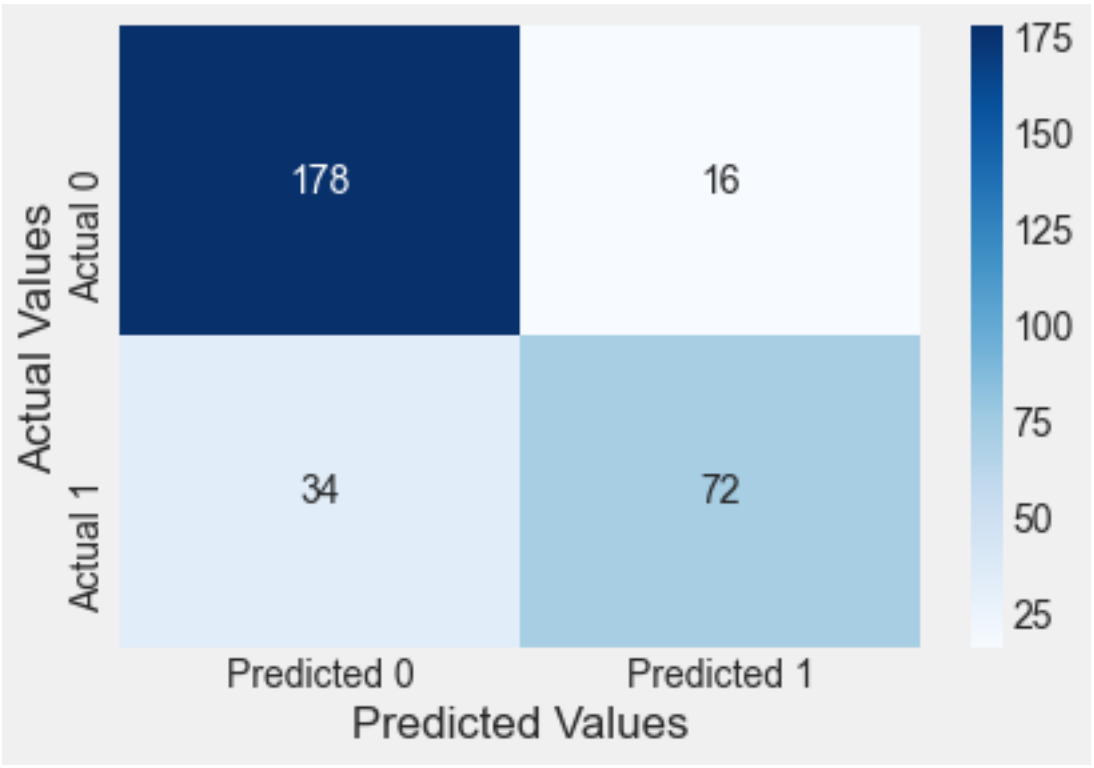
Table 4.6: Logit Regression Results

| | | | |
|---|---|---|---|
| Dep. Variable: | Purchased | No. Observations: | 300 |
| Model: | Logit | Df Residuals: | 297 |
| Method: | MLE | Df Model: | 2 |
| Date: | Tue, 14 Feb 2023 | Pseudo R-squ.: | 0.4474 |
| Time: | 12:03:29 | Log-Likelihood: | -107.67 |
| converged: | True | LL-Null: | -194.85 |
| Covariance Type: | nonrobust | LLR p-value: | 1.385e-38 |

| | coef | std err | z | P>\|z\| | [0.025 | 0.975] |
|---|---|---|---|---|---|---|
| Intercept | -11.9432 | 1.424 | -8.386 | 0.000 | -14.735 | -9.152 |
| Age | 0.2242 | 0.028 | 7.890 | 0.000 | 0.168 | 0.280 |
| EstimatedSalary | 3.48e-05 | 6.15e-06 | 5.660 | 0.000 | 2.27e-05 | 4.68e-05 |

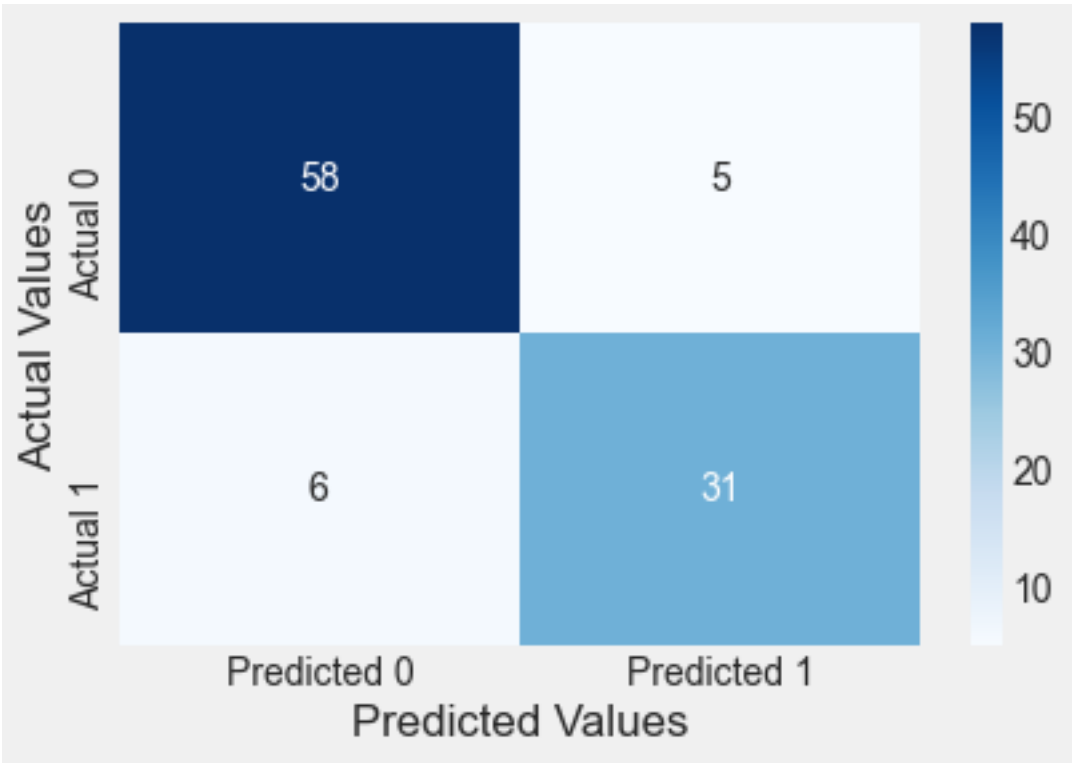
```
confusion_matrix_train(logit_model2)
```

```
Classification accuracy = 83.3%
```




```
confusion_matrix_test(test,test.Purchased,logit_model2)
```

```
Classification accuracy = 89.0%
```




The log likelihood of the model has increased, while also increasing the prediction accuracy on test data, which shows that the additional predictor is helping explain the response better, without overfitting the data.

**Include `Gender` as a predictor in the above model**

```
logit_model = sm.logit(formula = 'Purchased~Age+EstimatedSalary+Gender', data = train).fit()
logit_model.summary()
```

```
Optimization terminated successfully.
         Current function value: 0.357327
         Iterations 7
```

Table 4.8: Logit Regression Results

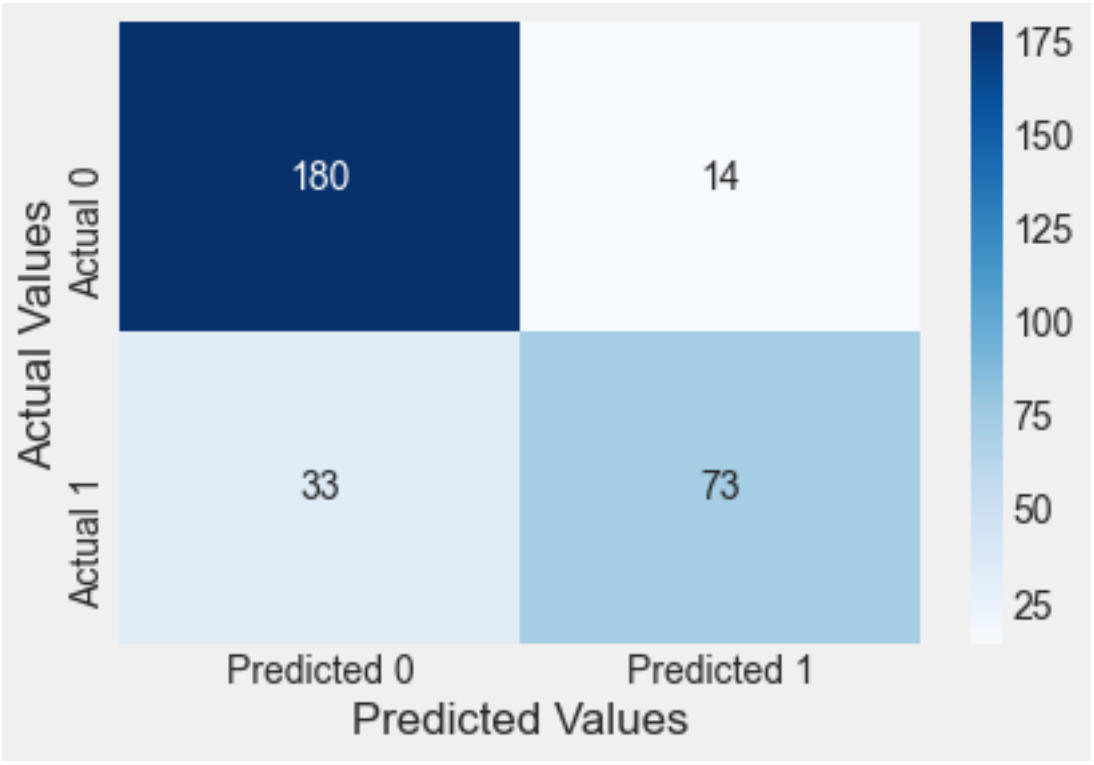
| | | | |
|---|---|---|---|
| Dep. Variable: | Purchased | No. Observations: | 300 |
| Model: | Logit | Df Residuals: | 296 |
| Method: | MLE | Df Model: | 3 |
| Date: | Tue, 14 Feb 2023 | Pseudo R-squ.: | 0.4498 |
| Time: | 12:17:28 | Log-Likelihood: | -107.20 |

| | | | |
|---|---|---|---|
| converged: | True | LL-Null: | -194.85 |
| Covariance Type: | nonrobust | LLR p-value: | 9.150e-38 |

| | coef | std err | z | P>\|z\| | [0.025 | 0.975] |
|---|---|---|---|---|---|---|
| Intercept | -12.2531 | 1.478 | -8.293 | 0.000 | -15.149 | -9.357 |
| Gender[T.Male] | 0.3356 | 0.346 | 0.970 | 0.332 | -0.342 | 1.013 |
| Age | 0.2275 | 0.029 | 7.888 | 0.000 | 0.171 | 0.284 |
| EstimatedSalary | 3.494e-05 | 6.17e-06 | 5.666 | 0.000 | 2.29e-05 | 4.7e-05 |

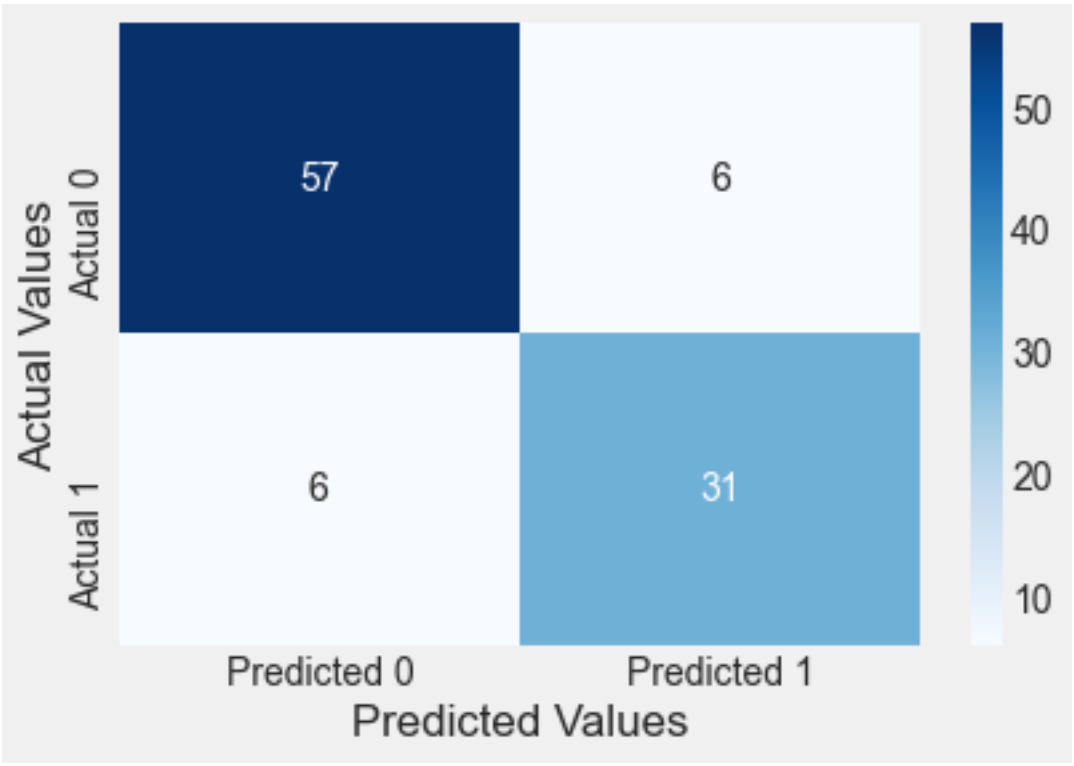
```
confusion_matrix_train(logit_model)
```

```
Classification accuracy = 84.3%
```




```
confusion_matrix_test(test,test.Purchased,logit_model)
```

```
Classification accuracy = 88.0%
```




`Gender` is a statistically insignificant predictor, and including it slightly lowers the classification accuracy on test data. Note that the classification accuracy on training data will continue to increase on adding more predictors, irrespective of their relevance *(similar to the idea of RSS on training data in linear regression)*.

**Is there a residual in logistic regression?**

No, since the response is assumed to have a Bernoulli distribution, instead of a normal distribution.

**Is the odds ratio for a unit increase in a predictor $X_j$, a constant (assuming that the rest of the predictors are held constant)?**

Yes, the odds ratio in this case will $e^{\beta_j}$

## 4.5 Variable transformations in logistic regression

Read the dataset *diabetes.csv* that contains if a person has diabetes (`Outcome = 1`) based on health parameters such as BMI, blood pressure, age etc. Develop a model to predict the probability of a person having diabetes based on their age.

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

```
data.head()
```

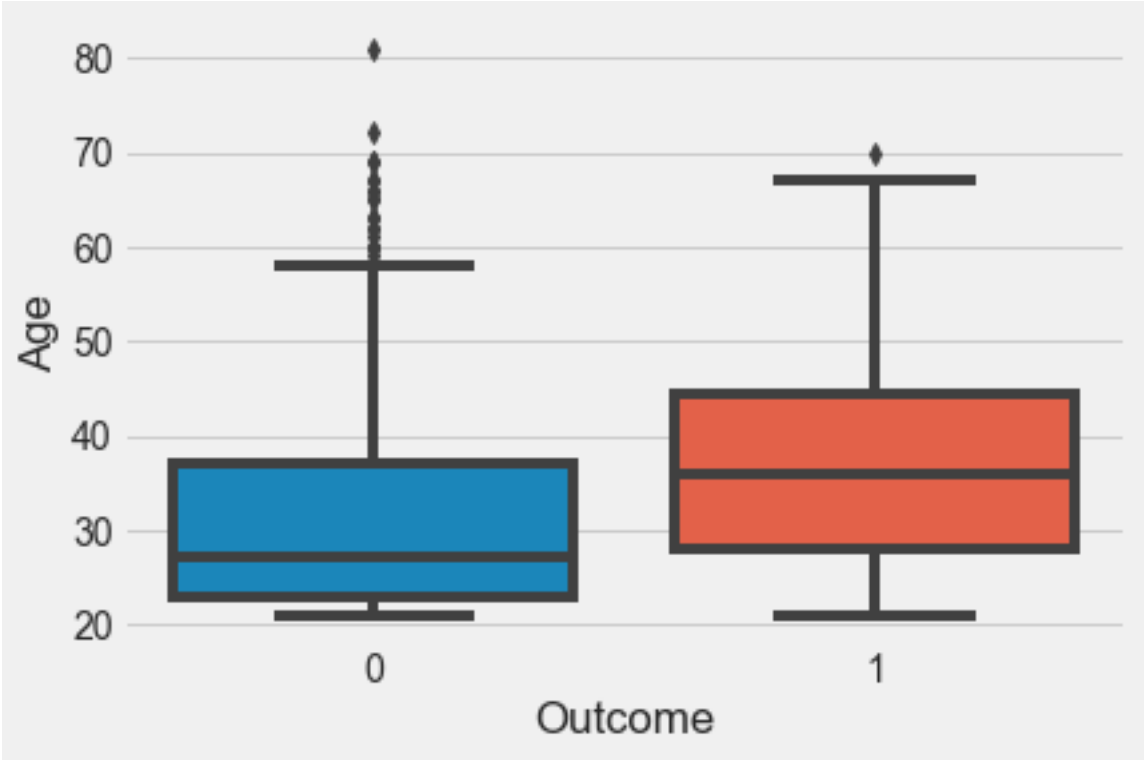
| | Pregnancies | Glucose | BloodPressure | SkinThickness | Insulin | BMI | DiabetesPedigreeFunction | Age |
|---|---|---|---|---|---|---|---|---|
| 0 | 6 | 148 | 72 | 35 | 0 | 33.6 | 0.627 | 50 |
| 1 | 1 | 85 | 66 | 29 | 0 | 26.6 | 0.351 | 31 |
| 2 | 8 | 183 | 64 | 0 | 0 | 23.3 | 0.672 | 32 |
| 3 | 1 | 89 | 66 | 23 | 94 | 28.1 | 0.167 | 21 |
| 4 | 0 | 137 | 40 | 35 | 168 | 43.1 | 2.288 | 33 |

Randomly select 80% of the observations to create a training dataset. Create a test dataset with the remaining 20% observations.

```
#Creating training and test datasets
np.random.seed(2)
train = data.sample(round(data.shape[0]*0.8))
test = data.drop(train.index)
```

Does `Age` seem to distinguish `Outcome` levels?

```
sns.boxplot(x = 'Outcome', y = 'Age', data = train)
```

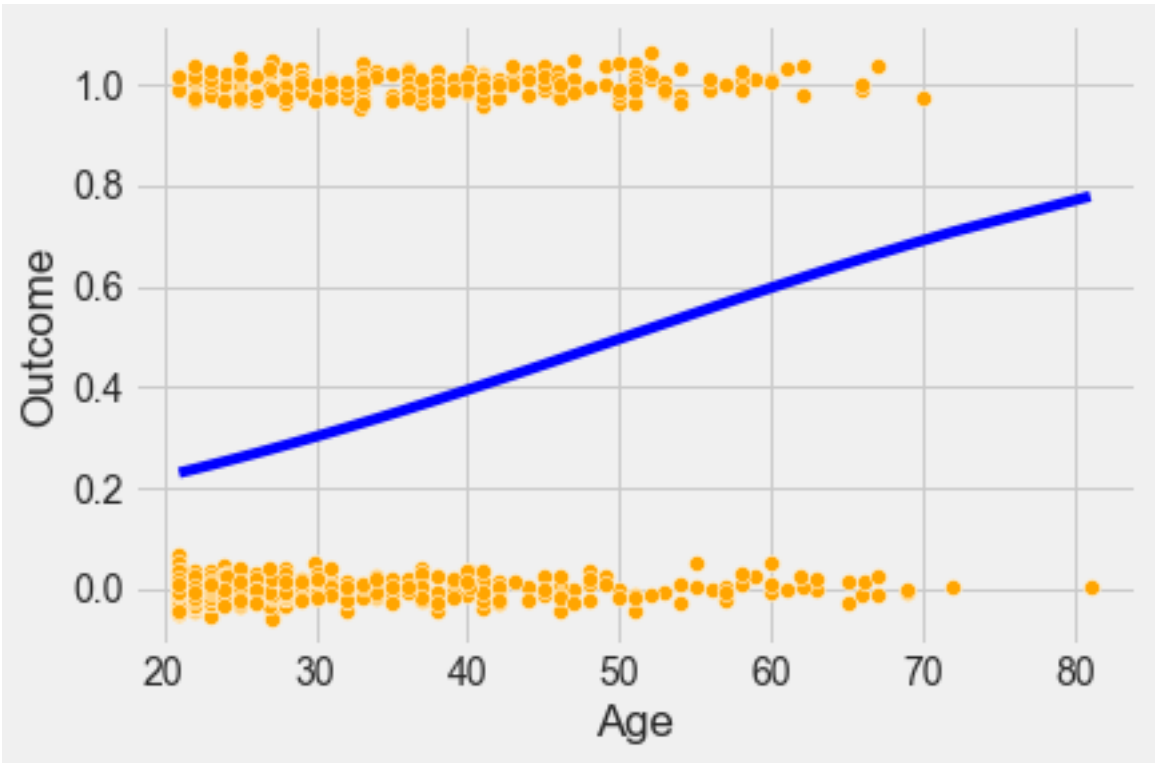



Yes it does!

Develop and visualize a logistic regression model to predict `Outcome` using `Age`.

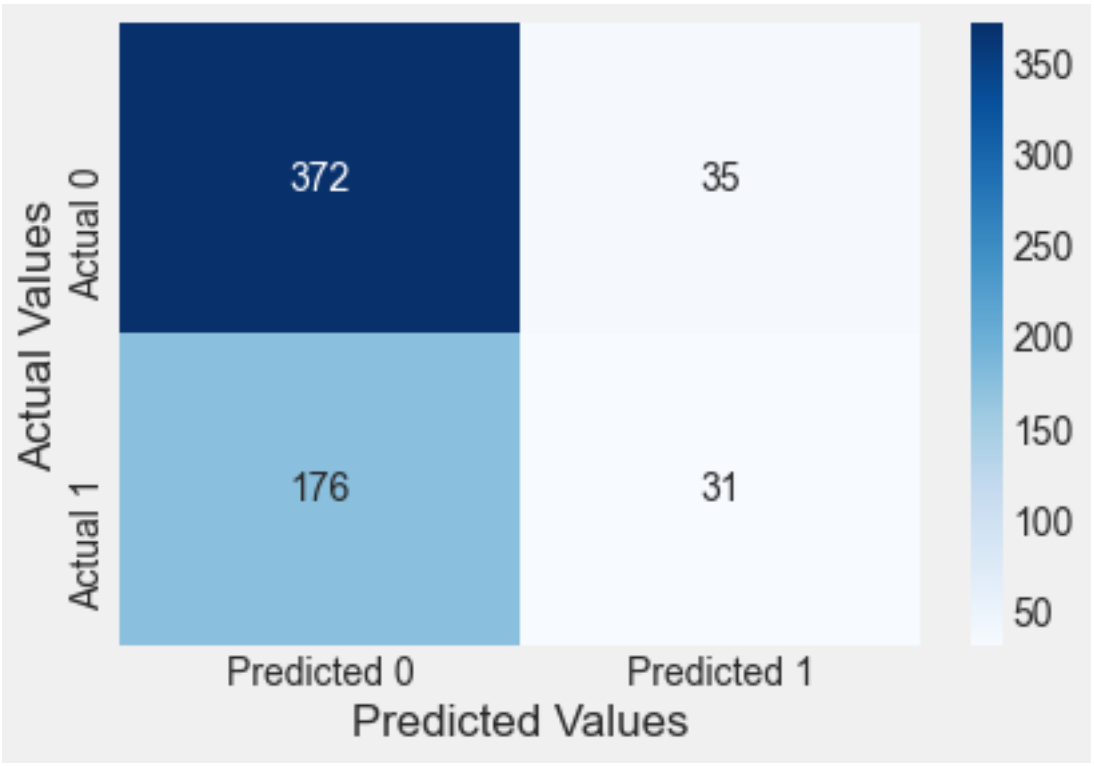
```
#Jittering points to better see the density of points in any given region of the plot
def jitter(values,j):
    return values + np.random.normal(j,0.02,values.shape)
sns.scatterplot(x = jitter(train.Age,0), y = jitter(train.Outcome,0), data = train, color =
logit_model = sm.logit(formula = 'Outcome~Age', data = train).fit()
sns.lineplot(x = 'Age', y= logit_model.predict(train), data = train, color = 'blue')
print(logit_model.llf) #Printing the log likelihood to compare it with the next model we buil
```

```
Optimization terminated successfully.
         Current function value: 0.612356
         Iterations 5
-375.9863802089716
```




```
confusion_matrix_train(logit_model)
```

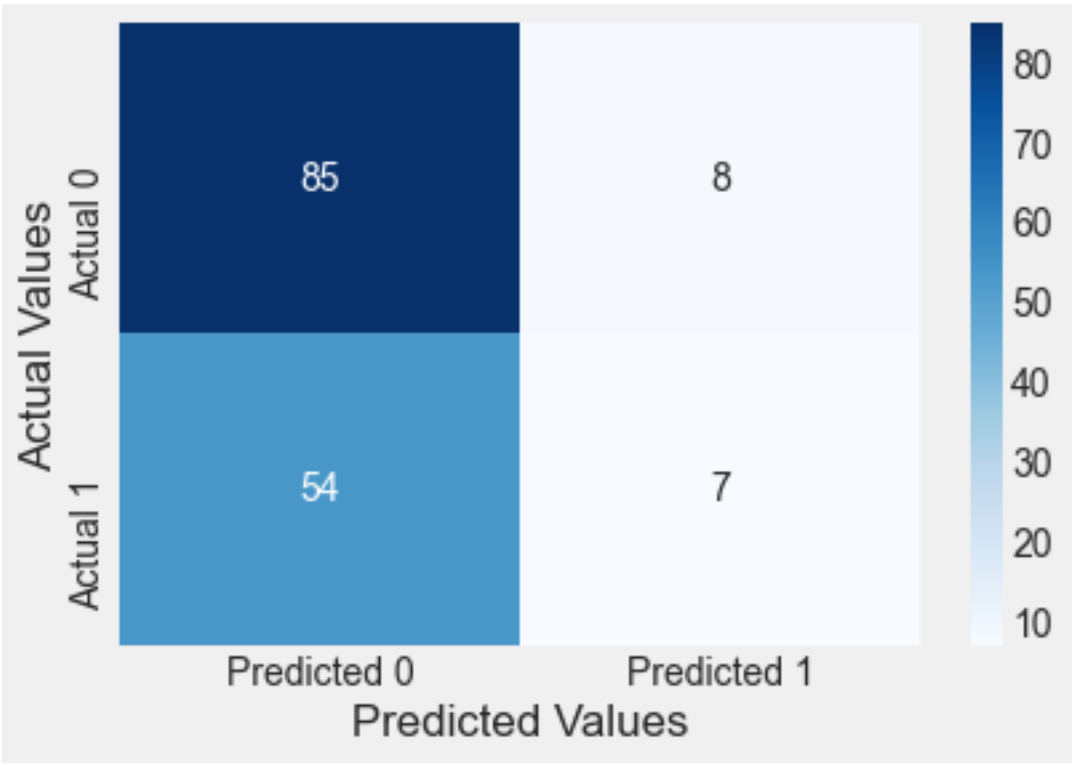
```
Classification accuracy = 65.6%
```




Classification accuracy on train data = 66%

```
confusion_matrix_test(test,test.Outcome,logit_model)
```

```
Classification accuracy = 59.7%
```




Classification accuracy on test data = 60%

Can a tranformation of `Age` provide a more accurate model?

Let us visualize how the probability of people having diabetes varies with `Age`. We will bin `Age` to get the percentage of people having diabetes within different `Age` bins.

```
#Binning Age
binned_age = pd.qcut(train['Age'],11,retbins=True)
train['age_binned'] = binned_age[0]
```

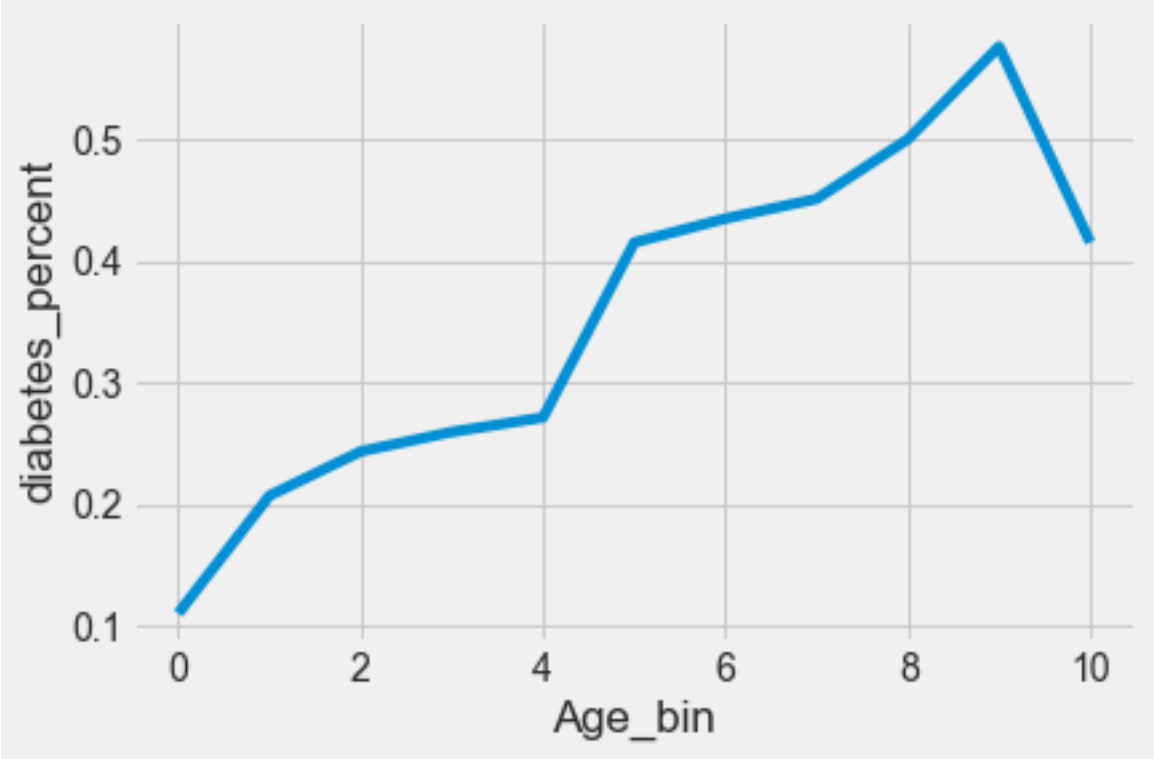
```
#Finding percentage of people having diabetes in each Age bin
age_data = train.groupby('age_binned')['Outcome'].agg([('diabetes_percent','mean'),('nobs','
age_data
```

| | age_binned | diabetes_percent | nobs |
|---|---|---|---|
| 0 | (20.999, 22.0] | 0.110092 | 109 |
| 1 | (22.0, 23.0] | 0.206897 | 29 |
| 2 | (23.0, 25.0] | 0.243243 | 74 |
| 3 | (25.0, 26.0] | 0.259259 | 27 |

| | age_binned | diabetes_percent | nobs |
|---|---|---|---|
| 4 | (26.0, 28.0] | 0.271186 | 59 |
| 5 | (28.0, 31.0] | 0.415094 | 53 |
| 6 | (31.0, 35.0] | 0.434783 | 46 |
| 7 | (35.0, 39.0] | 0.450980 | 51 |
| 8 | (39.0, 43.545] | 0.500000 | 54 |
| 9 | (43.545, 52.0] | 0.576271 | 59 |
| 10 | (52.0, 81.0] | 0.415094 | 53 |

```
#Visualizing percentage of people having diabetes with increasing Age (or Age bins)
sns.lineplot(x = age_data.index, y= age_data['diabetes_percent'])
plt.xlabel('Age_bin')
```

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



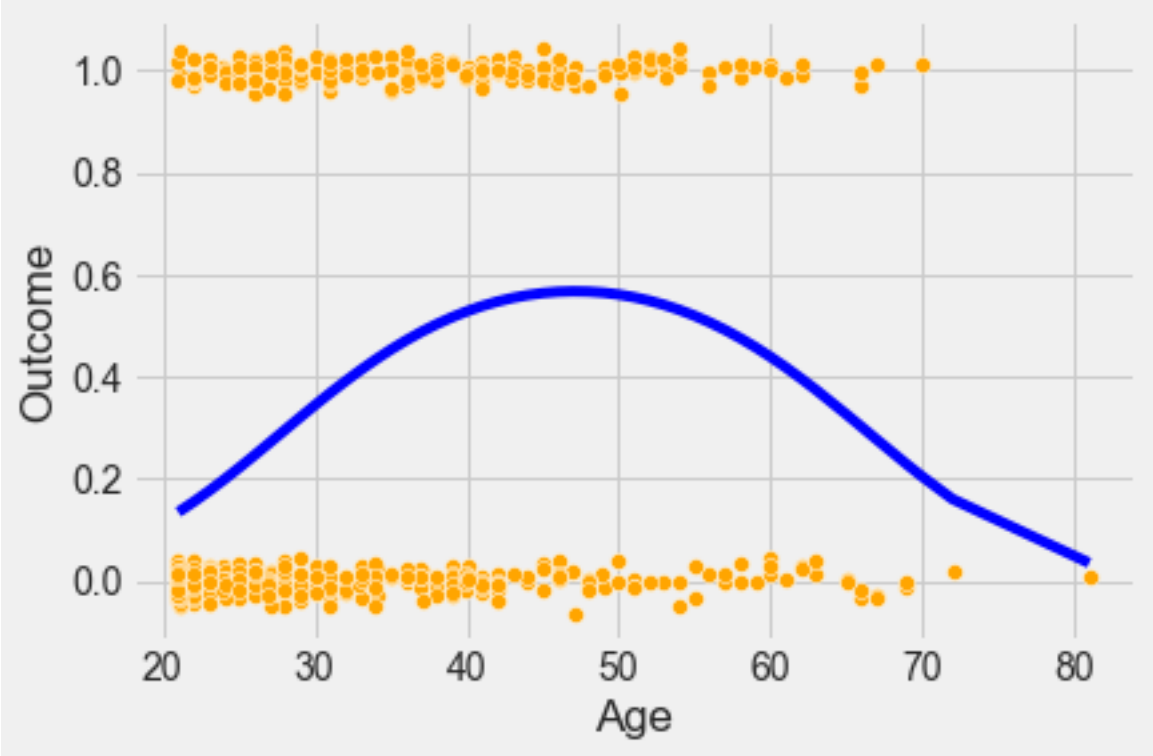

We observe that the probability of people having diabetes does **not** keep increasing monotonically with age. People with ages 52 and more have a lower probability of having diabetes than people in the immediately younger `Age` bin.

A quadratic transformation of `Age` may better fit the above trend

```
#Model with the quadratic transformation of Age
def jitter(values,j):
    return values + np.random.normal(j,0.02,values.shape)
sns.scatterplot(x = jitter(train.Age,0), y = jitter(train.Outcome,0), data = train, color =
logit_model = sm.logit(formula = 'Outcome~Age+I(Age**2)', data = train).fit()
sns.lineplot(x = 'Age', y= logit_model.predict(train), data = train, color = 'blue')
logit_model.llf
```

```
Optimization terminated successfully.
         Current function value: 0.586025
         Iterations 6
```

```
-359.81925590230185
```




```
logit_model.summary()
```

Table 4.12: Logit Regression Results

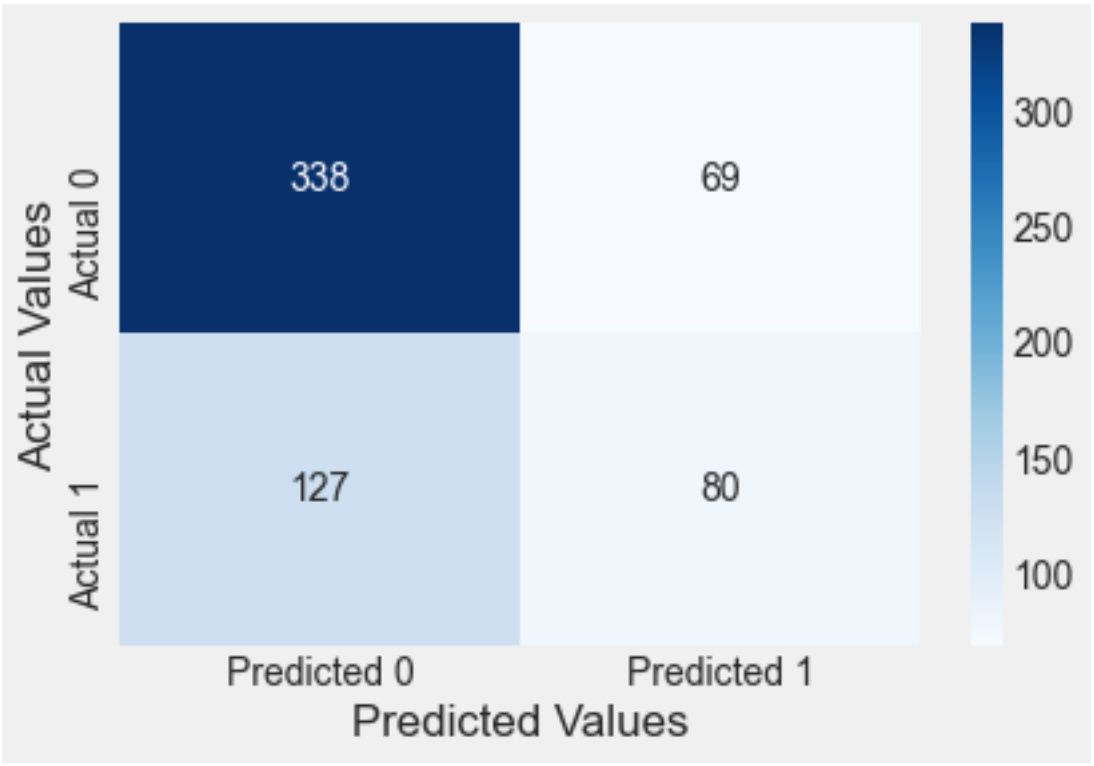
| | | | |
|---|---|---|---|
| Dep. Variable: | Outcome | No. Observations: | 614 |
| Model: | Logit | Df Residuals: | 611 |
| Method: | MLE | Df Model: | 2 |
| Date: | Tue, 14 Feb 2023 | Pseudo R-squ.: | 0.08307 |
| Time: | 12:25:54 | Log-Likelihood: | -359.82 |
| converged: | True | LL-Null: | -392.42 |
| Covariance Type: | nonrobust | LLR p-value: | 6.965e-15 |

| | coef | std err | z | P>\|z\| | [0.025 | 0.975] |
|---|---|---|---|---|---|---|
| Intercept | -6.6485 | 0.908 | -7.320 | 0.000 | -8.429 | -4.868 |
| Age | 0.2936 | 0.048 | 6.101 | 0.000 | 0.199 | 0.388 |
| I(Age ** 2) | -0.0031 | 0.001 | -5.280 | 0.000 | -0.004 | -0.002 |

The log likelihood of the model is higher and both the predictors are statistically significant indicating a better model fit. However, the model may also be overfitting. Let us check the model accuracy on test data.

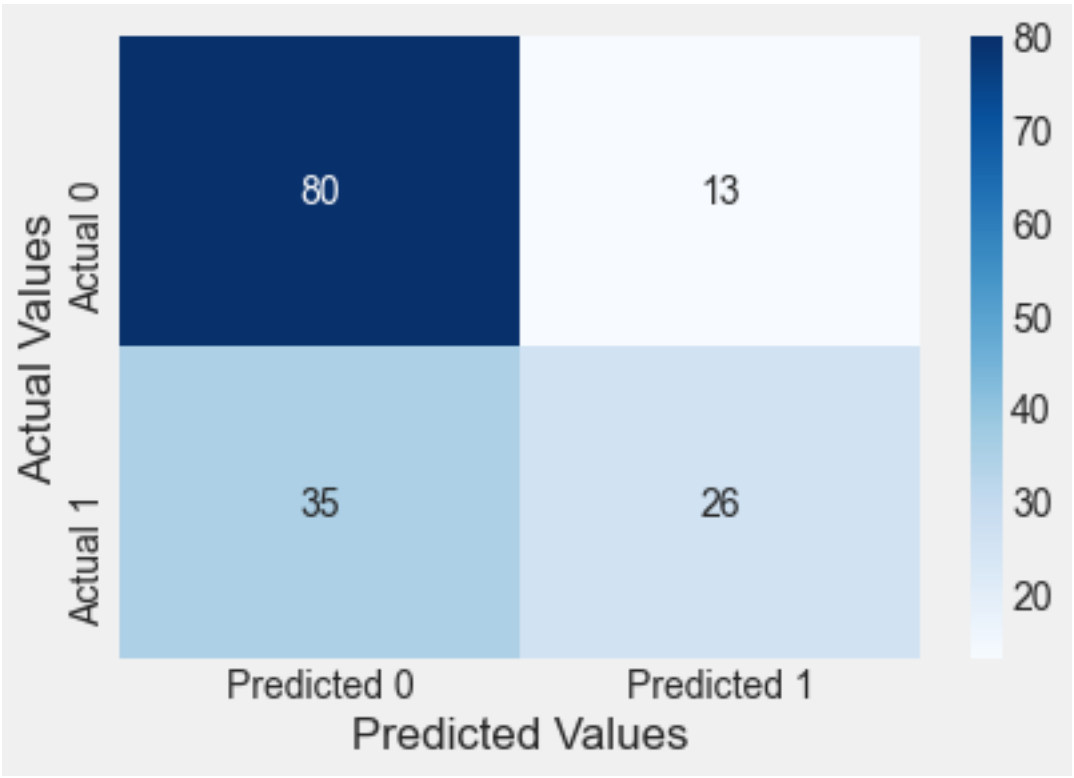
```
confusion_matrix_train(logit_model)
```

```
Classification accuracy = 68.1%
```




```
confusion_matrix_test(test,test.Outcome,logit_model)
```

```
Classification accuracy = 68.8%
```

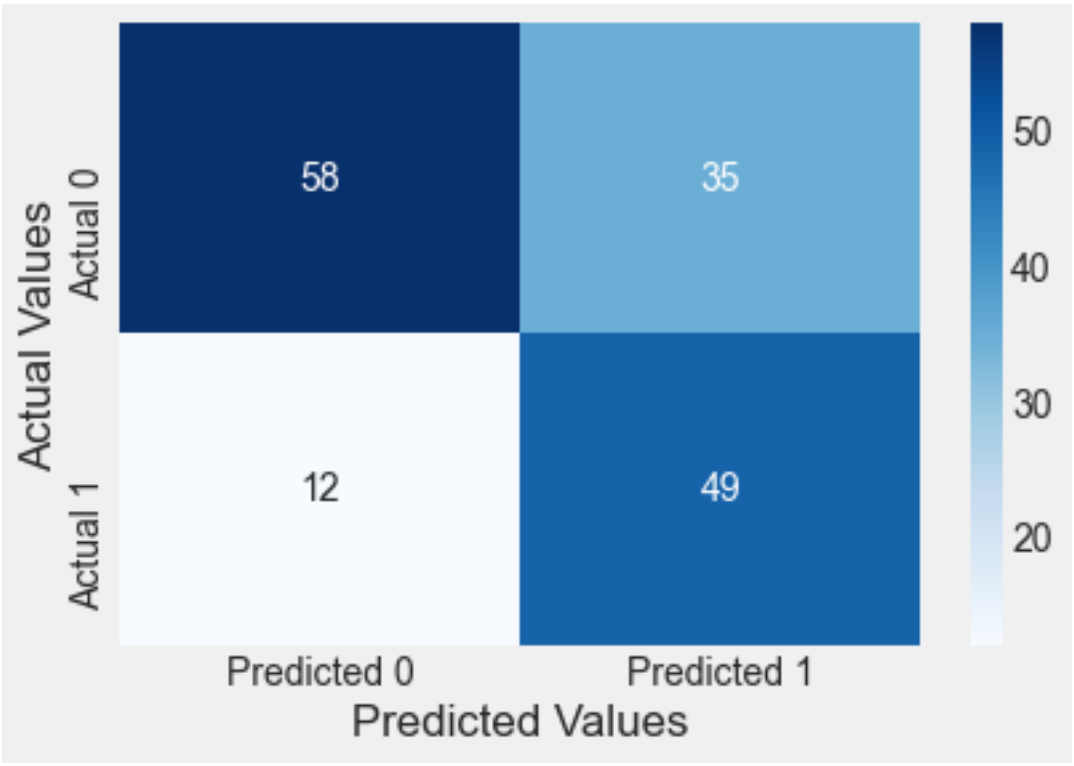



The classification accuracy on test data has increased to 69%. However, the number of *false positives* have increased. But in case of diabetes, *false negatives* are more concerning than *false positives*. This is because if a person has diabetes, and is told that they do not have diabetes, their condition may deteriorate. If a person does not have diabetes, and is told that they have diabetes, they may take unnecessary precautions or tests, but it will not be as harmful to the person as in the previous case. So, in this problem, we will be more focused on reducing the number of *false negatives*, instead of reducing the *false positives* or increasing the overall classification accuracy.

We can decrease the cutoff for classifying a person as having diabetes to reduce the number of false negatives.

```
#Reducing the cutoff for classifying a person as diabetic to 0.3 (instead of 0.5)
confusion_matrix_test(test,test.Outcome,logit_model,0.3)
```

```
Classification accuracy = 69.5%
```




Note that the changed cut-off reduced the number of *false negatives*, but at the cost of increasing the *false positives*. However, the stakeholders may prefer the reduced cut-off to be safer.

**Is there another way to transform `Age`?**

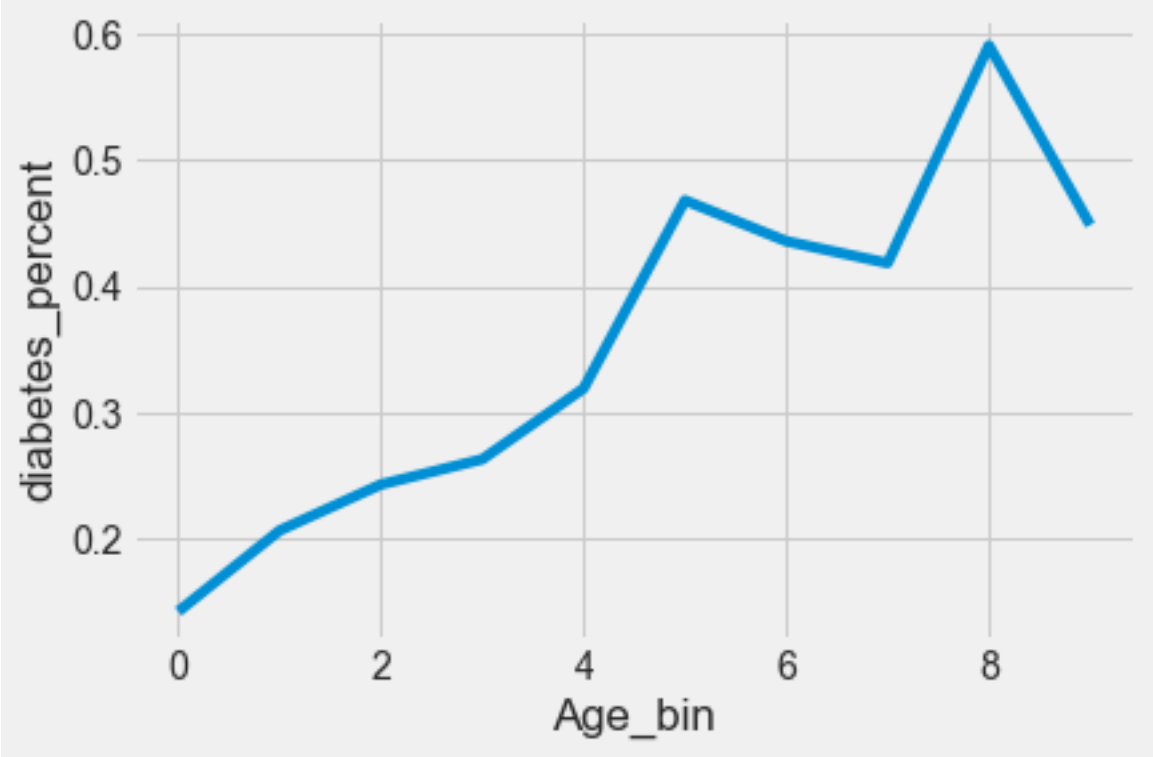
Yes, binning age into bins that have similar proportion of people with diabetes may provide a better model fit.

```
#Creating a function to bin age so that it can be applied to both the test and train datasets
def var_transform(data):
    binned_age = pd.qcut(train['Age'],10,retbins=True)
    bins = binned_age[1]
    data['age_binned'] = pd.cut(data['Age'],bins = bins)
    dum = pd.get_dummies(data.age_binned,drop_first = True)
    dum.columns = ['age'+str(x) for x in range(1,len(bins)-1)]
    data = pd.concat([data,dum], axis = 1)
    return data
```

```
#Binning age using the function var_transform()
train = var_transform(train)
test = var_transform(test)
```

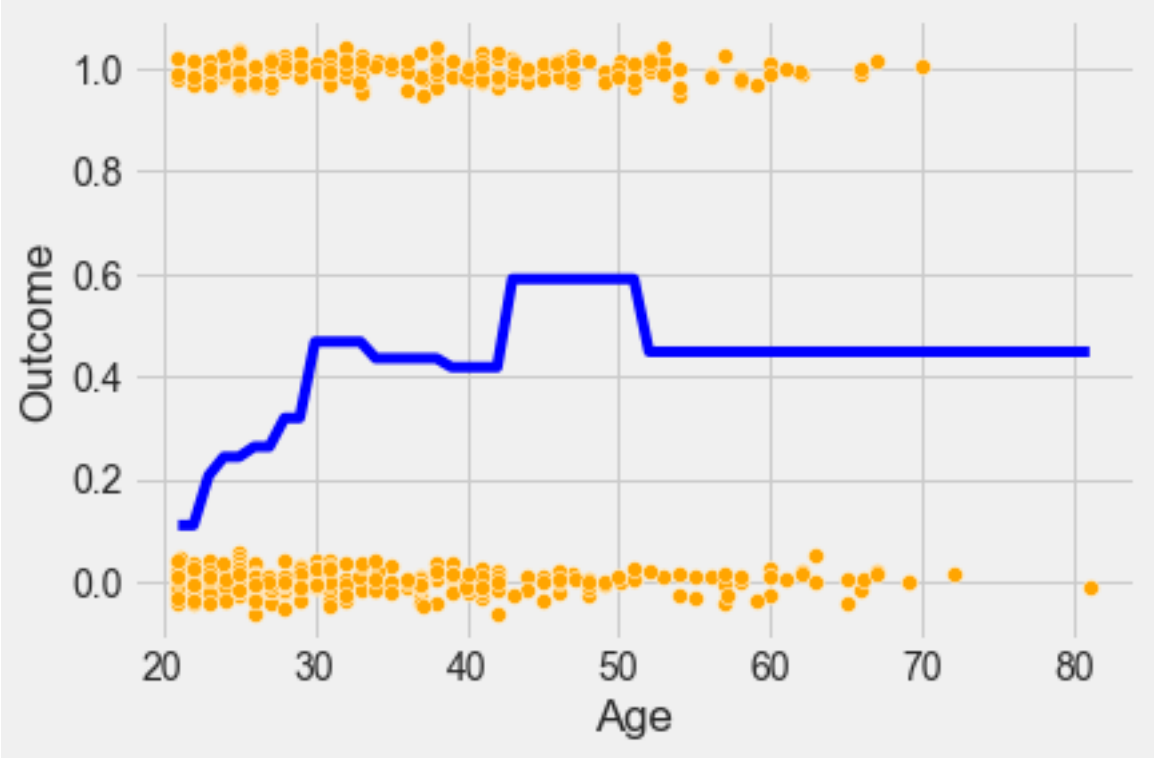
```
#Re-creating the plot of diabetes_percent vs age created earlier, just to check if the functi
age_data = train.groupby('age_binned')['Outcome'].agg([('diabetes_percent','mean'),('nobs','c
sns.lineplot(x = age_data.index, y= age_data['diabetes_percent'])
plt.xlabel('Age_bin')
```

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




```
#Model with binned Age
def jitter(values,j):
    return values + np.random.normal(j,0.02,values.shape)
sns.scatterplot(x = jitter(train.Age,0), y = jitter(train.Outcome,0), data = train, color =
logit_model = sm.logit(formula = 'Outcome~' + '+'.join(['age'+str(x) for x in range(1,10)]),
sns.lineplot(x = 'Age', y= logit_model.predict(train), data = train, color = 'blue')
```

```
Optimization terminated successfully.
         Current function value: 0.585956
         Iterations 6
```




```
logit_model.summary()
```

Table 4.14: Logit Regression Results

| | | | |
|---|---|---|---|
| Dep. Variable: | Outcome | No. Observations: | 614 |
| Model: | Logit | Df Residuals: | 604 |
| Method: | MLE | Df Model: | 9 |
| Date: | Sun, 19 Feb 2023 | Pseudo R-squ.: | 0.08318 |
| Time: | 14:19:51 | Log-Likelihood: | -359.78 |
| converged: | True | LL-Null: | -392.42 |
| Covariance Type: | nonrobust | LLR p-value: | 1.273e-10 |

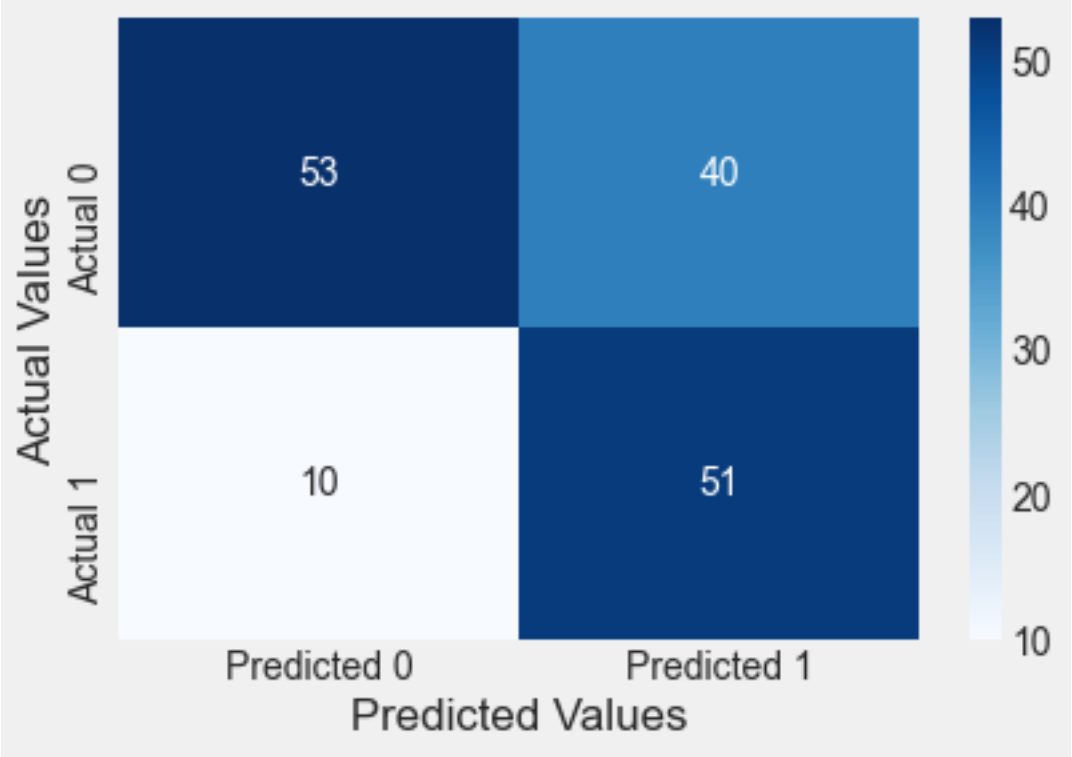
| | coef | std err | z | P>\|z\| | [0.025 | 0.975] |
|---|---|---|---|---|---|---|
| Intercept | -2.0898 | 0.306 | -6.829 | 0.000 | -2.690 | -1.490 |
| age1 | 0.7461 | 0.551 | 1.354 | 0.176 | -0.334 | 1.826 |
| age2 | 0.9548 | 0.409 | 2.336 | 0.019 | 0.154 | 1.756 |
| age3 | 1.0602 | 0.429 | 2.471 | 0.013 | 0.219 | 1.901 |
| age4 | 1.3321 | 0.438 | 3.044 | 0.002 | 0.474 | 2.190 |

| | | | | | | |
|---|---|---|---|---|---|---|
| age5 | 1.9606 | 0.398 | 4.926 | 0.000 | 1.180 | 2.741 |
| age6 | 1.8303 | 0.399 | 4.586 | 0.000 | 1.048 | 2.612 |
| age7 | 1.7596 | 0.410 | 4.288 | 0.000 | 0.955 | 2.564 |
| age8 | 2.4544 | 0.402 | 6.109 | 0.000 | 1.667 | 3.242 |
| age9 | 1.8822 | 0.404 | 4.657 | 0.000 | 1.090 | 2.674 |

Note that the probability of having diabetes for each age bin is a constant, as per the above plot.

```
confusion_matrix_test(test,test.Outcome,logit_model,0.3)
```

```
Classification accuracy = 67.5%
```




Binning `Age` provides a similar result as compared to the model with the quadratic transformation of `Age`.

```
train.head()
```

| | Pregnancies | Glucose | BloodPressure | SkinThickness | Insulin | BMI | DiabetesPedigreeFunction | A |
|---|---|---|---|---|---|---|---|---|
| 158 | 2 | 88 | 74 | 19 | 53 | 29.0 | 0.229 | 22 |
| 251 | 2 | 129 | 84 | 0 | 0 | 28.0 | 0.284 | 27 |
| 631 | 0 | 102 | 78 | 40 | 90 | 34.5 | 0.238 | 24 |
| 757 | 0 | 123 | 72 | 0 | 0 | 36.3 | 0.258 | 52 |
| 689 | 1 | 144 | 82 | 46 | 180 | 46.1 | 0.335 | 46 |

```
#Model with the quadratic transformation of Age and more predictors
logit_model_diabetes = sm.logit(formula = 'Outcome~Age+I(Age**2)+Glucose+BloodPressure+BMI+D
logit_model_diabetes.summary()
```

```
Optimization terminated successfully.
         Current function value: 0.470478
         Iterations 6
```

Table 4.17: Logit Regression Results

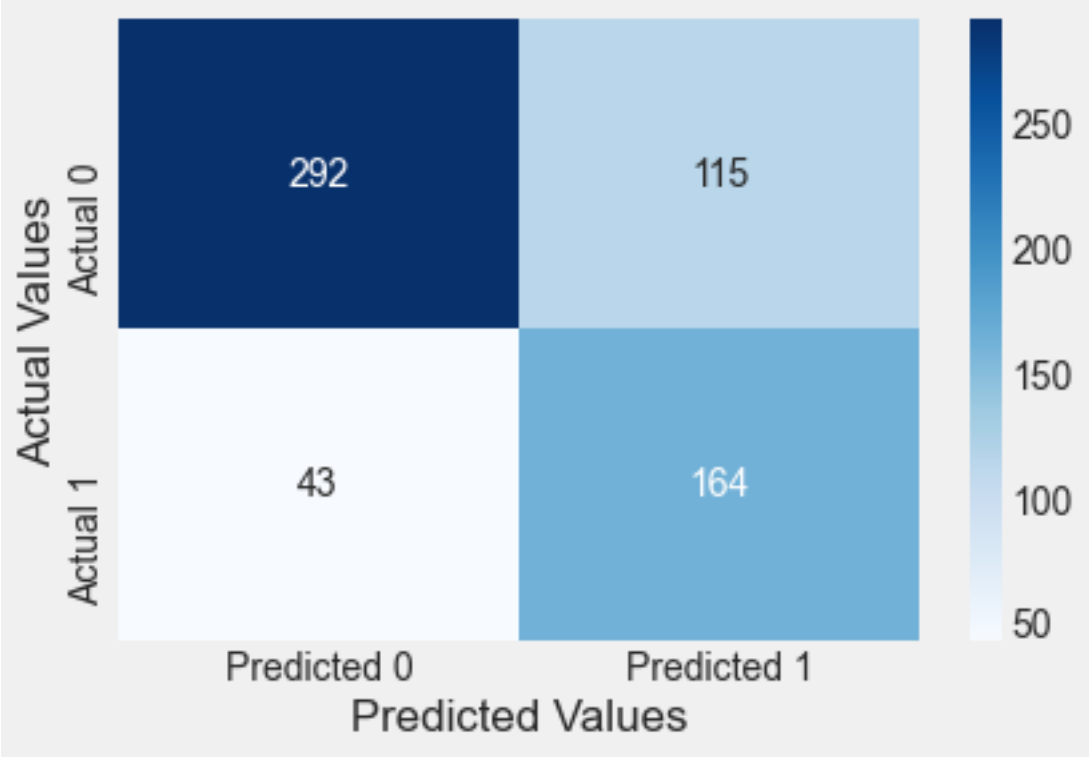
| | | | |
|---|---|---|---|
| Dep. Variable: | Outcome | No. Observations: | 614 |
| Model: | Logit | Df Residuals: | 607 |
| Method: | MLE | Df Model: | 6 |
| Date: | Thu, 23 Feb 2023 | Pseudo R-squ.: | 0.2639 |
| Time: | 10:26:00 | Log-Likelihood: | -288.87 |
| converged: | True | LL-Null: | -392.42 |
| Covariance Type: | nonrobust | LLR p-value: | 5.878e-42 |

| | coef | std err | z | P>\|z\| | [0.025 | 0.975] |
|---|---|---|---|---|---|---|
| Intercept | -12.3347 | 1.282 | -9.621 | 0.000 | -14.847 | -9.822 |
| Age | 0.2852 | 0.056 | 5.121 | 0.000 | 0.176 | 0.394 |
| I(Age ** 2) | -0.0030 | 0.001 | -4.453 | 0.000 | -0.004 | -0.002 |
| Glucose | 0.0309 | 0.004 | 8.199 | 0.000 | 0.024 | 0.038 |
| BloodPressure | -0.0141 | 0.006 | -2.426 | 0.015 | -0.025 | -0.003 |
| BMI | 0.0800 | 0.016 | 4.978 | 0.000 | 0.049 | 0.112 |
| DiabetesPedigreeFunction | 0.7138 | 0.322 | 2.213 | 0.027 | 0.082 | 1.346 |

Adding more predictors has increased the log likelihood of the model as expected.

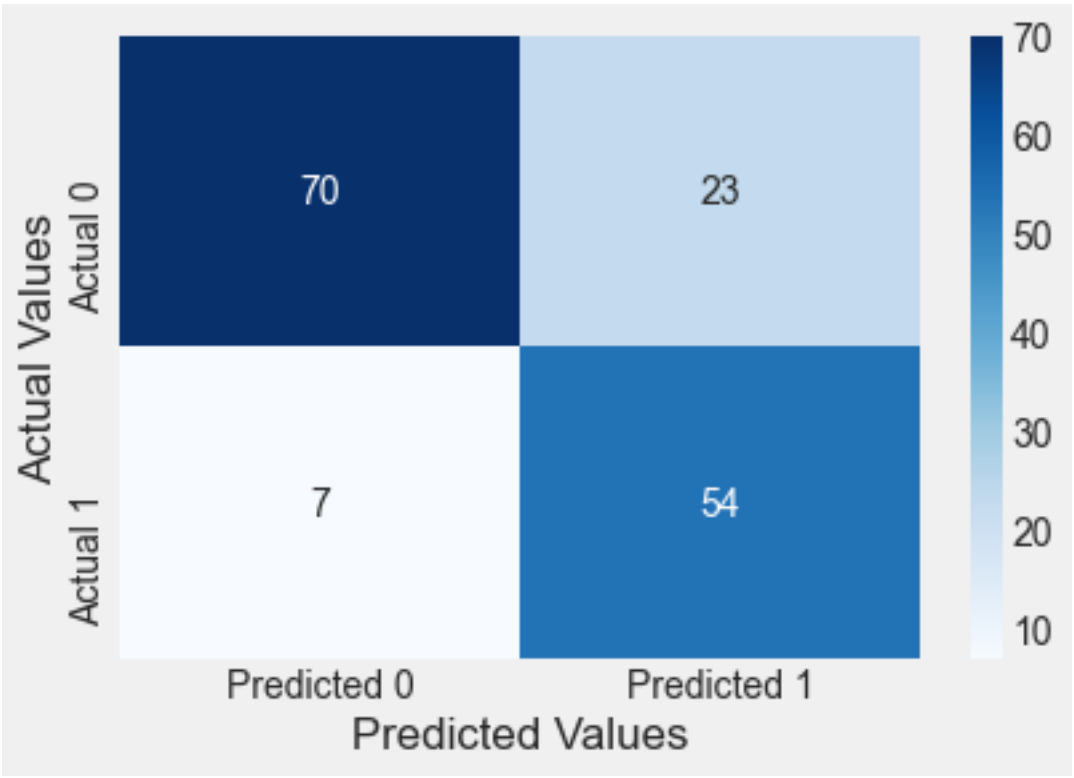
```
confusion_matrix_train(logit_model_diabetes,cutoff=0.3)
```

```
Classification accuracy = 74.3%
```




```
confusion_matrix_test(test,test.Outcome,logit_model_diabetes,0.3)
```

```
Classification accuracy = 80.5%
```




The model with more predictors also has lesser number of *false negatives*, and higher overall classification accuracy.

**How many bins must you make for `Age` to get the most accurate model?**
If the number of bins are too less, the trend may not be captured accurately. If the number of bins are too many, it may lead to overfitting of the model. There is an optimal value of the number of bins that captures the trend, but does not overfit. A couple of ways of estimating the optimal number of bins can be:

1. The number of bins for which the trend continues to be "almost" the same for several samples of the data.
2. Testing the model on multiple test datasets.

Optimizing the number of bins for each predictor may be a time-consuming exercises. You may do it for your course project. However, we will not do it here in the class notes.

## 4.6 Performance Measurement

We have already seen the confusion matrix, and classification accuracy. Now, let us see some other useful performance metrics that can be computed from the confusion matrix. The metrics

below are computed for the confusion matrix immediately above this section *(or the confusion matrix on test data corresponding to the model* ***`logit_model_diabetes`****).*

### 4.6.1 Precision-recall

**Precision** measures the accuracy of positive predictions. Also called the `precision` of the classifier

$$\text{precision} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Positives}}$$

==> `70.13%`

`Precision` is typically used with `recall` (`Sensitivity` or `True Positive Rate`). The ratio of positive instances that are correctly detected by the classifier.

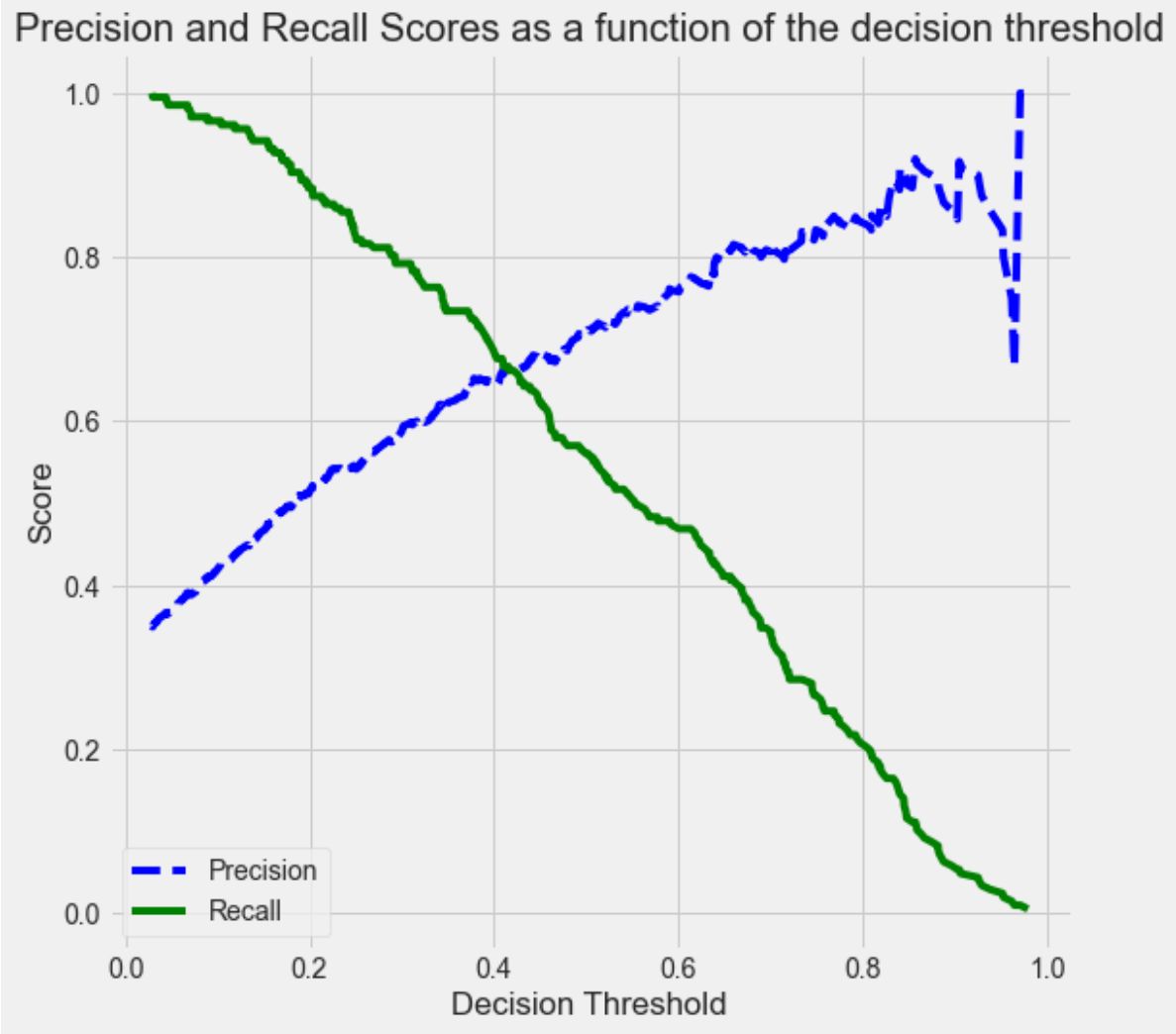
$$\text{recall} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Negatives}}$$

==> `88.52%`

**Precision / Recall Tradeoff**: Increasing precision reduces recall and vice versa.

**Visualize the precision-recall curve for the model `logit_model_diabetes`.**

```
y=train.Outcome
ypred = logit_model_diabetes.predict(train)
p, r, thresholds = precision_recall_curve(y, ypred)
def plot_precision_recall_vs_threshold(precisions, recalls, thresholds):
    plt.figure(figsize=(8, 8))
    plt.title("Precision and Recall Scores as a function of the decision threshold")
    plt.plot(thresholds, precisions[:-1], "b--", label="Precision")
    plt.plot(thresholds, recalls[:-1], "g-", label="Recall")
    plt.ylabel("Score")
    plt.xlabel("Decision Threshold")
    plt.legend(loc='best')
    plt.legend()
plot_precision_recall_vs_threshold(p, r, thresholds)
```




As the decision threshold probability increases, the precision increases, while the recall decreases.

**Q:** How are the values of the `thresholds` chosen to make the precision-recall curve?

**Hint:** Look at the documentation for `precision_recall_curve`.

### 4.6.2 The Receiver Operating Characteristics (ROC) Curve

A **ROC(Receiver Operator Characteristic Curve)** is a plot of sensitivity (True Positive Rate) on the y axis against (1−specificity) (False Positive Rate) on the x axis for varying values of the threshold t. The 45° diagonal line connecting (0,0) to (1,1) is the ROC curve

corresponding to random chance. The ROC curve for the gold standard is the line connecting (0,0) to (0,1) and (0,1) to (1,1).

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

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

An animation to demonstrate how an ROC curve relates to sensitivity and specificity for all possible cutoffs (Source)

**High Threshold:**

- High specificity
- Low sensitivity

**Low Threshold**

- Low specificity
- High sensitivity

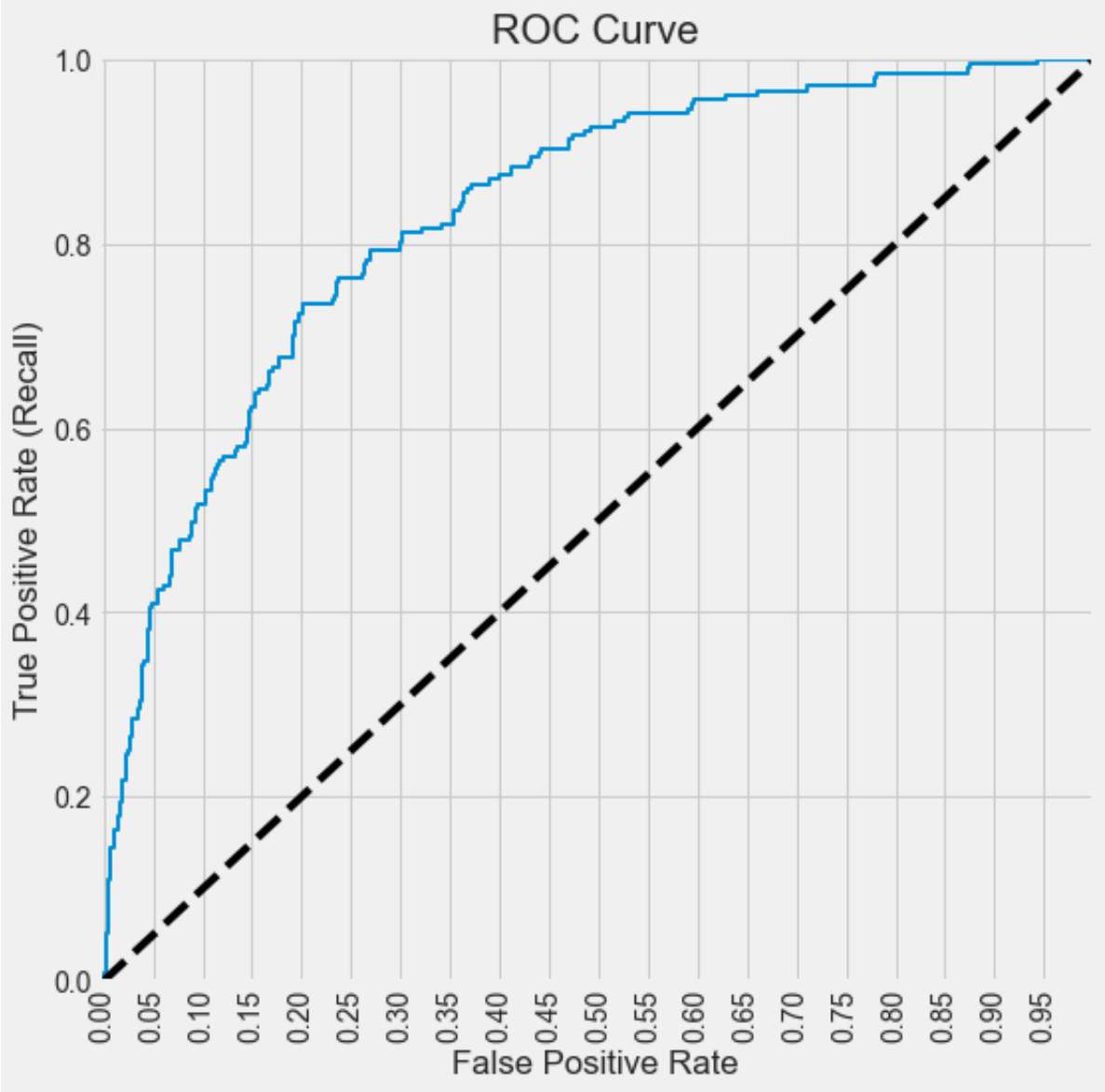
The area under ROC is called *Area Under the Curve(AUC)*. AUC gives the rate of successful classification by the logistic model. To get a more in-depth idea of what a ROC-AUC curve is and how is it calculated, here is a good blog link.

Here is good post by google developers on interpreting ROC-AUC, and its advantages / disadvantages.

**Visualize the ROC curve and compute the ROC-AUC for the model `logit_model_diabetes`.**

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

fpr, tpr, auc_thresholds = roc_curve(y, ypred)
plot_roc_curve(fpr, tpr)
```

```
0.8325914847653979
```



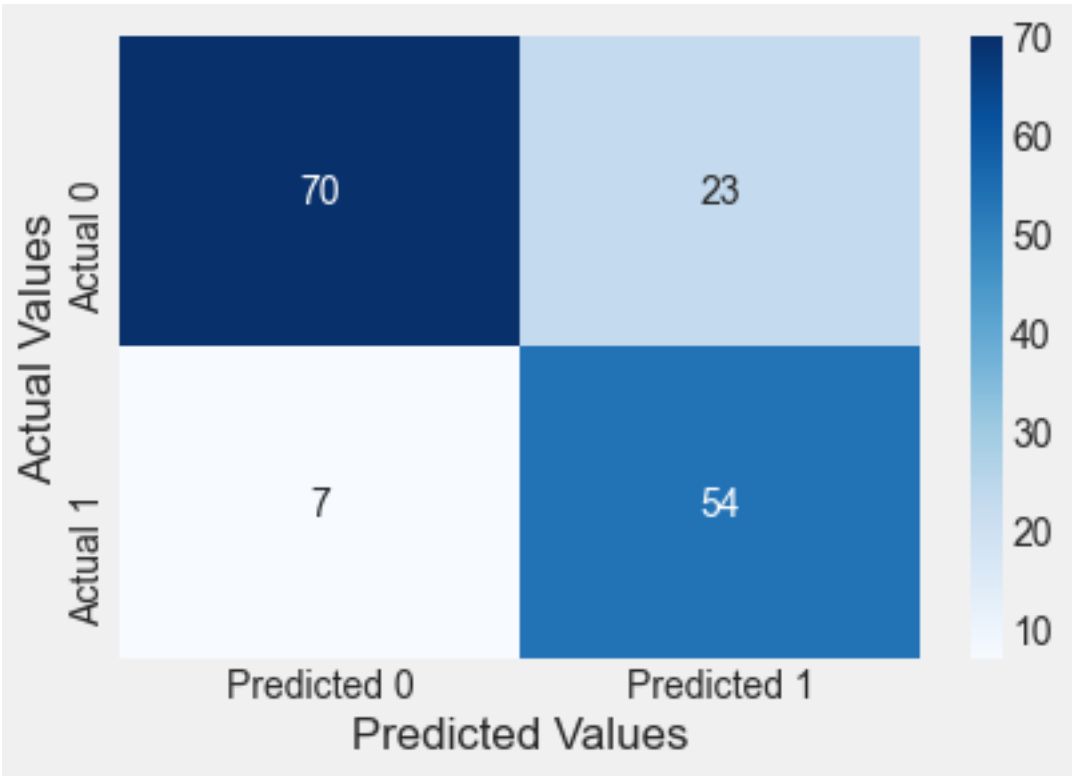

**Q:** How are the values of the `auc_thresholds` chosen to make the ROC curve? Why does it look like a step function?

Below is a function that prints the confusion matrix along with all the performance metrics we discussed above for a given decision threshold probability, on train / test data. Note that ROC-AUC does not depend on a decision threshold probability.

```
#Function to compute confusion matrix and prediction accuracy on test/train data
def confusion_matrix_data(data,actual_values,model,cutoff=0.5):
#Predict the values using the Logit model
    pred_values = model.predict(data)
# Specify the bins
    bins=np.array([0,cutoff,1])
#Confusion matrix
    cm = np.histogram2d(actual_values, pred_values, bins=bins)[0]
    cm_df = pd.DataFrame(cm)
    cm_df.columns = ['Predicted 0','Predicted 1']
    cm_df = cm_df.rename(index={0: 'Actual 0',1:'Actual 1'})
# Calculate the accuracy
    accuracy = (cm[0,0]+cm[1,1])/cm.sum()
    fnr = (cm[1,0])/(cm[1,0]+cm[1,1])
    precision = (cm[1,1])/(cm[0,1]+cm[1,1])
    fpr = (cm[0,1])/(cm[0,0]+cm[0,1])
    tpr = (cm[1,1])/(cm[1,0]+cm[1,1])
    fpr_roc, tpr_roc, auc_thresholds = roc_curve(actual_values, pred_values)
    auc_value = (auc(fpr_roc, tpr_roc))# AUC of ROC
    sns.heatmap(cm_df, annot=True, cmap='Blues', fmt='g')
    plt.ylabel("Actual Values")
    plt.xlabel("Predicted Values")
    print("Classification accuracy = {:.1%}".format(accuracy))
    print("Precision = {:.1%}".format(precision))
    print("TPR or Recall = {:.1%}".format(tpr))
    print("FNR = {:.1%}".format(fnr))
    print("FPR = {:.1%}".format(fpr))
    print("ROC-AUC = {:.1%}".format(auc_value))
```

```
confusion_matrix_data(test,test.Outcome,logit_model_diabetes,0.3)
```

```
Classification accuracy = 80.5%
Precision = 70.1%
TPR or Recall = 88.5%
FNR = 11.5%
FPR = 24.7%
ROC-AUC = 90.1%
```




## 4.7 sklearn

The `LogisticRegression()` function from the `linear_model` module of the `sklearn` library is used for fitting a logistic regression model. Note that the function as a default regularization parameter value set as `C = 1`. We'll understand the purpose of regularization later in the course.

```
train = pd.read_csv('./Datasets/Social_Network_Ads_train.csv') #Develop the model on train da
test = pd.read_csv('./Datasets/Social_Network_Ads_test.csv') #Test the model on test data

X_train = train[['Age']]
y_train = train['Purchased']

X_test = test[['Age']]
y_test = test['Purchased']

model = LogisticRegression(penalty=None) # We will talk about this input later in the quarte

model.fit(X_train, y_train)
```

```
y_pred = model.predict(X_test) # Note that in sklearn, .predict returns the classes directly

print("Accuracy = ",accuracy_score(test.Purchased, y_pred)*100, "%")

# To return the prediction probabilities, we need .predict_proba

y_pred_probs = model.predict_proba(X_test)

# First col: class 0 prob, second col: class 1 prob

# We will need the probs to try different thresholds - this will be necessary for the other m
```

```
Accuracy =  86.0 %
```

# 5 Ridge regression and Lasso

*Read section 6.2 of the book before using these notes.*

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

```
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.linear_model import Ridge, RidgeCV, Lasso, LassoCV, LogisticRegressionCV, Logist
from sklearn.preprocessing import StandardScaler
from sklearn.metrics import r2_score, accuracy_score
from sklearn.model_selection import cross_val_score, cross_val_predict
```

```
trainf = pd.read_csv('./Datasets/house_feature_train.csv')
trainp = pd.read_csv('./Datasets/house_price_train.csv')
testf = pd.read_csv('./Datasets/house_feature_test.csv')
testp = pd.read_csv('./Datasets/house_price_test.csv')
train = pd.merge(trainf,trainp)
test = pd.merge(testf,testp)
train.head()
```

| | house_id | house_age | distance_MRT | number_convenience_stores | latitude | longitude | house_pri |
|---|---|---|---|---|---|---|---|
| 0 | 210 | 5.2 | 390.5684 | 5 | 24.97937 | 121.54245 | 2724.84 |
| 1 | 190 | 35.3 | 616.5735 | 8 | 24.97945 | 121.53642 | 1789.29 |
| 2 | 328 | 15.9 | 1497.7130 | 3 | 24.97003 | 121.51696 | 556.96 |
| 3 | 5 | 7.1 | 2175.0300 | 3 | 24.96305 | 121.51254 | 1030.41 |
| 4 | 412 | 8.1 | 104.8101 | 5 | 24.96674 | 121.54067 | 2756.25 |

## 5.1 Ridge regression

Let us develop a ridge regression model to predict house price based on the five house features.

```
#Taking the log transform of house_price as house prices have a right-skewed distribution
y = np.log(train.house_price)
```

### 5.1.1 Standardizing the predictors

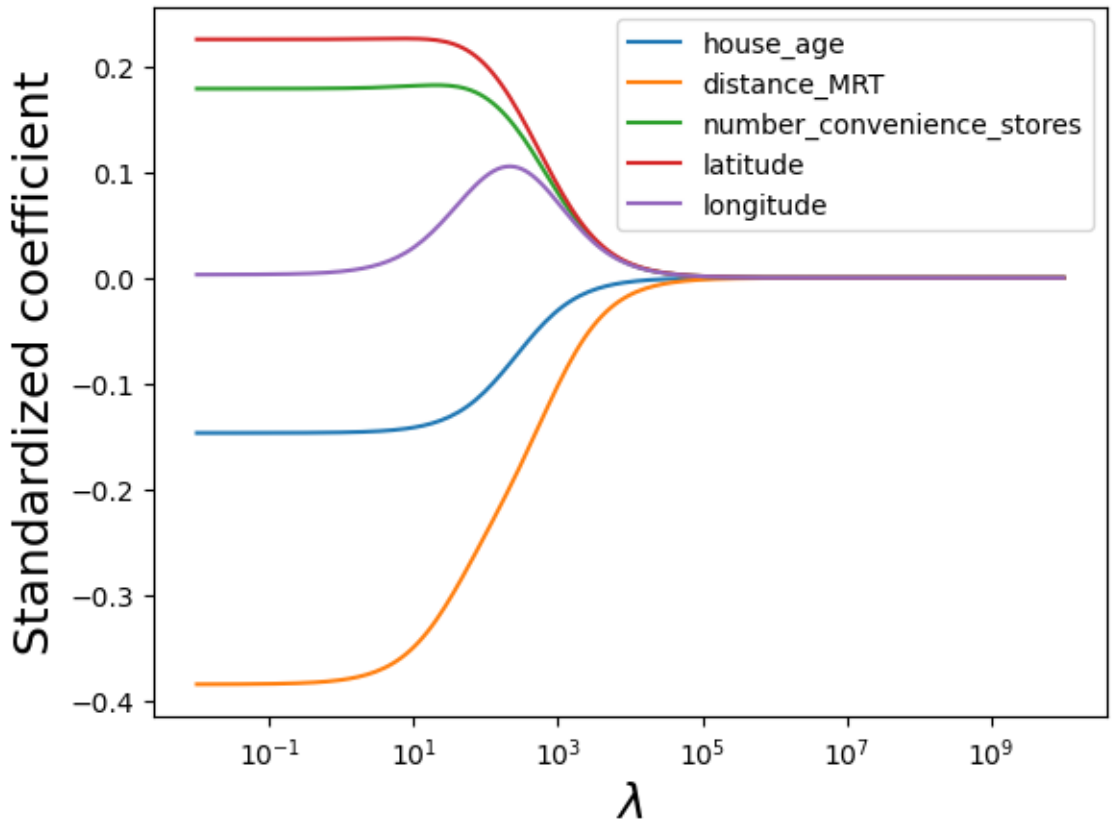
```
#Standardizing predictors so that each of them have zero mean and unit variance

#Filtering all predictors
X = train.iloc[:,1:6];

#Defining a scaler object
scaler = StandardScaler()

#The scaler object will contain the mean and variance of each column (predictor) of X.
#These values will be useful to scale test data based on the same mean and variance as obtai
scaler.fit(X)

#Using the scaler object (or the values of mean and variance stored in it) to standardize X
Xstd = scaler.transform(X)
```

### 5.1.2 Optimizing the tuning parameter

```
#The tuning parameter lambda is referred as alpha in sklearn

#Creating a range of values of the tuning parameter to visualize the ridge regression coeffi
#for different values of the tuning parameter
alphas = np.logspace(10,-2,200)
```

```
#Finding the ridge regression coefficients for increasing values of the tuning parameter
coefs = []
for a in alphas:
    ridge = Ridge(alpha = a)
    ridge.fit(Xstd, y)
    coefs.append(ridge.coef_)
```

```
#Visualizing the shrinkage in ridge regression coefficients with increasing values of the tu
plt.xlabel('xlabel', fontsize=18)
plt.ylabel('ylabel', fontsize=18)
plt.plot(alphas, coefs)
plt.xscale('log')
plt.xlabel('$\lambda$')
plt.ylabel('Standardized coefficient')
plt.legend(train.columns[1:6]);
```

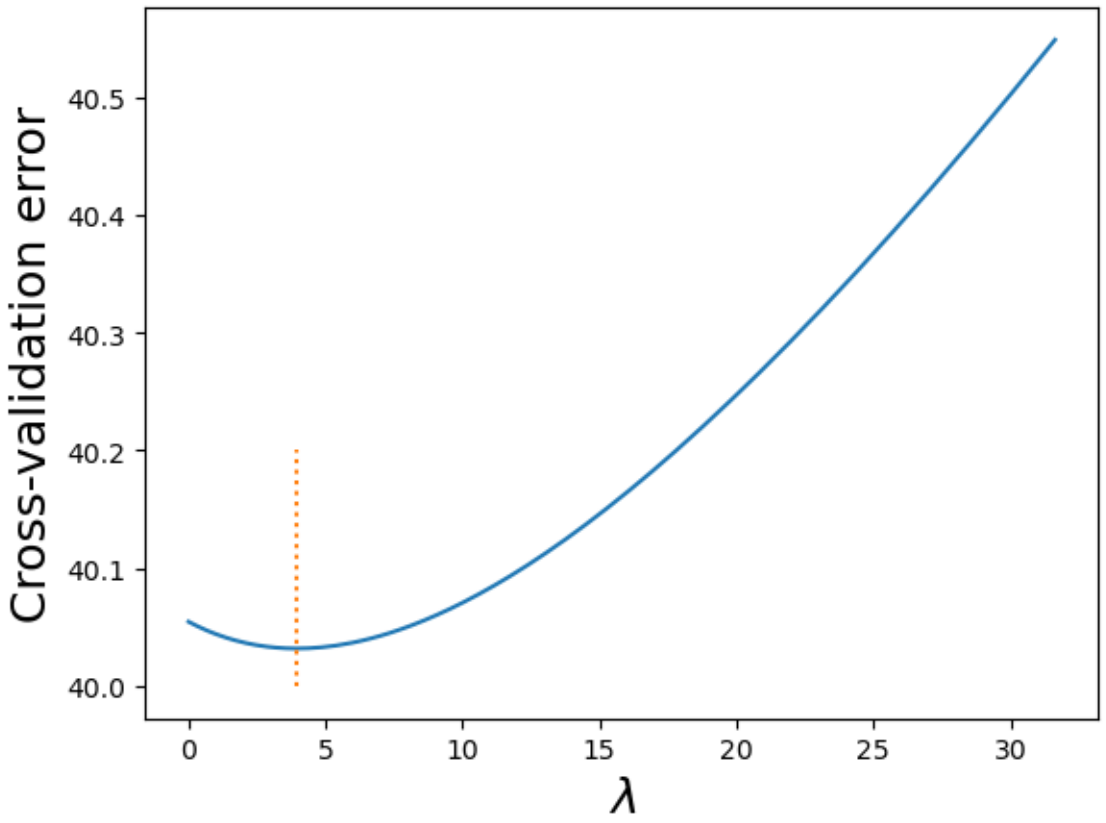



```
#Let us use cross validation to find the optimal value of the tuning parameter - lambda
#For the optimal lambda, the cross validation error will be the least

#Note that we are reducing the range of alpha so as to better visualize the minimum
alphas = np.logspace(1.5,-3,200)
ridgecv = RidgeCV(alphas = alphas,store_cv_values=True)
ridgecv.fit(Xstd, y)
```

```
#Optimal value of the tuning parameter - lambda
ridgecv.alpha_
```

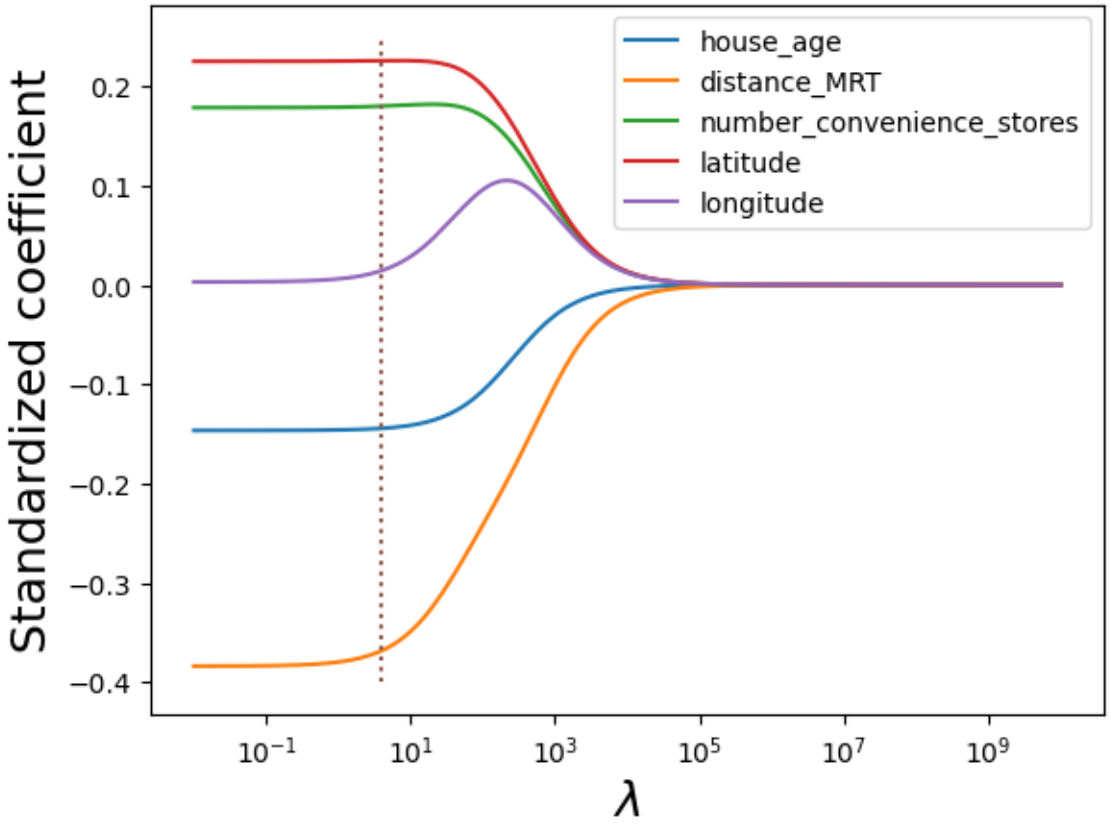
```
3.939829130085526
```

```
#Visualizing the LOOCV (leave one out cross validatation error vs lambda)
plt.xlabel('xlabel', fontsize=18)
plt.ylabel('ylabel', fontsize=18)
plt.plot(ridgecv.alphas,ridgecv.cv_values_.sum(axis=0))
plt.plot([ridgecv.alpha_,ridgecv.alpha_],[40,40.2],':')
plt.xlabel('$\lambda$')
plt.ylabel('Cross-validation error');
```




Note that the cross validation error is minimum at the optimal value of the tuning parameter.

```
#Visualizing the shrinkage in ridge regression coefficients with increasing values of the tu
alphas = np.logspace(10,-2,200)
plt.xlabel('xlabel', fontsize=18)
plt.ylabel('ylabel', fontsize=18)
plt.plot(alphas, coefs)
plt.plot([ridgecv.alpha_,ridgecv.alpha_],[-0.4,0.25],':')
plt.xscale('log')
plt.xlabel('$\lambda$')
plt.ylabel('Standardized coefficient')
plt.legend(train.columns[1:6]);
```




### 5.1.3 RMSE on test data

```
#Test dataset
Xtest = test.iloc[:,1:6]
```

```
#Standardizing test data
Xtest_std = scaler.transform(Xtest)
```

```
#Using the developed ridge regression model to predict on test data
ridge = Ridge(alpha = ridgecv.alpha_)
ridge.fit(Xstd, y)
pred=ridge.predict(Xtest_std)
```

```
#RMSE on test data
np.sqrt(((np.exp(pred)-test.house_price)**2).mean())
```

```
405.64878431933295
```

Note that the RMSE is similar to the one obtained using least squares regression on all the five predictors. This is because the coefficients were required to shrink very slightly for the best ridge regression fit. This may happen when we have a low number of predictors, where most of them are significant. Ridge regression is likely to perform better than least squares in case of a large number of predictors, where an OLS model will be prone to overfitting.

### 5.1.4 Model coefficients & $R$-squared

```
#Checking the coefficients of the ridge regression model
ridge.coef_
```

```
array([-0.14444475, -0.3683359 ,  0.17988341,  0.22567002,  0.01429926])
```

Note that none of the coefficients are shrunk to zero. The coefficient of `longitude` is smaller than the rest, but not zero.

```
#R-squared on train data for the ridge regression model
r2_score(ridge.predict(Xstd),y)
```

```
0.6993726041206049
```

```
#R-squared on test data for the ridge regression model
r2_score(pred,np.log(test.house_price))
```

```
0.757276231336096
```

## 5.2 Lasso

Let us develop a lasso model to predict house price based on the five house features.

### 5.2.1 Standardizing the predictors

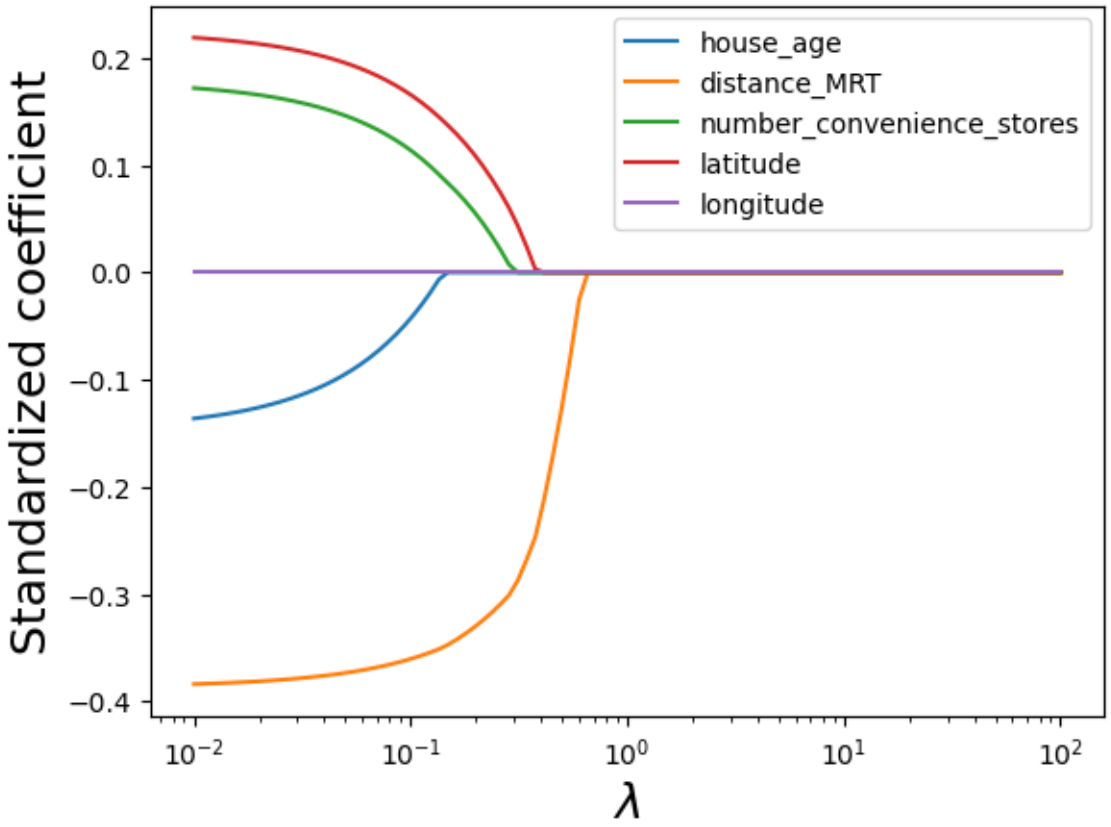
We have already standardized the predictors in the previous section. The standardized predictors are the NumPy array object `Xstd`.

### 5.2.2 Optimizing the tuning parameter

```
#Creating a range of values of the tuning parameter to visualize the lasso coefficients
#for different values of the tuning parameter
alphas = np.logspace(2,-2,100)
```

```
#Finding the lasso coefficients for increasing values of the tuning parameter
lasso = Lasso(max_iter = 10000)
coefs = []

for a in alphas:
    lasso.set_params(alpha=a)
    lasso.fit(Xstd, y)
    coefs.append(lasso.coef_)
```

```
#Visualizing the shrinkage in lasso coefficients with increasing values of the tuning parame
plt.xlabel('xlabel', fontsize=18)
plt.ylabel('ylabel', fontsize=18)
plt.plot(alphas, coefs)
plt.xscale('log')
plt.xlabel('$\lambda$')
plt.ylabel('Standardized coefficient')
plt.legend(train.columns[1:6]);
```

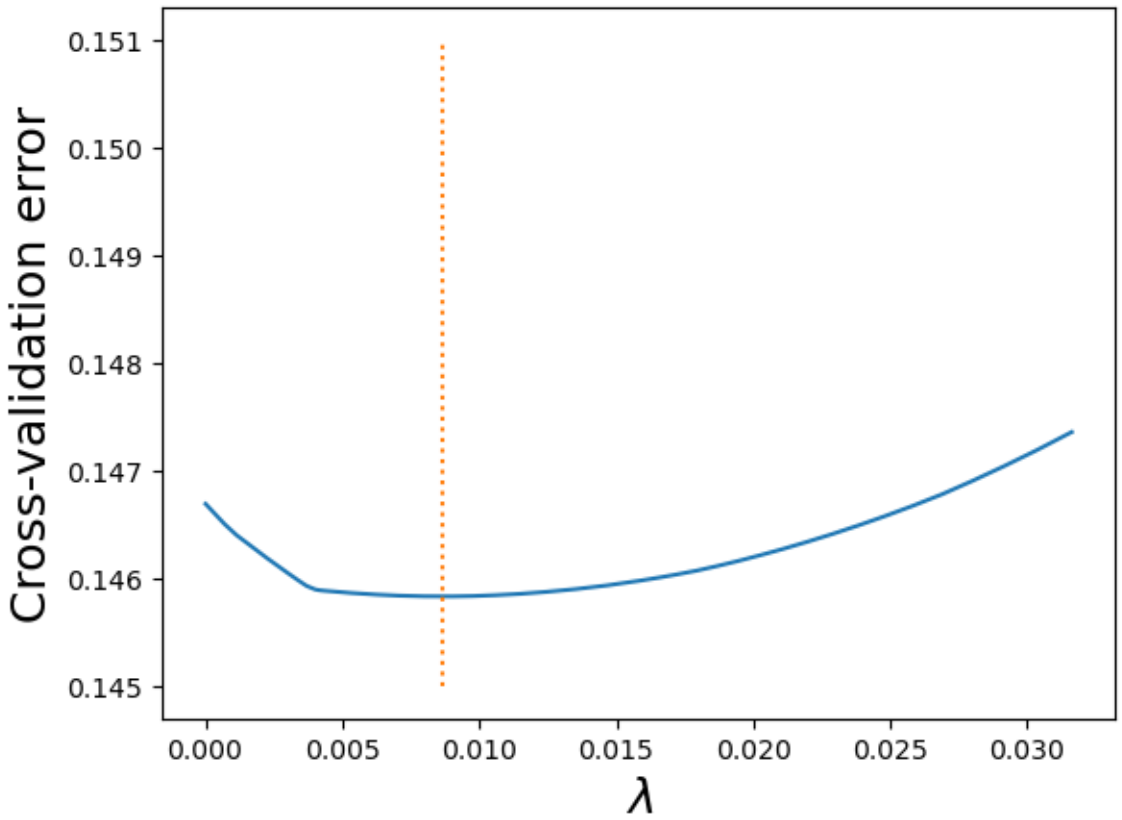



Note that lasso performs variable selection. For certain values of lambda, some of the predictor coefficients are zero, while others are non-zero. This is different than ridge regression, which only shrinks the coefficients, but doesn't do variable selection.

```
#Let us use cross validation to find the optimal value of the tuning parameter - lambda
#For the optimal lambda, the cross validation error will be the least

#Note that we are reducing the range of alpha so as to better visualize the minimum
alphas = np.logspace(-1.5,-5,200)
lassocv = LassoCV(alphas = alphas, cv = 10, max_iter = 100000)
lassocv.fit(Xstd, y)

#Optimal value of the tuning parameter - lamda
lassocv.alpha_
```

```
0.00865338307114046
```

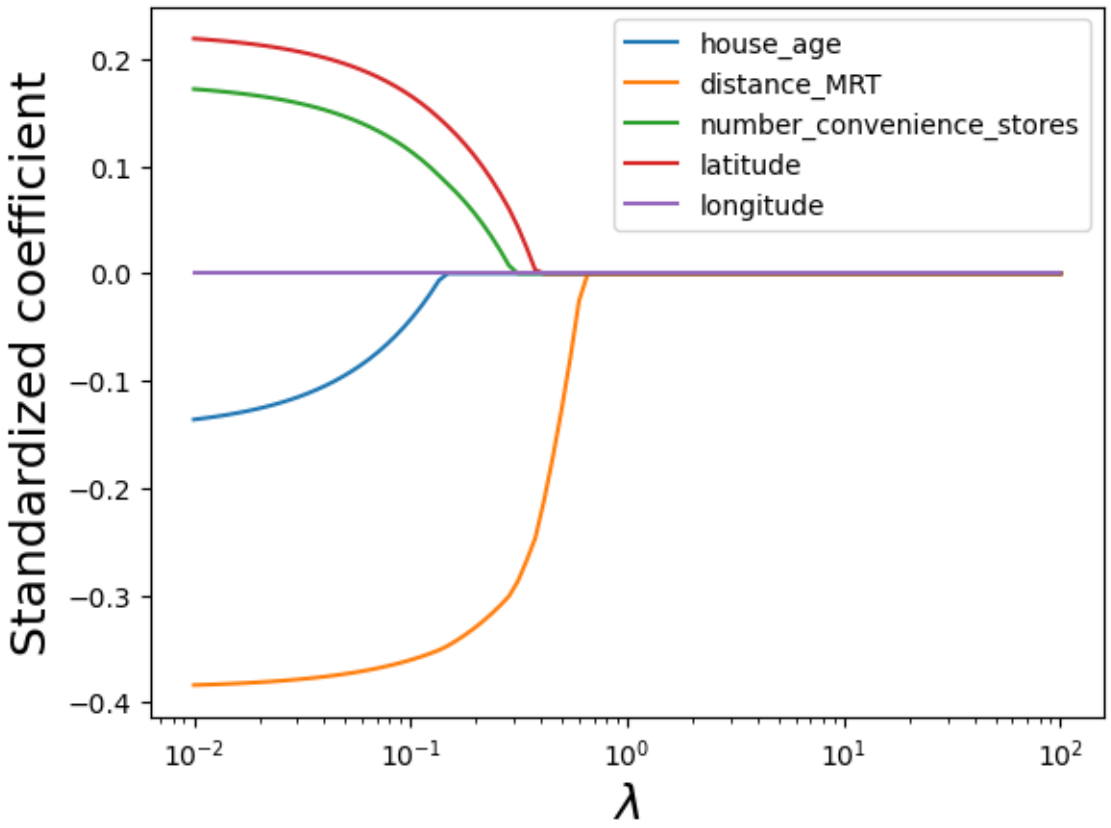
```
#Visualizing the LOOCV (leave one out cross validatation error vs lambda)
plt.xlabel('xlabel', fontsize=18)
plt.ylabel('ylabel', fontsize=18)
plt.plot(lassocv.alphas_,lassocv.mse_path_.mean(axis=1))
plt.plot([lassocv.alpha_,lassocv.alpha_],[0.145,0.151],':')
plt.xlabel('$\lambda$')
plt.ylabel('Cross-validation error');
```




The 10-fold cross validation error minimizes at lambda = 0.009.

```
#Visualizing the shrinkage in lasso coefficients with increasing values of the tuning paramet
alphas = np.logspace(2,-2,100)
plt.xlabel('xlabel', fontsize=18)
plt.ylabel('ylabel', fontsize=18)
plt.plot(alphas, coefs)
plt.xscale('log')
plt.xlabel('$\lambda$')
```

```
plt.ylabel('Standardized coefficient')
plt.legend(train.columns[1:6]);
```




### 5.2.3 RMSE on test data

```
#Using the developed lasso model to predict on test data
lasso = Lasso(alpha = lassocv.alpha_)
lasso.fit(Xstd, y)
pred=lasso.predict(Xtest_std)
```

```
#RMSE on test data
np.sqrt(((np.exp(pred)-test.house_price)**2).mean())
```

```
400.8580108804818
```

### 5.2.4 Model coefficients & $R$-squared

```
#Checking the coefficients of the lasso model
lasso.coef_
```

```
array([-0.13758288, -0.38414914,  0.17276584,  0.21970825,  0.        ])
```

Note that the coefficient of `longitude` is shrunk to zero. Lasso performs variable selection.

```
#R-squared on train data for the lasso model
r2_score(lasso.predict(Xstd),y)
```

```
0.6931007715680897
```

```
#R-squared on test data for the lasso model
r2_score(pred,np.log(test.house_price))
```

```
0.7526968660283655
```

## 5.3 Lasso/Ridge Classification

The Ridge and Lasso penalties are added from inside the same LogisticRegression object, they don't have their own objects like they do in regression.

```
# Data
train = pd.read_csv('Datasets/Social_Network_Ads_train.csv')
test = pd.read_csv('Datasets/Social_Network_Ads_test.csv')
```

```
# Predictors and response
X_train = train[['Age', 'EstimatedSalary']]
y_train = train['Purchased']

X_test = test[['Age', 'EstimatedSalary']]
y_test = test['Purchased']
```

```
# Creating the model
    # penalty=None means regular logistic Regression
    # penalty=l2 means Ridge Classification
    # penalty=l1 means Lasso Classification
    # C = 1/lambda

model = LogisticRegression(penalty='l2', C = 1)
```

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

# Train
model.fit(X_train_scaled, y_train)
y_pred = model.predict(X_test_scaled) # threshold = 0.5 here

# Evaluate
print(accuracy_score(test.Purchased, y_pred)*100)

# Probs
y_pred_probs = model.predict_proba(X_test_scaled)
```

```
88.0
```

### 5.3.1 Cross-validation to find optimal `C`

```
# a list of possible C values
Cs = np.logspace(-1,1)

# Cs =  the C values we want to try out
# cv = number of folds, 3,5,10 - if no input given, 5-fold
# penalty = Ridge or Lasso
model_cv = LogisticRegressionCV(Cs = Cs, cv=5, penalty='l2')

model_cv.fit(X_train_scaled, y_train)

model_cv.C_[0]
```

```
1.3894954943731375
```

```
model = LogisticRegression(penalty='l2', C = model_cv.C_[0])
model.fit(X_train_scaled, y_train)
y_pred = model.predict(X_test_scaled) # threshold = 0.5 here

# Evaluate
print(accuracy_score(test.Purchased, y_pred)*100)
```

```
88.0
```

# 6 Cross-validation

*Read section 5.1 of the book before using these notes.*

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

- The aim of the notebook is to introduce how to use some low-level cross-validation tools.
- Why? Because unlike Lasso, Ridge and LogisticRegression, most models in sklearn don't have a CV version.
- In that case, you need to CV yourself with the tools in this notebook.

```
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.linear_model import Ridge, Lasso, LogisticRegression # No CV versions of the obj
from sklearn.preprocessing import StandardScaler, PolynomialFeatures
from sklearn.metrics import mean_squared_error, mean_absolute_error, accuracy_score, roc_curv
precision_score, recall_score, confusion_matrix
from sklearn.model_selection import cross_val_score, cross_val_predict
```

## 6.1 Regression

```
trainf = pd.read_csv('Datasets/house_feature_train.csv')
trainp = pd.read_csv('Datasets/house_price_train.csv')
testf = pd.read_csv('Datasets/house_feature_test.csv')
testp = pd.read_csv('Datasets/house_price_test.csv')
train = pd.merge(trainf,trainp)
test = pd.merge(testf,testp)
train.head()
```

| | house_id | house_age | distance_MRT | number_convenience_stores | latitude | longitude | house_pri |
|---|---|---|---|---|---|---|---|
| 0 | 210 | 5.2 | 390.5684 | 5 | 24.97937 | 121.54245 | 2724.84 |
| 1 | 190 | 35.3 | 616.5735 | 8 | 24.97945 | 121.53642 | 1789.29 |
| 2 | 328 | 15.9 | 1497.7130 | 3 | 24.97003 | 121.51696 | 556.96 |
| 3 | 5 | 7.1 | 2175.0300 | 3 | 24.96305 | 121.51254 | 1030.41 |
| 4 | 412 | 8.1 | 104.8101 | 5 | 24.96674 | 121.54067 | 2756.25 |

```
# Data

# Train
y_train = np.log(train.house_price) # Response (log taken to account for the skewed dist. of
X_train = train.iloc[:,1:6] # Slice out the predictors

# Test
y_test = np.log(test.house_price) # Response (log taken to account for the skewed dist. of ho
X_test = test.iloc[:,1:6] # Slice out the predictor

# Scale both
scaler = StandardScaler()
scaler.fit(X_train)
X_train_scaled = scaler.transform(X_train)
X_test_scaled = scaler.transform(X_test)
```

```
# Let's tune the lambda of a Ridge model, with 5-fold CV.

# For that, we need to loop through lambda (alpha) values.
# However, we don't need to loop through folds - we will use a function for that! - cross_val

alphas = np.logspace(-1,1,200)

cv_results = []

for alpha in alphas: # For each alpha
    model = Ridge(alpha=alpha) # Create the model
    cv_results.append(cross_val_score(model, X_train_scaled, y_train, cv=5, scoring='neg_root

# Note that the input is the model object, the data, number of folds and the metric
# If you don't specify the scoring, it will use r-squared for regression and accuracy for cla
# The output is an array of k values, k being the number of folds (cv input)
```

```
# For each alpha value, 5 RMSE values

# Take the mean of each row to find avg cv score for each alpha
# Negative sign because the scoring input has "neg" in the previous cell
rmses = -np.array(cv_results).mean(axis=1)

# Index of the minimum CV RMSE
np.argmin(rmses)

alphas[np.argmin(rmses)]

# Note the same alpha as in RidgeCV example in the previous notebook
```

```
4.768611697714469
```

```
# Now we need to create one final Ridge model with the optimized alpha value

model = Ridge(alpha=alphas[np.argmin(rmses)])

model.fit(X_train_scaled, y_train)

# Predict
# Evaluate
```

```
Ridge(alpha=4.768611697714469)
```

## 6.2 Classification

```
# Data
train = pd.read_csv('Datasets/Social_Network_Ads_train.csv')
test = pd.read_csv('Datasets/Social_Network_Ads_test.csv')

# Predictors and response
X_train = train[['Age', 'EstimatedSalary']]
y_train = train['Purchased']

X_test = test[['Age', 'EstimatedSalary']]
y_test = test['Purchased']
```

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

```
# CV a logistic regression model

# a list of possible C values
Cs = [0.001, 0.01, 0.1, 1, 10, 100]

cv_results = []

for C in Cs:
    model = LogisticRegression(penalty='l2', C=C)
    cv_results.append(cross_val_score(model, X_train_scaled, y_train, cv=10))

# Scoring not given, default metric is accuracy (you can use recall, precision etc.)
```

```
# For each C, 10 accuracy values

accs = np.array(cv_results).mean(axis=1)

Cs[np.argmax(accs)] # best C - Same as the output of LogisticRegressionCV in the previous not

# Train the final model
# predict
# Evaluate
```

1

- Important question: How were these accuracies calculated? With a threhold of 0.5
- What if we want to change/optimize the threshold in this process as well? Then `cross_val_score()` is not enough, we need to change the function!

```
# CV a logistic regression model - but do not return the accuracy metric for each fold
    # Return the PREDICTIONS FOR EACH FOLD

# a list of possible C values
Cs = [0.001, 0.01, 0.1, 1, 10, 100, 1000]
```

```
cv_results = []

for C in Cs:
    model = LogisticRegression(penalty='l2', C=C)
    cv_results.append(cross_val_predict(model, X_train_scaled, y_train, cv=10, method='predi

# Cross_val_predict function has an optional input: method
```

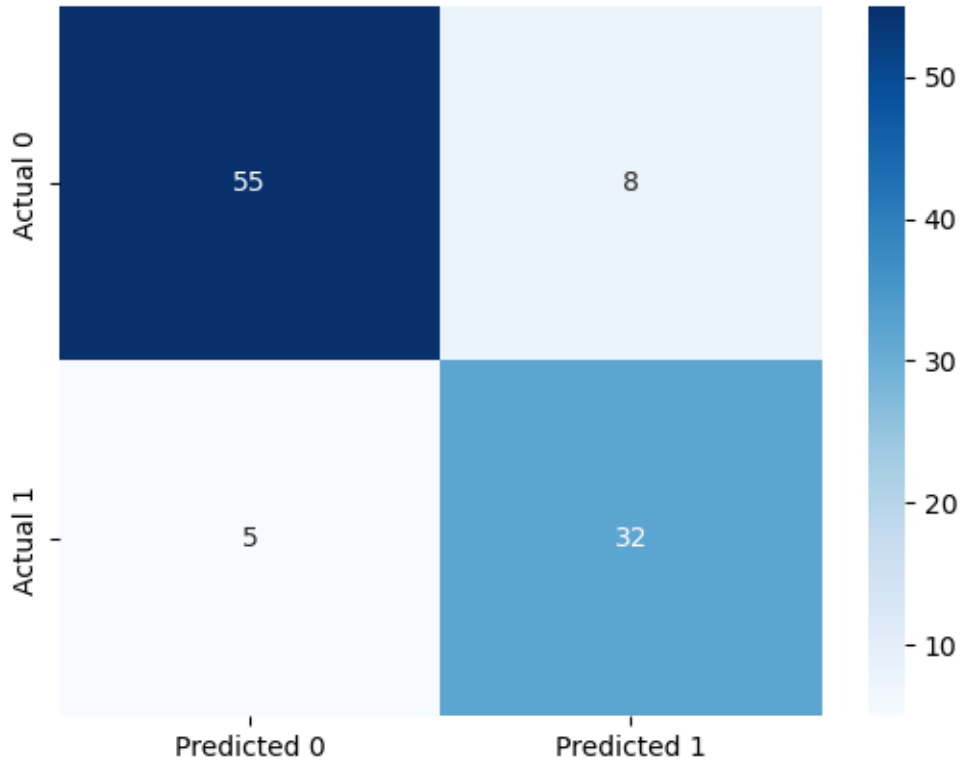
```
threshold_hyperparam_vals = np.arange(0,1.01,0.01)
C_hyperparam_vals = np.logspace(-3.5, 1)
accuracy_iter = pd.DataFrame(columns = {'threshold':[], 'C':[], 'accuracy':[]})
iter_number = 0

for c_val in C_hyperparam_vals:
    predicted_probability = cross_val_predict(LogisticRegression(C = c_val), X_train_scaled,
                                              y_train, cv = 5, method = 'predict_proba')

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

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

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

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

```
Optimal decision threshold =  0.41000000000000003
Optimal C =  0.06250551925273976
```

```
model = LogisticRegression(C = optimal_C).fit(X_train_scaled, y_train)
test_pred = model.predict_proba(X_test_scaled)[:,1]

y_pred_optimal_threshold = (test_pred > optimal_threshold).astype(int)

#Computing the accuracy
print("Accuracy: ",accuracy_score(y_pred_optimal_threshold, y_test)*100)

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

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

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

```
Accuracy:  87.0
ROC-AUC:  0.868940368940369
Precision:  0.8
Recall:  0.8648648648648649
```




- We will use `cross_val_score()` and `cross_val_predict()` repeatedly next quarter.
- There is a `cross_validate()` function that allows us to use multiple metrics at once (for example, accuracy and recall) - next quarter.

Find some more examples of using the cross validation and some other useful functions here.

# 7 Potential issues

*Read section 3.3.3 (4, 5, & 6) of the book before using these notes.*

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

Let us continue with the car price prediction example from the previous chapter.

```
import pandas as pd
import numpy as np
import statsmodels.formula.api as smf
import seaborn as sns
import matplotlib.pyplot as plt
import statsmodels.api as sm
from scipy import stats
from sklearn.model_selection import cross_val_predict
from patsy import dmatrices
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_squared_error
```

```
trainf = pd.read_csv('./Datasets/Car_features_train.csv')
trainp = pd.read_csv('./Datasets/Car_prices_train.csv')
testf = pd.read_csv('./Datasets/Car_features_test.csv')
testp = pd.read_csv('./Datasets/Car_prices_test.csv')
train = pd.merge(trainf,trainp)
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 |

```
# Considering the model developed to address assumptions in the previous chapter
# Model with an interaction term and a variable transformation term
ols_object = smf.ols(formula = 'np.log(price)~(year+engineSize+mileage+mpg)**2+I(mileage**2)
model_log = ols_object.fit()
model_log.summary()
```

| | | | |
|---|---|---|---|
| **Dep. Variable:** | np.log(price) | **R-squared:** | 0.803 |
| **Model:** | OLS | **Adj. R-squared:** | 0.803 |
| **Method:** | Least Squares | **F-statistic:** | 1834. |
| **Date:** | Sun, 10 Mar 2024 | **Prob (F-statistic):** | 0.00 |
| **Time:** | 16:51:01 | **Log-Likelihood:** | -1173.8 |
| **No. Observations:** | 4960 | **AIC:** | 2372. |
| **Df Residuals:** | 4948 | **BIC:** | 2450. |
| **Df Model:** | 11 | | |
| **Covariance Type:** | nonrobust | | |

| | **coef** | **std err** | **t** | **P> \|t\|** | **[0.025** | **0.975]** |
|---|---|---|---|---|---|---|
| **Intercept** | -238.2125 | 25.790 | -9.237 | 0.000 | -288.773 | -187.652 |
| **year** | 0.1227 | 0.013 | 9.608 | 0.000 | 0.098 | 0.148 |
| **engineSize** | 13.8349 | 5.795 | 2.387 | 0.017 | 2.475 | 25.195 |
| **mileage** | 0.0005 | 0.000 | 3.837 | 0.000 | 0.000 | 0.001 |
| **mpg** | -1.2446 | 0.345 | -3.610 | 0.000 | -1.921 | -0.569 |
| **year:engineSize** | -0.0067 | 0.003 | -2.324 | 0.020 | -0.012 | -0.001 |
| **year:mileage** | -2.67e-07 | 6.8e-08 | -3.923 | 0.000 | -4e-07 | -1.34e-07 |
| **year:mpg** | 0.0006 | 0.000 | 3.591 | 0.000 | 0.000 | 0.001 |
| **engineSize:mileage** | -2.668e-07 | 4.08e-07 | -0.654 | 0.513 | -1.07e-06 | 5.33e-07 |
| **engineSize:mpg** | 0.0028 | 0.000 | 6.842 | 0.000 | 0.002 | 0.004 |
| **mileage:mpg** | 7.235e-08 | 1.79e-08 | 4.036 | 0.000 | 3.72e-08 | 1.08e-07 |
| **I(mileage ** 2)** | 1.828e-11 | 5.64e-12 | 3.240 | 0.001 | 7.22e-12 | 2.93e-11 |

| | | | |
|---|---|---|---|
| **Omnibus:** | 711.514 | **Durbin-Watson:** | 0.498 |
| **Prob(Omnibus):** | 0.000 | **Jarque-Bera (JB):** | 2545.807 |
| **Skew:** | 0.699 | **Prob(JB):** | 0.00 |
| **Kurtosis:** | 6.220 | **Cond. No.** | 1.73e+13 |

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
[2] The condition number is large, 1.73e+13. This might indicate that there are strong multicollinearity or other numerical problems.

```
#Computing RMSE on test data
pred_price_log = model_log.predict(testf)
np.sqrt(((testp.price - np.exp(pred_price_log))**2).mean())
```

```
9094.209473232966
```

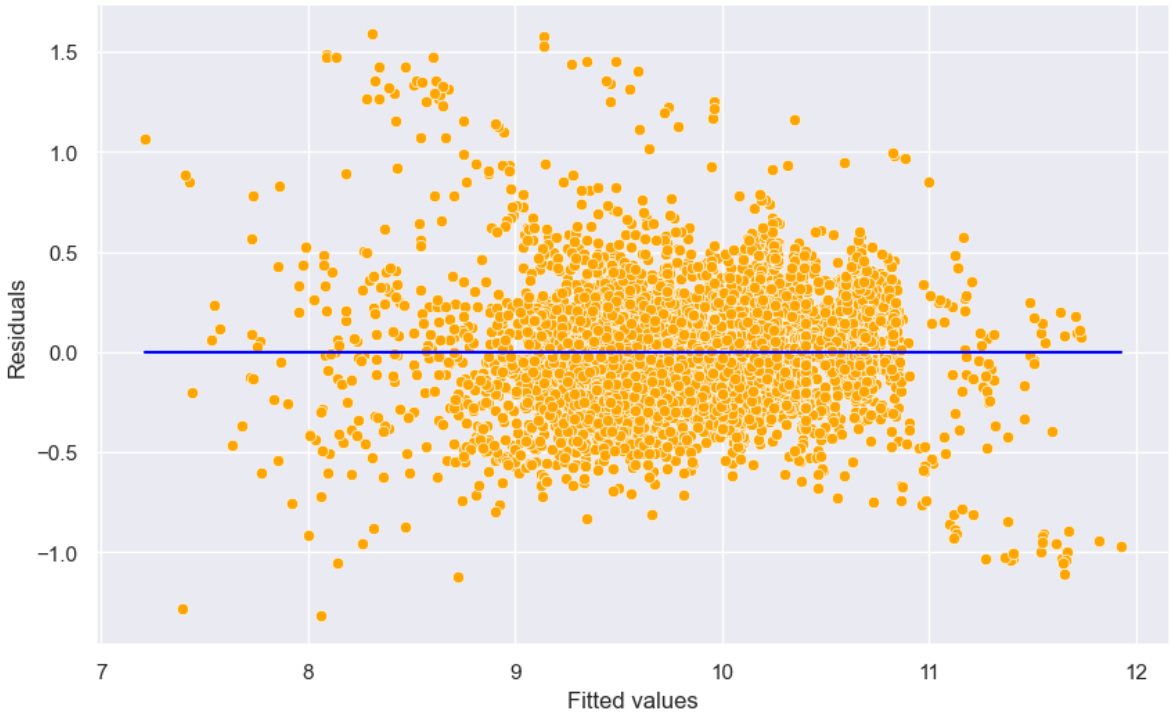
## 7.1 Outliers

An outlier is a point for which the true response ($y_i$) is far from the value predicted by the model. Residual plots can be used to identify outliers.

If the the response at the $i^{th}$ observation is $y_i$, the prediction is $\hat{y}_i$, then the residual $e_i$ is:

$$e_i = y_i - \hat{y}_i$$

```
#Plotting residuals vs fitted values
sns.set(rc={'figure.figsize':(10,6)})
sns.scatterplot(x = (model_log.fittedvalues), y=(model_log.resid),color = 'orange')
sns.lineplot(x = [model_log.fittedvalues.min(),model_log.fittedvalues.max()],y = [0,0],color
plt.xlabel('Fitted values')
plt.ylabel('Residuals');
```



Some of the errors may be high. However, it is difficult to decide how large a residual needs to be before we can consider a point to be an outlier. To address this problem, we have standardized residuals, which are defined as:

$$r_i = \frac{e_i}{RSE(\sqrt{1-h_{ii}})},$$

where $r_i$ is the standardized residual, $RSE$ is the residual standard error, and $h_{ii}$ is the leverage *(introduced in the next section)* of the $i^{th}$ observation.

Standardized residuals, allow the residuals to be compared on a *standard scale*.

**Issue with standardized residuals:**, If the observation corresponding to the standardized residual has a high leverage, then it will drag the regression line / plane / hyperplane towards it, thereby influencing the estimate of the residual itself.

**Studentized residuals:** To address the issue with standardized residuals, studentized residual for the $i^{th}$ observation is computed as the standardized residual, but with the $RSE$ (residual standard error) computed after removing the $i^{th}$ observation from the data. Studentized residual, $t_i$ for the $i^{th}$ observation is given as:

$$t_i = \frac{e_i}{RSE_i(\sqrt{1-h_{ii}})},$$

where $RSE_i$ is the residual standard error of the model developed on the data without the $i^{th}$ observation.

**Distribution of studentized residuals:** If the regression model is appropriate such that no case is outlying because of a change in the model, then each studentized residual will follow a $t$ distribution with ($n$–$p$–1) degrees of freedom.

As the studentized residuals follow a $t$ distribution, we can conduct a hypothesis test to identify whether an observation is an outlier or not for a given sigificance level. Note that the test will be two-sided since we are not concerned with the sign of the residuals, but only their absolute values.

In the current example, for a signficance level of 5%, the critical $t$-statistic is $t(1-\frac{\alpha}{2}, n-p-1)$, as calculated below.

```
n = train.shape[0]
p = model_log.df_model
alpha = 0.05

# Critical value
stats.t.ppf(1 - alpha/2, n - p - 1)
```

```
1.9604435402730618
```

If we were conducting the test for a single observation, we'll compare the studentized residual for that observation with the critical $t$-statistic, and if the residual is greater than the critical value, we'll consider that observation as an outlier.

However, typically, we'll be interested in conducting this test for all observations, and thus we'll need a more conservative critical value for the same signficance level. This critical value is given by the Bonferroni correction as $t(1-\frac{\alpha}{2n}, n-p-1)$.

Thus, the minimum value of studentized residual for which the observation will be classified as an outlier is:

```
critical_value = stats.t.ppf(1-alpha/(2*n), n - p - 1)
critical_value
```

```
4.4200129981725365
```

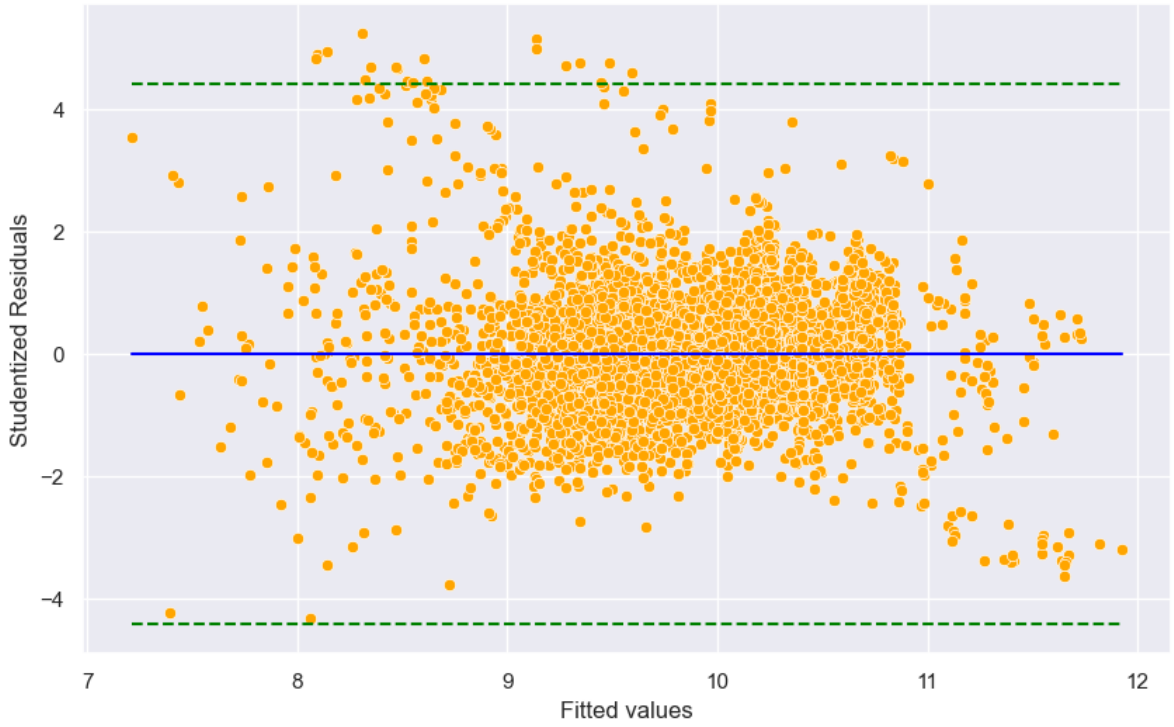
The studentized residuals can be obtained using the `outlier_test()` method of the object returned by the `fit()` method of an OLS object. Let us find the studentized residuals in our car `price` prediction model.

```
#Studentized residuals
out = model_log.outlier_test()
out
```

| | student_resid | unadj_p | bonf(p) |
|---|---|---|---|
| 0 | -1.164204 | 0.244398 | 1.0 |
| 1 | -0.801879 | 0.422661 | 1.0 |
| 2 | -1.263820 | 0.206354 | 1.0 |
| 3 | -0.614171 | 0.539131 | 1.0 |
| 4 | 0.027929 | 0.977720 | 1.0 |
| ... | ... | ... | ... |
| 4955 | -0.523361 | 0.600747 | 1.0 |
| 4956 | -0.509538 | 0.610398 | 1.0 |
| 4957 | -1.718808 | 0.085712 | 1.0 |
| 4958 | -0.077594 | 0.938154 | 1.0 |
| 4959 | -0.482388 | 0.629551 | 1.0 |

Studentized residuals are in the first column of the above table. Let us plot the studentized residuals against fitted values. In the figure below, the studentized residuals above the top dotted green line and below the bottom dotted green line are outliers.

```
#Plotting studentized residuals vs fitted values
sns.scatterplot(x = (model_log.fittedvalues), y=(out.student_resid),color = 'orange')
sns.lineplot(x = [model_log.fittedvalues.min(),model_log.fittedvalues.max()],y = [0,0],color
ax = sns.lineplot(x = [model_log.fittedvalues.min(),model_log.fittedvalues.max()],y = [criti
             color = 'green')
sns.lineplot(x = [model_log.fittedvalues.min(),model_log.fittedvalues.max()],y = [-critical_
             color = 'green')
ax.lines[1].set_linestyle("--")
ax.lines[2].set_linestyle("--")

plt.xlabel('Fitted values')
plt.ylabel('Studentized Residuals');
```




**Outliers:** Observations whose studentized residuals have a magnitude greater than $t(1 - \frac{\alpha}{2n}, n - p - 1)$.

**Impact of outliers:** Outliers do not have a large impact on the OLS line / plane / hyperplane as long as they don't have a high leverage *(discussed in the next section)*. However, outliers do inflate the residual standard error (RSE). RSE in turn is used to compute the standard errors of regression coefficients. As a result, statistically significant variables may appear to be insignificant, and $R^2$ may appear to be lower.

**Are there outliers in our example?**

```
#Number of points with absolute studentized residuals greater than critical_value
np.sum(np.abs(out.student_resid) > critical_value)
```

```
19
```

Let us analyze the outliers.

```
ind = (np.abs(out.student_resid) > critical_value)
pd.concat([train.loc[ind,:], np.exp(model_log.fittedvalues[ind])], axis = 1)
```

| | carID | brand | model | year | transmission | mileage | fuelType | tax | mpg | engineSize | price |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 2042 | 18228 | bmw | i3 | 2017 | Automatic | 24041 | Hybrid | 0 | 78.2726 | 0.0 | 2149 |
| 2046 | 17362 | bmw | i3 | 2016 | Automatic | 68000 | Hybrid | 0 | 78.0258 | 0.0 | 1599 |
| 2050 | 19224 | bmw | i3 | 2016 | Automatic | 20013 | Hybrid | 0 | 77.9310 | 0.0 | 1987 |
| 2051 | 13913 | bmw | i3 | 2014 | Automatic | 34539 | Hybrid | 0 | 78.3838 | 0.0 | 1449 |
| 2055 | 16512 | bmw | i3 | 2017 | Automatic | 28169 | Hybrid | 0 | 77.9799 | 0.0 | 2375 |
| 2059 | 15844 | bmw | i3 | 2016 | Automatic | 19995 | Hybrid | 0 | 78.2825 | 0.0 | 1985 |
| 2060 | 12107 | bmw | i3 | 2016 | Automatic | 8421 | Hybrid | 0 | 77.9125 | 0.0 | 1949 |
| 2061 | 18215 | bmw | i3 | 2014 | Automatic | 37161 | Hybrid | 0 | 77.7505 | 0.0 | 1418 |
| 2063 | 15617 | bmw | i3 | 2017 | Automatic | 41949 | Hybrid | 140 | 78.1907 | 0.0 | 1999 |
| 2064 | 18020 | bmw | i3 | 2015 | Automatic | 9886 | Hybrid | 0 | 78.1810 | 0.0 | 1748 |
| 2143 | 12972 | bmw | i8 | 2017 | Automatic | 9992 | Hybrid | 135 | 69.2767 | 1.5 | 5995 |
| 2144 | 13826 | bmw | i8 | 2015 | Automatic | 43323 | Hybrid | 0 | 69.2683 | 1.5 | 4499 |
| 2150 | 18949 | bmw | i8 | 2015 | Automatic | 43102 | Hybrid | 0 | 69.0922 | 1.5 | 4289 |
| 2151 | 18977 | bmw | i8 | 2016 | Automatic | 10087 | Hybrid | 0 | 68.9279 | 1.5 | 4899 |
| 2744 | 18866 | merc | M Class | 2004 | Automatic | 121000 | Diesel | 325 | 29.3713 | 2.7 | 1995 |
| 3548 | 13149 | audi | S4 | 2019 | Automatic | 4900 | Diesel | 145 | 40.7030 | 0.0 | 4500 |
| 4116 | 16420 | audi | SQ5 | 2020 | Automatic | 1500 | Diesel | 145 | 34.7968 | 0.0 | 5645 |
| 4117 | 17611 | audi | SQ5 | 2019 | Automatic | 1500 | Diesel | 145 | 34.5016 | 0.0 | 4880 |
| 4851 | 16577 | bmw | Z3 | 2002 | Automatic | 16500 | Petrol | 325 | 29.7614 | 2.2 | 1499 |

**Do you notice some unique characteristics of these observations due to which they may be outliers?**

**What methods you can propose to estimate the price of these outliers more accurately, which will also result in the overall reduction in RMSE?**

## 7.2 High leverage points

High leverage points are those with an unsual value of the predictor(s). They have the potential to have a relatively higher impact on the OLS line / plane / hyperplane, as compared to the outliers.

**Leverage statistic** (page 99 of the book): In order to quantify an observation's leverage, we compute the leverage statistic. A large value of this statistic indicates an observation with high leverage. For simple linear regression,

$$h_i = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum_{i'=1}^{n}(x_{i'} - \bar{x})^2}. \tag{7.1}$$

It is clear from this equation that $h_i$ increases with the distance of $x_i$ from $\bar{x}$. A large value of $h_i$ indicates that the $i^{th}$ observation is distance from the center of all the other observations in terms of predictor values.

The leverage statistic $h_i$ is always between $1/n$ and 1, and the average leverage for all the observations is always equal to $(p+1)/n$:

$$\bar{h} = \frac{p+1}{n} \tag{7.2}$$

So if a given observation has a leverage statistic that greatly exceeds $(p+1)/n$, then we may suspect that the corresponding point has high leverage.

If the $i^{th}$ observation has a large leverage $h_i$, it may exercise substantial leverage in determining the fitted value $\hat{Y}_i$, because:

- The fitted value $\hat{Y}_i$ is a linear combination of the observed $Y$ values, and $h_i$ is the weight of observation $Y_i$ in determining this fitted value.
- The larger the $h_i$, the smaller is the variance of the residual $e_i$, and the closer the fitted value $\hat{Y}_i$ will tend to be the observed value $Y_i$.

**Thumb rules:**

- A leverage $h_i$ is usually considered large if it is more than twice as large as the mean value $\bar{h}$.
- Another suggested guideline is that $h_i$ values exceeding 0.5 indicate **very high leverage**, whereas those between 0.2 and 0.5 indicate moderate leverage.

**Influential points:** Note that if a high leverage point falls in line with the regression line, then it will not affect the regression line. However, it may inflate $R$-squared and increase the significance of predictors. If a high leverage point falls away from the regression line, then it is also an outlier, and will affect the regression line. The points whose presence significantly affects the regression line are called influential points. A point that is both a high leverage point and an outlier is likely to be an influential point. However, a high leverage point is not necessarily an influential point.

*Source for influential points: https://online.stat.psu.edu/stat501/book/export/html/973*

Let us see if there are any high leverage points in our regression `model`.

```
#Model with an interaction term and a variable transformation term
ols_object = smf.ols(formula = 'np.log(price)~(year+engineSize+mileage+mpg)**2+I(mileage**2)
model_log = ols_object.fit()
model_log.summary()
```

| | | | |
|---|---|---|---|
| **Dep. Variable:** | np.log(price) | **R-squared:** | 0.803 |
| **Model:** | OLS | **Adj. R-squared:** | 0.803 |
| **Method:** | Least Squares | **F-statistic:** | 1834. |
| **Date:** | Sun, 10 Mar 2024 | **Prob (F-statistic):** | 0.00 |
| **Time:** | 16:53:39 | **Log-Likelihood:** | -1173.8 |
| **No. Observations:** | 4960 | **AIC:** | 2372. |
| **Df Residuals:** | 4948 | **BIC:** | 2450. |
| **Df Model:** | 11 | | |
| **Covariance Type:** | nonrobust | | |

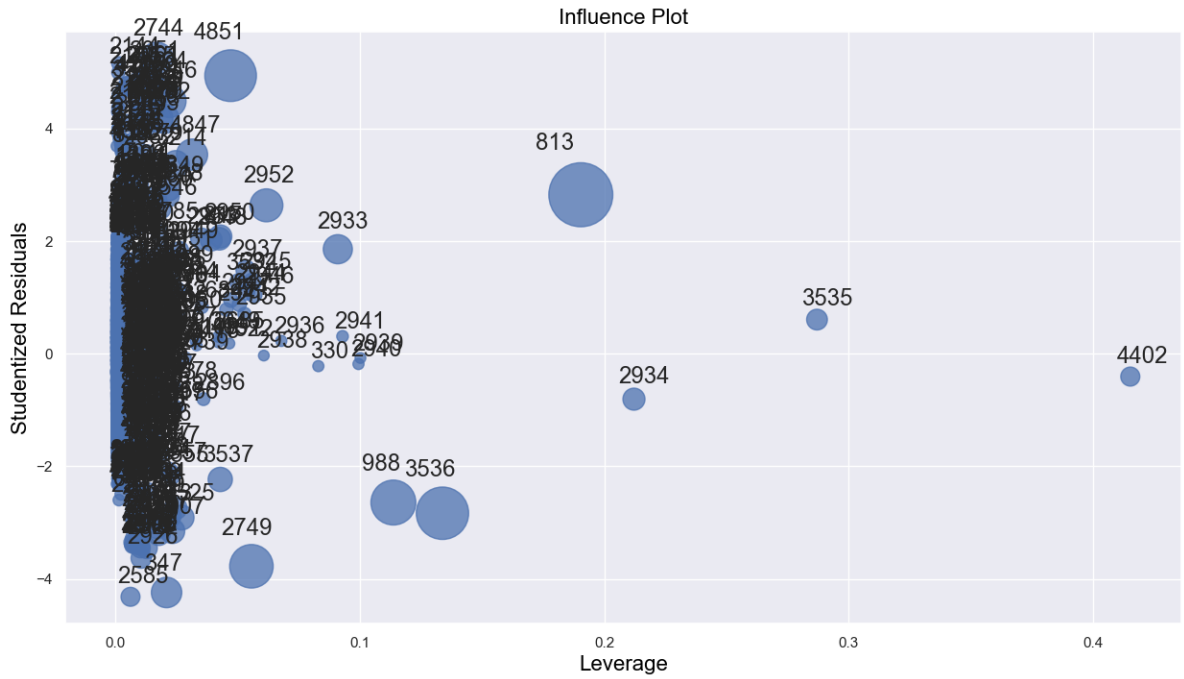
| | **coef** | **std err** | **t** | **P> \|t\|** | **[0.025** | **0.975]** |
|---|---|---|---|---|---|---|
| **Intercept** | -238.2125 | 25.790 | -9.237 | 0.000 | -288.773 | -187.652 |
| **year** | 0.1227 | 0.013 | 9.608 | 0.000 | 0.098 | 0.148 |
| **engineSize** | 13.8349 | 5.795 | 2.387 | 0.017 | 2.475 | 25.195 |
| **mileage** | 0.0005 | 0.000 | 3.837 | 0.000 | 0.000 | 0.001 |
| **mpg** | -1.2446 | 0.345 | -3.610 | 0.000 | -1.921 | -0.569 |
| **year:engineSize** | -0.0067 | 0.003 | -2.324 | 0.020 | -0.012 | -0.001 |
| **year:mileage** | -2.67e-07 | 6.8e-08 | -3.923 | 0.000 | -4e-07 | -1.34e-07 |
| **year:mpg** | 0.0006 | 0.000 | 3.591 | 0.000 | 0.000 | 0.001 |
| **engineSize:mileage** | -2.668e-07 | 4.08e-07 | -0.654 | 0.513 | -1.07e-06 | 5.33e-07 |
| **engineSize:mpg** | 0.0028 | 0.000 | 6.842 | 0.000 | 0.002 | 0.004 |
| **mileage:mpg** | 7.235e-08 | 1.79e-08 | 4.036 | 0.000 | 3.72e-08 | 1.08e-07 |
| **I(mileage ** 2)** | 1.828e-11 | 5.64e-12 | 3.240 | 0.001 | 7.22e-12 | 2.93e-11 |

| | | | |
|---|---|---|---|
| **Omnibus:** | 711.514 | **Durbin-Watson:** | 0.498 |
| **Prob(Omnibus):** | 0.000 | **Jarque-Bera (JB):** | 2545.807 |
| **Skew:** | 0.699 | **Prob(JB):** | 0.00 |
| **Kurtosis:** | 6.220 | **Cond. No.** | 1.73e+13 |

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
[2] The condition number is large, 1.73e+13. This might indicate that there are strong multicollinearity or other numerical problems.

```
#Computing the leverage statistic for each observation
influence = model_log.get_influence()
leverage = influence.hat_matrix_diag
```

```
#Visualizng leverage against studentized residuals
sns.set(rc={'figure.figsize':(15,8)})
sm.graphics.influence_plot(model_log);
```




Let us identify the high leverage points in the data, as they may be affecting the regression line if they are outliers as well, i.e., if they are influential points. Note that there is no defined threshold for a point to be classified as a high leverage point. Some statisticians consider points having twice the average leverage as high leverage points, some consider points having thrice the average leverage as high leverage points, and so on.

```
out = model_log.outlier_test()
```

```
#Average leverage of points
average_leverage = (model_log.df_model+1)/model_log.nobs
average_leverage
```

```
0.0024193548387096775
```

Let us consider points having four times the average leverage as high leverage points.

```
#We will remove all observations that have leverage higher than the threshold value.
high_leverage_threshold = 3*average_leverage
```

```
#Number of high leverage points in the dataset
np.sum(leverage>high_leverage_threshold)
```

```
269
```

### 7.2.1 Identifying extrapolation using leverage

Leverage can be used to check if prediction on a particular point will lead to extrapolation.

Below is the function that can be used to find the leverage at for a particular observation `xnew`. Note that `xnew` has to be a single-dimensional array, and `X` has to be the predictor matrix (also called the design matrix).

```
def leverage_compute(xnew, X):
    return(xnew.reshape(-1, 1).T.dot(np.linalg.inv(X.T.dot(X))).dot(xnew.reshape(-1, 1))[0][0
```

As expected, the function will return the same leverage as provided by the `hat_matrix_diag` attribute of the objected returned by the `get_influence()` method of `model_log` as shown below:

```
leverage[0]
```

```
0.0026426981240353694
```

As the observation for prediction is required we need to create the predictor matrix `X` to create all the observations with the interactions specified in the model.

```
y, X = dmatrices('np.log(price)~(year+engineSize+mileage+mpg)**2+I(mileage**2)', data = trai
```

```
leverage_compute(X[0,:], X)
```

```
0.0026426973869101977
```

If the leverage for a new observation is higher than the maximum leverage among all the observations in the training dataset, then prediction at the new observation will be extrapolation.

## 7.3 Influential points

Observations that are both high leverage points and outliers are influential points that may affect the regression line. Let's remove these influential points from the data and see if it improves the model prediction accuracy on test data.

```
#Dropping influential points from data
train_filtered = train.drop(np.intersect1d(np.where(np.abs(out.student_resid) > critical_valu
                                           (np.where(leverage>high_leverage_threshold)[0])))
```

Note that as the Bonferroni's critical value is very conservative estimate, we have rounded off the critical value to 4, instead of 4.42.

```
train_filtered.shape
```

```
(4948, 11)
```

```
#Number of points removed as they were influential
train.shape[0]-train_filtered.shape[0]
```

```
12
```

We removed 12 influential data points from the training data.

```
#Model after removing the influential observations
ols_object = smf.ols(formula = 'np.log(price)~(year+engineSize+mileage+mpg)**2+I(mileage**2)
model_log = ols_object.fit()
model_log.summary()
```

| | | | |
|---|---|---|---|
| **Dep. Variable:** | np.log(price) | **R-squared:** | 0.815 |
| **Model:** | OLS | **Adj. R-squared:** | 0.814 |
| **Method:** | Least Squares | **F-statistic:** | 1971. |
| **Date:** | Sun, 10 Mar 2024 | **Prob (F-statistic):** | 0.00 |
| **Time:** | 16:54:08 | **Log-Likelihood:** | -1027.9 |
| **No. Observations:** | 4948 | **AIC:** | 2080. |
| **Df Residuals:** | 4936 | **BIC:** | 2158. |
| **Df Model:** | 11 | | |
| **Covariance Type:** | nonrobust | | |

| | **coef** | **std err** | **t** | **P> \|t\|** | **[0.025** | **0.975]** |
|---|---|---|---|---|---|---|
| **Intercept** | -256.2339 | 25.421 | -10.080 | 0.000 | -306.070 | -206.398 |
| **year** | 0.1317 | 0.013 | 10.462 | 0.000 | 0.107 | 0.156 |
| **engineSize** | 18.4650 | 5.663 | 3.261 | 0.001 | 7.364 | 29.566 |
| **mileage** | 0.0006 | 0.000 | 4.288 | 0.000 | 0.000 | 0.001 |
| **mpg** | -1.1810 | 0.338 | -3.489 | 0.000 | -1.845 | -0.517 |
| **year:engineSize** | -0.0090 | 0.003 | -3.208 | 0.001 | -0.015 | -0.004 |
| **year:mileage** | -2.933e-07 | 6.7e-08 | -4.374 | 0.000 | -4.25e-07 | -1.62e-07 |
| **year:mpg** | 0.0006 | 0.000 | 3.458 | 0.001 | 0.000 | 0.001 |
| **engineSize:mileage** | -4.316e-07 | 4e-07 | -1.080 | 0.280 | -1.21e-06 | 3.52e-07 |
| **engineSize:mpg** | 0.0048 | 0.000 | 11.537 | 0.000 | 0.004 | 0.006 |
| **mileage:mpg** | 7.254e-08 | 1.75e-08 | 4.140 | 0.000 | 3.82e-08 | 1.07e-07 |
| **I(mileage ** 2)** | 1.668e-11 | 5.53e-12 | 3.017 | 0.003 | 5.84e-12 | 2.75e-11 |

| | | | |
|---|---|---|---|
| **Omnibus:** | 718.619 | **Durbin-Watson:** | 0.521 |
| **Prob(Omnibus):** | 0.000 | **Jarque-Bera (JB):** | 2512.509 |
| **Skew:** | 0.714 | **Prob(JB):** | 0.00 |
| **Kurtosis:** | 6.185 | **Cond. No.** | 1.75e+13 |

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
[2] The condition number is large, 1.75e+13. This might indicate that there are strong multicollinearity or other numerical problems.

Let us compare the square root of 5-fold cross-validated mean squared error of the model with and without the influential points.

```
y, X = dmatrices('np.log(price)~(year+engineSize+mileage+mpg)**2+I(mileage**2)', data = trai
np.sqrt(mean_squared_error(np.exp(cross_val_predict(LinearRegression(), X, y)), np.exp(y)))
```

```
9811.74078331643
```

```
y, X = dmatrices('np.log(price)~(year+engineSize+mileage+mpg)**2+I(mileage**2)', data = trai
np.sqrt(mean_squared_error(np.exp(cross_val_predict(LinearRegression(), X, y)), np.exp(y)))
```

```
9800.202063309154
```

**Why can't we use `cross_val_score()` instead of `cross_val_predict()` here?**

There seems to be a slight improvement in prediction error after removing influential points. Note that none of the points had "very high leverage", and thus the change is not substantial.

Note that we obtain a higher R-squared value of 81.5% as compared to 80% with the complete data. Removing the influential points helped obtain a slightly better model fit. However, that may also happen just by reducing observations.

```
#Computing RMSE on test data
pred_price_log = model_log.predict(testf)
np.sqrt(((testp.price - np.exp(pred_price_log))**2).mean())
```

```
8922.977452912108
```

The RMSE on test data has also reduced. This shows that some of the influential points were impacting the regression line. With those points removed, the model better captures the general trend in the data.

### 7.3.1 Influence on single fitted value (DFFITS)

- A useful measure of the influence that the $i^{th}$ observation has on the fitted value $\hat{Y}_i$ is:

$$(DFFITS)_i = \frac{\hat{Y}_i - \hat{Y}_{i(i)}}{\sqrt{MSE_i h_i}} \tag{7.3}$$

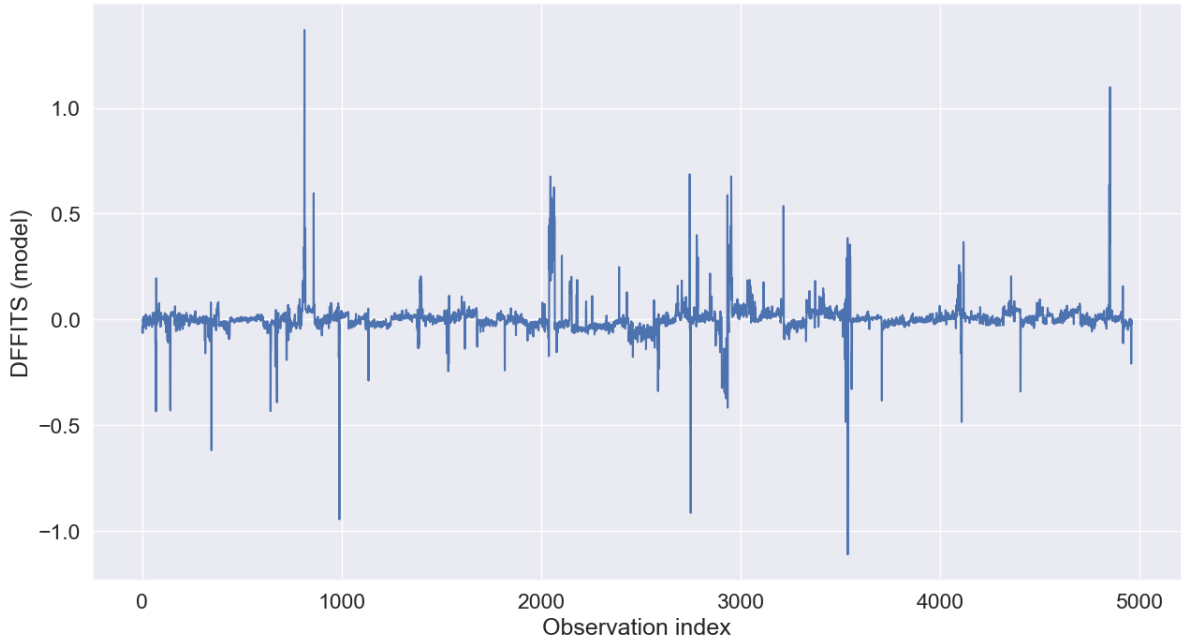
- Note that the denominator in the above fraction is the estimated standard deviation of $\hat{Y}_i$, but uses the error mean square when the $i^{th}$ observation is omitted.
- $DFFITS$ for the $i^{th}$ observation represents the number of estimated standard deviations of $\hat{Y}_i$ that the fitted value $\hat{Y}_i$ increases or decreases with the inclusion of the $i^{th}$ observation in fitting the regression model.
- It can be shown that:

$$(DFFITS)_i = t_i \sqrt{\frac{h_i}{1-h_i}} \tag{7.4}$$

where $t_i$ is the studentized deleted residual for the $i^{th}$ observation.

- We can see that if an observation has high leverage and is an outlier, it is likely to be influential
- For large datasets, an observation is considered influential if the magnitude of $DFFITS$ for it exceeds $2\sqrt{\frac{p}{n}}$

```
sns.set(font_scale =1.5)
sns.lineplot(x = range(train.shape[0]), y = influence.dffits[0])
plt.xlabel('Observation index')
plt.ylabel('DFFITS (model)');
```




**Let us analyze the point with the highest $DFFITS$.**

```
np.where(influence.dffits[0]>1)
```

```
(array([ 813, 4851], dtype=int64),)
```

```
train.loc[813,:]
```

```
carID                12454
brand                   vw
model            Caravelle
year                  2012
transmission     Semi-Auto
mileage             212000
fuelType            Diesel
tax                    325
mpg                34.4424
engineSize             2.0
price                11995
Name: 813, dtype: object
```

```
train.loc[train.model == ' Caravelle','mileage'].describe()
```

```
count        65.000000
mean      25638.692308
std       42954.135726
min          10.000000
25%        3252.000000
50%        6900.000000
75%       30414.000000
max      212000.000000
Name: mileage, dtype: float64
```

```
# Prediction with model developed based on all points
ols_object = smf.ols(formula = 'np.log(price)~(year+engineSize+mileage+mpg)**2+I(mileage**2)
                     data = train)
model_log = ols_object.fit();
np.exp(model_log.predict(train.loc[[813],:]))
```

```
813    5502.647323
dtype: float64
```

```
# Prediction with model developed based on all points except the 813th point
ols_object = smf.ols(formula = 'np.log(price)~(year+engineSize+mileage+mpg)**2+I(mileage**2)
                     data = train.drop(index = 813))
model_log = ols_object.fit();
np.exp(model_log.predict(train.loc[[813],:]))
```

```
813    4581.374593
dtype: float64
```

Let us see the leverage and studentized residual for this observation.

```
# Leverage
leverage[813]
```

```
0.19038697461006687
```

```
# Studentized residual
out.student_resid[813]
```

```
2.823478041409651
```

**Do you notice what may be contributing to the high influence of this point?**

### 7.3.2 Influence on all fitted values (Cook's distance)

In contrast to $DFFITS$, which considers the influence of the $i^{th}$ observation on the fitted value $\hat{Y}_i$, Cook's distance considers the influence of the $i^{th}$ observation on all $n$ the fitted values:

$$D_i = \frac{\sum_{j=1}^{n}(\hat{Y}_j - \hat{Y}_{j(i)})^2}{pMSE} \tag{7.5}$$

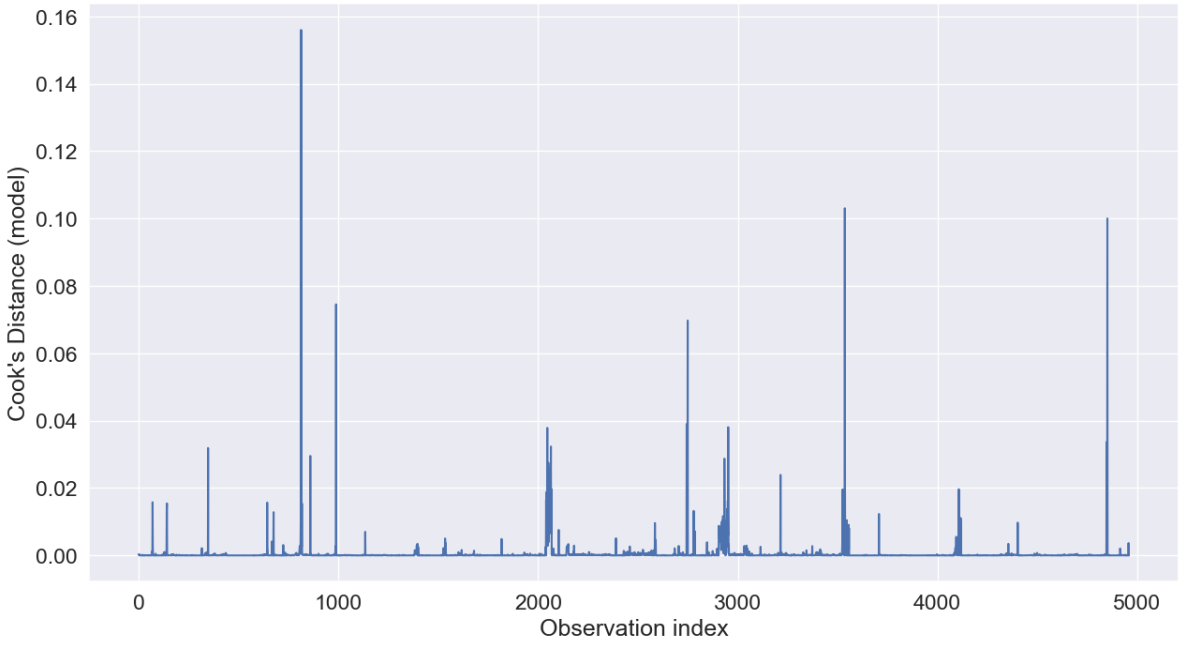
It can be shown that:

$$D_i = \frac{e_i^2}{pMSE}\left[\frac{h_i}{(1-h_i)^2}\right] \tag{7.6}$$

The larger $h_i$ or $e_i$, the larger is $D_i$. $D_i$ can be related to the $F(p, n-p)$ distribution. If the percentile value is 50% or more, the observation is considered as highly influential.

Cook's distance is considered high if it is greater than 0.5 and extreme if it is greater than 1.

```
sns.set(font_scale =1.5)
sns.lineplot(x = range(train.shape[0]), y = influence.cooks_distance[0])
plt.xlabel('Observation index')
plt.ylabel("Cook's Distance (model)");
```




```
# Point with the highest Cook's distance
np.where(influence.cooks_distance[0]>0.15)
```

```
(array([813], dtype=int64),)
```

The critical Cook's distance value for a point to be highly influential in this dataset is:

```
stats.f.ppf(0.5, 11, 4949)
```

```
0.9402181103263811
```

Thus, we don't have any highly influential points in the dataset.

### 7.3.3 Influence on regression coefficients (DFBETAS)

- $DFBETAS$ measures the influence of the $i^{th}$ observation on the regression coefficient.
- $DFBETAS$ of the $i^{th}$ observation on the $k^{th}$ regression coefficient is:

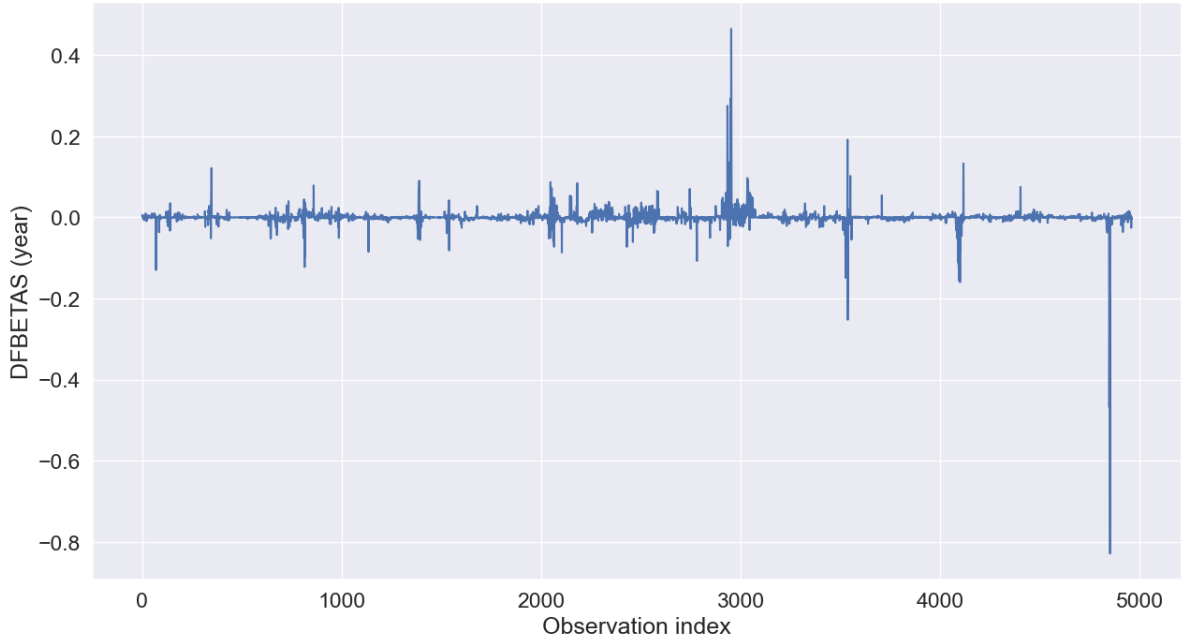
$$(DFBETAS)_{k(i)} = \frac{\hat{\beta}_k - \hat{\beta}_{k(i)}}{\sqrt{MSE_i c_k}} \tag{7.7}$$

where $c_k$ is the $k^{th}$ diagonal element of $(X^T X)^{-1}$.

For large datasets, an observation is considered influential if $DFBETAS$ exceeds $\frac{2}{\sqrt{n}}$.

Below is the plot of $DFBETAS$ for the `year` predictor against the observation index.

```
sns.set(font_scale =1.5)
sns.lineplot(x = range(train.shape[0]), y = influence.dfbetas[:,1])
plt.xlabel('Observation index')
plt.ylabel("DFBETAS (year)");
```




Let us analyze the point with the highest magnitude of $DFBETAS$.

```
np.where(influence.dfbetas[:,1]<-0.8)
```

```
(array([4851], dtype=int64),)
```

```
train.year.describe()
```

```
count    4960.000000
mean     2016.737903
std         2.884035
min      1997.000000
25%      2016.000000
50%      2017.000000
75%      2019.000000
max      2020.000000
Name: year, dtype: float64
```

```
train.loc[train.year<=2002,:]
```

| | carID | brand | model | year | transmission | mileage | fuelType | tax | mpg | engineSize | pri |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 330 | 13200 | audi | A8 | 1997 | Automatic | 122000 | Petrol | 265 | 19.3511 | 4.2 | 465 |
| 732 | 13988 | vw | Beetle | 2001 | Manual | 47729 | Petrol | 330 | 32.5910 | 2.0 | 249 |
| 3157 | 18794 | ford | Puma | 2002 | Manual | 108000 | Petrol | 230 | 38.5757 | 1.7 | 219 |
| 3525 | 19395 | merc | S Class | 2001 | Automatic | 108800 | Diesel | 325 | 31.5473 | 3.2 | 169 |
| 3532 | 17531 | merc | S Class | 1999 | Automatic | 34000 | Petrol | 145 | 24.8735 | 3.2 | 599 |
| 3533 | 18761 | merc | S Class | 2001 | Automatic | 66000 | Petrol | 570 | 24.7744 | 3.2 | 449 |
| 3535 | 18813 | merc | S Class | 1998 | Automatic | 43534 | Petrol | 265 | 23.2962 | 6.0 | 199 |
| 3536 | 17891 | merc | S Class | 2002 | Automatic | 24000 | Petrol | 570 | 20.7968 | 5.0 | 699 |
| 3707 | 18746 | hyundi | Santa Fe | 2002 | Manual | 94000 | Petrol | 325 | 30.2671 | 2.4 | 120 |
| 4091 | 12995 | merc | SLK | 1998 | Automatic | 113557 | Petrol | 265 | 31.8368 | 2.3 | 199 |
| 4094 | 19585 | merc | SLK | 2001 | Automatic | 69234 | Petrol | 325 | 30.8839 | 2.0 | 399 |
| 4096 | 14265 | merc | SLK | 2001 | Automatic | 48172 | Petrol | 325 | 29.7058 | 2.3 | 399 |
| 4097 | 15821 | merc | SLK | 2002 | Automatic | 61400 | Petrol | 325 | 29.6568 | 2.3 | 399 |
| 4098 | 13021 | merc | SLK | 2001 | Automatic | 91000 | Petrol | 325 | 30.3248 | 2.3 | 395 |
| 4099 | 12660 | merc | SLK | 2001 | Automatic | 42087 | Petrol | 325 | 29.9404 | 2.3 | 449 |
| 4101 | 17521 | merc | SLK | 2002 | Automatic | 75034 | Petrol | 325 | 30.1380 | 2.3 | 499 |
| 4107 | 13977 | merc | SLK | 2000 | Automatic | 87000 | Petrol | 265 | 27.2998 | 3.2 | 149 |
| 4108 | 18679 | merc | SLK | 2000 | Automatic | 113237 | Petrol | 270 | 26.8765 | 3.2 | 399 |
| 4109 | 14598 | merc | SLK | 2001 | Automatic | 64476 | Petrol | 325 | 27.4628 | 3.2 | 499 |
| 4847 | 17268 | bmw | Z3 | 1997 | Manual | 49000 | Petrol | 270 | 34.9548 | 1.9 | 395 |
| 4848 | 12137 | bmw | Z3 | 1999 | Manual | 58000 | Petrol | 270 | 35.3077 | 1.9 | 395 |
| 4849 | 13288 | bmw | Z3 | 1999 | Manual | 74282 | Petrol | 245 | 35.4143 | 1.9 | 399 |
| 4850 | 19172 | bmw | Z3 | 2001 | Manual | 60000 | Petrol | 325 | 30.7305 | 2.2 | 595 |
| 4851 | 16577 | bmw | Z3 | 2002 | Automatic | 16500 | Petrol | 325 | 29.7614 | 2.2 | 149 |

Let us see the leverage and studentized residual for this observation.

```
# Leverage
leverage[4851]
```

```
0.047120455781282225
```

```
# Studentized residual
out.student_resid[4851]
```

```
4.938606329343604
```

**Do you see what makes this point influential?**

## 7.4 Collinearity

Collinearity refers to the situation when two or more predictor variables have a high linear association. Linear association between a pair of variables can be measured by the correlation coefficient. Thus the correlation matrix can indicate some potential collinearity problems.

### 7.4.1 Why and how is collinearity a problem

*(Source: page 100-101 of book)*

The presence of collinearity can pose problems in the regression context, since it can be difficult to separate out the individual effects of collinear variables on the response.

Since collinearity reduces the accuracy of the estimates of the regression coefficients, it causes the standard error for $\widehat{\beta}_j$ to grow. Recall that the t-statistic for each predictor is calculated by dividing $\widehat{\beta}_j$ by its standard error. Consequently, collinearity results in a decline in the $t$-statistic. As a result, **in the presence of collinearity, we may fail to reject $H_0 : \beta_j = 0$. This means that the power of the hypothesis test—the probability of correctly detecting a non-zero coefficient—is reduced by collinearity.**

### 7.4.2 How to measure collinearity/multicollinearity

*(Source: page 102 of book)*

Unfortunately, not all collinearity problems can be detected by inspection of the correlation matrix: it is possible for collinearity to exist between three or more variables even if no pair of variables has a particularly high correlation. We call this situation multicollinearity. Instead of inspecting the correlation matrix, a better way to assess multicollinearity is to compute the variance inflation factor (VIF). The VIF is variance inflation factor the ratio of the variance of $\hat{\beta}_j$ when fitting the full model divided by the variance of $\hat{\beta}_j$ if fit on its own. The smallest possible value for VIF is 1, which indicates the complete absence of collinearity. Typically in practice there is a small amount of collinearity among the predictors. As a rule of thumb, a **VIF value that exceeds 5 or 10 indicates a problematic amount of collinearity.**

The estimated variance of the coefficient $\beta_j$, of the $j^{th}$ predictor $X_j$, can be expressed as:

$$\hat{var}(\hat{\beta}_j) = \frac{(\hat{\sigma})^2}{(n-1)\hat{var}(X_j)} \cdot \frac{1}{1 - R^2_{X_j|X_{-j}}},$$

where $R^2_{X_j|X_{-j}}$ is the $R$-squared for the regression of $X_j$ on the other covariates (a regression that does not involve the response variable $Y$).

In case of simple linear regression, the variance expression in the equation above does not contain the term $\frac{1}{1-R^2_{X_j|X_{-j}}}$, as there is only one predictor. However, in case of multiple linear regression, the variance of the estimate of the $j^{th}$ coefficient ($\hat{\beta}_j$) gets inflated by a factor of $\frac{1}{1-R^2_{X_j|X_{-j}}}$ *(Note that in the complete absence of collinearity,* $R^2_{X_j|X_{-j}} = 0$*, and the value of this factor will be 1).*

Thus, the Variance inflation factor, or the VIF for the estimated coefficient of the $j^{th}$ predictor $X_j$ is:

$$VIF(\hat{\beta}_j) = \frac{1}{1 - R^2_{X_j|X_{-j}}} \tag{7.8}$$

```
#Correlation matrix
train.corr()
```

| | carID | year | mileage | tax | mpg | engineSize | price |
|---|---|---|---|---|---|---|---|
| carID | 1.000000 | 0.006251 | -0.001320 | 0.023806 | -0.010774 | 0.011365 | 0.012129 |
| year | 0.006251 | 1.000000 | -0.768058 | -0.205902 | -0.057093 | 0.014623 | 0.501296 |
| mileage | -0.001320 | -0.768058 | 1.000000 | 0.133744 | 0.125376 | -0.006459 | -0.478705 |

| | carID | year | mileage | tax | mpg | engineSize | price |
|---|---|---|---|---|---|---|---|
| tax | 0.023806 | -0.205902 | 0.133744 | 1.000000 | -0.488002 | 0.465282 | 0.144652 |
| mpg | -0.010774 | -0.057093 | 0.125376 | -0.488002 | 1.000000 | -0.419417 | -0.369919 |
| engineSize | 0.011365 | 0.014623 | -0.006459 | 0.465282 | -0.419417 | 1.000000 | 0.624899 |
| price | 0.012129 | 0.501296 | -0.478705 | 0.144652 | -0.369919 | 0.624899 | 1.000000 |

Let us compute the Variance Inflation Factor (VIF) for the four predictors.

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

```
X.columns[1:]
```

```
Index(['year', 'mileage', 'engineSize'], dtype='object')
```

```
from statsmodels.stats.outliers_influence import variance_inflation_factor
from statsmodels.tools.tools import add_constant
X = add_constant(X)
vif_data = pd.DataFrame()
vif_data["feature"] = X.columns

for i in range(len(X.columns)):
    vif_data.loc[i,'VIF'] = variance_inflation_factor(X.values, i)

print(vif_data)
```

```
      feature           VIF
0       const  1.201579e+06
1         mpg  1.243040e+00
2        year  2.452891e+00
3     mileage  2.490210e+00
4  engineSize  1.219170e+00
```

As all the values of VIF are close to one, we do not have the problem of multicollinearity in the model. Note that the VIF of `year` and `mileage` is relatively high as they are the most correlated.

**Q1:** Why is the VIF of the constant so high?

**Q2:** Why do we need to include the constant while finding the VIF?

### 7.4.3 Manual computation of VIF

```
#Manually computing the VIF for year
ols_object = smf.ols(formula = 'price~mpg', data = train)
model_log = ols_object.fit()
model_log.summary()
```

| | | | |
|---|---|---|---|
| **Dep. Variable:** | price | **R-squared:** | 0.137 |
| **Model:** | OLS | **Adj. R-squared:** | 0.137 |
| **Method:** | Least Squares | **F-statistic:** | 786.0 |
| **Date:** | Wed, 06 Mar 2024 | **Prob (F-statistic):** | 1.14e-160 |
| **Time:** | 17:04:39 | **Log-Likelihood:** | -54812. |
| **No. Observations:** | 4960 | **AIC:** | 1.096e+05 |
| **Df Residuals:** | 4958 | **BIC:** | 1.096e+05 |
| **Df Model:** | 1 | | |
| **Covariance Type:** | nonrobust | | |

| | **coef** | **std err** | **t** | **P> \|t\|** | **[0.025** | **0.975]** |
|---|---|---|---|---|---|---|
| **Intercept** | 4.144e+04 | 676.445 | 61.258 | 0.000 | 4.01e+04 | 4.28e+04 |
| **mpg** | -374.2975 | 13.351 | -28.036 | 0.000 | -400.471 | -348.124 |

| | | | |
|---|---|---|---|
| **Omnibus:** | 2132.208 | **Durbin-Watson:** | 0.320 |
| **Prob(Omnibus):** | 0.000 | **Jarque-Bera (JB):** | 13751.995 |
| **Skew:** | 1.942 | **Prob(JB):** | 0.00 |
| **Kurtosis:** | 10.174 | **Cond. No.** | 158. |

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.

```
(13.351/9.338)**2
```

```
2.044183378279958
```

```
#Manually computing the VIF for year
ols_object = smf.ols(formula = 'price~year+mpg+engineSize+mileage', data = train)
model_log = ols_object.fit()
model_log.summary()
```

| | | | |
|---|---|---|---|
| **Dep. Variable:** | price | **R-squared:** | 0.660 |
| **Model:** | OLS | **Adj. R-squared:** | 0.660 |
| **Method:** | Least Squares | **F-statistic:** | 2410. |
| **Date:** | Wed, 06 Mar 2024 | **Prob (F-statistic):** | 0.00 |
| **Time:** | 17:01:18 | **Log-Likelihood:** | -52497. |
| **No. Observations:** | 4960 | **AIC:** | 1.050e+05 |
| **Df Residuals:** | 4955 | **BIC:** | 1.050e+05 |
| **Df Model:** | 4 | | |
| **Covariance Type:** | nonrobust | | |

| | **coef** | **std err** | **t** | **P> \|t\|** | **[0.025** | **0.975]** |
|---|---|---|---|---|---|---|
| **Intercept** | -3.661e+06 | 1.49e+05 | -24.593 | 0.000 | -3.95e+06 | -3.37e+06 |
| **year** | 1817.7366 | 73.751 | 24.647 | 0.000 | 1673.151 | 1962.322 |
| **mpg** | -79.3126 | 9.338 | -8.493 | 0.000 | -97.620 | -61.006 |
| **engineSize** | 1.218e+04 | 189.969 | 64.107 | 0.000 | 1.18e+04 | 1.26e+04 |
| **mileage** | -0.1474 | 0.009 | -16.817 | 0.000 | -0.165 | -0.130 |

| | | | |
|---|---|---|---|
| **Omnibus:** | 2450.973 | **Durbin-Watson:** | 0.541 |
| **Prob(Omnibus):** | 0.000 | **Jarque-Bera (JB):** | 31060.548 |
| **Skew:** | 2.045 | **Prob(JB):** | 0.00 |
| **Kurtosis:** | 14.557 | **Cond. No.** | 3.83e+07 |

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
[2] The condition number is large, 3.83e+07. This might indicate that there are strong multicollinearity or other numerical problems.

```
#Manually computing the VIF for year
ols_object = smf.ols(formula = 'year~mpg+engineSize+mileage', data = train)
model_log = ols_object.fit()
model_log.summary()
```

| | | | |
|---|---|---|---|
| **Dep. Variable:** | year | **R-squared:** | 0.592 |
| **Model:** | OLS | **Adj. R-squared:** | 0.592 |
| **Method:** | Least Squares | **F-statistic:** | 2400. |
| **Date:** | Wed, 06 Mar 2024 | **Prob (F-statistic):** | 0.00 |
| **Time:** | 17:00:13 | **Log-Likelihood:** | -10066. |
| **No. Observations:** | 4960 | **AIC:** | 2.014e+04 |
| **Df Residuals:** | 4956 | **BIC:** | 2.017e+04 |
| **Df Model:** | 3 | | |
| **Covariance Type:** | nonrobust | | |

| | coef | std err | t | P> \|t\| | [0.025 | 0.975] |
|---|---|---|---|---|---|---|
| **Intercept** | 2018.3135 | 0.140 | 1.44e+04 | 0.000 | 2018.039 | 2018.588 |
| **mpg** | 0.0095 | 0.002 | 5.301 | 0.000 | 0.006 | 0.013 |
| **engineSize** | 0.1171 | 0.037 | 3.203 | 0.001 | 0.045 | 0.189 |
| **mileage** | -9.139e-05 | 1.08e-06 | -84.615 | 0.000 | -9.35e-05 | -8.93e-05 |

| | | | |
|---|---|---|---|
| **Omnibus:** | 2949.664 | **Durbin-Watson:** | 1.161 |
| **Prob(Omnibus):** | 0.000 | **Jarque-Bera (JB):** | 63773.271 |
| **Skew:** | -2.426 | **Prob(JB):** | 0.00 |
| **Kurtosis:** | 19.883 | **Cond. No.** | 1.91e+05 |

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
[2] The condition number is large, 1.91e+05. This might indicate that there are strong multicollinearity or other numerical problems.

```
#VIF for year
1/(1-0.592)
```

```
2.4509803921568625
```

Note that year and mileage have a high linear correlation. Removing one of them should decrease the standard error of the coefficient of the other, without significanty decrease R-squared.

```
ols_object = smf.ols(formula = 'price~mpg+engineSize+mileage+year', data = train)
model_log = ols_object.fit()
model_log.summary()
```

Table 7.6: OLS Regression Results

| | | | |
|---|---|---|---|
| Dep. Variable: | price | R-squared: | 0.660 |
| Model: | OLS | Adj. R-squared: | 0.660 |
| Method: | Least Squares | F-statistic: | 2410. |
| Date: | Tue, 07 Feb 2023 | Prob (F-statistic): | 0.00 |
| Time: | 21:39:45 | Log-Likelihood: | -52497. |
| No. Observations: | 4960 | AIC: | 1.050e+05 |
| Df Residuals: | 4955 | BIC: | 1.050e+05 |
| Df Model: | 4 | | |
| Covariance Type: | nonrobust | | |

| | coef | std err | t | P>\|t\| | [0.025 | 0.975] |
|---|---|---|---|---|---|---|
| Intercept | -3.661e+06 | 1.49e+05 | -24.593 | 0.000 | -3.95e+06 | -3.37e+06 |
| mpg | -79.3126 | 9.338 | -8.493 | 0.000 | -97.620 | -61.006 |
| engineSize | 1.218e+04 | 189.969 | 64.107 | 0.000 | 1.18e+04 | 1.26e+04 |
| mileage | -0.1474 | 0.009 | -16.817 | 0.000 | -0.165 | -0.130 |
| year | 1817.7366 | 73.751 | 24.647 | 0.000 | 1673.151 | 1962.322 |

| | | | |
|---|---|---|---|
| Omnibus: | 2450.973 | Durbin-Watson: | 0.541 |
| Prob(Omnibus): | 0.000 | Jarque-Bera (JB): | 31060.548 |
| Skew: | 2.045 | Prob(JB): | 0.00 |
| Kurtosis: | 14.557 | Cond. No. | 3.83e+07 |

Removing mileage from the above regression.

```
ols_object = smf.ols(formula = 'price~mpg+engineSize+year', data = train)
model_log = ols_object.fit()
model_log.summary()
```

Table 7.9: OLS Regression Results

| | | | |
|---|---|---|---|
| Dep. Variable: | price | R-squared: | 0.641 |
| Model: | OLS | Adj. R-squared: | 0.641 |
| Method: | Least Squares | F-statistic: | 2951. |
| Date: | Tue, 07 Feb 2023 | Prob (F-statistic): | 0.00 |
| Time: | 21:40:00 | Log-Likelihood: | -52635. |
| No. Observations: | 4960 | AIC: | 1.053e+05 |
| Df Residuals: | 4956 | BIC: | 1.053e+05 |
| Df Model: | 3 | | |
| Covariance Type: | nonrobust | | |

| | coef | std err | t | P>\|t\| | [0.025 | 0.975] |
|---|---|---|---|---|---|---|
| Intercept | -5.586e+06 | 9.78e+04 | -57.098 | 0.000 | -5.78e+06 | -5.39e+06 |
| mpg | -101.9120 | 9.500 | -10.727 | 0.000 | -120.536 | -83.288 |
| engineSize | 1.196e+04 | 194.848 | 61.392 | 0.000 | 1.16e+04 | 1.23e+04 |
| year | 2771.1844 | 48.492 | 57.147 | 0.000 | 2676.118 | 2866.251 |

| | | | |
|---|---|---|---|
| Omnibus: | 2389.075 | Durbin-Watson: | 0.528 |
| Prob(Omnibus): | 0.000 | Jarque-Bera (JB): | 26920.051 |
| Skew: | 2.018 | Prob(JB): | 0.00 |
| Kurtosis: | 13.675 | Cond. No. | 1.41e+06 |

Note that the standard error of the coefficient of *year* has reduced from 73 to 48, without any large reduction in R-squared.

### 7.4.4 When can we overlook multicollinearity?

- The severity of the problems increases with the degree of the multicollinearity. Therefore, if there is only moderate multicollinearity *(5 < VIF < 10)*, we may overlook it.
- Multicollinearity affects only the standard errors of the coefficients of collinear predictors. Therefore, if multicollinearity is not present for the predictors that we are particularly interested in, we may not need to resolve it.
- Multicollinearity affects the standard error of the coefficients and thereby their $p$-values, but in general, it does not influence the prediction accuracy, except in the case that the coefficients are so unstable that the predictions are outside of the domain space of the response. If our sole aim is prediction, and we don't wish to infer the statistical significance of predictors, then we may avoid addressing multicollinearity. "*The fact that some or all predictor variables are correlated among themselves does not, in general, inhibit our ability to obtain a good fit nor does it tend to affect inferences about mean responses or predictions of new observations, provided these inferences are made within the region of observations" - Neter, John, Michael H. Kutner, Christopher J. Nachtsheim, and William Wasserman. "Applied linear statistical models." (1996): 318.*