Data Science II with python (Class notes)

STAT 303-2

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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!

Part I

Linear regression

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: $\widehat{price}$ = -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.

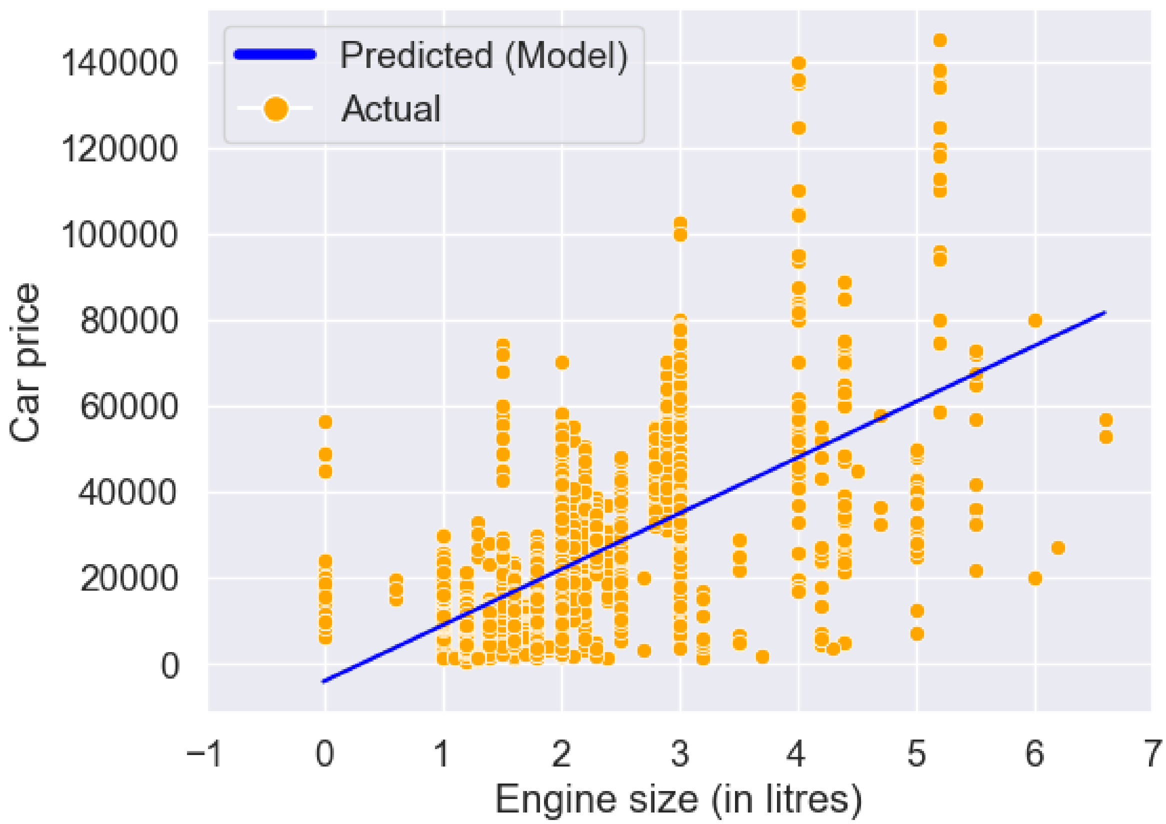
The coefficients can also be returned directly usign the `params` attribute of the `model` object returned by the `fit()` method of the `ols` class:

```
model.params
```

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

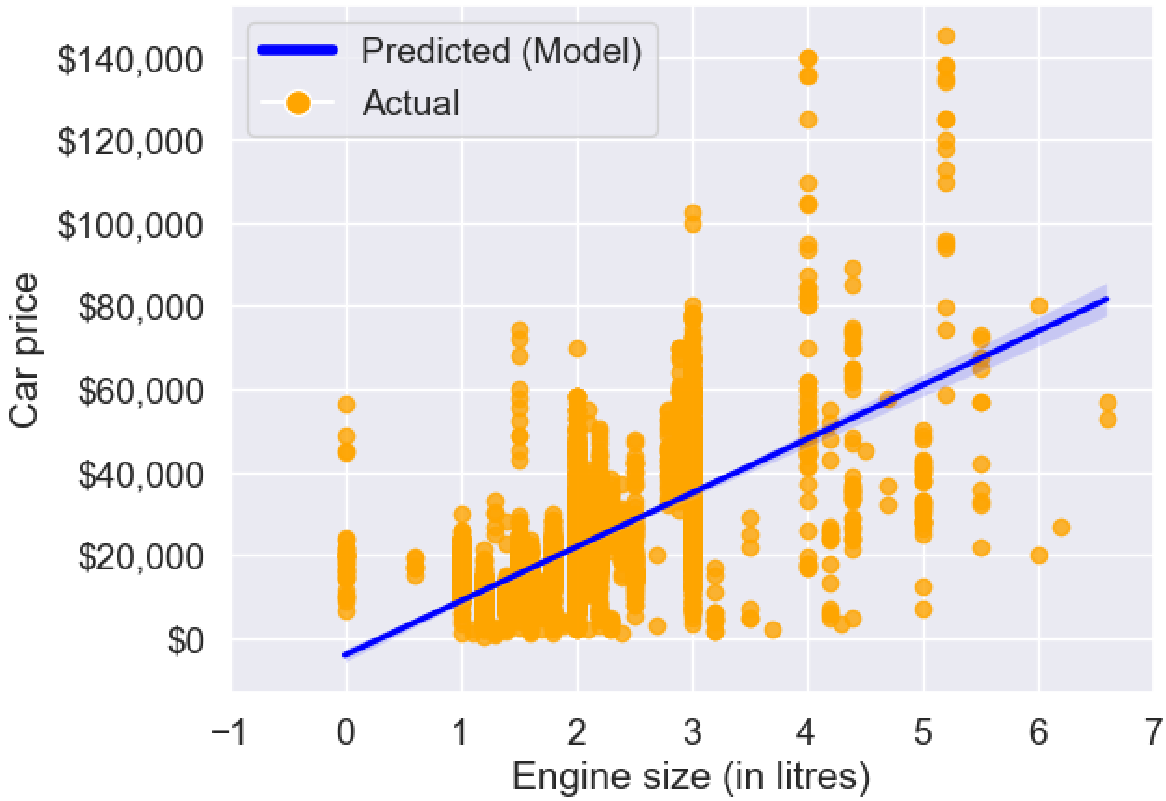
Visualize the regression line

```
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={"col
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 imp
```



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.

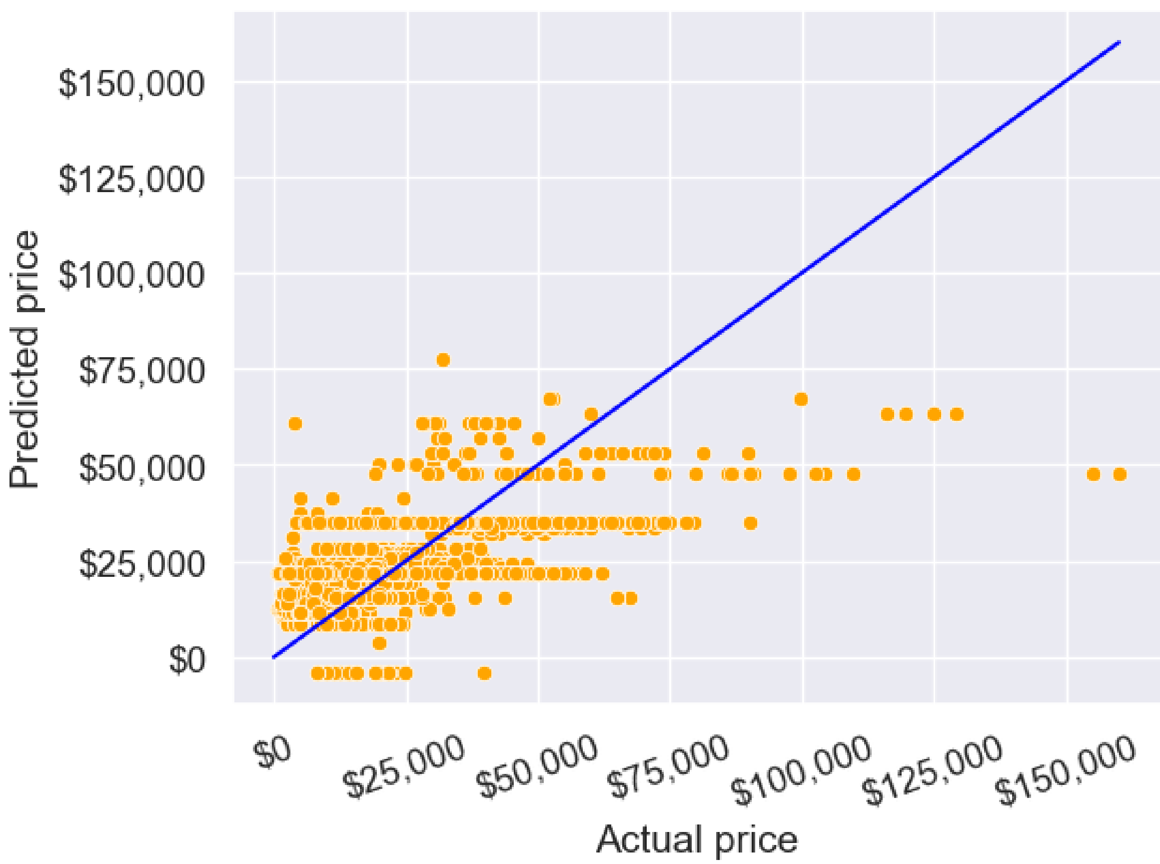
```
# Read the test data
testf = pd.read_csv('./Datasets/Car_features_test.csv') # Predictors
```

```
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 'engin
```

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 confiden
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

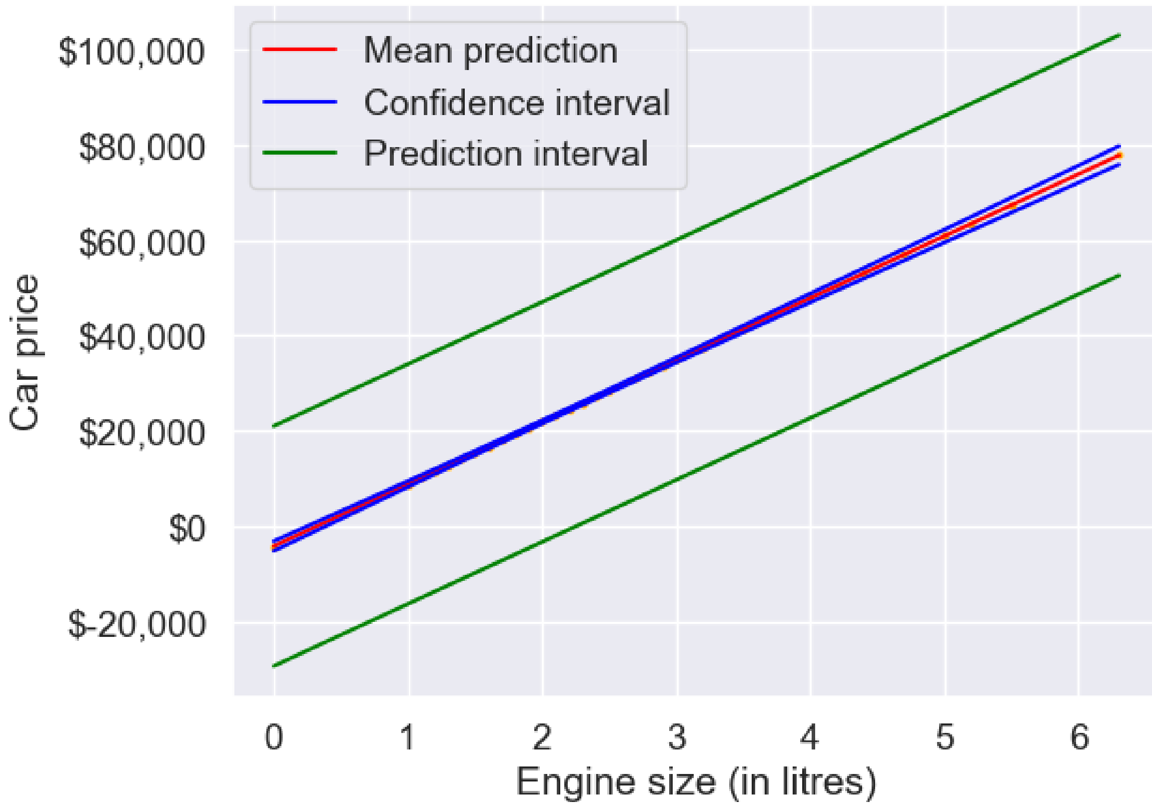
	mean	mean_se	mean_ci_lower	mean_ci_upper	obs_ci_lower	obs_ci_upper
2668	34842.807319	271.666459	34310.220826	35375.393812	9723.677232	59961.937406
2669	8866.245277	316.580850	8245.606701	9486.883853	-16254.905974	33987.396528
2670	21854.526298	184.135754	21493.538727	22215.513869	-3261.551421	46970.604017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

```python
# 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.

```python
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
```

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
4	18492	bmw	6 Series	2015	Automatic	62953	Diesel	160	51.4903	3.0	18990

```
#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()
```

Table 2.2: 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, 27 Dec 2022	Prob (F-statistic):	0.00
Time:	01:07:25	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

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

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

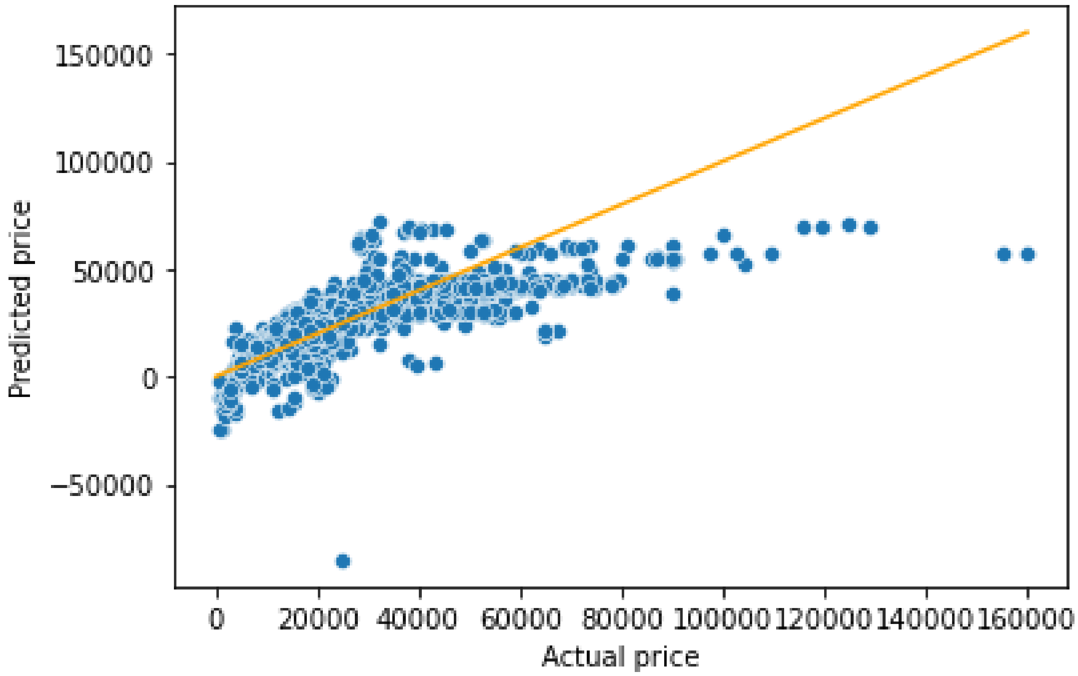
```
testf = pd.read_csv('./Datasets/Car_features_test.csv')
testp = pd.read_csv('./Datasets/Car_prices_test.csv')
```

```
#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 'engin
```

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

```
sns.scatterplot(x = testp.price, y = pred_price)
#In case of a perfect prediction, all the points must lie on the line x = y.
sns.lineplot(x = [0,testp.price.max()], y = [0,testp.price.max()],color='orange') #Plotting t
plt.xlabel('Actual price')
plt.ylabel('Predicted price')
```

```
Text(0, 0.5, 'Predicted price')
```



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 R2 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
```

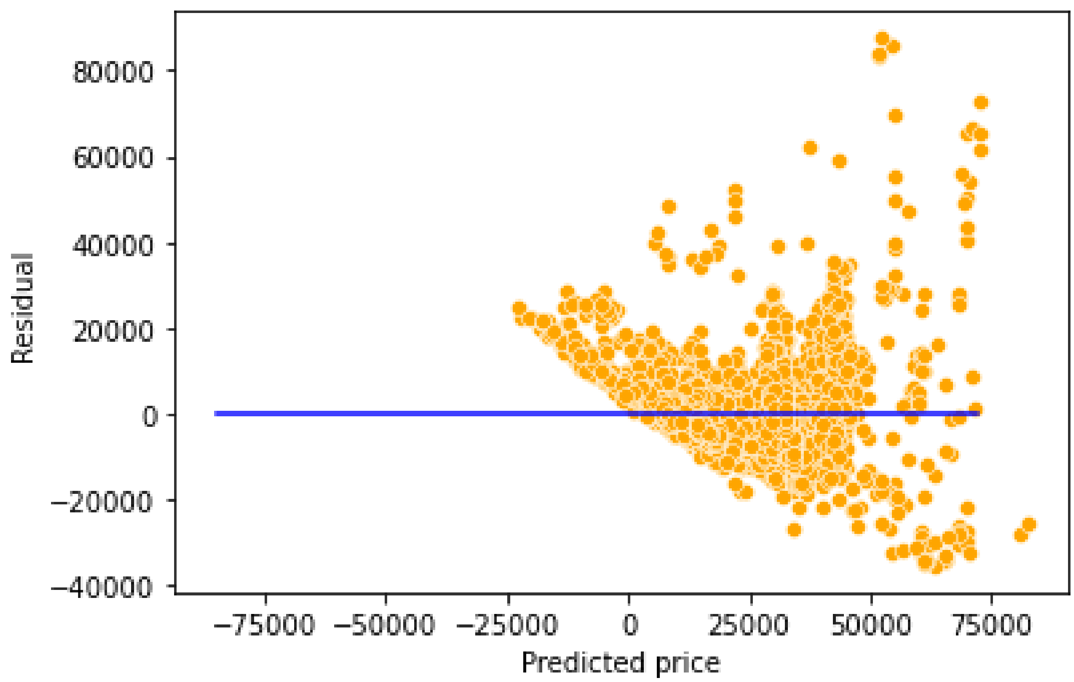
What is the residual standard error based on the training data?

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

```
9563.74782917604
```

```
sns.scatterplot(x = model.fittedvalues, y=model.resid,color = 'orange')
sns.lineplot(x = [pred_price.min(),pred_price.max()],y = [0,0],color = 'blue')
plt.xlabel('Predicted price')
plt.ylabel('Residual')
```

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



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 2.5: 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-squared). 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-squared.