Data Science III with python (Class notes)

STAT 303-3

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3/24/23

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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 Introduction to Scikit-learn

```
# Importing necessary libraries
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
```

```
# sklearn has 100s of models - grouped in sublibraries, such as linear_model
from sklearn.linear_model import LogisticRegression, LinearRegression
# sklearn also has many tools for cleaning/processing data, also grouped in sublibraries
from sklearn.model_selection import train_test_split # splitting one dataset into train an
from sklearn.metrics import accuracy_score, mean_absolute_error, mean_squared_error, r2_sc
from sklearn.preprocessing import StandardScaler
```

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

```
# Separating the predictors and response - THIS IS HOW ALL SKLEARN OBJECTS ACCEPT DATA (di
y = data.Outcome
X = data.drop("Outcome", axis = 1)
```

```
# Creating training and test data
    # 80-20 split, which is usual - 70-30 split is also fine, 90-10 is fine if the dataset
    # random_state to set a random seed for the splitting - reproducible results
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.2, random_state =
# stratify
```

```
# With linear/logistic regression in scikit-learn, especially when the predictors have dif
# of magn., scaling is necessary. This is to enable the training algo. which we did not co
scaler = StandardScaler().fit(X_train)
X_train_scaled = scaler.transform(X_train)
X_test_scaled = scaler.transform(X_test) # Do NOT refit the scaler with the test data, jus
```

```python
X_train = X_train_scaled
X_test = X_test_scaled
```

```python
# Create a model - not trained yet
logreg = LogisticRegression()

# Train the model
logreg.fit(X_train, y_train)

# Test the model - prediction - two ways to go
y_pred = logreg.predict(X_test) # Get the predicted classes first
print(accuracy_score(y_pred, y_test)*100) # Use the predicted and true classes for accurac
```

```
73.37662337662337
```

```python
print(logreg.score(X_test, y_test)*100) # Use .score with test predictors and response to
                                            # Implements the same thing under the hood
```

```
73.37662337662337
```

```python
print(logreg.coef_) # Use coef_ to return the coefficients - only log reg inference you ca
```

```
[[ 0.32572891  1.20110566 -0.32046591  0.06849882 -0.21727131  0.72619528
   0.40088897  0.29698818]]
```

```python
# all metrics exist in sklearn
from sklearn.metrics import precision_score, recall_score, confusion_matrix

print(confusion_matrix(y_test, y_pred))
print(precision_score(y_test, y_pred))
print(recall_score(y_test, y_pred))

# What we covered today:
    # A recap of Log. Reg. with sklearn
        # Separate the predictors and response (if necessary)
        # Split the data into train and test (if necessary)

        # Create a model
```

```
        # Train with .fit
        # Predict with .predict or get the accuracy with .score
        # Use sklearn metrics with y_pred and y_test


        # Same idea with LinearRegression()
        # .score returns r-squared by default
        # use the appropriate metrics!


########################################################################################
```

```
[[87 17]
 [24 26]]
0.6046511627906976
0.52
```

```
# More details on the LogisticRegression model:
    # Inputs - for regularization and
    # prediction prob.s instead of classes - so we can change the thresholds

# .predict_proba returns the prob.s for both classes
    # Two cols for two classes
    # Apply your threshold to y_pred_probs[1] (second col)
y_pred_probs = logreg.predict_proba(X_test)

cutoff = 0.3

y_pred2 = y_pred_probs[:,1] > cutoff
y_pred2 = y_pred2.astype(int)

print(confusion_matrix(y_test, y_pred2))
print(precision_score(y_test, y_pred2))
print(recall_score(y_test, y_pred2))
```

```
[[78 26]
 [15 35]]
0.5737704918032787
0.7
```

```
# Test accuracy stayed the same - reg was not very necessary

# Too much reg
logreg2 = LogisticRegression(C=1e-10)
logreg2.fit(X_train, y_train)
y_pred = logreg2.predict(X_test) # Get the predicted classes first
print(accuracy_score(y_pred, y_test)*100)

# Test accuracy is even lower - too much reg caused underfitting


# The key to take full advantage of sklearn models is their inputs
    # Always read the doc
    # In Log Reg, you can switch to Lasso with penalty = 'l1' - for variable selection
    # For no regression, besides what we did above, you can use penalty = None

# Recall that C, or lambda, is a hyperparameter, which is optimized with cross-validation
    # There is LogisticRegressionCV, just like LassoCV and RidgeCV
    # Works the exact same way - check LassoCV and RidgeCV notes

# For all the sklearn models we will create in this course, there will be hyperparameters.
    # Mostly more than one for each model
    # These hyperparameters will determine how much regularization the model will have
    # These models will not have a CV version
    # So, we need to use two sklearn tools that implement cross-validation
        # cross_val_score - now
        # GridSearchCV - later when we get to trees and tree-based models

from sklearn.model_selection import cross_val_score

val_scores = []

hyperparam_vals = 10**np.linspace(-5, 10)

for c_val in hyperparam_vals: # For each possible C value in your grid
    logreg_model = LogisticRegression(C=c_val) # Create a model with the C value

    val_scores.append(cross_val_score(logreg_model, X_train, y_train, scoring='accuracy',
```

```
import matplotlib.pyplot as plt

plt.plot(hyperparam_vals, np.mean(np.array(val_scores), axis=1))
plt.xlabel('possible C value')
plt.ylabel('avg 5-fold CV value')
plt.xscale('log')
plt.show()


# Train the best model with the hyperparam val that returns the highest average accuracy
logreg_model_best = LogisticRegression(C=hyperparam_vals[np.argmax(np.mean(np.array(val_sc

# .fit
# .predict & .predict_proba
# .score
# ...

# Log. reg. has one hyperparameter - C.
# More complex models will have more
# If we have two hyperparams - we can use a nested loop and cross_val_score
    # or we can use GridSearchCV - more on that when we get to trees and tree-based models
```

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*

```
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~engineSize', data = train)
```

```python
#Using the fit() function of the 'ols' class to fit the model
model = ols_object.fit()
```

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

Table 1.2: OLS Regression Results

Dep. Variable:	price	R-squared:	0.390
Model:	OLS	Adj. R-squared:	0.390
Method:	Least Squares	F-statistic:	3177.
Date:	Thu, 19 Jan 2023	Prob (F-statistic):	0.00
Time:	16:44:04	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

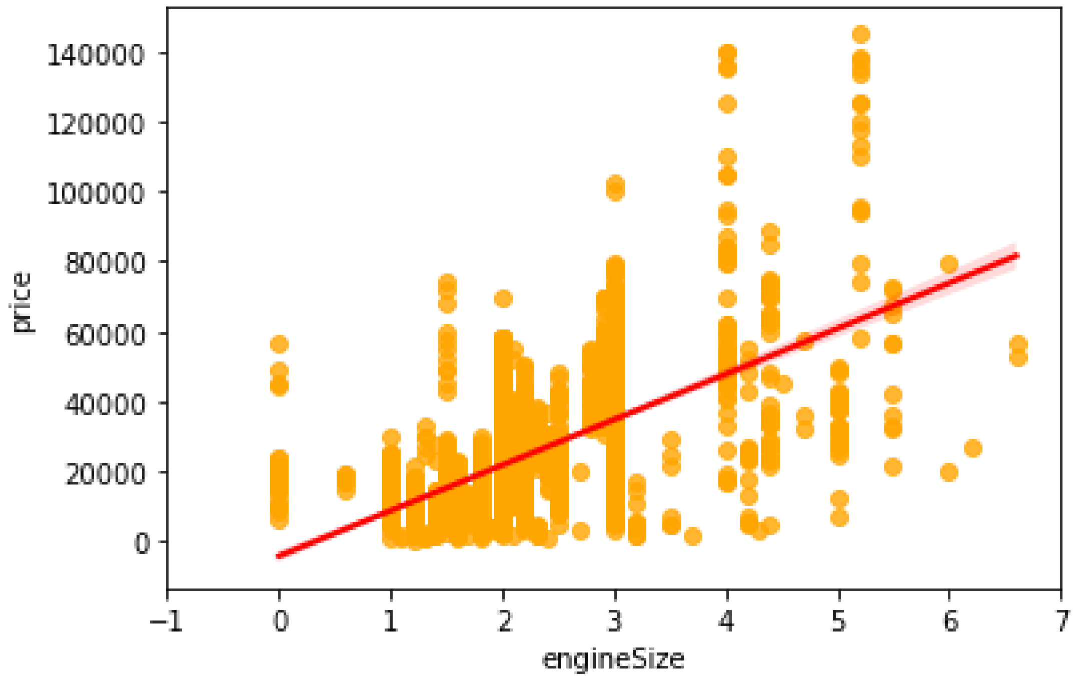
Omnibus:	1271.986	Durbin-Watson:	0.517
Prob(Omnibus):	0.000	Jarque-Bera (JB):	6490.719
Skew:	1.137	Prob(JB):	0.00
Kurtosis:	8.122	Cond. No.	7.64

The model equation is: car price = -4122.0357 + 12990 * engineSize

Visualize the regression line

```python
sns.regplot(x = 'engineSize', y = 'price', data = train, color = 'orange',line_kws={"color
plt.xlim(-1,7)
#Note that some of the engineSize values are 0. They are incorrect, and should ideally be
```

```
(-1.0, 7.0)
```



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

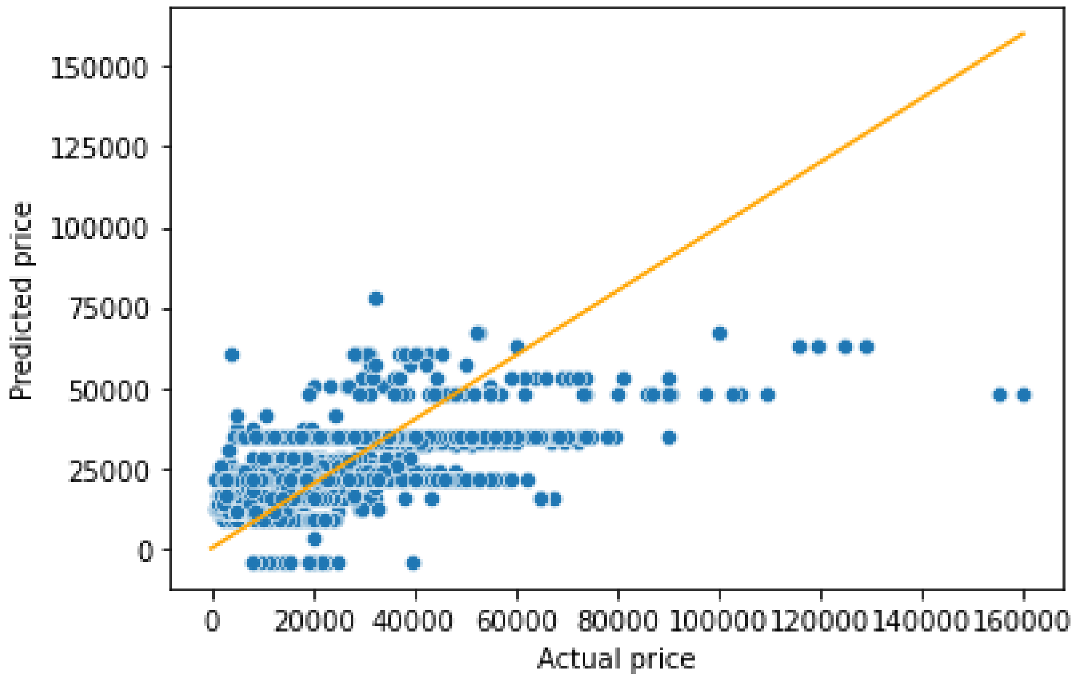
```
testf = pd.read_csv('./Datasets/Car_features_test.csv')
testp = pd.read_csv('./Datasets/Car_prices_test.csv')
```

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

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') #Plottin
plt.xlabel('Actual price')
plt.ylabel('Predicted price')
```

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



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?

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

```
12995.1064515487
```

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)
```

```
12810.109175214136
```

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 interva
intervals = model.get_prediction(testf)
```

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

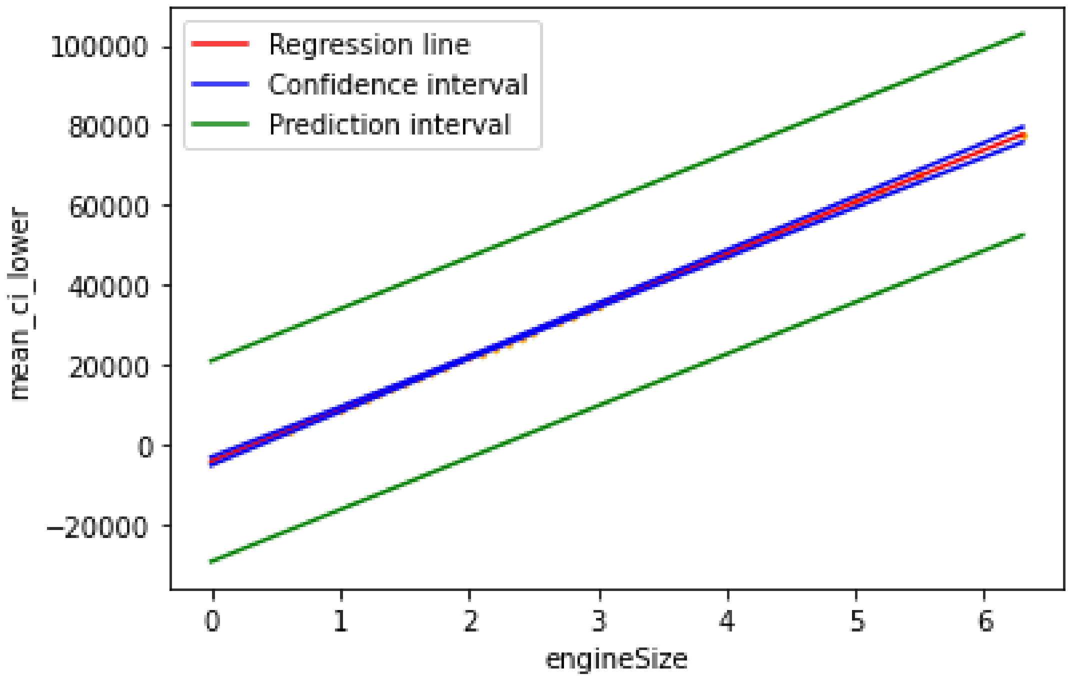
	mean	mean_se	mean_ci_lower	mean_ci_upper	obs_ci_lower	obs_ci_upper
0	34842.807319	271.666459	34310.220826	35375.393812	9723.677232	59961.937406
1	34842.807319	271.666459	34310.220826	35375.393812	9723.677232	59961.937406
2	34842.807319	271.666459	34310.220826	35375.393812	9723.677232	59961.937406
3	8866.245277	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
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)
```

```
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',label=
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')
plt.legend(labels=["Regression line","Confidence interval", "Prediction interval"])
```

```
<matplotlib.legend.Legend at 0x26a3a32c550>
```



Regression line
Confidence interval
Prediction interval
100000
80000
60000
40000
20000
0
−20000
mean_ci_lower
0
1
2
3
4
5
6
engineSize

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.

```
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*

```
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
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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*

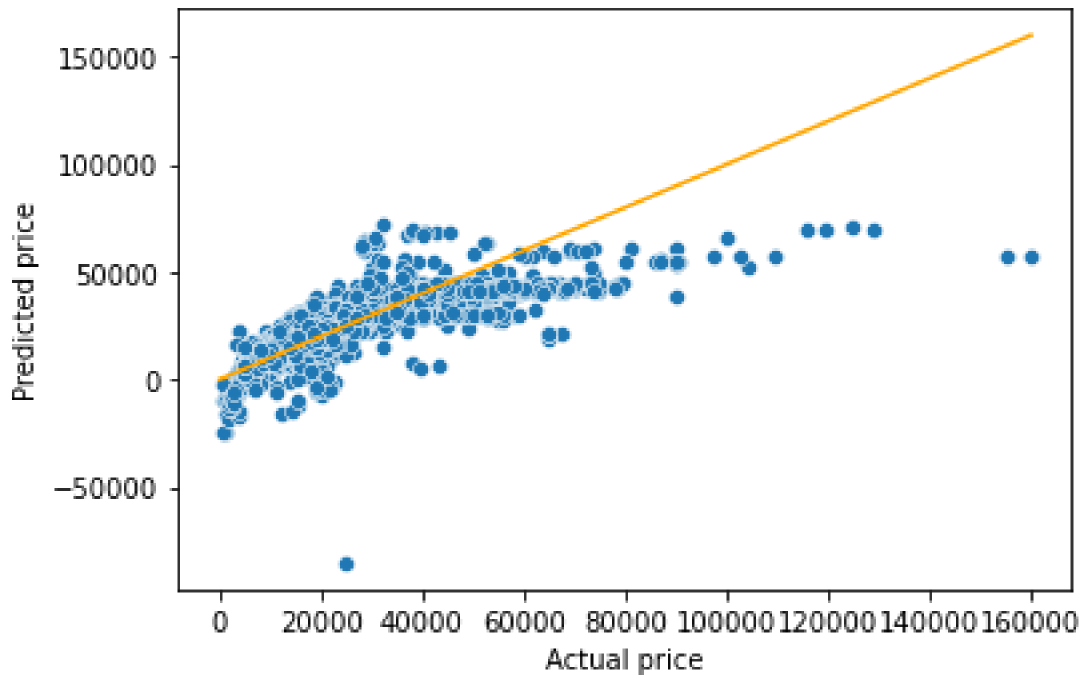
```
testf = pd.read_csv('./Datasets/Car_features_test.csv')
testp = pd.read_csv('./Datasets/Car_prices_test.csv')
```

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

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') #Plottin
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
```

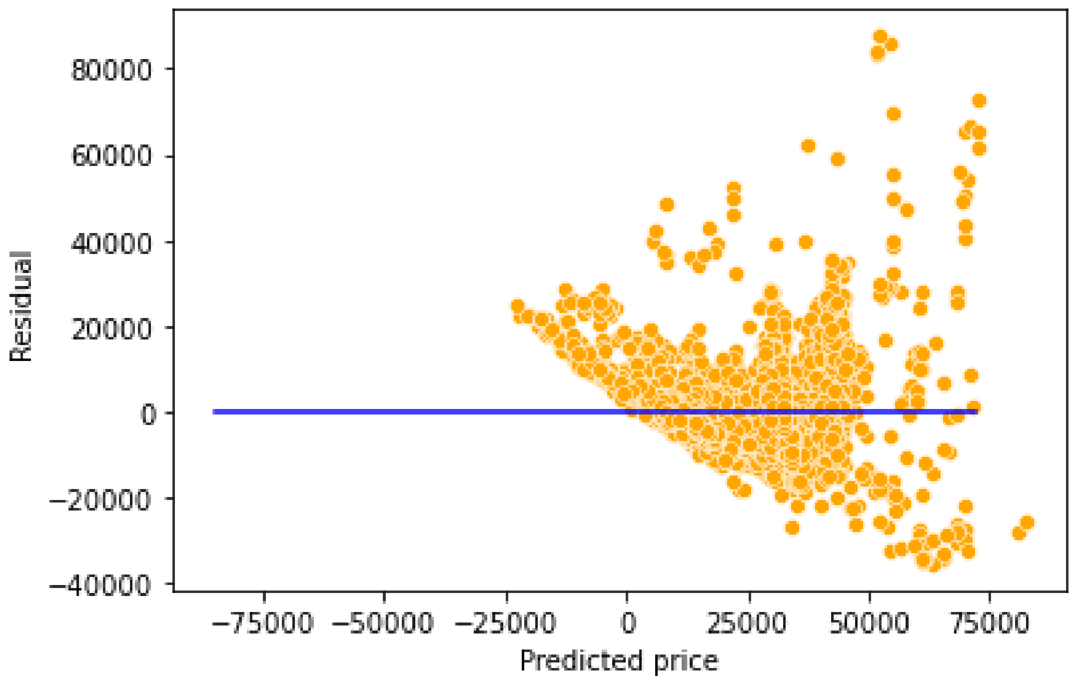
What is the residual standard error based on the training data?

```
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.

A Datasets, assignment and project files

Datasets used in the book, assignment files, project files, and prediction problems report tempate can be found here

References