2.2.2. Import libraries and load data

Get ready by importing the APIs needed from respective libraries.

```
# %load ../standard_import.txt
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import axes3d

from sklearn.linear_model import LinearRegression
from statsmodels.formula.api import ols

%matplotlib inline
```

Load Datasets

Load the Advertising dataset.

```
data_url = "https://github.com/pykale/transparentML/raw/main/data/Advertising.csv"
advertising_df = pd.read_csv(data_url, header=0, index_col=0)
```

To accommodate multiple predictor variables, one option is to run simple linear regression separately for each predictor variable.

The following code runs a simple linear regression model of **radio**, and **newspaper** onto **sales** using **statsmodels**, respectively (Table 3.3 in the textbook).

```
est = ols("Sales ~ Radio", advertising_df).fit()
est.summary().tables[1]
```

```
             coef   std err       t    P>|t|   [0.025    0.975]
Intercept  9.3116    0.563   16.542   0.000    8.202    10.422
    Radio  0.2025    0.020    9.921   0.000    0.162     0.243
```

```
est = ols("Sales ~ Newspaper", advertising_df).fit()
est.summary().tables[1]
```

```
              coef   std err       t    P>|t|   [0.025    0.975]
 Intercept  12.3514    0.621  19.876   0.000   11.126    13.577
Newspaper   0.0547    0.017   3.300   0.001    0.022     0.087
```

However, fitting a separate simple linear regression model for each predictor is problematic: 1) It is unclear how to make a single prediction given the three advertising media budgets; 2) each separate linear regression model ignores the effect of the other two predictors, which can lead to misleading estimates.

A better approach is to use *multiple linear regression*. Multiple linear regression is an extension of simple linear regression. It allows us to predict a quantitative response using more than one predictor variable. The equation for a multiple linear regression model with D predictor variables is given by:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_D x_D + \epsilon, \tag{2.13}$$

where y is the response, $x_1, x_2, \ldots, x_D$ are the D predictors, D is the total number of predictor variables (features), and ϵ is the error term. The βs are called the *regression coefficients*, where β_0 is the bias (intercept), and $\beta_1, \beta_2, \ldots, \beta_D$ are the weights (slopes). Considering N samples, the equation can be written in matrix form as:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}, \tag{2.14}$$

where $\mathbf{y}$ is an $N \times 1$ vector of responses, $\mathbf{X}$ is an $N \times (D+1)$ matrix of predictors, $\boldsymbol{\beta}$ is a $(D+1) \times 1$ vector of regression coefficients, and $\boldsymbol{\epsilon}$ is an $N \times 1$ vector of errors. The predictor (feature) matrix $\mathbf{X}$ contains a column of 1s to account for the intercept. The vector $\boldsymbol{\beta}$ contains the intercept in the first position and the slopes for the remaining D predictors. The vector $\boldsymbol{\epsilon}$ contains the error terms for each observation.

Using the **Advertising** dataset as an example, we can fit a multiple linear regression model to the three predictor variables **TV**, **radio** and **newspaper** to predict **sales** as follows:

$$\text{Sales} = \beta_0 + \beta_1 \times \text{TV} + \beta_2 \times \text{Radio} + \beta_3 \times \text{Newspaper} + \epsilon. \tag{2.15}$$

2.2.3. Estimating the regression coefficients

Similar to simple linear regression, we can estimate the regression coefficients using least squares. The least squares estimates for the regression coefficients are given by:

$$\begin{aligned} \text{RSS} &= \sum_{i=1}^{N} (y_i - \hat{y}_i)^2 \\ &= \sum_{i=1}^{N} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i1} - \hat{\beta}_2 x_{i2} - \ldots - \hat{\beta}_D x_{iD})^2, \end{aligned} \tag{2.16}$$

where y_i is the ith response, $\hat{y}_i$ is the ith predicted response, $\hat{\beta}_0$ is the intercept, $\hat{\beta}_1$ is the slope for x_{i1}, $\hat{\beta}_2$ is the slope for x_{i2}, and so on. $\hat{\beta}$s are the least squares estimates for the regression coefficients, which can be obtained in matrix form as:

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}. \tag{2.17}$$

The following code run a multiple linear regression model to regress **TV**, **radio** and **newspaper** onto **sales** using **statsmodels**, and display the learnt coefficients (Table 3.4 in the textbook).

```
est = ols("Sales ~ TV + Radio + Newspaper", advertising_df).fit()
est.summary()
```

```
     Dep. Variable:             Sales          R-squared:     0.897
            Model:                OLS     Adj. R-squared:     0.896
           Method:      Least Squares        F-statistic:     570.3
             Date:   Tue, 06 Feb 2024  Prob (F-statistic):  1.58e-96
             Time:           20:20:20     Log-Likelihood:   -386.18
 No. Observations:                200                AIC:     780.4
     Df Residuals:                196                BIC:     793.6
         Df Model:                  3
  Covariance Type:          nonrobust

OLS Regression Results

                 coef  std err       t   P>|t|  [0.025  0.975]
   Intercept   2.9389    0.312   9.422   0.000   2.324   3.554
          TV   0.0458    0.001  32.809   0.000   0.043   0.049
       Radio   0.1885    0.009  21.893   0.000   0.172   0.206
   Newspaper  -0.0010    0.006  -0.177   0.860  -0.013   0.011

       Omnibus:  60.414    Durbin-Watson:    2.084
 Prob(Omnibus):   0.000  Jarque-Bera (JB):  151.241
          Skew:  -1.327         Prob(JB):  1.44e-33
      Kurtosis:   6.332         Cond. No.     454.

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

2.2.4. Interpreting the results

Wehaveinterpreted the results ofsimple linear regressionin the previous section. The interpretation of the results of multiple linear regression is similar. The only difference is that there are now three coefficients to interpret.

Challenge

Interpret the results of the multiple linear regression model above based on the previous section and then click the following to compare the provided interpretation with yours.

How to interpret the results?

We interpret these results above as follows:

- For a given (i.e. fixed) amount of **TV** and **newspaper** advertising budgets, spending an additional $1,000 on **radio** advertising is associated with approximately 189 units of additional **sales** (*recall the units of the variables*).
- Comparing these coefficients to the estimates in simple linear regression, we notice that the multiple regression coefficient estimates for **TV** and **radio** are pretty similar to the simple linear regression coefficient estimates. However, while the **newspaper** regression coefficient estimate in simple linear regression was significantly non-zero, the coefficient estimate for **newspaper** in the multiple regression model is close to zero, and the corresponding *p*-value is no longer significant, with a value around 0.86.
- This illustrates that the simple and multiple regression coefficients can be quite different. This difference stems from the fact that in the simple regression case, the slope term represents the average increase in product sales associated with a $1,000 increase in newspaper advertising, ignoring other predictors such as **TV** and **radio**. By contrast, in the multiple regression setting, the coefficient for **newspaper** represents the average increase in product **sales** associated with increasing **newspaper** spending by $1,000 while holding **TV** and **radio**fixed.

Why the relationship between **sales** and **newspaper** are opposite in the simple linear regression and multiple linear regression? Use following code displays the correlation matrix of the **Advertising** dataset for further analysis.

```
advertising_df.corr()
```

	TV	Radio	Newspaper	Sales
TV	1.000000	0.054809	0.056648	0.782224
Radio	0.054809	1.000000	0.354104	0.576223
Newspaper	0.056648	0.354104	1.000000	0.228299
Sales	0.782224	0.576223	0.228299	1.000000

How to interpret the results?

The correlation between **radio** and **newspaper** is 0.35, which is much higher than the other pair-wise correlations among the three medias. This indicates that in those markets spending more on **newspaper** (**radio**) advertising, there is a tendency to spend more on **radio** (**newspaper**) advertising as well.
Now suppose that the multiple regression is correct and **newspaper** advertising is not associated with sales, but **radio** advertising is associated with **sales**. Then in markets where we spend more on **radio**, our sales will tend to be higher. As our correlation matrix shows, we also tend to spend more on **newspaper** advertising in those same markets. Hence, in a simple linear regression which only examines sales versus **newspaper**, we will observe that higher values of **newspaper** tend to be associated with higher values of **sales**, even though **newspaper** advertising is not directly associated with **sales**. So **newspaper** advertising is a surrogate for **radio** advertising; **newspaper** gets “credit” for the association between **radio** on **sales**.

- Backward selection. We begin with a model containing all predictors, and then consider removing predictors one at a time until no predictors remain. The worst single predictor is removed from the model, and the process is repeated until no predictors remain in the model. This is also a greedy algorithm, and it is not guaranteed to find the best model containing a subset of the predictors.
- Mixed selection. We begin with some initial model containing a subset of the predictors. We then consider adding or removing each predictor individually, and retain the best model that results. This is also a greedy algorithm, and it is not guaranteed to find the best model containing a subset of the predictors.

2.2.5.3. How well does the model fit the data?

Similar to simple linear regression. We can answer this question by computing the R^2 and RSE statistics. The R^2 for multiple linear regression is defined in the same way as in simple linear regression as:

$$R^2 = 1 - \frac{\text{RSS}}{\text{TSS}} = 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y})^2}. \quad (2.19)$$

The $R2$ statistic provides an indication of the proportion of the variance in the response that is predictable from the predictors. In this the $R2$ statistic is 0.897, which indicates that 89.7% of the variance in **sales** is predictable from **TV**, **radio**, and **newspaper**.

The RSE for multiple linear regression is defined as:

$$\text{RSE} = \sqrt{\frac{\text{RSS}}{N - D - 1}} = \sqrt{\frac{\sum (y_i - \hat{y}_i)^2}{N - D - 1}}. \quad (2.20)$$

You can verify that when $D=1$, the RSE for multiple linear regression is the same as the RSE for simple linear regression.

Run the following code to fit and then evaluate a multiple linear regression model using **scikit-learn**:

Firstly, fit a linear regression to **sales** using **TV** and **radio** as predictors.

```
regr = LinearRegression()

X = advertising_df[["Radio", "TV"]].values
y = advertising_df.Sales
regr.fit(X, y)
print(regr.coef_)
print(regr.intercept_)
```

```
[0.18799423 0.04575482]
2.9210999124051398
```

Find out the min/max values of Radio & TV to set up the grid (range) for plotting.

```
advertising_df[["Radio", "TV"]].describe()
```

	Radio	TV
count	200.000000	200.000000
mean	23.264000	147.042500
std	14.846809	85.854236
min	0.000000	0.700000
25%	9.975000	74.375000
50%	22.900000	149.750000
75%	36.525000	218.825000
max	49.600000	296.400000

Create a coordinate grid

```
radio = np.arange(0, 50)
tv = np.arange(0, 300)

beta_1, beta_2 = np.meshgrid(radio, tv, indexing="xy")
Z = np.zeros((tv.size, radio.size))
for (i, j), v in np.ndenumerate(Z):

    Z[i, j] = (
        regr.intercept_ + beta_1[i, j] * regr.coef_[0] + beta_2[i, j]              *
regr.coef_[1]
    )
```

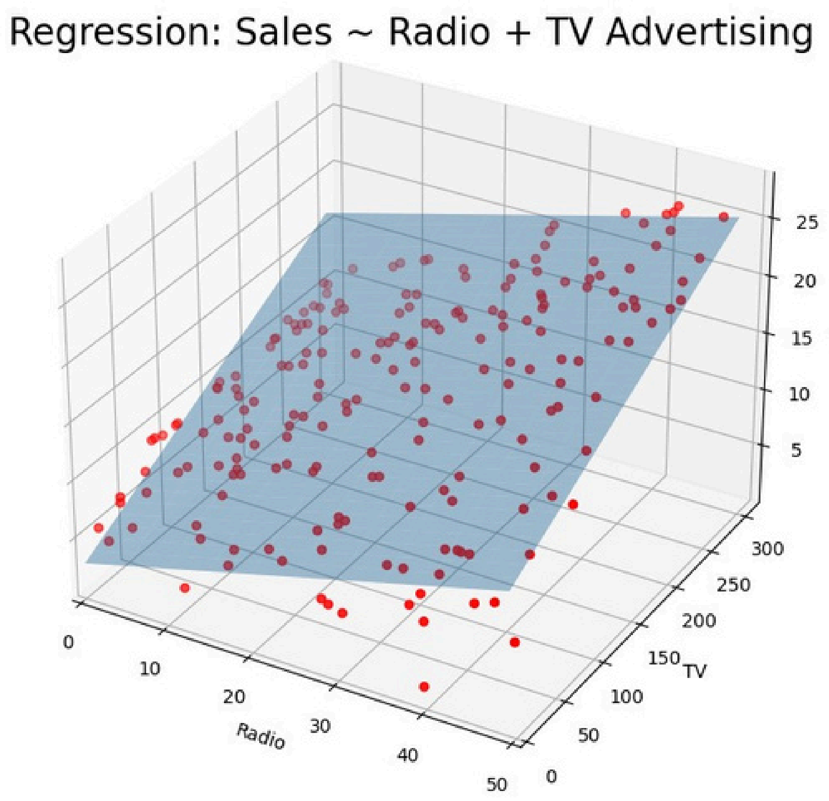
Create 3D plot of `sales` vs `TV` and `radio`.

```
# Create plot
fig = plt.figure(figsize=(10, 6))
fig.suptitle("Regression: Sales ~ Radio + TV Advertising", fontsize=20)

ax = axes3d.Axes3D(fig, auto_add_to_figure=False)
fig.add_axes(ax)

ax.plot_surface(beta_1, beta_2, Z, rstride=10, cstride=5, alpha=0.4)
ax.scatter3D(advertising_df.Radio, advertising_df.TV, advertising_df.Sales, c="r")

ax.set_xlabel("Radio")
ax.set_xlim(0, 50)
ax.set_ylabel("TV")
ax.set_ylim(bottom=0)
ax.set_zlabel("Sales")
plt.show()
```



2.2.5.4. Given a set of predictor values, what response value should we predict, and how accurate is our prediction?

Once we have fit a multiple linear regression model, we can use the model to make predictions of the response for a given set of predictor values.

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_D x_D. \tag{2.21}$$

However, we must be careful when making predictions, because the observed values of the predictors may not have been part of the data used to fit the model. In this case, the prediction may not be very accurate and using a confidence interval can help quantify the uncertainty associated with the prediction.

2.2.6. Exercise

1. All the following exercises involve the use of the Carseats dataset. Fit a multiple regression model to predict Sales using Price, Income, and CompPrice. Hint: See section 2.2.5.

```
# Write your code below to answer the question
```

Compare your answer with the reference solution below

```
import pandas as pd
import numpy as np
from sklearn.preprocessing import StandardScaler
from sklearn.linear_model import LinearRegression

# Load data
carseats_df = pd.read_csv(
    "https://github.com/pykale/transparentML/raw/main/data/Carseats.csv"
)
regr    =    LinearRegression()    X    =    carseats_df[["Price",    "Income",

"CompPrice"]].values
y = carseats_df.Sales
regr.fit(X, y)
print("Regression model slop/coeffcient (weight):", regr.coef_)
print("Regression model intercept (bias):", regr.intercept_)
```

```
Regression model slop/coeffcient (weight): [-0.08719674          0.01525145     0.09278583]
Regression model intercept (bias): 4.950235603666373
```

i. How well does the model fit the data?

```
# Write your code below to answer the question
```

Compare your answer with the reference solution below

```
from sklearn.metrics import mean_squared_error, r2_score

y_pred = regr.predict(X)
print("R2 score:", r2_score(y, y_pred))

# The model didn't fit the data well as the R2 score is still way below 1.
```

```
R2 score: 0.3805237817874102
```

ii. Does multiple linear regression help the model fit the data better than simpler linear regression (see simple linear regression exercises).

Compare your answer with the solution below

Yes. The $R2$score has increased in multiple linear regression, and the MSE has decreased, which means the model performed better than simpler linear regression in terms of fitting the data.

iii. Write out the model in equation form.

Compare your answer with the solution below

$$\hat{y}\hat{}=4.95+(-0.08719674*Price)+(0.01525145*Income)+(0.09278583*CompPrice)$$

2. Find the correlation between Sales, Price, Income, and CompPrice and interpret the result. Hint: See section 2.2.4.

```
# Write your code below to answer the question
```

Compare your answer with the reference solution below

```
carseats_df[["Sales", "Price", "Income", "CompPrice"]].corr()
# The correlation between Price and CompPrice is 0.58, which is much higher than
the other pair-wise correlations. This indicates that by increasing the component
price(Price) of a caraseat, there is a tendency for the overall price(CompPrice)
to increase as well.
```

	Sales	Price	Income	CompPrice
Sales	1.000000	-0.444951	0.151951	0.064079
Price	-0.444951	1.000000	-0.056698	0.584848
Income	0.151951	-0.056698	1.000000	-0.080653
CompPrice	0.064079	0.584848	-0.080653	1.000000

3. Perform a multiple linear regression using statsmodels library with Sales as the response and Price, Income, and CompPrice as predictors. Use the summary() function to print the results. Compare the regression coefficients/weights with Exercise 1. Hint: See section 2.2.3.

```
# Write your code below to answer the question
```

Compare your answer with the reference solution below

```
import patsy
import statsmodels.api as sm

f = "Sales ~ Price + Income + CompPrice"
y, X = patsy.dmatrices(f, carseats_df, return_type="dataframe")

model = sm.OLS(y, X).fit()
print(model.summary())
# The regression coeffcients are same as scikit learn model
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                  Sales   R-squared:                       0.381
Model:                            OLS   Adj. R-squared:                  0.376
Method:                 Least Squares   F-statistic:                     81.08
Date:                Tue, 06 Feb 2024   Prob (F-statistic):           6.52e-41
Time:                        20:20:20   Log-Likelihood:                -886.58
No. Observations:                 400   AIC:                             1781.
Df Residuals:                     396   BIC:                             1797.
Df Model:                           3
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
Intercept      4.9502      0.981      5.044      0.000       3.021       6.880
Price         -0.0872      0.006    -14.991      0.000      -0.099      -0.076
Income         0.0153      0.004      3.809      0.000       0.007       0.023
CompPrice      0.0928      0.009     10.315      0.000       0.075       0.110
==============================================================================
Omnibus:                        7.331   Durbin-Watson:                   1.884
Prob(Omnibus):                  0.026   Jarque-Bera (JB):                7.077
Skew:                           0.285   Prob(JB):                       0.0291
Kurtosis:                       2.683   Cond. No.                     1.63e+03
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
[2] The condition number is large, 1.63e+03. This might indicate that there are
strong multicollinearity or other numerical problems.
```

4. From the model fitted in Exercise 3, for which predictors can you reject the null hypothesis $H0 : \beta j = 0$? Hint: See section 2.2.5.

```
# Write your code below to answer the question
```

Compare your answer with the reference solution below