C2_W2_Assignment

October 23, 2024

1 Optimization Using Gradient Descent: Linear Regression

In this assignment, you will build a simple linear regression model to predict sales based on TV marketing expenses. You will investigate three different approaches to this problem. You will use `NumPy` and `Scikit-Learn` linear regression models, as well as construct and optimize the sum of squares cost function with gradient descent from scratch.

2 Table of Contents

2.1 Packages

Load the required packages:

[1]:
```python
import numpy as np
# A library for programmatic plot generation.
import matplotlib.pyplot as plt
# A library for data manipulation and analysis.
import pandas as pd
# LinearRegression from sklearn.
from sklearn.linear_model import LinearRegression
```

Import the unit tests defined for this notebook.

[2]:
```python
import w2_unittest
```

## 1 - Open the Dataset and State the Problem

In this lab, you will build a linear regression model for a simple Kaggle dataset, saved in a file `data/tvmarketing.csv`. The dataset has only two fields: TV marketing expenses (`TV`) and sales amount (`Sales`).

### Exercise 1

Use `pandas` function `pd.read_csv` to open the .csv file the from the `path`.

```
[3]: path = "data/tvmarketing.csv"

     ### START CODE HERE ### (~ 1 line of code)
     adv = pd.read_csv(path)
     ### END CODE HERE ###
```

```
[4]: # Print some part of the dataset.
     adv.head()
```

```
[4]:       TV  Sales
     0  230.1   22.1
     1   44.5   10.4
     2   17.2    9.3
     3  151.5   18.5
     4  180.8   12.9
```

Expected Output

```
    TV   Sales
0   230.1   22.1
1   44.5    10.4
2   17.2    9.3
3   151.5   18.5
4   180.8   12.9
```

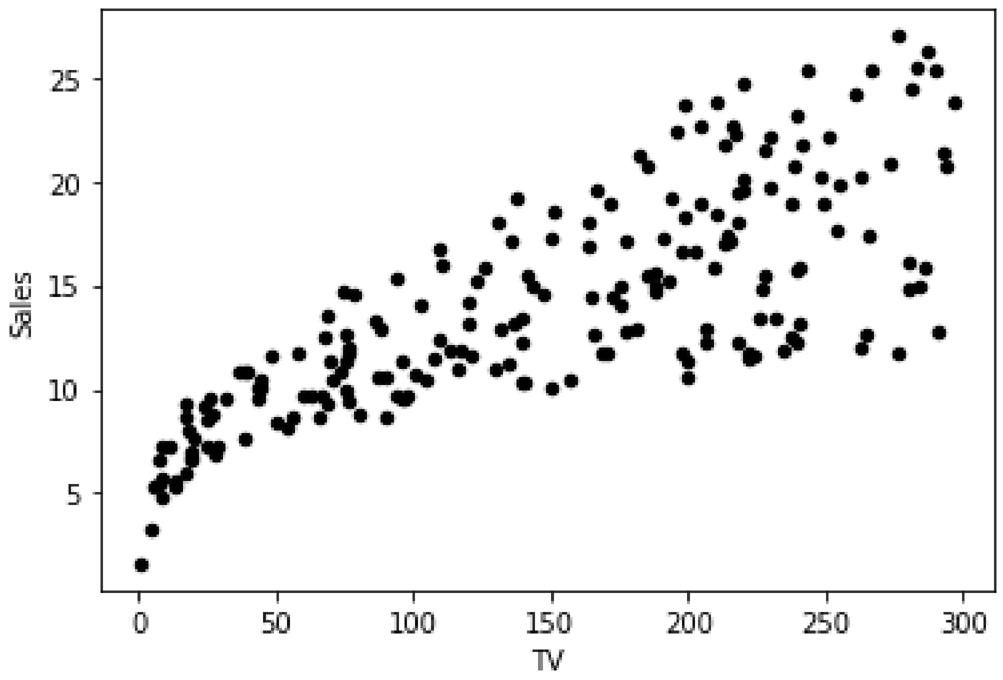
```
[5]: w2_unittest.test_load_data(adv)
```

```
 All tests passed
```

`pandas` has a function to make plots from the DataFrame fields. By default, matplotlib is used at the backend. Let's use it here:

```
[6]: adv.plot(x='TV', y='Sales', kind='scatter', c='black')
```

```
[6]: <AxesSubplot: xlabel='TV', ylabel='Sales'>
```



You can use this dataset to solve a simple problem with linear regression: given a TV marketing budget, predict sales.

## 2 - Linear Regression in Python with `NumPy` and `Scikit-Learn`

Save the required field of the DataFrame into variables `X` and `Y`:

[7]:
```
X = adv['TV']
Y = adv['Sales']
```

### 2.1 - Linear Regression with `NumPy`

You can use the function `np.polyfit(x, y, deg)` to fit a polynomial of degree `deg` to points (x, y), minimising the sum of squared errors. You can read more in the documentation. Taking `deg = 1` you can obtain the slope `m` and the intercept `b` of the linear regression line:

[8]:
```
m_numpy, b_numpy = np.polyfit(X, Y, 1)

print(f"Linear regression with NumPy. Slope: {m_numpy}. Intercept: {b_numpy}")
```

```
Linear regression with NumPy. Slope: 0.04753664043301978. Intercept:
7.032593549127698
```

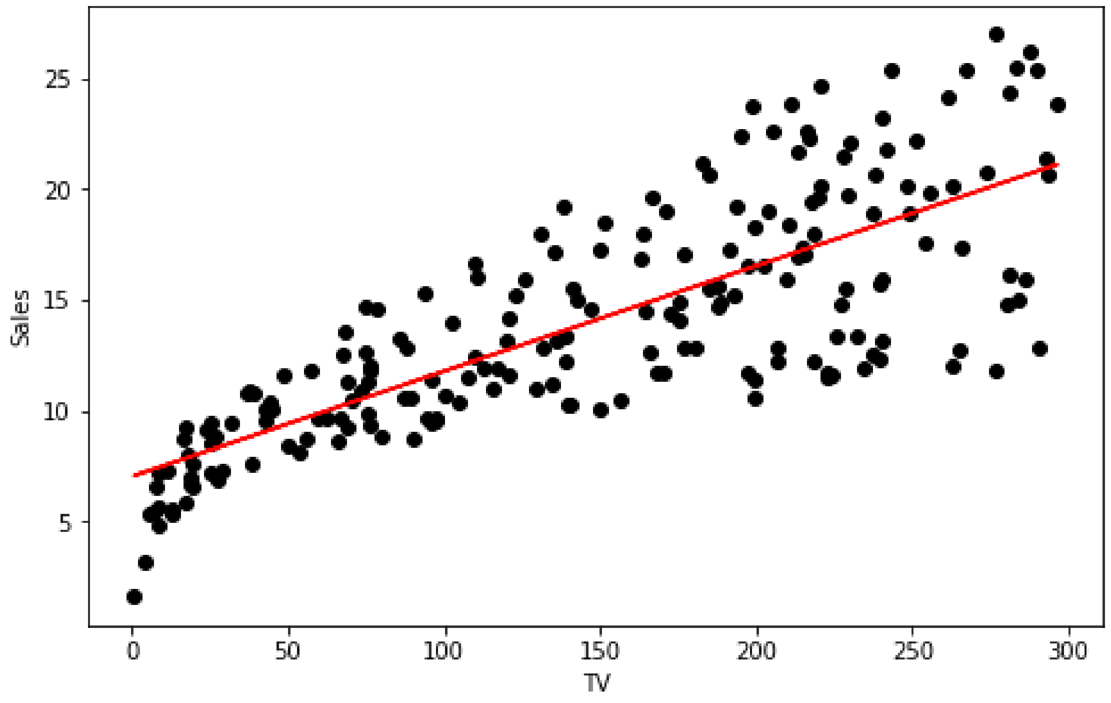
Note: `NumPy` documentation suggests the `Polynomial.fit` class method as recommended for new code as it is more stable numerically. But in this simple example, you can stick to the `np.polyfit` function for simplicity.

You can plot the linear regression line by running the following code. The regression line is red.

[9]:
```
def plot_linear_regression(X, Y, x_label, y_label, m, b, X_pred=np.array([]),␣
↪Y_pred=np.array([])):
    fig, ax = plt.subplots(1,1,figsize=(8,5))
    ax.plot(X, Y, 'o', color='black')
    ax.set_xlabel(x_label)
    ax.set_ylabel(y_label)

    ax.plot(X, m*X + b, color='red')
    # Plot prediction points (empty arrays by default - the predictions will be␣
↪calculated later).
    ax.plot(X_pred, Y_pred, 'o', color='blue', markersize=8)

plot_linear_regression(X, Y, 'TV', 'Sales', m_numpy, b_numpy)
```



### Exercise 2

Make predictions substituting the obtained slope and intercept coefficients into the equation $Y = mX + b$, given an array of X values.

[10]:
```
# This is organised as a function only for grading purposes.
def pred_numpy(m, b, X):
    ### START CODE HERE ### (~ 1 line of code)
    Y = m * X + b
    ### END CODE HERE ###
    return Y
```

[11]:
```
X_pred = np.array([50, 120, 280])
Y_pred_numpy = pred_numpy(m_numpy, b_numpy, X_pred)

print(f"TV marketing expenses:\n{X_pred}")
print(f"Predictions of sales using NumPy linear regression:\n{Y_pred_numpy}")
```

```
TV marketing expenses:
[ 50 120 280]
Predictions of sales using NumPy linear regression:
[ 9.40942557 12.7369904  20.34285287]
```

Expected Output

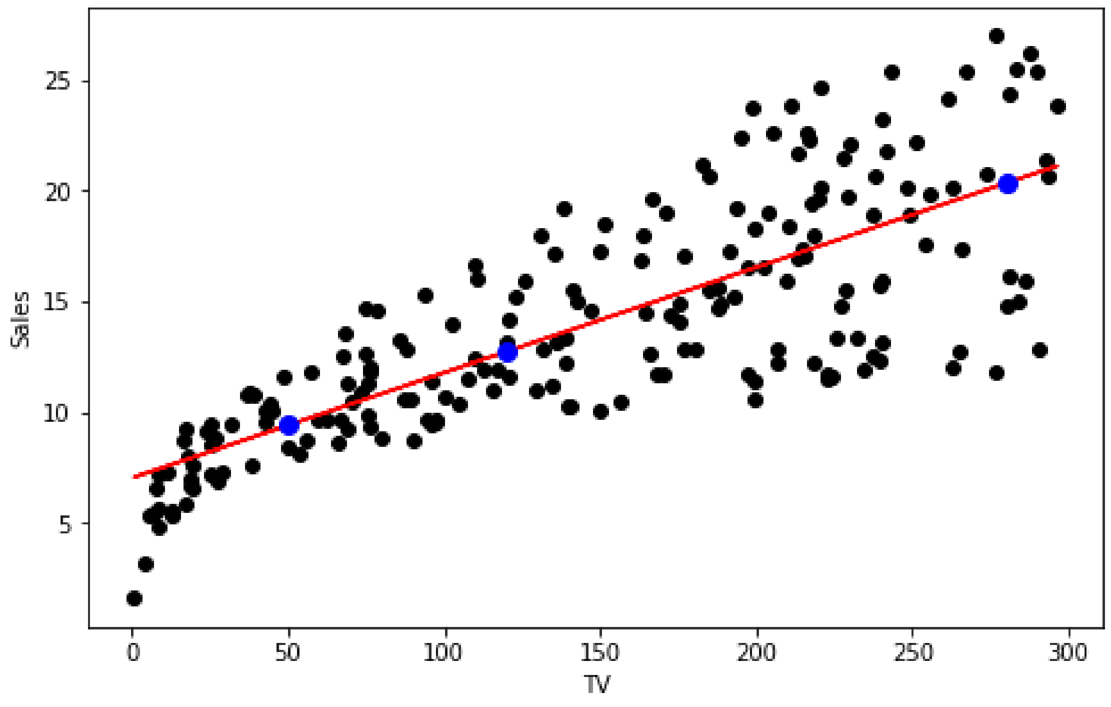
```
TV marketing expenses:
[ 50 120 280]
Predictions of sales using NumPy linear regression:
[ 9.40942557 12.7369904  20.34285287]
```

[12]:
```
w2_unittest.test_pred_numpy(pred_numpy)
```

```
 All tests passed
```

Now you can add the prediction points to the plot (blue dots).

[13]:
```
plot_linear_regression(X, Y, 'TV', 'Sales', m_numpy, b_numpy, X_pred,␣
 ↪Y_pred_numpy)
```



### 2.2 - Linear Regression with `Scikit-Learn`

`Scikit-Learn` is an open-source machine learning library that supports supervised and unsupervised learning. It also provides various tools for model fitting, data preprocessing, model selection, model evaluation, and many other utilities. `Scikit-learn` provides dozens of built-in machine learning algorithms and models, called **estimators**. Each estimator can be fitted to some data using its `fit` method. Full documentation can be found here.

Create an estimator object for a linear regression model:

[14]:
```
lr_sklearn = LinearRegression()
```

The estimator can learn from data calling the `fit` function. However, trying to run the following code you will get an error, as the data needs to be reshaped into 2D array:

[15]:
```
print(f"Shape of X array: {X.shape}")
print(f"Shape of Y array: {Y.shape}")

try:
    lr_sklearn.fit(X, Y)
except ValueError as err:
    print(err)
```

```
Shape of X array: (200,)
Shape of Y array: (200,)
Expected 2D array, got 1D array instead:
array=[230.1  44.5  17.2 151.5 180.8   8.7  57.5 120.2   8.6 199.8  66.1 214.7
  23.8  97.5 204.1 195.4  67.8 281.4  69.2 147.3 218.4 237.4  13.2 228.3
  62.3 262.9 142.9 240.1 248.8  70.6 292.9 112.9  97.2 265.6  95.7 290.7
 266.9  74.7  43.1 228.  202.5 177.  293.6 206.9  25.1 175.1  89.7 239.9
 227.2  66.9 199.8 100.4 216.4 182.6 262.7 198.9   7.3 136.2 210.8 210.7
  53.5 261.3 239.3 102.7 131.1  69.   31.5 139.3 237.4 216.8 199.1 109.8
  26.8 129.4 213.4  16.9  27.5 120.5   5.4 116.   76.4 239.8  75.3  68.4
 213.5 193.2  76.3 110.7  88.3 109.8 134.3  28.6 217.7 250.9 107.4 163.3
 197.6 184.9 289.7 135.2 222.4 296.4 280.2 187.9 238.2 137.9  25.   90.4
  13.1 255.4 225.8 241.7 175.7 209.6  78.2  75.1 139.2  76.4 125.7  19.4
 141.3  18.8 224.  123.1 229.5  87.2   7.8  80.2 220.3  59.6   0.7 265.2
   8.4 219.8  36.9  48.3  25.6 273.7  43.  184.9  73.4 193.7 220.5 104.6
  96.2 140.3 240.1 243.2  38.   44.7 280.7 121.  197.6 171.3 187.8   4.1
  93.9 149.8  11.7 131.7 172.5  85.7 188.4 163.5 117.2 234.5  17.9 206.8
 215.4 284.3  50.  164.5  19.6 168.4 222.4 276.9 248.4 170.2 276.7 165.6
 156.6 218.5  56.2 287.6 253.8 205.  139.5 191.1 286.   18.7  39.5  75.5
  17.2 166.8 149.7  38.2  94.2 177.  283.6 232.1].
Reshape your data either using array.reshape(-1, 1) if your data has a single
feature or array.reshape(1, -1) if it contains a single sample.
```

You can increase the dimension of the array by one with `reshape` function, or there is another

another way to do it:

[16]:
```
X_sklearn = X[:, np.newaxis]
Y_sklearn = Y[:, np.newaxis]

print(f"Shape of new X array: {X_sklearn.shape}")
print(f"Shape of new Y array: {Y_sklearn.shape}")
```

```
Shape of new X array: (200, 1)
Shape of new Y array: (200, 1)
```

### Exercise 3

Fit the linear regression model passing `X_sklearn` and `Y_sklearn` arrays into the function `lr_sklearn.fit`.

[17]:
```
### START CODE HERE ### (~ 1 line of code)
lr_sklearn.fit(X_sklearn, Y_sklearn)
### END CODE HERE ###
```

[17]:
```
LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None, normalize=False)
```

[18]:
```
m_sklearn = lr_sklearn.coef_
b_sklearn = lr_sklearn.intercept_

print(f"Linear regression using Scikit-Learn. Slope: {m_sklearn}. Intercept:␣
 ↪{b_sklearn}")
```

```
Linear regression using Scikit-Learn. Slope: [[0.04753664]]. Intercept:
[7.03259355]
```

Expected Output

```
Linear regression using Scikit-Learn. Slope: [[0.04753664]]. Intercept: [7.03259355]
```

[19]:
```
w2_unittest.test_sklearn_fit(lr_sklearn)
```

```
 All tests passed
```

Note that you have got the same result as with the `NumPy` function `polyfit`. Now, to make predictions it is convenient to use `Scikit-Learn` function `predict`.

### Exercise 4

Increase the dimension of the X array using the function `np.newaxis` (see an example above) and pass the result to the `lr_sklearn.predict` function to make predictions.

[20]:
```
# This is organised as a function only for grading purposes.
def pred_sklearn(X, lr_sklearn):
    ### START CODE HERE ### (~ 2 lines of code)
    X_2D = X[:, np.newaxis]
    Y = lr_sklearn.predict(X_2D)
    ### END CODE HERE ###

    return Y
```

[21]:
```
Y_pred_sklearn = pred_sklearn(X_pred, lr_sklearn)

print(f"TV marketing expenses:\n{X_pred}")
print(f"Predictions of sales using Scikit_Learn linear regression:
 ↪\n{Y_pred_sklearn.T}")
```

```
TV marketing expenses:
[ 50 120 280]
Predictions of sales using Scikit_Learn linear regression:
[[ 9.40942557 12.7369904  20.34285287]]
```

Expected Output

```
TV marketing expenses:
[ 50 120 280]
Predictions of sales using Scikit_Learn linear regression:
[[ 9.40942557 12.7369904  20.34285287]]
```

[22]:
```
w2_unittest.test_sklearn_predict(pred_sklearn, lr_sklearn)
```

```
 All tests passed
```

The predicted values are also the same.

## 3 - Linear Regression using Gradient Descent

Functions to fit the models automatically are convenient to use, but for an in-depth understanding of the model and the maths behind it is good to implement an algorithm by yourself. Let's try to find linear regression coefficients m and b, by minimising the difference between original values $y^{(i)}$ and predicted values $\hat{y}^{(i)}$ with the **loss function** $L\left(w, b\right) = \frac{1}{2}\left(\hat{y}^{(i)} - y^{(i)}\right)^2$ for each of the training examples. Division by 2 is taken just for scaling purposes, you will see the reason below, calculating partial derivatives.

To compare the resulting vector of the predictions $\hat{Y}$ with the vector Y of original values $y^{(i)}$, you can take an average of the loss function values for each of the training examples:

$$E\left(m, b\right) = \frac{1}{2n}\sum_{i=1}^{n} \left(\hat{y}^{(i)} - y^{(i)}\right)^2 = \frac{1}{2n}\sum_{i=1}^{n} \left(mx^{(i)}+b - y^{(i)}\right)^2, \tag{1}$$

where n is a number of data points. This function is called the sum of squares **cost function**. To use gradient descent algorithm, calculate partial derivatives as:

$$\frac{\partial E}{\partial m} = \frac{1}{n}\sum_{i=1}^{n}\left(mx^{(i)} + b - y^{(i)}\right)x^{(i)}, \tag{1}$$

$$\frac{\partial E}{\partial b} = \frac{1}{n}\sum_{i=1}^{n}\left(mx^{(i)} + b - y^{(i)}\right), \tag{2}$$

and update the parameters iteratively using the expressions

$$m = m - \alpha\frac{\partial E}{\partial m}, \tag{2}$$

$$b = b - \alpha\frac{\partial E}{\partial b}, \tag{3}$$

where α is the learning rate.

Original arrays `X` and `Y` have different units. To make gradient descent algorithm efficient, you need to bring them to the same units. A common approach to it is called **normalization**: substract the mean value of the array from each of the elements in the array and divide them by standard deviation (a statistical measure of the amount of dispersion of a set of values). If you are not familiar with mean and standard deviation, do not worry about this for now - this is covered in the next Course of Specialization.

Normalization is not compulsory - gradient descent would work without it. But due to different units of `X` and `Y`, the cost function will be much steeper. Then you would need to take a significantly smaller learning rate α, and the algorithm will require thousands of iterations to converge instead of a few dozens. Normalization helps to increase the efficiency of the gradient descent algorithm.

Normalization is implemented in the following code:

[23]:
```
X_norm = (X - np.mean(X))/np.std(X)
Y_norm = (Y - np.mean(Y))/np.std(Y)
```

Define cost function according to the equation (1):

[24]:
```
def E(m, b, X, Y):
    return 1/(2*len(Y))*np.sum((m*X + b - Y)**2)
```

### Exercise 5

Define functions `dEdm` and `dEdb` to calculate partial derivatives according to the equations (2). This can be done using vector form of the input data `X` and `Y`.

[25]:
```
def dEdm(m, b, X, Y):
    ### START CODE HERE ### (~ 1 line of code)
    # Use the following line as a hint, replacing all None.
    res = 1/len(Y)*np.dot((m * X + b - Y), X)
    ### END CODE HERE ###
    return res


def dEdb(m, b, X, Y):
    ### START CODE HERE ### (~ 1 line of code)
    # Replace None writing the required expression fully.
    res = 1/len(Y) * np.sum(m * X + b - Y)
    ### END CODE HERE ###

    return res
```

[26]:
```
print(dEdm(0, 0, X_norm, Y_norm))
print(dEdb(0, 0, X_norm, Y_norm))
print(dEdm(1, 5, X_norm, Y_norm))
print(dEdb(1, 5, X_norm, Y_norm))
```

```
-0.7822244248616067
5.151434834260726e-16
0.21777557513839355
5.000000000000001
```

Expected Output

```
-0.7822244248616067
5.098005351200641e-16
0.21777557513839355
5.000000000000002
```

[27]:
```
w2_unittest.test_partial_derivatives(dEdm, dEdb, X_norm, Y_norm)
```

```
 All tests passed
```

### Exercise 6

Implement gradient descent using expressions (3):

$$m = m - \alpha \frac{\partial E}{\partial m}, \tag{3}$$
$$b = b - \alpha \frac{\partial E}{\partial b}, \tag{4}$$

where α is the `learning_rate`.

[28]:
```
def gradient_descent(dEdm, dEdb, m, b, X, Y, learning_rate = 0.001,␣
↪num_iterations = 1000, print_cost=False):
    for iteration in range(num_iterations):
        ### START CODE HERE ### (~ 2 lines of code)
        m_new = m - learning_rate * dEdm(m, b, X, Y)
        b_new = b - learning_rate * dEdb(m, b, X, Y)
        ### END CODE HERE ###
        m = m_new
        b = b_new
        if print_cost:
            print (f"Cost after iteration {iteration}: {E(m, b, X, Y)}")

    return m, b
```

[29]:
```
print(gradient_descent(dEdm, dEdb, 0, 0, X_norm, Y_norm))
print(gradient_descent(dEdm, dEdb, 1, 5, X_norm, Y_norm, learning_rate = 0.01,␣
 ↪num_iterations = 10))
```

```
(0.49460408269589495, -3.4915181856831644e-16)
(0.9791767513915026, 4.521910375044022)
```

Expected Output

```
(0.49460408269589495, -3.489285249624889e-16)
(0.9791767513915026, 4.521910375044022)
```

[30]:
```
w2_unittest.test_gradient_descent(gradient_descent, dEdm, dEdb, X_norm, Y_norm)
```

```
 All tests passed
```

Now run the gradient descent method starting from the initial point $(m_0, b_0) = (0, 0)$.

[31]:
```
m_initial = 0; b_initial = 0; num_iterations = 30; learning_rate = 1.2
m_gd, b_gd = gradient_descent(dEdm, dEdb, m_initial, b_initial,
                              X_norm, Y_norm, learning_rate, num_iterations,␣
 ↪print_cost=True)

print(f"Gradient descent result: m_min, b_min = {m_gd}, {b_gd}")
```

```
Cost after iteration 0: 0.20629997559196597
Cost after iteration 1: 0.19455197461564464
Cost after iteration 2: 0.19408205457659178
Cost after iteration 3: 0.19406325777502967
Cost after iteration 4: 0.19406250590296714
Cost after iteration 5: 0.19406247582808467
Cost after iteration 6: 0.19406247462508938
Cost after iteration 7: 0.19406247457696957
Cost after iteration 8: 0.19406247457504477
Cost after iteration 9: 0.19406247457496775
Cost after iteration 10: 0.1940624745749647
Cost after iteration 11: 0.19406247457496456
Cost after iteration 12: 0.19406247457496456
Cost after iteration 13: 0.19406247457496456
Cost after iteration 14: 0.19406247457496456
Cost after iteration 15: 0.19406247457496456
Cost after iteration 16: 0.19406247457496456
Cost after iteration 17: 0.19406247457496456
Cost after iteration 18: 0.19406247457496456
Cost after iteration 19: 0.19406247457496456
Cost after iteration 20: 0.19406247457496456
Cost after iteration 21: 0.19406247457496456
Cost after iteration 22: 0.19406247457496456
Cost after iteration 23: 0.19406247457496456
Cost after iteration 24: 0.19406247457496456
Cost after iteration 25: 0.19406247457496456
Cost after iteration 26: 0.19406247457496456
Cost after iteration 27: 0.19406247457496456
Cost after iteration 28: 0.19406247457496456
Cost after iteration 29: 0.19406247457496456
Gradient descent result: m_min, b_min = 0.7822244248616068,
-6.075140390748858e-16
```

Remember, that the initial datasets were normalized. To make the predictions, you need to normalize `X_pred` array, calculate `Y_pred` with the linear regression coefficients `m_gd`, `b_gd` and then **denormalize** the result (perform the reverse process of normalization):

[32]:
```
X_pred = np.array([50, 120, 280])
# Use the same mean and standard deviation of the original training array X
X_pred_norm = (X_pred - np.mean(X))/np.std(X)
Y_pred_gd_norm = m_gd * X_pred_norm + b_gd
# Use the same mean and standard deviation of the original training array Y
Y_pred_gd = Y_pred_gd_norm * np.std(Y) + np.mean(Y)

print(f"TV marketing expenses:\n{X_pred}")
print(f"Predictions of sales using Scikit_Learn linear regression:
 ↪\n{Y_pred_sklearn.T}")
print(f"Predictions of sales using Gradient Descent:\n{Y_pred_gd}")
```

```
TV marketing expenses:
[ 50 120 280]
Predictions of sales using Scikit_Learn linear regression:
[[ 9.40942557 12.7369904  20.34285287]]
Predictions of sales using Gradient Descent:
[ 9.40942557 12.7369904  20.34285287]
```

You should have gotten similar results as in the previous sections.

Well done! Now you know how gradient descent algorithm can be applied to train a real model. Reproducing results manually for a simple case should give you extra confidence that you understand what happends under the hood of commonly used functions.

[ ]:
```

```