Linear supervised regression

0. Import library

Import library

```
# Import libraries

# math library
import numpy as np

# visualization library
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('png2x','pdf')
import matplotlib.pyplot as plt

# machine learning library
from sklearn.linear_model import LinearRegression

# 3d visualization
from mpl_toolkits.mplot3d import axes3d

# computational time
import time

```

1. Load dataset

Load a set of data pairs $\{x_i, y_i\}_{i=1}^n$ where x represents label and y represents target.

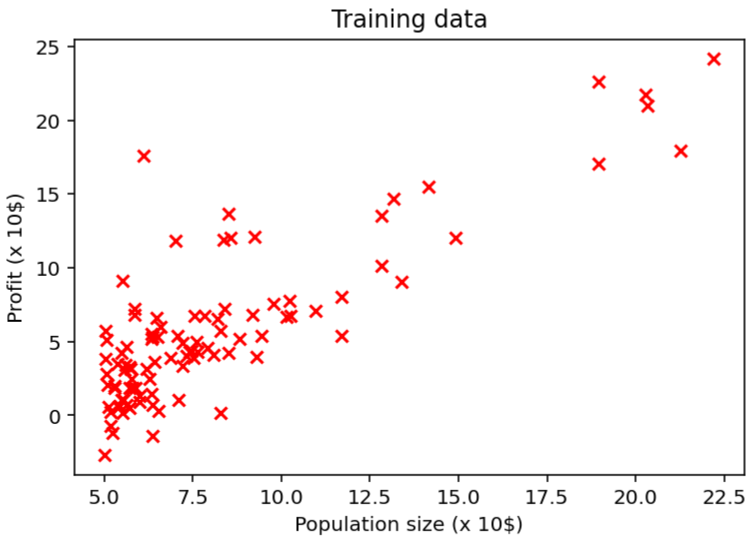
```python
# import data with numpy
data = np.loadtxt('profit_population.txt', delimiter=',')

```

2. Explore the dataset distribution

Plot the training data points.

```python
x_train = data[:,0]
y_train = data[:,1]

plt.title('Training data')
plt.xlabel('Population size (x 10$)')
plt.ylabel('Profit (x 10$)')
plt.scatter(x_train, y_train, c = 'r', marker = 'x')
```

```
<matplotlib.collections.PathCollection at 0x7fab6a068208>
```



3. Define the linear prediction function

$$f_w(x) = w_0 + w_1 x$$

Vectorized implementation:

$$f_w(x) = Xw$$

with

$$X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \\ 1 & x_n \end{bmatrix} \quad \text{and} \quad w = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix} \quad \Rightarrow \quad f_w(x) = Xw = \begin{bmatrix} w_0 + w_1 x_1 \\ w_0 + w_1 x_2 \\ \vdots \\ w_0 + w_1 x_n \end{bmatrix}$$

```
# construct data matrix
X = np.ones((len(x_train), 2))
for i in range(len(X)):
    X[i][1] = x_train[i]

# parameters vector
w = [1, 1]

# predictive function definition
def f_pred(X,w):

    f = np.dot(X,w)

    return f

# Test predicitive function
y_pred = f_pred(X,w)

```

4. Define the linear regression loss

$$L(w) = \frac{1}{n} \sum_{i=1}^{n} \left(f_w(x_i) - y_i \right)^2$$

Vectorized implementation:

$$L(w) = \frac{1}{n}(Xw - y)^T (Xw - y)$$

with

$$Xw = \begin{bmatrix} w_0 + w_1 x_1 \\ w_0 + w_1 x_2 \\ \vdots \\ w_0 + w_1 x_n \end{bmatrix} \quad \text{and} \quad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

Implement the vectorized version of the linear regression loss function

```
# loss function definition
def loss_mse(y_pred,y):

    loss = np.sum((y_pred - y) ** 2) / len(y)
    return loss


# Test loss function
y = y_train
y_pred = f_pred(X,w)
loss = loss_mse(y_pred,y)
```

5. Define the gradient of the linear regression loss

Vectorized implementation: Given the loss

$$L(w) = \frac{1}{n}(Xw - y)^T(Xw - y)$$

The gradient is given by

$$\frac{\partial}{\partial w}L(w) = \frac{2}{n}X^T(Xw - y)$$

Implement the vectorized version of the gradient of the linear regression loss function.

```
# gradient function definition
def grad_loss(y_pred,y,X):

    grad = np.dot(X.T, y_pred - y) / len(X) * 2

    return grad


# Test grad function
y_pred = f_pred(X,w)
grad = grad_loss(y_pred,y,X)
```

6. Implement the gradient descent algorithm

- Vectorized implementation:

$$w^{k+1} = w^k - \tau\frac{2}{n}X^T(Xw^k - y)$$

Implement the vectorized version of the gradient descent function.

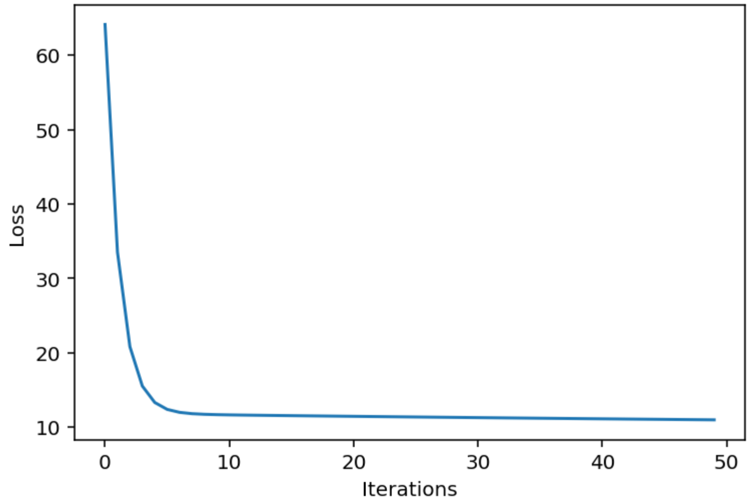
Plot the loss values $L(w^k)$ with respect to iteration k the number of iterations.

```
# gradient descent function definition
def grad_desc(X, y, w_init, tau, max_iter):
```

```
    L_iters = [] # record the loss values
    w_iters = [] # record the parameter values
    w = w_init # initialization

    for i in range(max_iter): # loop over the iterations
        tmp = []
        y_pred = f_pred(X,w) # linear predicition function
        grad_f = grad_loss(y_pred, y, X) # gradient of the loss

        for j in range(len(w)):
            w[j] = w[j] - tau * grad_f[j] # update rule of gradient descent
            tmp.append(w[j])

        w_iters.append(tmp) # save the current w value
        L_iters.append(loss_mse(y_pred, y)) # save the current loss value

    return w, L_iters, w_iters


# run gradient descent algorithm
start = time.time()
w_init = [0, 0]
tau = 0.01
max_iter = 50

w, L_iters, w_iters = grad_desc(X, y, w_init, tau, max_iter)

print('Time=',time.time() - start) # plot the computational cost
print(L_iters[-1] ) # plot the last value of the loss
print(w) # plot the last value of the parameter w


# plot
plt.figure(2)
plt.plot([i for i in range(len(L_iters))], L_iters) # plot the loss curve
plt.xlabel('Iterations')
plt.ylabel('Loss')
```

```
plt.ylabel('Loss')
plt.show()
```

```
Time= 0.0014889240264892578
10.973835031833165
[-0.5770974029560515, 0.8596358917014932]
```

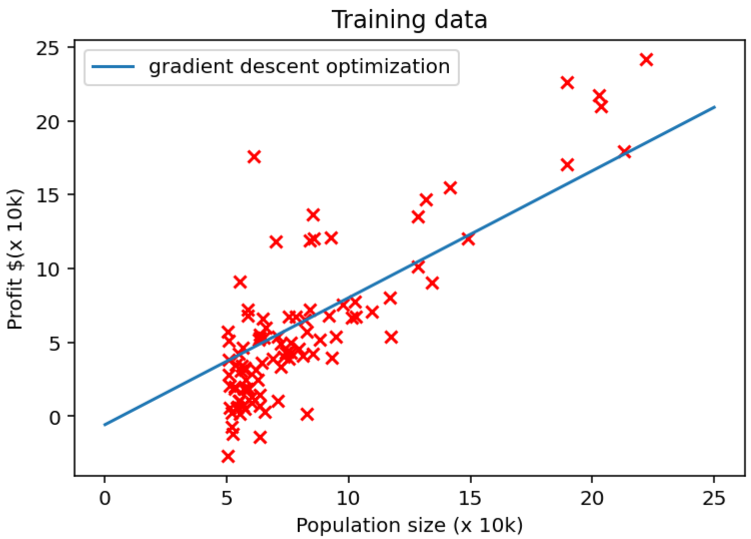


7. Plot the linear prediction function

$$f_w(x) = w_0 + w_1 x$$

```
# linear regression model
x_pred = np.linspace(0,25,100) # define the domain of the prediction function
y_pred = x_pred * w[1] + w[0]
# plot
plt.figure(3)
plt.scatter(x_train, y_train, c='r', marker = 'x')
plt.plot(x_pred, y_pred, label ='gradient descent optimization' )
plt.legend(loc='best')
plt.title('Training data')
plt.xlabel('Population size (x 10k)')
plt.ylabel('Profit $(x 10k)')
plt.show()
```

```
plt.show()
```



8. Comparison with Scikit-learn linear regression algorithm

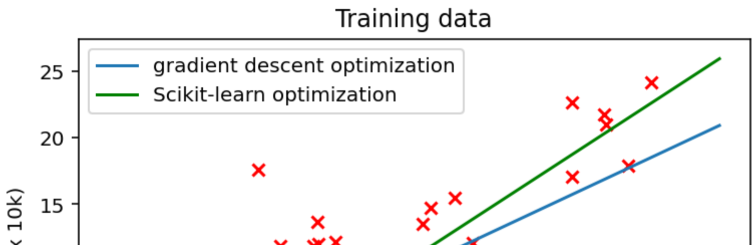
Compare with the Scikit-learn solution

```
# run linear regression with scikit-learn
start = time.time()
lin_reg_sklearn = LinearRegression()
sklearn_x_train = x_train.reshape(len(x_train), 1)
sklearn_y_train = y_train.reshape(len(y_train), 1)

lin_reg_sklearn.fit(sklearn_x_train,sklearn_y_train) # learn the model parameters
print('Time=',time.time() - start)


# compute loss value
w_sklearn = np.zeros([2,1])
w_sklearn[0,0] = lin_reg_sklearn.intercept_
w_sklearn[1,0] = lin_reg_sklearn.coef_
```

```
print(w_sklearn)

loss_sklearn = lin_reg_sklearn.score(sklearn_x_train, sklearn_y_train) # compute the loss from the sklearn solution

print('loss sklearn=',loss_sklearn)
print('loss gradient descent=',L_iters[-1])


# plot
y_pred_sklearn = lin_reg_sklearn.predict(np.linspace(0,25,100).reshape(100, 1))
```

```
Time= 0.0016458034515380859
[[-3.89578088]
 [ 1.19303364]]
loss sklearn= 0.7020315537841397
loss gradient descent= 10.973835031833165
```

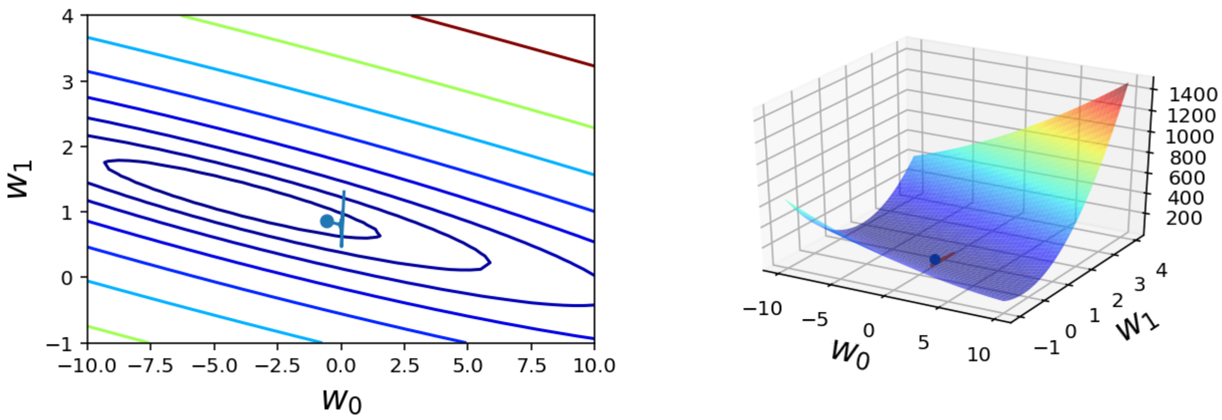
```
plt.figure(3)

plt.scatter(x_train, y_train, c='r', marker = 'x')
plt.plot(x_pred, y_pred, label ='gradient descent optimization' )
plt.plot(x_pred, y_pred_sklearn, c = 'g' ,label = 'Scikit-learn optimization' )
plt.legend(loc='best')
plt.title('Training data')
plt.xlabel('Population size (x 10k)')
plt.ylabel('Profit $(x 10k)')
plt.show()
```



9. Plot the loss surface, the contours of the loss and the gradient descent steps


```
# Create grid coordinates for plotting a range of L(w0,w1)-values
B0 = np.linspace(-10, 10, 50)
B1 = np.linspace(-1, 4, 50)

xx, yy = np.meshgrid(B0, B1, indexing='xy')
Z = np.zeros((B0.size,B1.size))

    # Calculate loss values based on L(w0,w1)-values
for (i,j),v in np.ndenumerate(Z):
    contour_pred = x_train * B1[i] + B0[j]
    Z[i,j] = np.sum((contour_pred - y) ** 2) / len(y)
    # 3D visualization
fig = plt.figure(figsize=(10,3))
ax1 = fig.add_subplot(121)
ax2 = fig.add_subplot(122, projection='3d')

    # Left plot
CS = ax1.contour(xx, yy, Z, np.logspace(-2, 3, 20), cmap=plt.cm.jet)
ax1.scatter(w[0], w[1])
ax1.plot(np.array(w_iters)[:,0],np.array(w_iters)[:,1]) # plot the loss curve

# Right plot
ax2.plot_surface(xx, yy, Z, rstride=1, cstride=1, alpha=0.6, cmap=plt.cm.jet)
ax2.set_zlabel('Loss $L(w_0,w_1)$')
ax2.set_zlim(Z.min(),Z.max())
ax2.plot(np.array(w_iters)[:,0],np.array(w_iters)[:,1])
```

```
ax2.scatter(w[0], w[1])

# settings common to both plots
for ax in fig.axes:
    ax.set_xlabel(r'$w_0$', fontsize=17)
    ax.set_ylabel(r'$w_1$', fontsize=17)
```

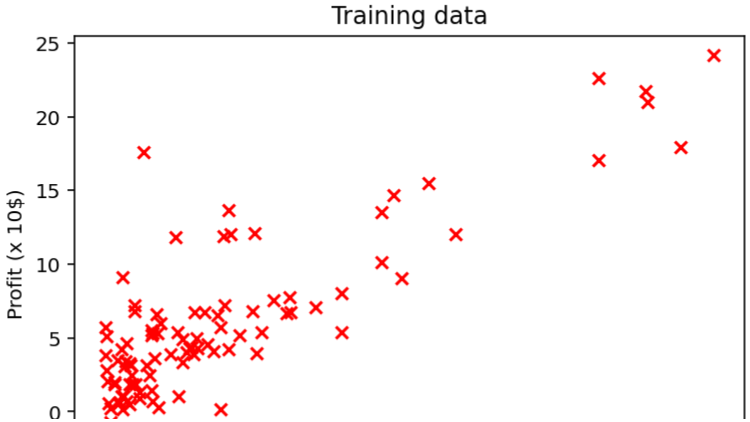


Output results

1. Plot the training data (1pt)

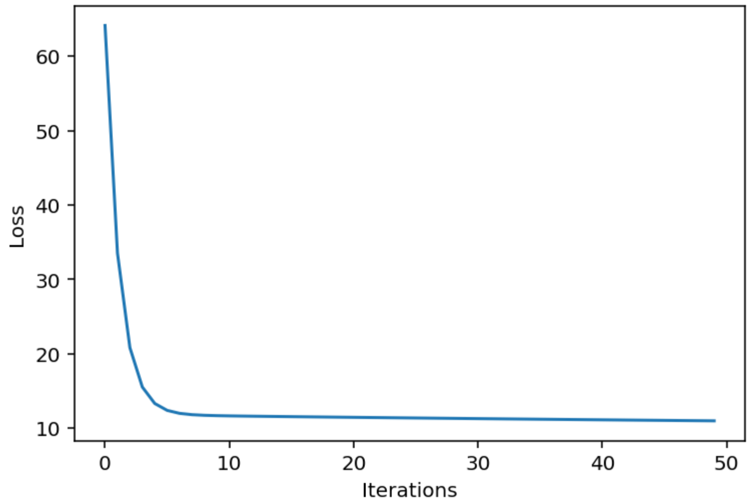
```
plt.title('Training data')
plt.xlabel('Population size (x 10$)')
plt.ylabel('Profit (x 10$)')
plt.scatter(x_train, y_train, c = 'r', marker = 'x')
```

<matplotlib.collections.PathCollection at 0x7fab654a5668>



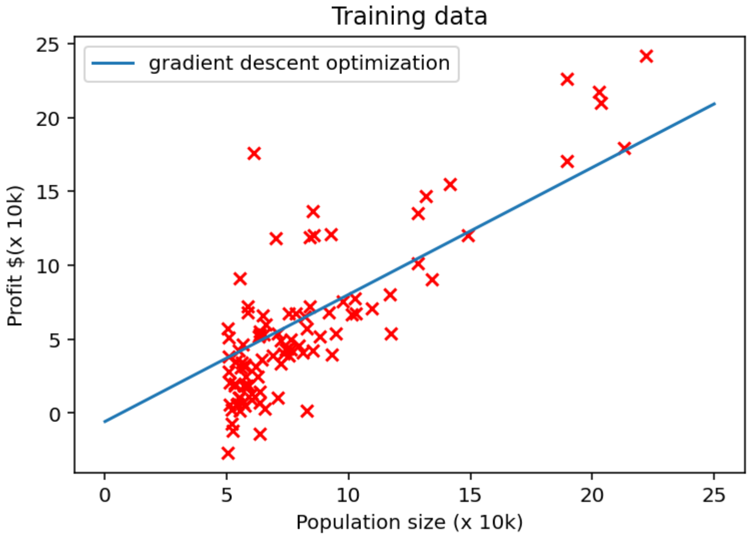
2. Plot the loss curve in the course of gradient descent (2pt)

```
plt.figure(2)
plt.plot([i for i in range(len(L_iters))], L_iters) # plot the loss curve
plt.xlabel('Iterations')
plt.ylabel('Loss')
plt.show()
```



3. Plot the prediction function superimposed on the training data (2pt)

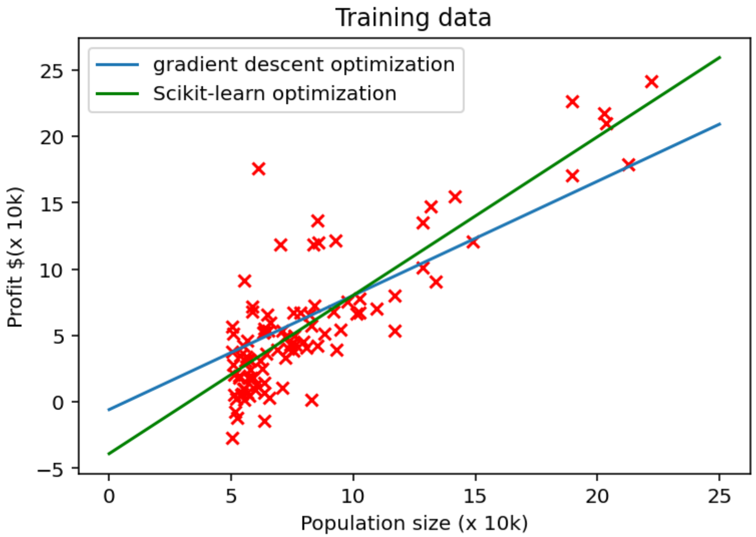
```
plt.scatter(x_train, y_train, c='r', marker = 'x')
plt.plot(x_pred, y_pred, label ='gradient descent optimization' )
plt.legend(loc='best')
plt.title('Training data')
plt.xlabel('Population size (x 10k)')
plt.ylabel('Profit $(x 10k)')
plt.show()
```



4. Plot the prediction functions obtained by both the Scikit-learn linear regression solution and the gradient descent superimposed on the training data (2pt)

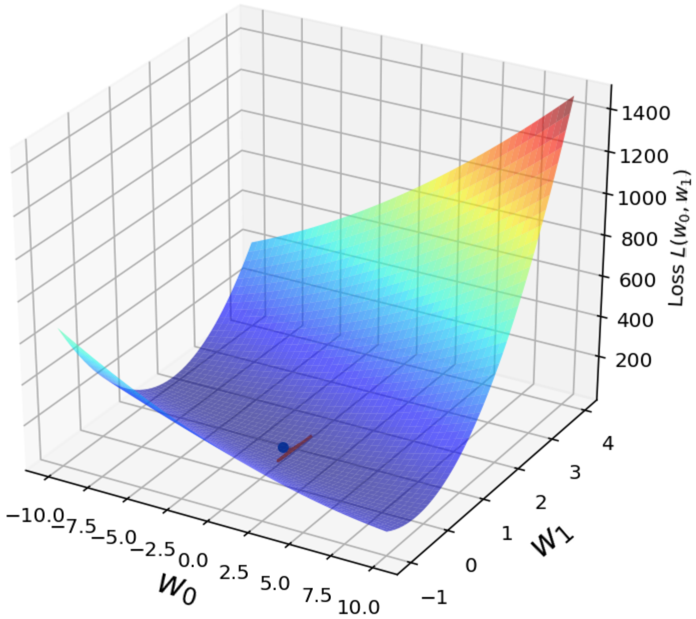
```
plt.scatter(x_train, y_train, c='r', marker = 'x')
plt.plot(x_pred, y_pred, label ='gradient descent optimization' )
plt.plot(x_pred, y_pred_sklearn, c = 'g' ,label = 'Scikit-learn optimization' )
```

```
plt.legend(loc='best')
plt.title('Training data')
plt.xlabel('Population size (x 10k)')
plt.ylabel('Profit $(x 10k)')
plt.show()
```



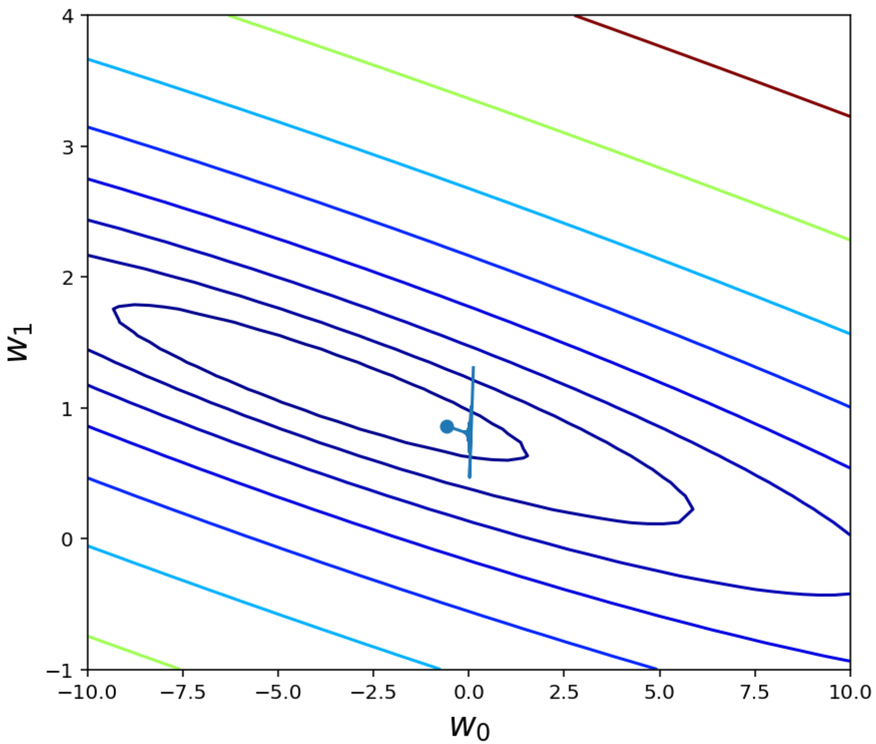
5. Plot the loss surface (right) and the path of the gradient descent (2pt)

```
fig = plt.figure(figsize=(15,6))
ax2 = fig.add_subplot(122, projection='3d')
ax2.plot_surface(xx, yy, Z, rstride=1, cstride=1, alpha=0.6, cmap=plt.cm.jet)
ax2.set_zlabel('Loss $L(w_0,w_1)$')
ax2.set_zlim(Z.min(),Z.max())
ax2.plot(np.array(w_iters)[:,0],np.array(w_iters)[:,1])
ax2.scatter(w[0], w[1])

for ax in fig.axes:
    ax.set_xlabel(r'$w_0$', fontsize=17)
    ax.set_ylabel(r'$w_1$', fontsize=17)
```



6. Plot the contour of the loss surface (left) and the path of the gradient descent (2pt)

```python
fig = plt.figure(figsize=(15,6))
ax1 = fig.add_subplot(121)

CS = ax1.contour(xx, yy, Z, np.logspace(-2, 3, 20), cmap=plt.cm.jet)
ax1.scatter(w[0], w[1])
ax1.plot(np.array(w_iters)[:,0],np.array(w_iters)[:,1]) # plot the loss curve

for ax in fig.axes:
    ax.set_xlabel(r'$w_0$', fontsize=17)
    ax.set_ylabel(r'$w_1$', fontsize=17)
```


4
3
2
1
0
−1
w_1
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
10.0
w_0