assignment_02_assignment-02-b

September 15, 2020

0.1 Linear supervised regression

0.2 0. Import library

Import library

[5]:
```
# 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
```

0.3 1. Load dataset

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

[6]:
```
# import data with numpy
data = np.loadtxt('profit_population.txt', delimiter=',')
```

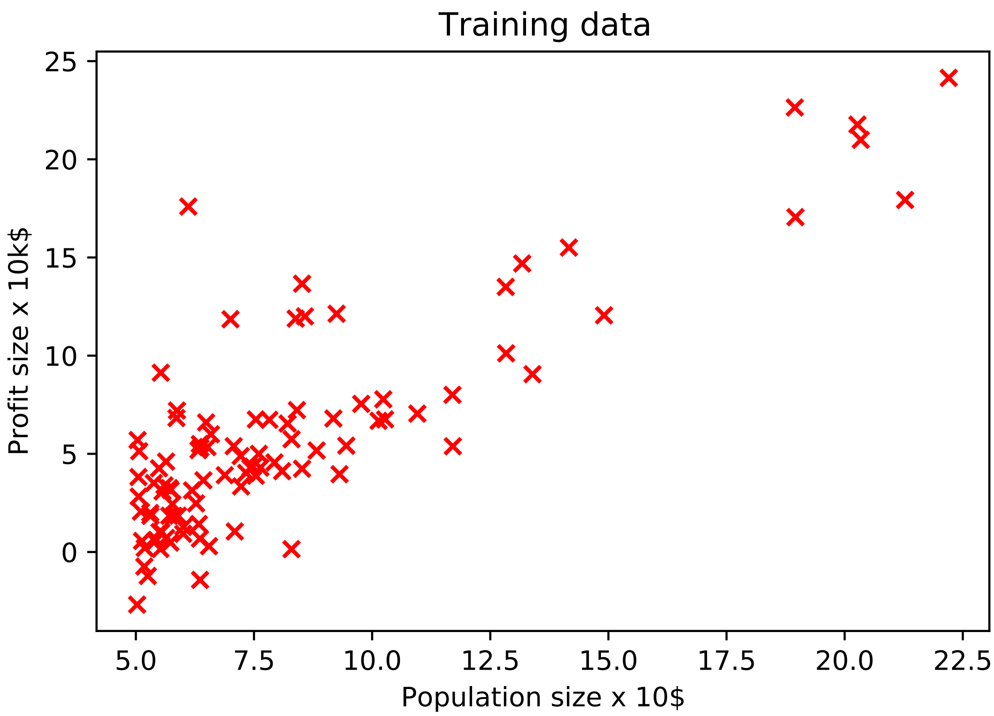
0.4 2. Explore the dataset distribution

Plot the training data points.

[7]:
```
x_train = data[:,0]
y_train = data[:,1]
```

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

[7]: <matplotlib.collections.PathCollection at 0x7fd40f0ab9e8>



0.5 3. Define the linear prediction function

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

0.5.1 Vectorized implementation:

$$f_w(x) = Xw$$

with

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

Implement the vectorized version of the linear predictive function.

[8]:
```python
# construct data matrix
X = np.append(np.ones(x_train.size).reshape(-1, 1), np.array(x_train).
 ↪reshape(-1, 1) , axis = 1)
```

```
# parameters vector
w = np.array([[0], [0]])

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

    f = np.dot(X, w)

    return f

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

0.6 4. Define the linear regression loss

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

0.6.1 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.

[9]:
```
# loss function definition
def loss_mse(y_pred,y):

    temp_y = y_pred - y
    loss = np.dot(temp_y.T, temp_y) / y_pred.size

    return loss


# Test loss function
y = np.array(y_train).reshape(-1, 1)# label
y_pred = f_pred(X, w)# prediction

loss = loss_mse(y_pred,y)
print(loss)
```

```
[[64.14546775]]
```

0.7 5. Define the gradient of the linear regression loss

0.7.1 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.

[10]:
```
# gradient function definition
def grad_loss(y_pred,y,X):

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


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

0.8 6. Implement the gradient descent algorithm

- Vectorized implementation:

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

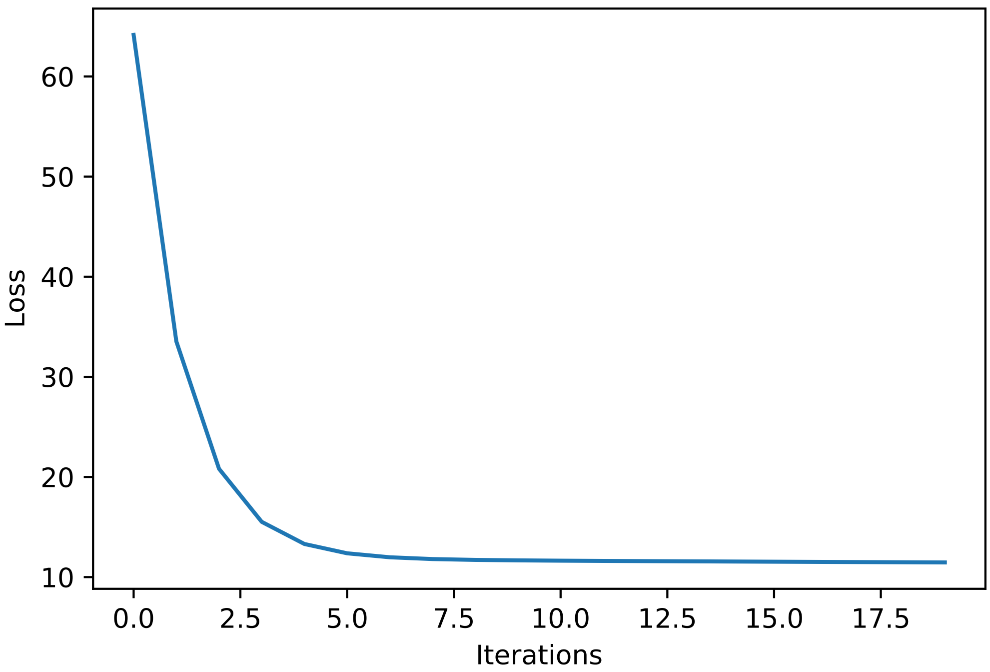
0.8.1 Implement the vectorized version of the gradient descent function.

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

[11]:
```
# gradient descent function definition
def grad_desc(X, y, w_init, tau, max_iter):

    L_iters = np.empty((max_iter, 1))# record the loss values
    w_iters = np.empty((max_iter, 2))# record the parameter values
    w = w_init # initialization

    for i in range(max_iter): # loop over the iterations

        y_pred = f_pred(X, w)# linear predicition function
        grad_f = grad_loss(y_pred,y,X)# gradient of the loss
        w = w - tau * grad_f# update rule of gradient descent
        L_iters[i] = loss_mse(y_pred,y)# save the current loss value
        w_iters[i,:] = w.T# save the current w value
```

```python
    return w, L_iters, w_iters


# run gradient descent algorithm
start = time.time()
w_init = np.array([[0],[0]])
tau = 0.01
max_iter = 20

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[max_iter-1][0]) # plot the last value of the loss
print(w) # plot the last value of the parameter w


# plot
plt.figure(2)
plt.plot(L_iters) # plot the loss curve
plt.xlabel('Iterations')
plt.ylabel('Loss')
plt.show()
```

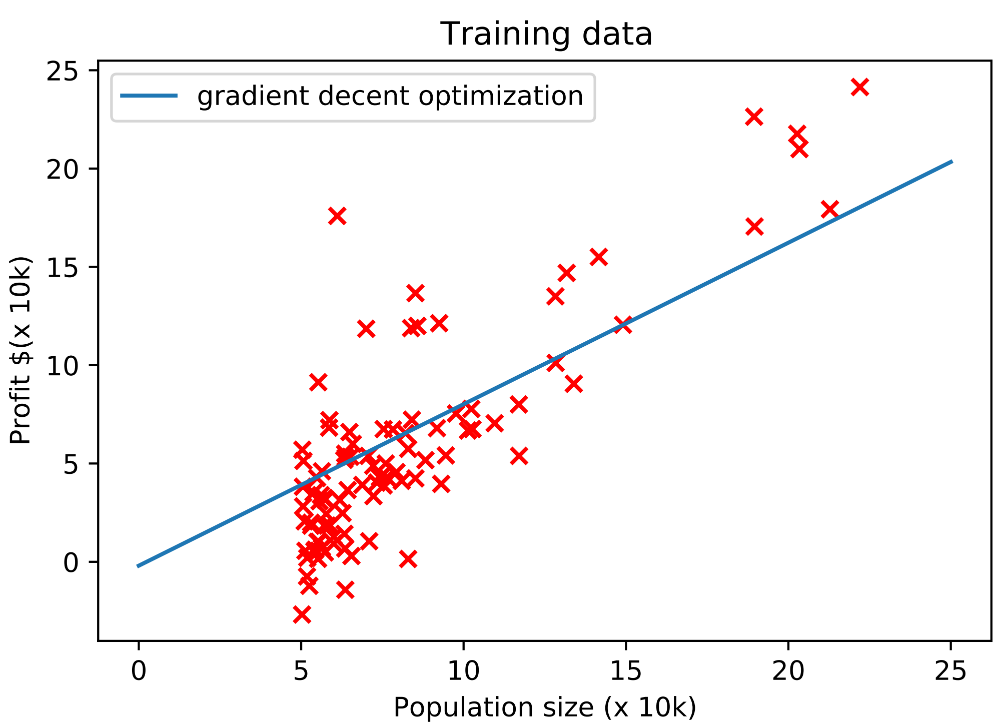
```
Time= 0.0014061927795410156
11.462600167377458
[[-0.19732262]
 [ 0.82136091]]
```



0.9 7. Plot the linear prediction function

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

[14]:
```
# linear regression model
x_pred = np.linspace(0,25,100) # define the domain of the prediction function
x_pred = np.append(np.ones(x_pred.size).reshape(-1, 1), np.array(x_pred).
 ↪reshape(-1, 1) , axis = 1)
y_pred = f_pred(x_pred, w)# compute the prediction values within the given␣
 ↪domain x_pred

# plot
plt.figure(3)
plt.scatter(x_train, y_train, c = 'r', marker = 'x')
line1, = plt.plot(x_pred[:, 1], y_pred)
plt.legend(handles = (line1,), prop={'size': 10}, labels = ['gradient decent␣
 ↪optimization'], loc='upper left')
plt.title('Training data')
plt.xlabel('Population size (x 10k)')
plt.ylabel('Profit $(x 10k)')
plt.show()
```



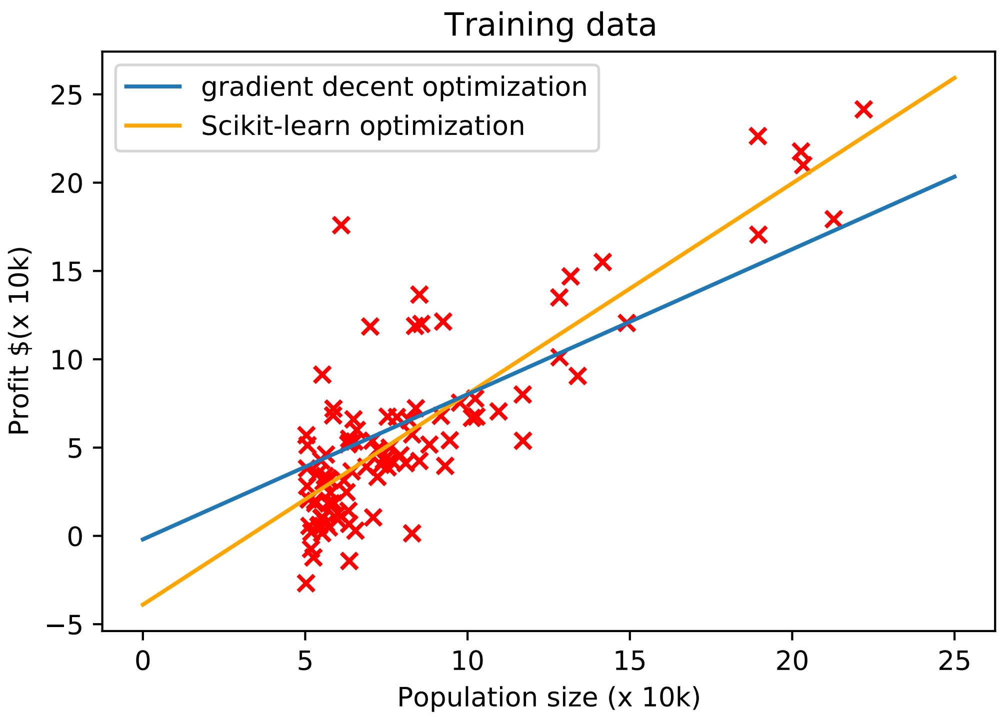
0.10 8. Comparison with Scikit-learn linear regression algorithm

0.10.1 Compare with the Scikit-learn solution

[15]:
```
# run linear regression with scikit-learn
start = time.time()
lin_reg_sklearn = LinearRegression()
lin_reg_sklearn.fit(np.array(x_train).reshape(-1, 1), np.array(y_train).
 ↪reshape(-1, 1)) # 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)

y_pred_sklearn = lin_reg_sklearn.predict(np.array(x_train).reshape(-1, 1))
loss_sklearn = loss_mse(y_pred_sklearn, y) # compute the loss from the sklearn␣
 ↪solution

print('loss sklearn=',loss_sklearn)
print('loss gradient descent=',L_iters[-1][0])


# plot
x_pred_sklearn = np.linspace(0,25,100)
y_pred_sklearn = lin_reg_sklearn.predict(np.array(x_pred_sklearn).reshape(-1,␣
 ↪1))# prediction obtained by the sklearn library

plt.figure(3)

line2, = plt.plot(x_pred_sklearn, y_pred_sklearn, c = 'orange')
line1, = plt.plot(x_pred[:, 1], y_pred)
plt.scatter(x_train, y_train, c = 'r', marker = 'x')
plt.legend(handles = (line1, line2), prop={'size': 10}, labels = ['gradient␣
 ↪decent optimization', 'Scikit-learn optimization'], loc='upper left')
plt.title('Training data')
plt.xlabel('Population size (x 10k)')
plt.ylabel('Profit $(x 10k)')
plt.show()
```

```
Time= 0.023693561553955078
[[-3.89578088]
 [ 1.19303364]]
loss sklearn= [[8.95394275]]
```

```
loss gradient descent= 11.462600167377458
```



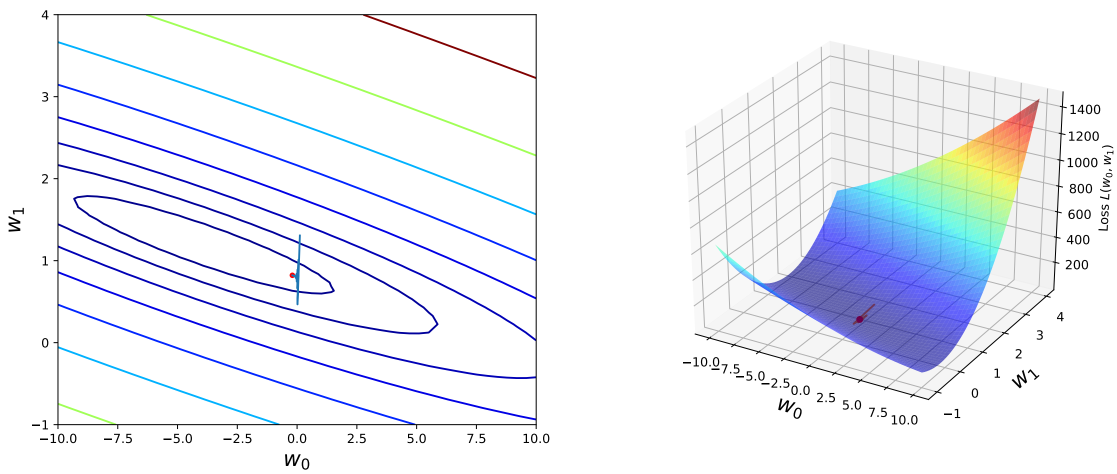
0.11 9. Plot the loss surface, the contours of the loss and the gradient descent steps

[53]:
```
# plot gradient descent
def plot_gradient_descent(X,y,w_init,tau,max_iter):

    def f_pred(X,w):

        f = np.dot(X, w)

        return f

    def loss_mse(y_pred,y):

        temp_y = y_pred - y
        loss = np.dot(temp_y.T, temp_y) / y_pred.size

        return loss

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

```
    L_iters = np.empty((max_iter, 1))# record the loss values
    w_iters = np.empty((max_iter, 2))# record the parameter values
    w = w_init # initialization

    for i in range(max_iter): # loop over the iterations

        y_pred = f_pred(X, w)# linear predicition function
        grad_f = grad_loss(y_pred,y,X)# gradient of the loss
        w = w - tau * grad_f# update rule of gradient descent
        L_iters[i] = loss_mse(y_pred,y)# save the current loss value
        w_iters[i,:] = w.T# save the current w value

    return w, L_iters, w_iters

# run gradient descent
w, L_iters, w_iters = grad_desc(X, y, w_init, tau, max_iter)

# 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
w_B = np.empty([2,1], dtype=float)
for (i,j),v in np.ndenumerate(Z):
    w_B[0][0] = B0[j]
    w_B[1][0] = B1[i]
    y_B = f_pred(X, w_B)
    Z[i,j] = loss_mse(y_B, y)


# 3D visualization
fig = plt.figure(figsize=(15,6))
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], L_iters[max_iter - 1][0],  c = 'r') # ????
ax1.plot(w_iters[:, 0], w_iters[:, 1])

# 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())

    # plot gradient descent
    Z2 = np.zeros([max_iter])
    w0 = np.empty(max_iter)
    w1 = np.empty(max_iter)
    for i in range(max_iter):
        w0[i] = w_iters[i][0]
        w1[i] = w_iters[i][1]
        Z2[i] = L_iters[i][0]

    ax2.plot(w0, w1, Z2)
    ax2.scatter(w[0], w[1], L_iters[max_iter - 1][0],  c = 'r') # ???

    # 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)
```

[63]:
```
# run plot_gradient_descent function
w_init = np.array([[0], [0]])
tau = 0.01
max_iter = 20
X = np.append(np.ones(x_train.size).reshape(-1, 1), np.array(x_train).
 ↪reshape(-1, 1) , axis = 1)
y = np.array(y_train).reshape(-1, 1)

plot_gradient_descent(X,y,w_init,tau,max_iter)
```

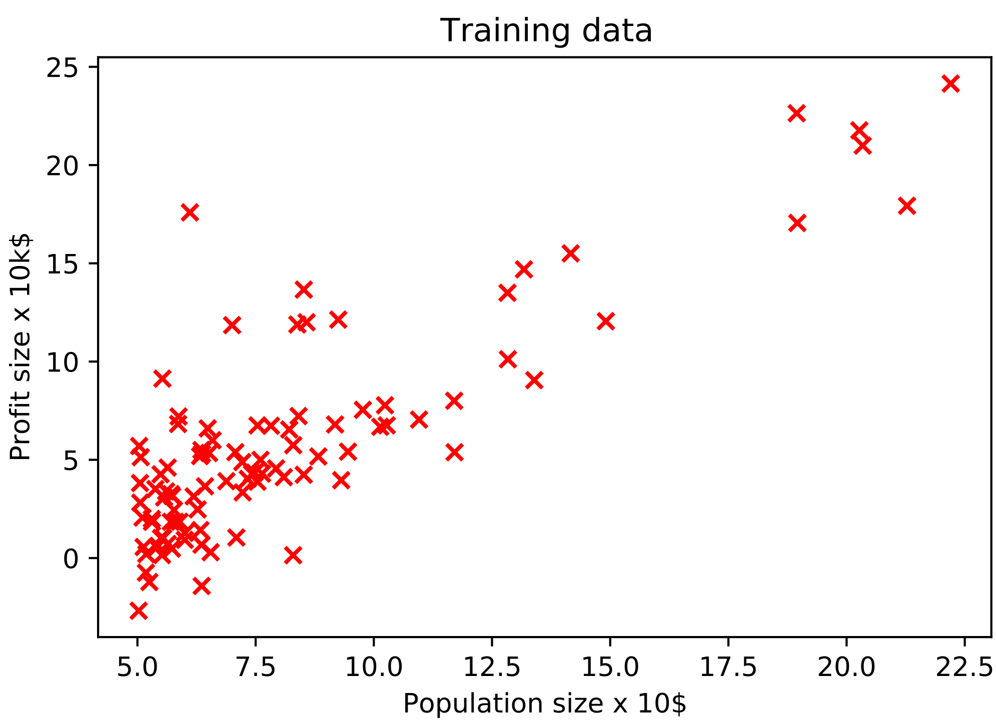


1 Output results

1.1 1. Plot the training data (1pt)

[ ]:
```
x_train = data[:,0]
y_train = data[:,1]
plt.title('Training data')
plt.xlabel('Population size x 10$')
plt.ylabel('Profit size x 10k$')
plt.scatter(x_train, y_train, c = 'r', marker = 'x')
```

[ ]: `<matplotlib.collections.PathCollection at 0x7f0dad652198>`

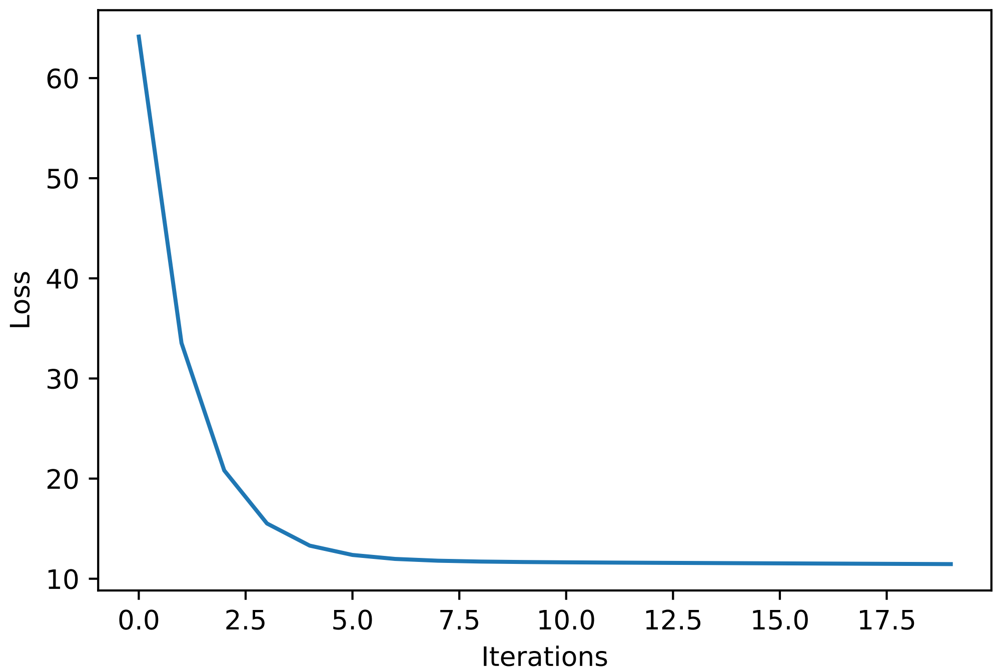


1.2 2. Plot the loss curve in the course of gradient descent (2pt)

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

    L_iters = np.empty((max_iter, 1))# record the loss values
    w_iters = np.empty((max_iter, 2))# record the parameter values
    w = w_init # initialization

    for i in range(max_iter): # loop over the iterations
```

```
        y_pred = f_pred(X, w)# linear predicition function
        grad_f = grad_loss(y_pred,y,X)# gradient of the loss
        w = w - tau * grad_f# update rule of gradient descent
        L_iters[i] = loss_mse(y_pred,y)# save the current loss value
        w_iters[i,:] = w.T# save the current w value

    return w, L_iters, w_iters


# run gradient descent algorithm
start = time.time()
w_init = np.array([[0],[0]])
tau = 0.01
max_iter = 20

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[max_iter-1][0]) # plot the last value of the loss
print(w) # plot the last value of the parameter w


# plot
plt.figure(2)
plt.plot(L_iters) # plot the loss curve
plt.xlabel('Iterations')
plt.ylabel('Loss')
plt.show()
```

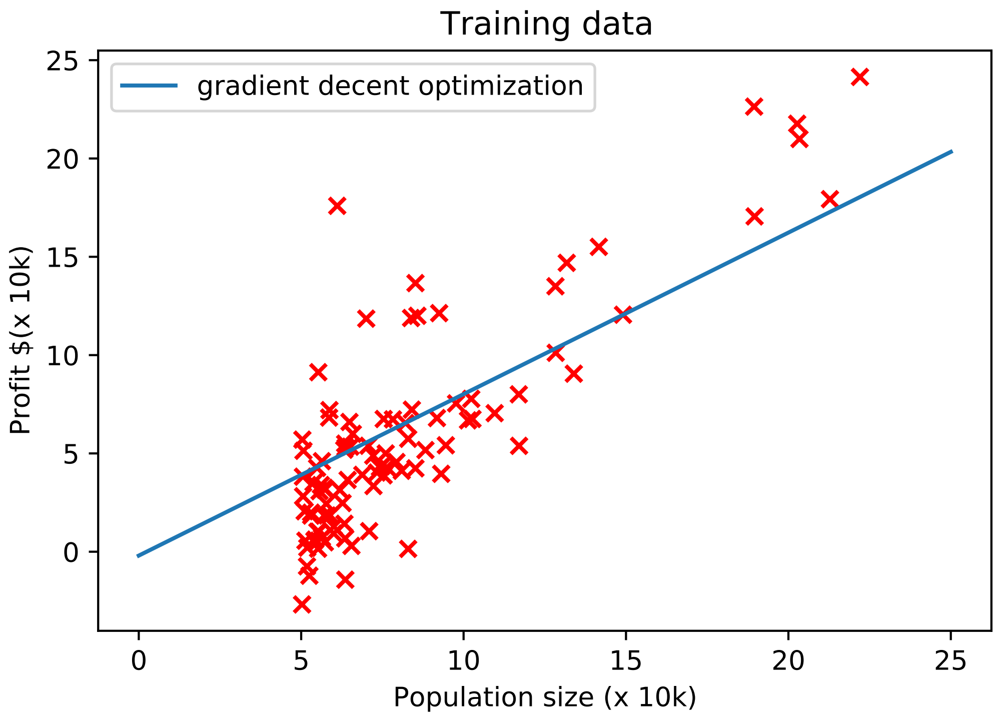
```
Time= 0.0012981891632080078
11.462600167377458
[[-0.19732262]
 [ 0.82136091]]
```



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

[ ]:
```
# linear regression model
x_pred = np.linspace(0,25,100) # define the domain of the prediction function
x_pred = np.append(np.ones(x_pred.size).reshape(-1, 1), np.array(x_pred).
 ↪reshape(-1, 1) , axis = 1)
y_pred = f_pred(x_pred, w)# compute the prediction values within the given␣
 ↪domain x_pred

print(x_pred.shape)
print(y_pred.shape)
# plot
plt.figure(3)
plt.scatter(x_train, y_train, c = 'r', marker = 'x')
line = plt.plot(x_pred[:, 1], y_pred)
plt.legend(handles = (line), prop={'size': 10}, labels = ['gradient decent␣
 ↪optimization'], loc='upper left')
plt.title('Training data')
plt.xlabel('Population size (x 10k)')
plt.ylabel('Profit $(x 10k)')
plt.show()
```

```
(100, 2)
(100, 1)
```

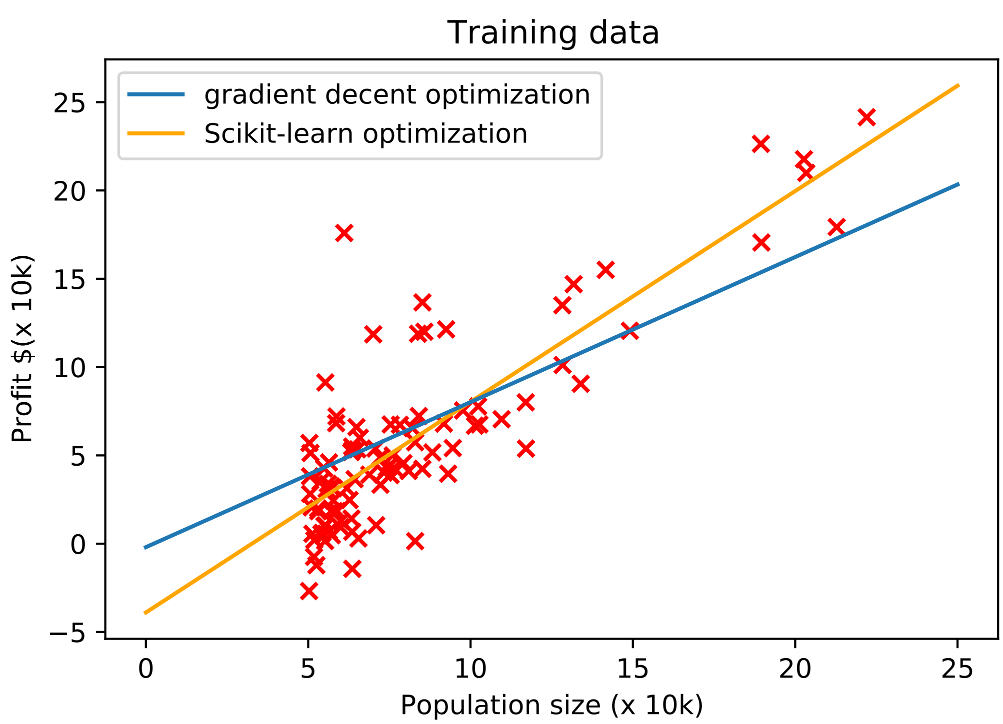


1.4 4. Plot the prediction functions obtained by both the Scikit-learn linear regression solution and the gradient descent superimposed on the training data (2pt)

[ ]:
```
# run linear regression with scikit-learn
start = time.time()
lin_reg_sklearn = LinearRegression()
lin_reg_sklearn.fit(np.array(x_train).reshape(-1, 1), np.array(y_train).
 ↪reshape(-1, 1)) # 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)

y_pred_sklearn = lin_reg_sklearn.predict(np.array(x_train).reshape(-1, 1))
loss_sklearn = loss_mse(y_pred_sklearn, y) # compute the loss from the sklearn␣
 ↪solution

print('loss sklearn=',loss_sklearn)
```

```
print('loss gradient descent=',L_iters[-1][0])


# plot
x_pred_sklearn = np.linspace(0,25,100)
y_pred_sklearn = lin_reg_sklearn.predict(np.array(x_pred_sklearn).reshape(-1,␣
↪1))# prediction obtained by the sklearn library

plt.figure(3)

line2, = plt.plot(x_pred_sklearn, y_pred_sklearn, c = 'orange')
line1, = plt.plot(x_pred[:, 1], y_pred)
plt.scatter(x_train, y_train, c = 'r', marker = 'x')
plt.legend(handles = (line1, line2), prop={'size': 10}, labels = ['gradient␣
↪decent optimization', 'Scikit-learn optimization'], loc='upper left')
plt.title('Training data')
plt.xlabel('Population size (x 10k)')
plt.ylabel('Profit $(x 10k)')
plt.show()
```

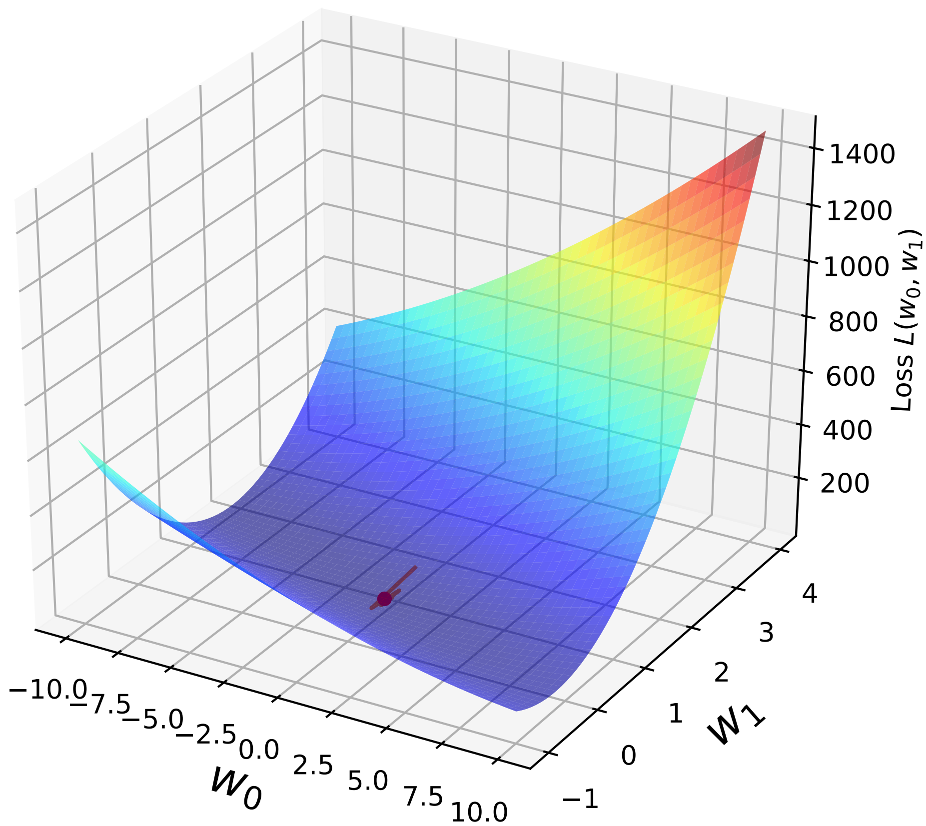
```
Time= 0.001325368881225586
[[-3.89578088]
 [ 1.19303364]]
loss sklearn= [[8.95394275]]
loss gradient descent= 11.462600167377458
```



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

[66]:
```python
# plot gradient descent
def plot_3d_gradient_descent(X,y,w_init,tau,max_iter):

    def f_pred(X,w):

        f = np.dot(X, w)

        return f

    def loss_mse(y_pred,y):

        temp_y = y_pred - y
        loss = np.dot(temp_y.T, temp_y) / y_pred.size

        return loss

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

        L_iters = np.empty((max_iter, 1))# record the loss values
        w_iters = np.empty((max_iter, 2))# record the parameter values
        w = w_init # initialization

        for i in range(max_iter): # loop over the iterations

            y_pred = f_pred(X, w)# linear predicition function
            grad_f = grad_loss(y_pred,y,X)# gradient of the loss
            w = w - tau * grad_f# update rule of gradient descent
            L_iters[i] = loss_mse(y_pred,y)# save the current loss value
            w_iters[i,:] = w.T# save the current w value

        return w, L_iters, w_iters

    # run gradient descent
    w, L_iters, w_iters = grad_desc(X, y, w_init, tau, max_iter)

    # 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
    w_B = np.empty([2,1], dtype=float)
    for (i,j),v in np.ndenumerate(Z):
        w_B[0][0] = B0[j]
        w_B[1][0] = B1[i]
        y_B = f_pred(X, w_B)
        Z[i,j] = loss_mse(y_B, y)


    # 3D visualization
    fig = plt.figure(figsize=(15,6))
    ax2 = fig.add_subplot(122, projection='3d')

    # 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())

    # plot gradient descent
    Z2 = np.zeros([max_iter])
    w0 = np.empty(max_iter)
    w1 = np.empty(max_iter)
    for i in range(max_iter):
        w0[i] = w_iters[i][0]
        w1[i] = w_iters[i][1]
        Z2[i] = L_iters[i][0]

    ax2.plot(w0, w1, Z2)
    ax2.scatter(w[0], w[1], L_iters[max_iter - 1][0],  c = 'r') # ???

    # 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)


# run plot_gradient_descent function
w_init = np.array([[0], [0]])
tau = 0.01
max_iter = 20
X = np.append(np.ones(x_train.size).reshape(-1, 1), np.array(x_train).
 ↪reshape(-1, 1) , axis = 1)
y = np.array(y_train).reshape(-1, 1)

plot_3d_gradient_descent(X,y,w_init,tau,max_iter)
```



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

[68]:
```
# plot gradient descent
def plot_contuor_gradient_descent(X,y,w_init,tau,max_iter):

    def f_pred(X,w):

        f = np.dot(X, w)

        return f

    def loss_mse(y_pred,y):

        temp_y = y_pred - y
        loss = np.dot(temp_y.T, temp_y) / y_pred.size

        return loss
```

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

    L_iters = np.empty((max_iter, 1))# record the loss values
    w_iters = np.empty((max_iter, 2))# record the parameter values
    w = w_init # initialization

    for i in range(max_iter): # loop over the iterations

        y_pred = f_pred(X, w)# linear predicition function
        grad_f = grad_loss(y_pred,y,X)# gradient of the loss
        w = w - tau * grad_f# update rule of gradient descent
        L_iters[i] = loss_mse(y_pred,y)# save the current loss value
        w_iters[i,:] = w.T# save the current w value

    return w, L_iters, w_iters

# run gradient descent
w, L_iters, w_iters = grad_desc(X, y, w_init, tau, max_iter)

# 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
w_B = np.empty([2,1], dtype=float)
for (i,j),v in np.ndenumerate(Z):
    w_B[0][0] = B0[j]
    w_B[1][0] = B1[i]
    y_B = f_pred(X, w_B)
    Z[i,j] = loss_mse(y_B, y)


# 3D visualization
fig = plt.figure(figsize=(15,6))
ax1 = fig.add_subplot(121)

# Left plot
CS = ax1.contour(xx, yy, Z, np.logspace(-2, 3, 20), cmap=plt.cm.jet)
ax1.scatter(w[0], w[1], L_iters[max_iter - 1][0],  c = 'r') # ????
ax1.plot(w_iters[:, 0], w_iters[:, 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)

# run plot_gradient_descent function
w_init = np.array([[0], [0]])
tau = 0.01
max_iter = 20
X = np.append(np.ones(x_train.size).reshape(-1, 1), np.array(x_train).
 ↪reshape(-1, 1) , axis = 1)
y = np.array(y_train).reshape(-1, 1)

plot_contuor_gradient_descent(X,y,w_init,tau,max_iter)
```