sheet04_solutions

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##Submitted by: **Group Name:**MI 4

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[1]:
```
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
```

$$E(w_{t+1}) = E(w_t) + \nabla E \cdot (-\eta_t d_t) + \frac{1}{2}(-\eta_t d_t)^T H(-\eta_t d_t) + \frac{1}{3!}E^{(3)}(w_t)(-\eta_t d_t)...,$$

where the fourth and next terms would need to be expanded with Frechet Derivative and cubic and higher order form. \

Fortunately, we are interested only in first three terms of the Taylor expansion.

$$\Delta E^T \leq 0$$

$$\Delta E^T \approx -E(w_t) + E(w_t) + \nabla E \cdot (-\eta_t d_t) + (-\eta_t d_t)H(-\eta_t d_t)$$

Using ineqality above, taking the scalar η in front of each term and dividing by η, we get (the product with Hessiannon is non zero for non-zero d, because H is positive definite)

$$\eta_t \leq \frac{\nabla E d_t}{d_t H d_t}$$

As E^T has a minimum at an unknown w^*, it's gradient is 0 there. Taylor approximation is equal to

$$E^T_{w_{t+1}} \approx E^T_{[w_t]} + \frac{1}{2}(w_{t+1} - w_t)^T H(w_{t+1} - w_t)$$

$$\nabla E^T_{[w_{t+1}]} = \nabla E^T_{[w_t]} + \frac{1}{2} * 2H(-\eta_t d_t) \tag{@}$$

If we want in next step get as close as possible to w^*, we shall assume that left side of equation is 0. Putting symbol * over η.

$$\eta_t^* H(-d_t) = d_t.$$

To calculate $\eta \in \mathbb{R}$ from this vector equation, we can take a dot product with d_t (or with $\nabla E^T_{w_t}$) from left side, to get real numbers. We can use the equality $d^T d = ||d||^2$.

$$-\eta_t^* (\nabla E^T_{w_t})^T H(d_t) = \nabla E^T_{w_t} \cdot d_t$$

Now, there is no point of taking d_t perpendicular to gradiant (don't go up!), hence the Hesian thing is non-zero (positive definite, bilinear form) and we can divide.

$$\eta_t^* = -\frac{\nabla E^T_{w_t} \cdot d_t}{(\nabla E^T_{w_t})^T H(d_t)}$$

Let's check! If such η^* really minimalize avarage cost function E, the ortogonality of direction d with gradient at the new point w_{t+1} should hold. It would mean, that level of E is tangent to direction d. So w_{t+1} is critical. Knowing, that E is convex we would be sure of minimality.

$$d_t \cdot \nabla E^T_w|_{w_{t+1}} \stackrel{?}{=} 0$$

Using definitions of η^*, and if direction is gradient $d_t = -\nabla E^T_{w_t} = -Hw_t$ (what if it is not gradient??) and equation (@), we have

$$d_t \cdot \nabla E^T|_{w_{t+1}} = d_t \cdot Hw_{t+1} =$$
$$= d_t \cdot H(w_t + \eta^* d_t) = d_t \nabla E^T_{w_t} + \eta^* d_t^T H d_t = d_t \cdot d_t - ||d_t||^2 = 0$$

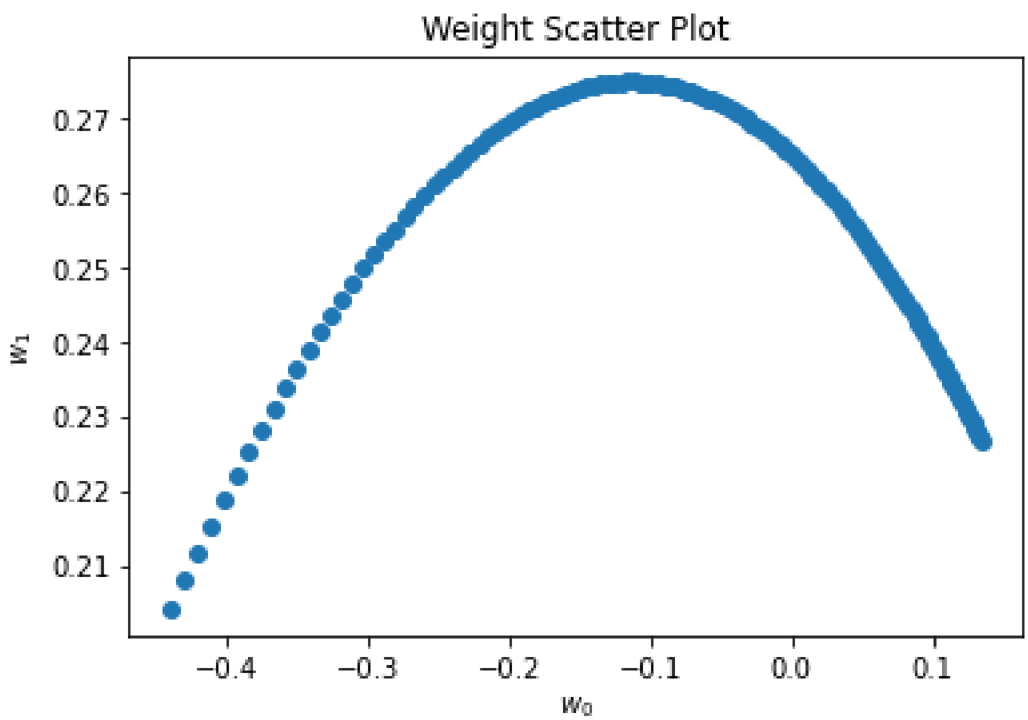
Part (**a**) : Gradient Descent

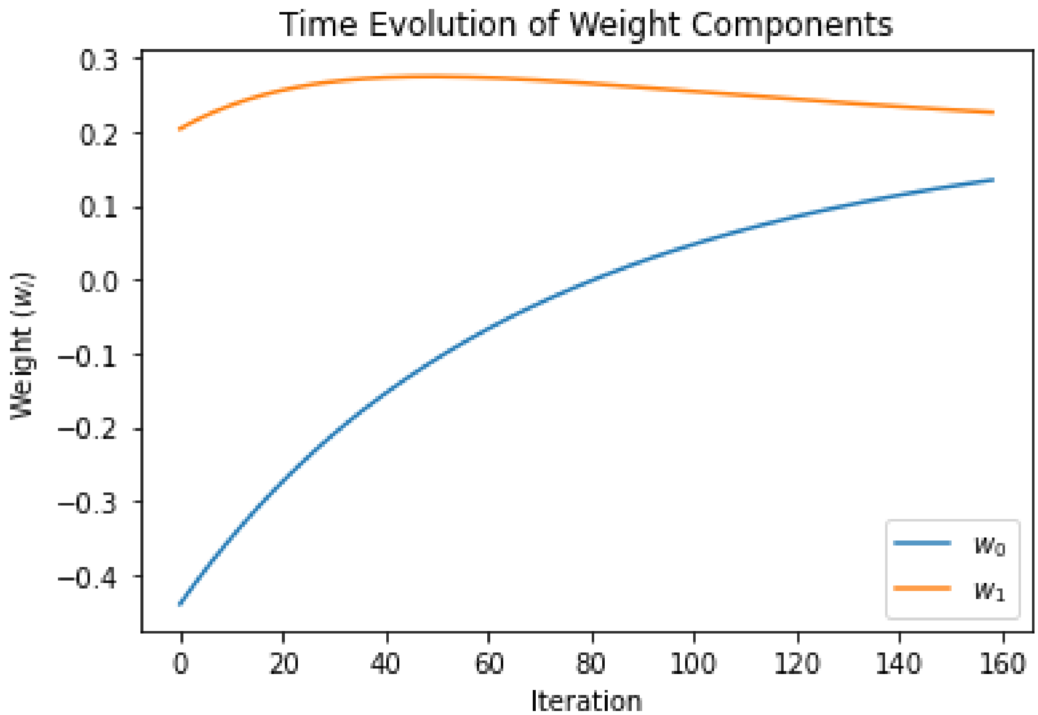
[2]:
```
# Initialise training data and weight matrix

X = np.array([ [1 ,  -1] , [1, 0.3] , [1 , 2] ]).T
Y = np.array([-0.1, 0.5, 0.5])

w_init = np.array([-0.45, 0.2]).T
```

[3]:
```python
# (a) Gradient Descent

def gradient_descent(X, Y, w_init, max_iter, lr = 0.001):

    w= w_init.copy()

    mse_history=[]
    stopping_criteria=True
    w0_history = []
    w1_history = []
    iter = 0

    H = np.dot(X, X.T)

    while iter < max_iter and stopping_criteria:
        g = np.dot(H,w) - np.dot(X, Y.T)
        w = w - lr*g


        Y_pred  = np.dot(w, X)
        mse=np.square(np.subtract(Y, Y_pred)).mean()
        # print(mse)
        mse_history+=[mse]


        #stopping criterion
        if iter>0:
            mse_new=mse_history[iter]
            mse_old=mse_history[iter-1]
            if ((abs(mse_new-mse_old))/mse_old)<=0.005:
              stopping_criteria=False

        w0_history += [w[0]]
        w1_history += [w[1]]
        iter += 1


    return w0_history , w1_history, mse_history
```

[4]:
```python
w0_history , w1_history, mse_history = gradient_descent(X, Y, w_init, max_iter␣
↪= 1_000, lr = 0.005)

plt.scatter(w0_history , w1_history)
plt.xlabel('$w_0$')
plt.ylabel('$w_1$')
plt.title('Weight Scatter Plot')
```

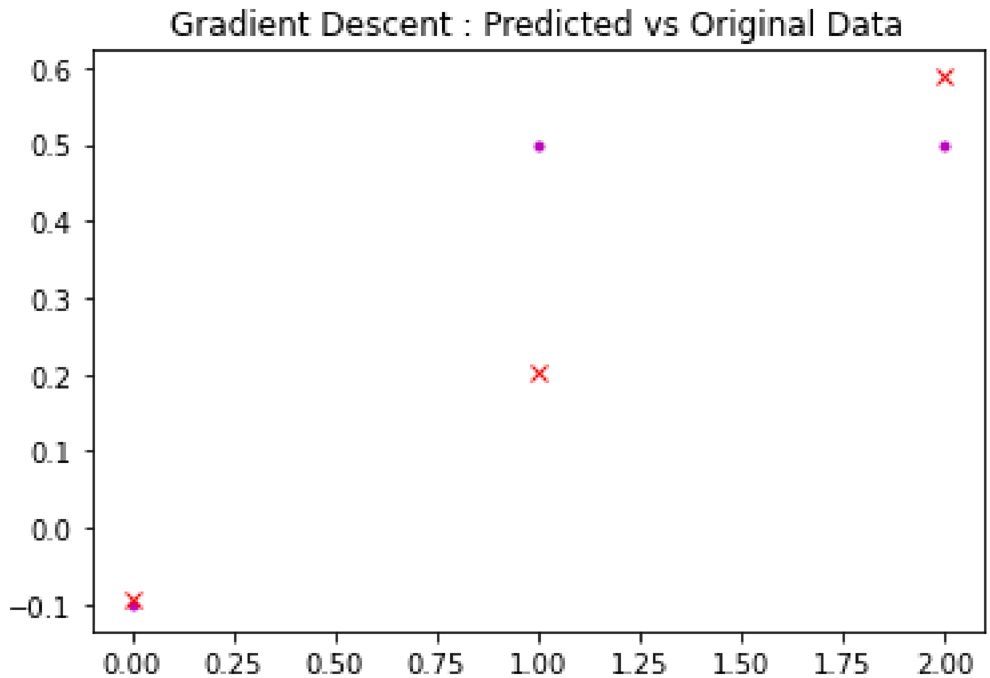
```
plt.show()

plt.plot(w0_history , label = '$w_0$')
plt.plot(w1_history , label = '$w_1$')
plt.ylabel('Weight ($w_i$) ')
plt.xlabel('Iteration')
plt.title('Time Evolution of Weight Components')
lgd = plt.legend()
plt.show()
```





As we can see, the weight vector components eventually stabilise when some optima (minima) has been found in the parameter weight space.

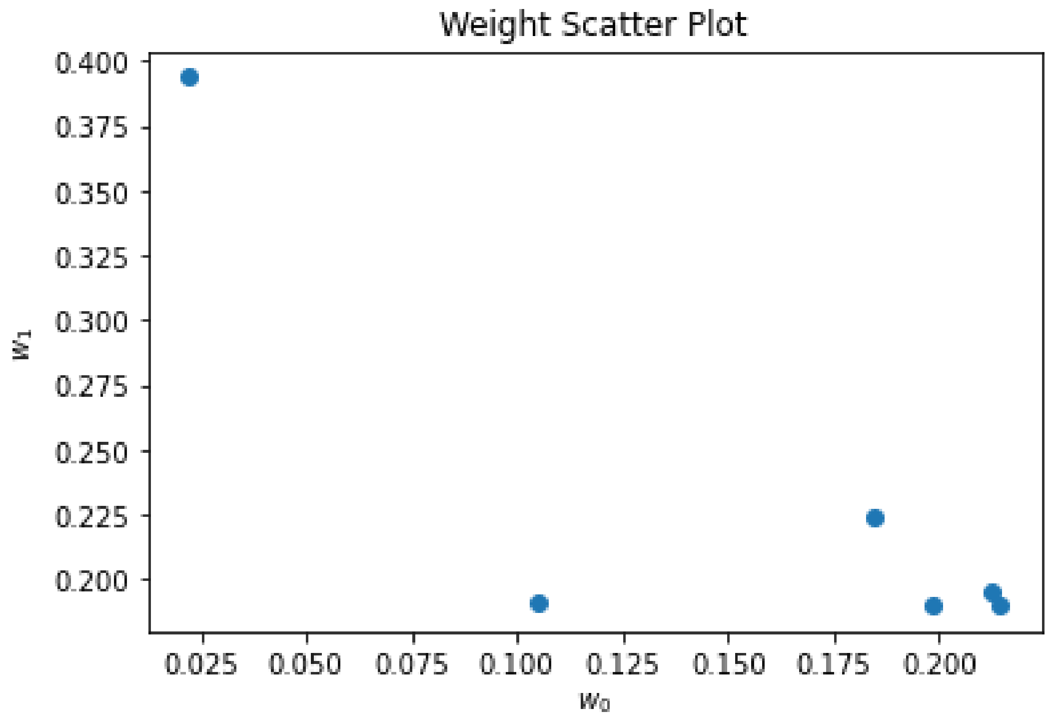
[5]:
```
w_final = np.array([w0_history[-1] , w1_history[-1] ]).T

Y_pred  = np.dot(w_final, X)
plt.plot(Y, '.m' , label = 'Data')
plt.plot(Y_pred, 'xr', label = 'Predicted')
plt.title('Gradient Descent : Predicted vs Original Data')
plt.show()
```

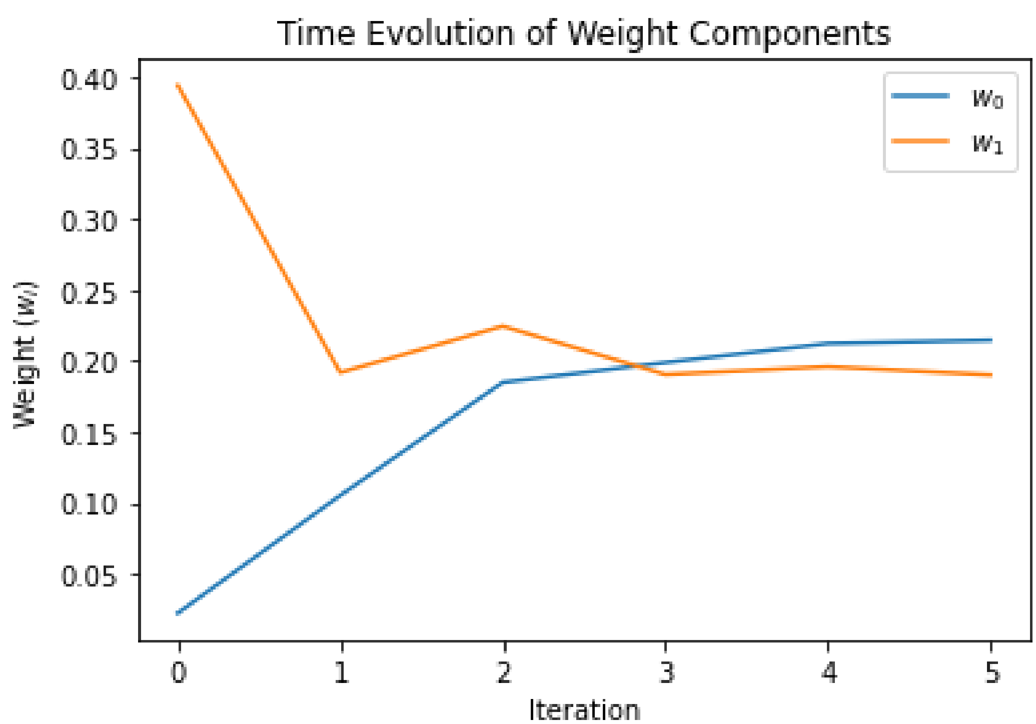


[6]:
```
# (b) Line search
def line_search(X, Y, w_init, max_iter, stopping = True):

    w= w_init.copy()

    w0_history = []
    w1_history = []
    mse_history=[]
    iter = 0
    stopping_criteria=True

    H = np.dot(X, X.T)

    while iter < max_iter and stopping and stopping_criteria:
        g = np.dot(H,w) - np.dot(X, Y.T)
        lr = np.dot(g.T,g)/np.dot(g.T, np.dot(H, g))
        w = w - np.multiply(lr, g, dtype=np.longdouble)

        Y_pred  = np.dot(w, X)
        mse=np.square(np.subtract(Y, Y_pred)).mean()
        # print(mse)
        mse_history+=[mse]
```

```
        #stopping criterion
        if iter>0:
            mse_new=mse_history[iter]
            mse_old=mse_history[iter-1]
            if ((abs(mse_new-mse_old))/mse_old)<=0.005:
              stopping_criteria=False

        w0_history += [w[0]]
        w1_history += [w[1]]
        iter += 1


    return w0_history , w1_history, mse_history
```

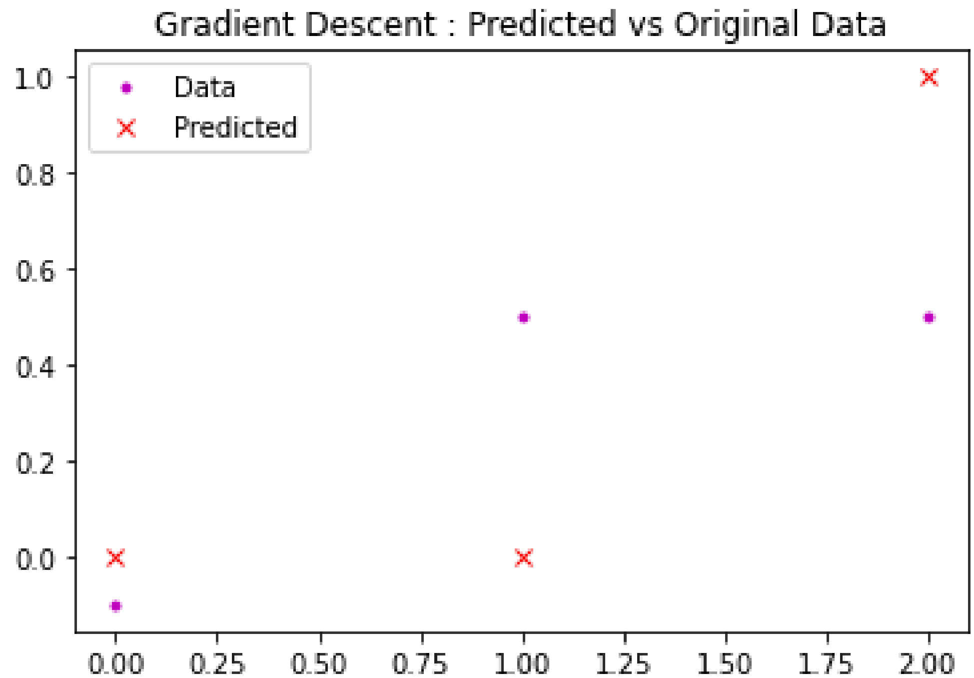
[7]:
```
w0_history , w1_history, mse_history = line_search(X, Y, w_init, max_iter = 50)

plt.scatter(w0_history , w1_history)
plt.xlabel('$w_0$')
plt.ylabel('$w_1$')
plt.title('Weight Scatter Plot')

plt.show()

plt.plot(w0_history , label = '$w_0$')
plt.plot(w1_history , label = '$w_1$')
plt.ylabel('Weight ($w_i$) ')
plt.xlabel('Iteration')
plt.title('Time Evolution of Weight Components')
plt.legend()
plt.show()
```


Weight Scatter Plot
0.400
0.375
0.350
0.325
0.300
0.275
0.250
0.225
0.200
w_1
0.025
0.050
0.075
0.100
0.125
0.150
0.175
0.200
w_0


Time Evolution of Weight Components
w_0
w_1
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
Weight (w_i)
0
1
2
3
4
5
Iteration

[8]:

```
w_final = np.array([w0_history[-1] , w1_history[-1] ]).T

Y_pred  = np.dot(w_final, X)
plt.plot(Y, '.m' , label = 'Data')
plt.plot(Y_pred.round(), 'xr', label = 'Predicted')
plt.title('Gradient Descent : Predicted vs Original Data')
plt.legend()
plt.show()
```



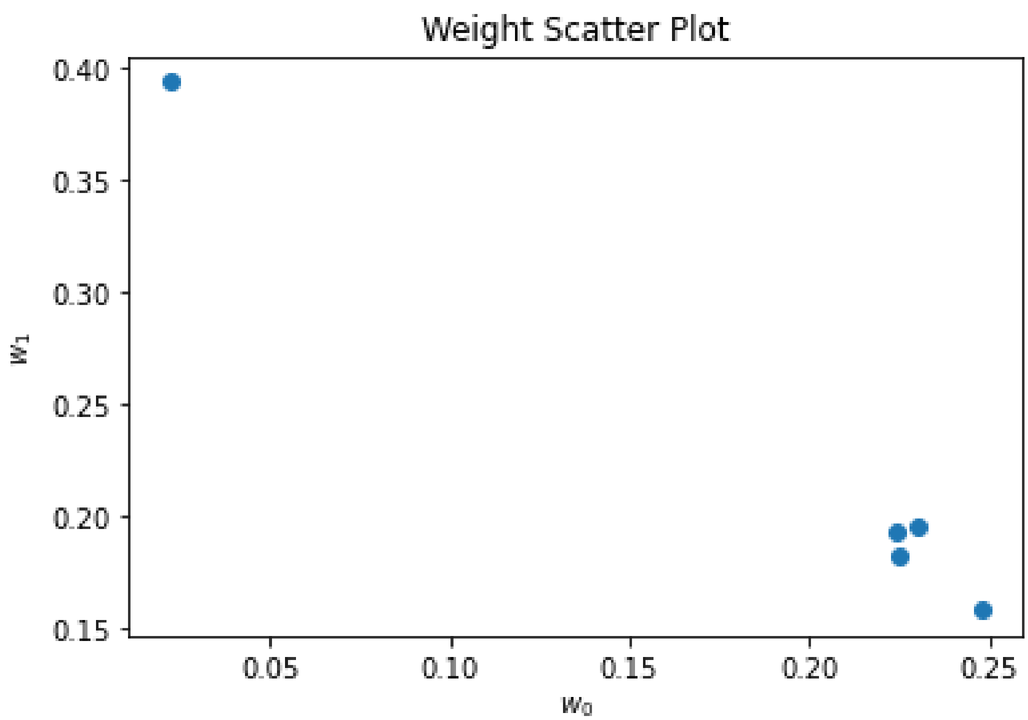
[9]:

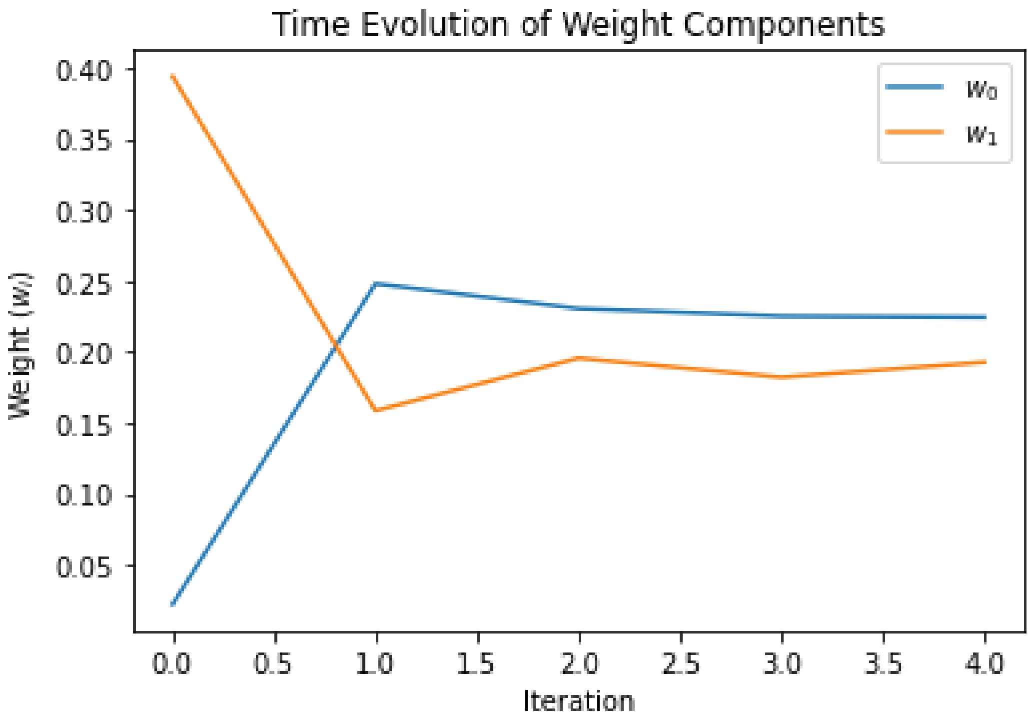
```
# (c) Conjugate Gradient
def conjugate_gradient(X, Y, w_init, max_iter, stopping = True):

    w= w_init.copy()

    mse_history=[]

    w0_history = []
    w1_history = []
    iter = 0
    stopping_criteria=True

    H = np.dot(X, X.T)
```

```
    while iter < max_iter and stopping and stopping_criteria:
      if iter==0:
        g_old = np.dot(H,w) - np.dot(X, Y.T)
        d=-g_old
        lr = -np.dot(d.T,g_old)/np.dot(d.T, np.dot(H, d))
        w= w + lr*d
        g_new = np.dot(H,w) - np.dot(X, Y.T)
        beta=-np.dot(g_new.T,g_new)/np.dot(g_old.T,g_old)
        d=g_new+beta*d
        g_old=g_new
      else:
        lr =-np.dot(d.T,d)/np.dot(d.T, np.dot(H, d))
        w = w + lr*d
        g_new = np.dot(H,w) - np.dot(X, Y.T)
        beta=-np.dot(g_new.T,g_new)/np.dot(g_old.T,g_old)
        d=g_new+beta*d
        g_old=g_new

      Y_pred  = np.dot(w, X)
      mse=np.square(np.subtract(Y, Y_pred)).mean()
      mse_history+=[mse]


      #stopping criterion
      if iter>0:
          mse_new=mse_history[iter]
          mse_old=mse_history[iter-1]
          if ((abs(mse_new-mse_old))/mse_old)<=0.005:
            stopping_criteria=False


      w0_history += [w[0]]
      w1_history += [w[1]]


      iter += 1


    return w0_history , w1_history, mse_history
```

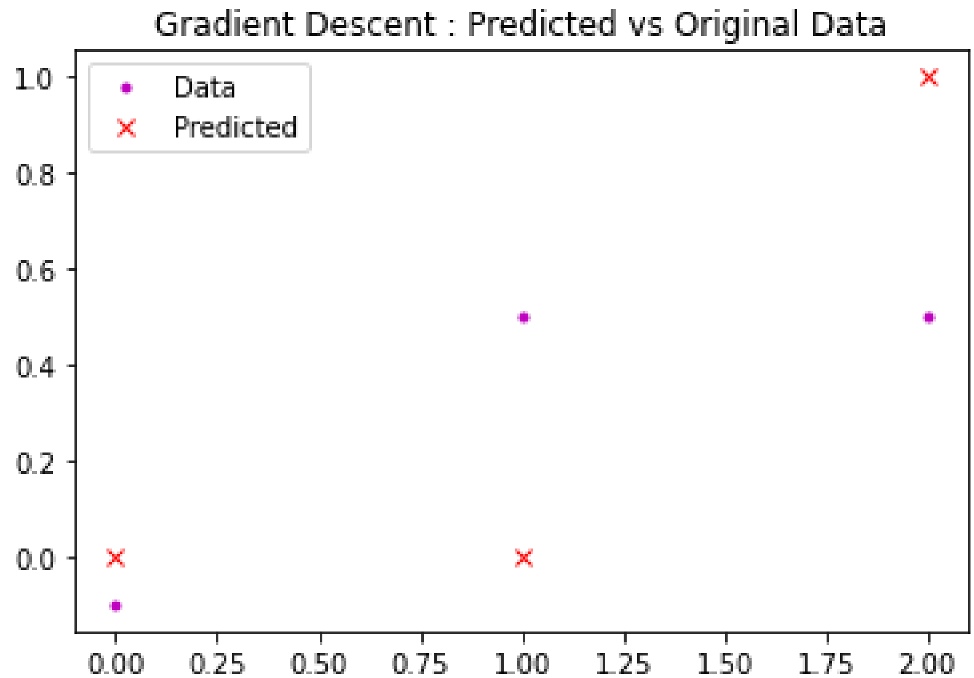
[10]:
```
w0_history , w1_history, mse_history = conjugate_gradient(X, Y, w_init,␣
 ↪max_iter = 50)

plt.scatter(w0_history , w1_history)
plt.xlabel('$w_0$')
plt.ylabel('$w_1$')
```

```
plt.title('Weight Scatter Plot')

plt.show()

plt.plot(w0_history , label = '$w_0$')
plt.plot(w1_history , label = '$w_1$')
plt.ylabel('Weight ($w_i$) ')
plt.xlabel('Iteration')
plt.title('Time Evolution of Weight Components')
plt.legend()
plt.show()
```

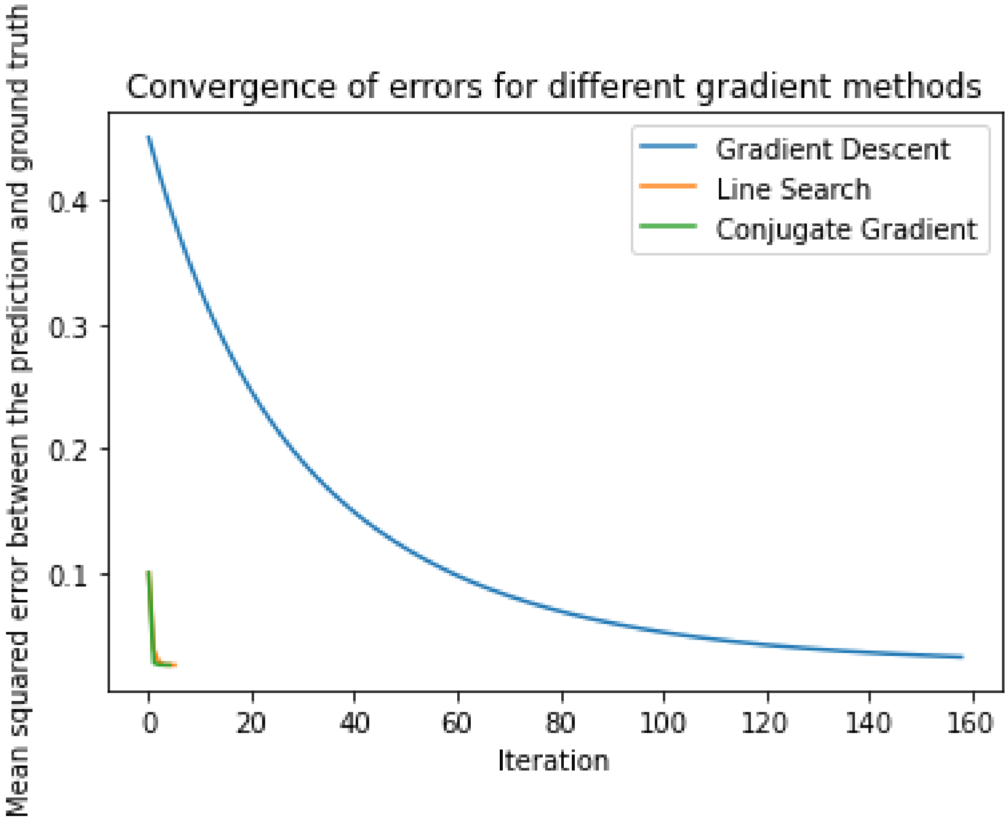




[11]:
```
w_final = np.array([w0_history[-1] , w1_history[-1] ]).T

Y_pred  = np.dot(w_final, X)
plt.plot(Y, '.m' , label = 'Data')
plt.plot(Y_pred.round(), 'xr', label = 'Predicted')
plt.title('Gradient Descent : Predicted vs Original Data')
plt.legend()
plt.show()
```



[12]:
```
w0_history , w1_history, mse_history_gd = gradient_descent(X, Y, w_init,␣
↪max_iter = 1_000, lr = 0.005)
w0_history , w1_history, mse_history_ls = line_search(X, Y, w_init, max_iter =␣
↪50)
w0_history , w1_history, mse_history_cg = conjugate_gradient(X, Y, w_init,␣
↪max_iter = 50)

plt.plot(mse_history_gd,label='Gradient Descent')
plt.plot(mse_history_ls,label='Line Search')
plt.plot(mse_history_cg, label= 'Conjugate Gradient')
plt.ylabel('Mean squared error between the prediction and ground truth ')
plt.xlabel('Iteration')
plt.title('Convergence of errors for different gradient methods')
plt.legend()
plt.show()
```



It can be seen from the above plot that the line search and conjugate gradient methods help the error to converge in a very less number of iterations compared to the general gradient descent method.