CS 559 - Fall 2021

Homework #4

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(1) Comparing Gradient Descent and Newton's method

The objective function is:

$$f(x,y) = -\log(1 - x - y) - \log x - \log y$$

with domain D = (x, y) : x + y, x + y < 1, x > 0, y > 0

GRADIENT CALCULATIONS:

$$d_x f = \frac{\partial f(x,y)}{\partial x} = -\frac{1}{1-x-y} * (-1) - \frac{1}{x}$$

$$= \frac{1}{1-x-y} - \frac{1}{x}$$

$$d_y f = \frac{\partial f(x,y)}{\partial y} = -\frac{1}{1-x-y} * (-1) - \frac{1}{y}$$

$$= \frac{1}{1-x-y} - \frac{1}{y}$$

$$G = (d_x f \quad d_y f) = \left(\frac{1}{1 - x - y} - \frac{1}{x} \quad \frac{1}{1 - x - y} - \frac{1}{y}\right)$$

HESSIAN CALCULATIONS

$$H = \begin{pmatrix} d_{xx}f & d_{xy}f \\ d_{yx}f & d_{yy}f \end{pmatrix}$$

$$d_{xx}f = \frac{\partial(d_x f)}{\partial x} = -\frac{1}{(1 - x - y)^2} * (-1) + \frac{1}{x^2} = \frac{1}{(1 - x - y)^2} + \frac{1}{x^2}$$

$$d_{xy}f = \frac{\partial(d_x f)}{\partial y} = -\frac{1}{(1 - x - y)^2} * (-1) + 0 = \frac{1}{(1 - x - y)^2}$$

$$d_{yx}f = \frac{\partial(d_y f)}{\partial x} = -\frac{1}{(1 - x - y)^2} * (-1) + 0 = \frac{1}{(1 - x - y)^2}$$

$$d_{yy}f = \frac{\partial(d_y f)}{\partial y} = -\frac{1}{(1 - x - y)^2} * (-1) + \frac{1}{y^2} = frac1(1 - x - y)^2 + \frac{1}{y^2}$$

$$H = \begin{pmatrix} \frac{1}{(1-x-y)^2} + \frac{1}{x^2} & \frac{1}{(1-x-y)^2} \\ \frac{1}{(1-x-y)^2} & \frac{1}{(1-x-y)^2} + \frac{1}{y^2} \end{pmatrix}$$

The initial point w_0 is (0.19, 0.02) and the learning rate η is 0.02.

Results: Refer Fig. (1, 2)

Generally, the notion is that Gradient Descent can go zigzag in the trajectory before it converges to the global minimum and may take a longer time to converge than the Newton method.

But for the given objective function, we can observe that Gradient Descent (GD) does not depict the zigzag behavior and rather it converges much much faster than Newton Method. For GD, it takes around 10 iterations to converge whereas it takes around 400 iterations for the Newton's method to converge. We observe the same phenomenon with a different learning rate also.

(2) Linear Least Squares Fit

CLOSED FORM SOLUTION

For the equation $y = w_1x + w_0$, we can find w_1 and w_0 using the following equations:

$$w_1 = \frac{N\sum(xy) - \sum x \cdot \sum y}{N\sum x^2 - (\sum x)^2}$$
$$w_0 = \frac{\sum y - N\sum x}{N}$$

GRADIENT DESCENT METHOD

Energy function is given by:

$$f(w_1, w_0) = \sum_{i=1}^{50} (y_i - (w_1 x_i + w_0))^2$$

The partial derivatives are given by:

$$\frac{\partial f}{\partial w_1} = \sum_{i=1}^{50} 2(w_0 + w_1 x_i - y_i)(x_i)$$
$$\frac{\partial f}{\partial w_0} = \sum_{i=1}^{50} 2(w_0 + w_1 x_i - y_i)$$

The weights are updated according to the following equations:

$$w_1 = w_1 - \eta * \frac{\partial f}{\partial w_1}$$
$$w_0 = w_0 - \eta * \frac{\partial f}{\partial w_0}$$

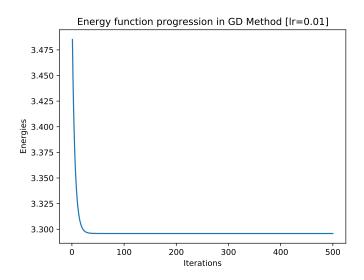
Results: Refer Fig. (3)

 $w_1 = 1.0124815602408974, w_0 = -0.2820802313809418$

 $w_1 = 0.9946671535014963, w_0 = 0.3175021482094951$

From the plot [3], we can observe that both the above methods could almost fit the datapoints and the line curves obtained using the two methods are almost indistinguishable. The weights mentioned above are almost equal in their w_1 parameter (which is the slope of the line) and there is only a slight difference in the w_0 (which is the intercept) and therefore, the line curves almost overlap.

In conclusion, both methods work fine in the given case where the objective function is bit simple and the number of datapoints are very less and the problem is univariate regression. In more complex cases, particularly when the objective function is non-convex, the closed form solution may not be available and in some other cases where the problem is multivariate with large number of datapoints, the closed form solution again may require tremendous mathematical calculations. In all those cases, gradient descent proves a better strategy due to its simple iterative way of approximating the weights.



Trajectory following by points in GD Method [Ir=0.01]

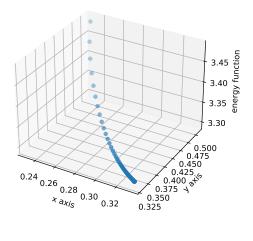
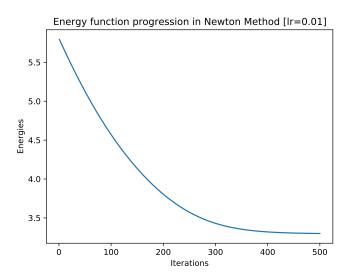


Figure 1: Gradient Descent Method



Trajectory following by points in Newton Method [Ir=0.01]

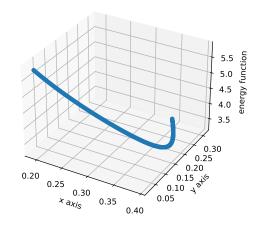


Figure 2: Newton's Method

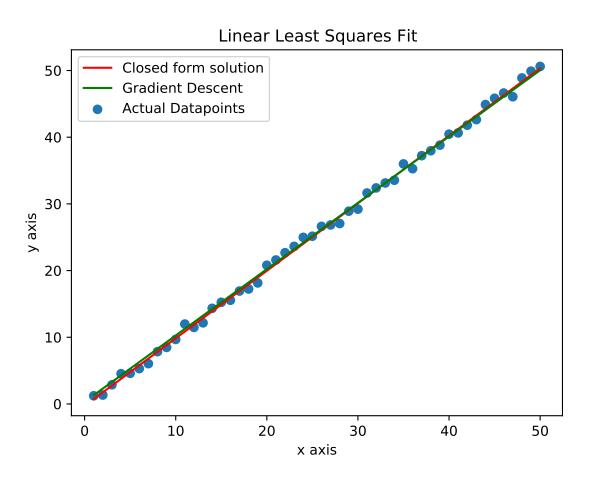


Figure 3: Least Squares Fit using usingusing (a) Closed form solution, (b) Gradient Descent

Code for (Q1)

```
import math, numpy as np, matplotlib.pyplot as plt
def objective_function(x, y):
   return -math.log(1 - x - y) - math.log(x) - math.log(y)
def gradient_function(x, y):
   return [(1/(1-x-y))-1/x, (1/(1-x-y))-1/y]
def hessian_function(x, y):
   return [[1/(x*x) + 1/(1-x-y)**2, 1/(1-x-y)**2], [1/(1-x-y)**2,
      1/(1-x-y)**2 + 1/(y*y)]]
x_0, y_0 = 0.19, 0.02 # Initial point
method = 'GD' # or 'Newton'
for eta in [1e-2]:
   x, y, E = [], [], []
   x_i = x_0; y_i = y_0
   iterations = 0
   while iterations < 500:</pre>
      g = gradient_function(x_i, y_i)
      if method == 'GD': # Gradient Descent
         delta = g
                     # Newton's Method
      else:
         H = hessian_function(x_i, y_i)
         H_inv = np.linalg.inv(np.array(H))
         delta = H_inv @ np.array(g)
      # update
      x_i = x_i - eta * delta[0]
      y_i = y_i - eta * delta[1]
         E_i = objective_function(x_i, y_i)
      except ValueError:
         E_i = 0
      E.append(E_i)
      x.append(x_i)
      y.append(y_i)
      iterations +=1
   # Plot Energy function
   epoch_arr = list(range(1, iterations+1))
   plt.figure()
   plt.xlabel('Iterations')
   plt.ylabel('Energies')
   plt.plot(epoch_arr, E)
   plt.title('Energy function progression in {} Method
       [lr={}]'.format(method, eta))
   plt.savefig('{}_Energy_x_{}_y_{}_eta_{}.pdf'.format(method, x_0, y_0,
      eta))
   # Plot Trajectory
   fig = plt.figure()
   ax = fig.add_subplot(111, projection='3d')
   ax.set_ylabel('y axis')
   ax.set_xlabel('x axis')
   ax.set_zlabel('energy function')
```

```
plt.title('Trajectory following by points in {} Method
    [lr={}]'.format(method, eta))
ax.scatter(x, y, E)
plt.savefig('{}_Trajectory_x_{}_{quad}).pdf'.format(method, x_0, y_0, eta))
```

Code for (Q2)

```
import math, numpy as np, matplotlib.pyplot as plt
np.random.seed(111)
x = np.array([i+1 for i in range(50)])
u = np.random.uniform(-1, 1, 50)
y = np.array([u_i + i + 1 for i, u_i in enumerate(u)])
    = len(x)
sum_x = np.sum(x)
sum_y = np.sum(y)
sum_x_2 = np.sum([x_i**2 for x_i in x])
sum_x_y = np.sum([x_i*y_i for x_i, y_i in zip(x, y)])
\# Linear least squares fit given by y = w1x + w0
w1 = (N*sum_x_y - sum_x*sum_y)/(N*sum_x_2 - sum_x**2)
w0 = (sum_y - w1*sum_x)/N
print(w1, w0)
# Plot
plt.figure()
plt.xlabel('x axis')
plt.ylabel('y axis')
plt.title('Linear Least Squares Fit')
plt.scatter(x, y)
plt.plot(x, w0 + w1 * x, 'r')
## Linear least squares fit using Gradient Descent
def gradient_function(w0, w1):
   # Objective function = \sum_{i=1}^{50} (y_i - w0 - w1*x_i)**2
   pred = w0 + w1 * x
   g_w0 = 2 * np.sum(pred - y)
   g_w1 = 2 * (pred - y) @ x
   return [g_w0, g_w1]
# initialize parameters
w0_i, w1_i = np.random.uniform(0, 1, 2)
w0_arr, w1_arr, E = [], [], []
iterations = 0; eta = 1e-5
w0 = w0_i; w1 = w1_i
# gradient descent loop
while iterations < 1000:</pre>
   g = gradient_function(w0, w1)
   w0 = w0 - eta * g[0]
  w1 = w1 - eta * g[1]
   iterations += 1
   E.append(np.sum((y - w0 - w1*x)**2)) # Energy function
print(w1, w0)
# plot
plt.plot(x, w0 + w1 * x, 'g')
plt.legend(['Closed form solution', 'Gradient Descent', 'Actual
   Datapoints'])
plt.savefig('least_squares_fit.pdf')
```