CA7-steepest-descent-instructor

November 7, 2019

```
In [1]: import numpy as np
    import numpy.linalg as la
    import scipy.optimize as opt
    import matplotlib.pyplot as plt
```

1 Steepest Descent in Machine Learning

Recall that steepest descent is an optimization algorithm that computes the minimum of a function by

$$x_{k+1} = x_k - \alpha_k \nabla f(x_k),$$

where x_k is the solution at step k, and α_k is a line search parameter that is computed by solving the 1-dimensional optimization problem

$$\alpha_k = \min_{\alpha_k} f(x_k - \alpha_k \nabla f(x_k))$$

We will explore how we can use steepest descent in machine learning.

1.1 1) Example 1: Linear Regression

In this first example, we will use steepest descent to compute a linear regression (line of best fit) model over some data.

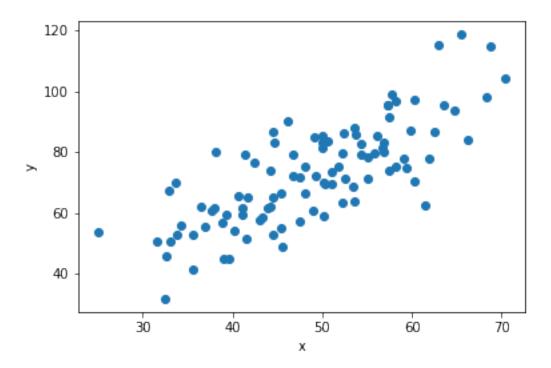
(This isn't the only way of computing the line of best fit and later on in the course we will explore other methods for accomplishing this same task.)

The data that we will be working with is an $n \times 2$ numpy array where each row represents an (x_i, y_i) pair.

```
In [2]: data = np.genfromtxt('data.csv', delimiter=',')
```

Plot the data to see what it looks like.

```
In [3]: plt.scatter(data[:,0], data[:,1])
        plt.xlabel('x')
        plt.ylabel('y')
        plt.show()
```



The first step in applying steepest descent is to formulate a function that we want to minimize. To compute the line of best fit, we want to construct a line (y = mx + b) and minimize the error between this line and the data points. Therefore, we want to minimize the sum of square error:

$$E(m,b) = \frac{1}{N} \sum_{i=1}^{N} (y_i - (mx_i + b))^2$$

that can be written as a unconstrained optimization problem:

$$\min_{m,b} E(m,b)$$

Since we will be using steepest descent to solve this optimization problem, we need to be able to evaluate E and ∇E .

a) Let's write a function to compute the error E(m,b). The function will have the following signature:

```
def E(mb, data):
```

```
# Compute error in the linear regression model using the sum of square error formula
# mb: Numpy array of length 2 with first entry as m and second entry as b
# data: 2D Numpy array of length nx2 where each row represents an (xi,yi) pair with n data p
# totalError: Scalar output of sum of square error formula
totalError = ...
return totalError
```

```
In [4]: #clear
    def E(mb, data):
        # Compute error in the linear regression model using the sum of square error formula
        # mb: Numpy array of length 2 with first entry as m and second entry as b
        # data: 2D Numpy array of length nx2 where each row represents an (xi,yi) pair with
        # totalError: Scalar output of sum of square error formula
        n,_ = data.shape
        m = mb[0]
        b = mb[1]
        totalError = np.sum((data[:,1] - (m*data[:,0]+b))**2)
        return totalError/n
```

You can try m = 1 and b = 2 as arguments to help debugging your code snippet. Your function should return 594.259213603709.

```
In [5]: #clear
    m = 1.
    b = 2.
    mb = np.array([m,b])
    print(E(mb, data))

594.259213603709
```

 $b_gradient = 0.$

b) Now that we the function that we want to minimize, we need to compute it's gradient ∇E .

You should compute the analytical form of these derivatives by hand (it is a good practice!) You can also later compare your results with SymPy. Note that the independent variables are m and b. The function should have the following signature:

```
def gradE(mb, data):
    # Compute the gradient of the error in the linear regression model
    # mb: Numpy array of length 2 with first entry as m and second entry as b
    # data: 2D Numpy array of length nx2 where each row represents an (xi,yi) pair with n data p
    # grad: Numpy array of length 2 with first entry as partial derivative with respect to m
            and second entry as partial derivative with respect to b
    m_gradient = ...
    b_gradient = ...
    grad = np.array([m_gradient, b_gradient])
    return grad
In [6]: #clear
        def gradE(mb, data):
           n = data.shape[0]
            m = mb[0]
            b = mb[1]
            m_gradient = 0.
```

```
for i in range(n):
    x = data[i,0]
    y = data[i,1]
    m_gradient += (2./n) * (-x*(y - (m*x+b)))
    b_gradient += (2./n) * (-1.*(y - (m*x+b)))
return np.array([m_gradient, b_gradient])
```

You can try m = 1 and b = 2 as arguments to help debugging your code snippet. Your function should return [-2192.94722958 -43.55341818].

The last thing that we need before we can write a function for steepest descent, is to solve a 1-dimensional optimization problem to solve for the line search parameter. However, in machine learning we want to avoid this and employ a heuristic approach.

Instead, we will pick a "learning rate" and use that instead of a line search parameter.

```
In [8]: learning_rate = 0.0001
```

We should now have everything that we need to use steepest descent.

1.1.1 Steepest descent using a fixed learning rate

Let's write a function for steepest descent with the following signature:

```
def steepest_descent(mb, learning_rate, data, num_iterations):
    # mb: Numpy array of length 2 containing initial guess for parameters m and b
    # learning_rate: Scalar with the learning rate that will be applied to steepest descent
    # data: 2D Numpy array of length nx2 where each row represents an (xi,yi) pair with n data p
    # num_iterations: Integer with the number of iterations to run steepest descent
    # mb_list: list that contains the history of values [m,b] for each iteration
    return mb_list
```

Note that in the above, we are not imposing a tolerance as stopping criteria, but instead letting the algorithm iterates for a fixed number of steps (num_iterations).

```
In [9]: #clear
    def steepest_descent(mb,learning_rate, data, num_iterations):
        mbs = [mb]
        x = mb
        for i in range(num_iterations):
            alpha = learning_rate # modify this line
            x = x - alpha * gradE(x, data)
            mbs.append(x)
        return mbs
```

Now, we have everything we need to compute a line of best fit for a given data set. Let's assume that our initial guess for the linear regression model is 0, meaning that

```
m = 0.
b = 0.
```

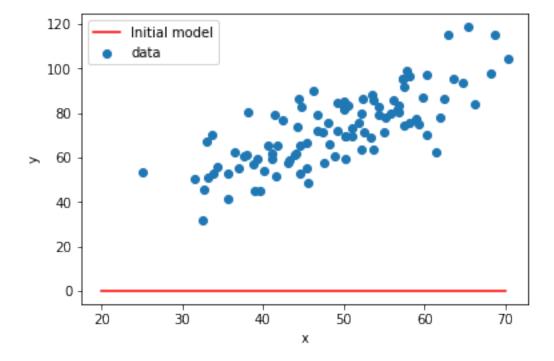
Let's plot the data again but now with our model to see what the initial line of best fit looks like.

```
In [10]: # Initial guess for m and b
    mb_initial = np.array([0.,0.])

# Line y = mx + b

xs = np.linspace(20,70,num=1000)
ys = mb_initial[0]*xs + mb_initial[1]

plt.scatter(data[:,0], data[:,1], label = 'data')
plt.plot(xs,ys,'r', label = 'Initial model')
plt.legend()
plt.xlabel('x')
plt.ylabel('y')
plt.show()
```

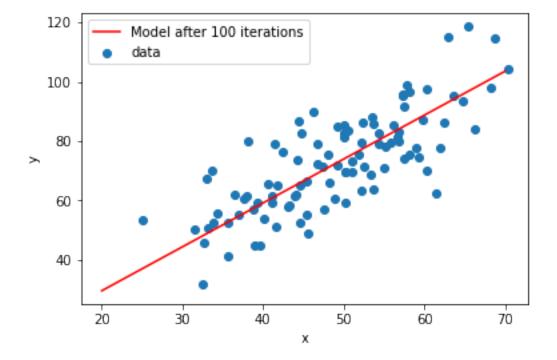


Perform 100 iterations of steepest descent and plot the model (line) with the optimized values of *m* and *b*.

```
In [11]: #clear
    mb_list = steepest_descent(mb_initial, 0.0001, data, num_iterations=100)
    mb_final = mb_list[-1]

    xs = np.linspace(20,70,num=1000)
    ys = mb_final[0]*xs + mb_final[1]

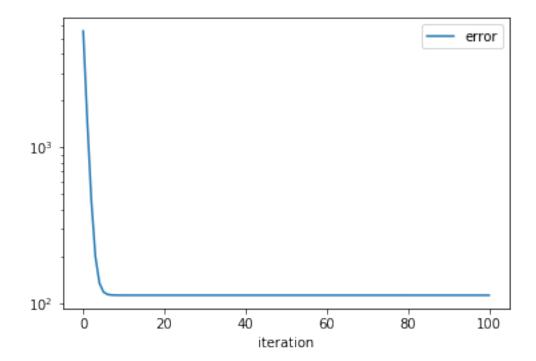
    plt.scatter(data[:,0], data[:,1], label = 'data')
    plt.plot(xs,ys,'r', label = 'Model after 100 iterations')
    plt.xlabel('x')
    plt.ylabel('y')
    plt.legend()
    plt.show()
```



Let's investigate the error in the model to see how steepest descent is minimizing the function. Compute the error (using the function E) for each update of m and b that was stored as a return value in steepest_descent. Store the error for each iteration in the list error. Note: you could have included this calculation inside your steepest_descent function.

```
In [12]: #clear
    errors = []
    for mb in mb_list:
        errors.append(E(mb, data))
```

Plot the error at each iteration.



It looks like the algorithm didn't need all the 100 iterations. Can you think of a better stopping criteria? Try that later (for now, let's just move on to the next section).

1.1.2 Steepest descent - what happens when we change the learning rate?

For all these experiments, we stated that learning_rate = 0.0001. What would happen if we were to increase or decrease the learning rate?

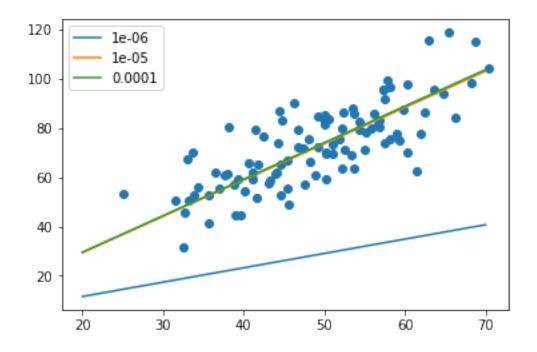
Run the steps above for the learning rates [1e-6, 1e-5, 1e-4]. Save the values of m and b obtained for the three different learning rates.

- 1) Plot the data and the model (lines) for the three different values of learning_rate
- 2) Plot the error for the three different values of learning_rate

```
In [14]: #clear
    learning_rates = [1e-6, 1e-5, 1e-4]
    mbs = []
    for learning_rate in learning_rates:
        mb = steepest_descent(mb_initial, learning_rate, data, num_iterations=100)
        mbs.append(mb)
```

```
xs = np.linspace(20,70,num=1000)
fig = plt.figure()
ax = fig.add_subplot(111)
ax.scatter(data[:,0], data[:,1])

for mb,learning_rate in zip(mbs, learning_rates):
    ys = mb[-1][0]*xs + mb[-1][1]
    plt.plot(xs,ys, label = learning_rate)
    plt.draw()
plt.legend()
plt.show()
```

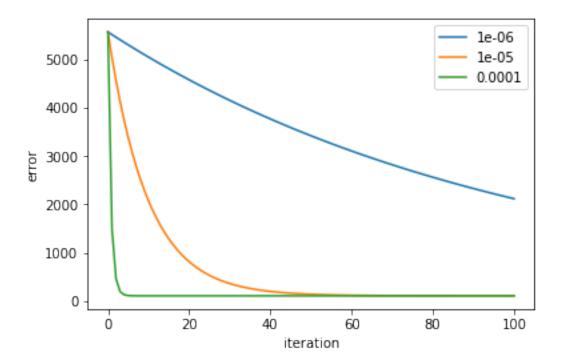


```
In [15]: #clear
    errors = []

for mb_per_lr in mbs:
    error = []
    for mb in mb_per_lr:
        error.append(E(mb,data))
    errors.append(error)

for error, lr in zip(errors, learning_rates):
    plt.plot(error, label = lr)
    plt.xlabel('iteration')
    plt.ylabel('error')
```

```
plt.legend()
plt.show()
```



As we can see from the above plots, the number of steps for convergence will change depending on the learning_rate.

1.1.3 Steepest descent using golden-section search

In class, we learned about golden-section search for solving for the line search parameter. How can we use it to compute the parameter α in steepest descent for this example?

We need to first create a wrapper function so that we can minimize $f(x_k - \alpha \nabla f(x_k))$ with respect to α .

Create a new steepest descent function to compute the line search parameter. Use scipy.optimize.golden to compute α .

```
alpha = opt.golden(objective_1d, args = (mb,data))
```

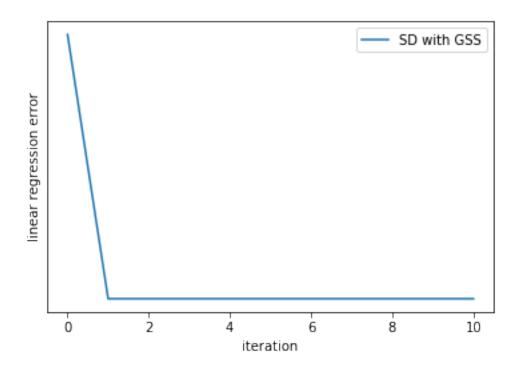
The steepest descent function signature should be:

```
def steepest_descent_gss(mb, data, num_iterations):
    # mb: Numpy array of length 2 containing initial guess for parameters m and b
```

```
# data: 2D Numpy array of length nx2 where each row represents an (xi,yi) pair with n data p
# num_iterations: Integer with the number of iterations to run steepest descent
# mb_list: list that contains the history of values [m,b] for each iteration
return mb_list

In [17]: #clear
    def steepest_descent_gss(mb, data, num_iterations):
        mbs = [mb]
        for i in range(num_iterations):
            alpha = opt.golden(objective_1d, args = (mb,data))
            mb = mb - alpha * gradE(mb, data)
            mbs.append(mb)
        return mbs
```

Plot the error of using golden-section search for the line search parameter and compare the results with using a learning rate. Does this improve the convergence? How many iterations does it take for steepest descent to converge?



In practice, we don't use golden-section search in machine learning and instead we employ the heuristic that we described earlier of using a learning rate (note that the learning rate is not fixed, but updated using different methods). Why would we want use a learning rate over a line search parameter?

1.2 Example 2: Location of Cities

http://www.benfrederickson.com/numerical-optimization/

In this example, given data on the distance between different cities, we want map out the cities by finding their locations in a 2-dimensional coordinate system.

Below is an example of distance data that we may have available that will allow us to map a list of cities.

Let's load the data that we will be working with in this example. city_data is an $n \times n$ numpy array where n is the number of cities. city_data will store the table of distances between cities similar to the one above.

```
In [20]: city_data = np.load('city_data.npy')
```

Before we start working with the data, we need to normalize the data by dividing by the largest element. This will allow us to more easily generate an initial guess for the location of each city.

```
In [21]: city_data = city_data/np.max(city_data)
```

Below is a list of cities that we want to locate on a map.

	Atlanta	Chicago	Denver	Houston	Los Angeles	Miami	New York	San Francisco	Seattle	Washington, DC
Atlanta	0	587	1212	701	1936	604	748	2139	2182	543
Chicago	587	0	920	940	1745	1188	713	1858	1737	597
Denver	1212	920	0	879	831	1726	1631	949	1021	1494
Houston	701	940	879	0	1374	968	1420	1645	1891	1220
Los Angeles	1936	1745	831	1374	0	2339	2451	347	959	2300
Miami	604	1188	1726	968	2339	0	1092	2594	2734	923
New York	748	713	1631	1420	2451	1092	0	2571	2408	205
San Francisco	2139	1858	949	1645	347	2594	2571	0	678	2442
Seattle	2182	1737	1021	1891	959	2734	2408	678	0	2329
Washington, DC	543	597	1494	1220	2300	923	205	2442	2329	0

Table of Distances Between Various Cities

```
In [22]: city_names = [
             "Vancouver",
             "Portland",
             "New York",
             "Miami",
             "Mexico City",
             "Los Angeles",
             "Toronto",
             "Panama City",
             "Winnipeg",
             "Montreal",
             "San Francisco",
             "Calgary",
             "Chicago",
             "Halifax",
             "New Orleans",
             "Saskatoon",
             "Guatemala City",
             "Santa Fe",
             "Austin",
             "Edmonton",
             "Washington",
             "Phoenix",
             "Atlanta",
             "Seattle",
             "Denver"
           ]
```

Similar to the first example, the first step is to define the function that we need to minimize.

One way to formulate this problem is using the following loss function:

$$loss(\mathbf{X}) = \sum_{i} \sum_{j} ((\mathbf{X}_{i} - \mathbf{X}_{j})^{T} (\mathbf{X}_{i} - \mathbf{X}_{j}) - D_{ij}^{2})^{2}$$

- X_i and X_j are the positions for cities i and j. Each position X has two components, the x and y coordinates.
 ** These are the variables we want to find! **
- $(\mathbf{X}_i \mathbf{X}_j)^T (\mathbf{X}_i \mathbf{X}_j)$ is the squared-distance between cities i and j, given the positions \mathbf{X}_i and \mathbf{X}_j .
- D_{ij} is the known distance between cities i and j. ** These are the given (known) variables provided in city_data.**

The loss function measures how much the actual location and the guess location differ. The optimization problem becomes:

$$\min_{\boldsymbol{X}} \mathit{loss}(\boldsymbol{X})$$

Assume that the location of cities is stored as $city_loc$, a 1D numpy array of size 2n, such that the x-coordinate of a given city is stored first followed by it's y-coordinate.

I.e.

$$city_loc = \begin{bmatrix} X_1[0] \\ X_1[1] \\ \vdots \\ X_n[0] \\ X_n[1] \end{bmatrix}$$

For example, if we had the cities Los Angeles, San Francisco and Chicago with their locations (0.2,0.1),(0.2,0.5),(0.6,0.7), respectively, then city_loc would be

$$city_loc = \begin{bmatrix} 0.2\\0.1\\0.2\\0.5\\0.6\\0.7 \end{bmatrix}.$$

Write the loss function defined above, with the following signature:

```
def loss(city_loc, city_data):
```

```
# city_loc: Numpy array of length 2n containing the x- and y-coordinates of all the cities
# city_data: 2D Numpy array of length nxn containing the table of distances between cities
# totalLoss: Scalar with the output of the loss function for a given set of locations of cit
return totalLoss
```

```
In [23]: #clear
          def loss(city_loc, city_data):
          totalLoss = 0.
          n = len(city_loc)//2
```

```
for i in range(n):
    for j in range(n):
        xij = city_loc[2*i:2*i+2] - city_loc[2*j:2*j+2]
        totalLoss += ( np.inner(xij,xij) - city_data[i,j]**2)**2
return totalLoss
```

Before we move on, let's check that our loss function is correct.

Check the output of your function on the following inputs. The loss function should evaluate to 0.2691297854852331.

Now that we have the function that we want to minimize, we need to compute it's gradient to use steepest descent.

$$\frac{\partial loss}{\partial X_k} = \sum_{i} -4((X_i - X_k)^T (X_i - X_k) - D_{ik}^2)(X_i - X_k) + \sum_{j} 4((X_k - X_j)^T (X_k - X_j) D_{kj}^2)(X_k - X_j)$$

We will give you one way to evaluate the gradient below. After lecture, make sure you can write this function for yourself. It is important to know how to obtain gradient of functions.

```
In [25]: def gradientLoss(city_loc, city_data):
    n = len(city_loc)
    grad = np.zeros(n)

for k in range(n//2):
    for i in range(n//2):
        xik = city_loc[2*i:2*i+2] - city_loc[2*k:2*k+2]
        grad[2*k:2*k+2] += -4 * (np.dot(xik,xik) - city_data[i,k]**2) * xik

for j in range(n//2):
        xkj = city_loc[2*k:2*k+2] - city_loc[2*j:2*j+2]
        grad[2*k:2*k+2] += 4 * (np.dot(xkj,xkj) - city_data[k,j]**2) * xkj
    return grad
```

Let's check that our gradient function is correct. Using the same input as we used in testing our loss function, the resulting gradient should be

```
[ 0.14328835 -0.27303188 1.05797149 1.01695016 -1.20125985 -0.74391827].
```

We should now have everything that we need to use steepest descent if we use a learning rate instead of a line search parameter.

1.2.1 Steepest descent using learning rate

Write a function to run steepest descent for this problem.

- Store the solution after each iteration of steepest descent in a list called city_loc_history. To make plotting easier, we will reshape city_loc when we store it so that it is of shape $n \times 2$ instead of 2n.
- Store the loss function after each iteration in a list called loss_history.
- Your algorithm should not exceed a given maximum number of iterations.
- In addition, you should add a convergence stopping criteria. Here assume that the change in the loss function from one iteration to the other should be smaller than a given tolerance tol.

```
def steepest_descent(city_loc, learning_rate, city_data, num_iterations, tol):
    # compute num_iterations of steepest_descent
    city_loc_history = [city_loc.reshape(-1,2)]
    loss_history = []
    for i in range(num_iterations):
        # write step of steepest descent here
        loss_history.append( ... )
        city_loc_history.append(city_loc.reshape(-1,2))
        if (check if tolerance is reached):
            break
    return city_loc_history, loss_history
In [27]: #clear
         def steepest_descent(city_loc, learning_rate, city_data, num_iterations, tol):
             city_history = [city_loc.reshape(-1,2)]
             loss_history = []
             for i in range(num_iterations):
                 loss_history.append( loss(city_loc, city_data) )
                 city_loc = city_loc - learning_rate * gradientLoss(city_loc, city_data)
                 city_history.append(city_loc.reshape(-1,2))
                 if (i > 0):
                     error = abs(loss_history[-2] - loss_history[-1])
```

```
if ( error < tol ) :
    break
return city_history, loss_history</pre>
```

Using your steepest_descent function, find the location of each city. Use a random initial guess for the location of each of the cities and use the following parameters.

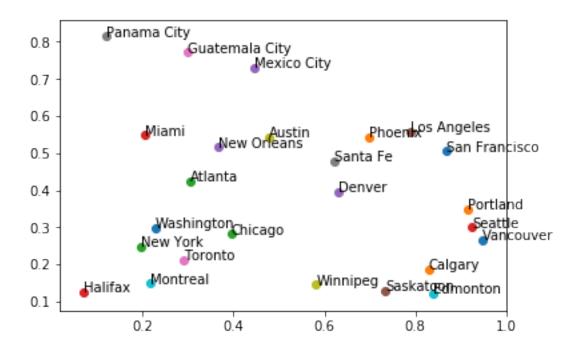
We can use the np.dstack function to change the list of city locations into a numpy array. We will have a 3D numpy array with dimensions $n \times 2 \times num_iterations$.

```
In [29]: city_loc_history = np.dstack(city_loc_history)
```

Now let's display the location of each of the cities. Note, you can use plt.text to display the name of the city on the plot next to its location instead of using a legend. The following code snippet will plot the final location of the cities if we assume that we stored the result of steepest descent as city_loc_history.

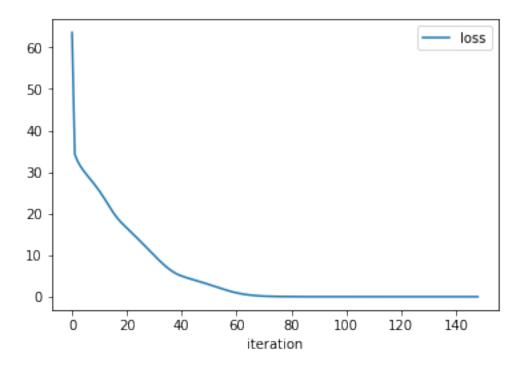
```
In [30]: num_cities = city_loc_history.shape[0]

for i in range(num_cities):
    plt.scatter(city_loc_history[i,0,-1], city_loc_history[i,1,-1])
    plt.text(city_loc_history[i,0,-1], city_loc_history[i,1,-1], city_names[i])
    plt.show()
```



Does your plot make sense? Keep in mind that we aren't keeping track of orientation (we don't have a fixed point for the origin) so you may need to "rotate" or "invert" your plot (mentally) for it to make sense. Or if you want an extra challenge for after class, you can modify the optimization problem to include a fixed origin:-)

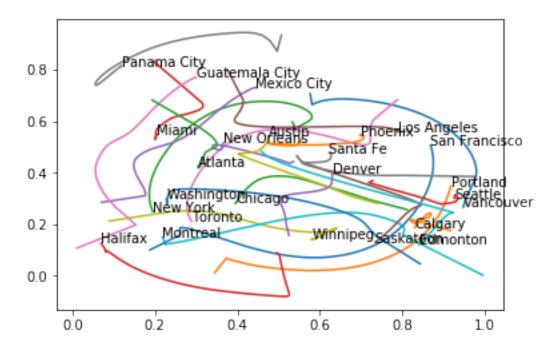
You can plot the history of the loss function, and observe the convergence of the optimization (you can also try with semilogy)



Let's also include how location of each of the cities changes throughout the optimization iterations. The following code snippet assumes that the output for steepest descent is stored in city_loc_history and is a numpy array of shape $n \times 2 \times num_iterations$

```
In [32]: num_cities = city_loc_history.shape[0]

for i in range(num_cities):
    plt.plot(city_loc_history[i,0,:], city_loc_history[i,1,:])
    plt.text(city_loc_history[i,0,-1], city_loc_history[i,1,-1], city_names[i])
    plt.show()
```



The plot looks too cluttered, right? Repeat the same experiment but use a smaller number of cities. But don't forget to normalize the smaller data set. Use 10 cities for this smaller experiment.

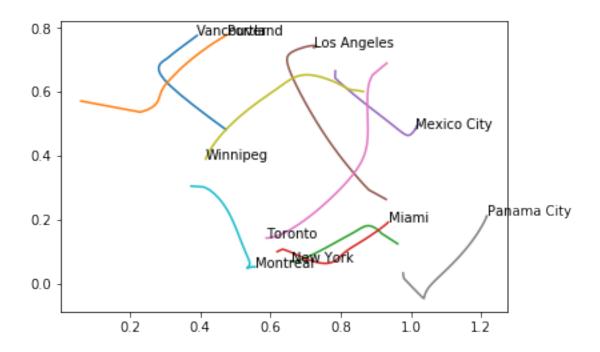
```
In [33]: #clear
    city_data2 = city_data[:10,:10]/np.max(city_data[:10,:10])
    city_loc2 = np.random.rand(2*city_data2.shape[0])

learning_rate = 0.01
    num_iterations = 300
    tol = 1e-8

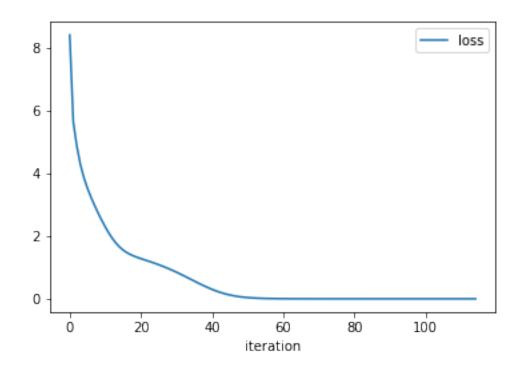
city_loc_hist2, loss_hist_2 = steepest_descent(city_loc2, learning_rate, city_data2, nu city_loc_hist2 = np.dstack(city_loc_hist2)

num_cities = city_loc_hist2.shape[0]
for i in range(num_cities):
    plt.plot(city_loc_hist2[i,0,:], city_loc_hist2[i,1,:])
    plt.text(city_loc_hist2[i,0,-1], city_loc_hist2[i,1,-1], city_names[i])
```

plt.show()



Let's see how the loss changes after each iteration. Plot the loss_history variable.



Repeat the same experiment but try different values for the learning rate. What happens when we decrease the learning rate? Do we need more iterations? What happens when we increase the learning rate? Do we need more or less iterations?

1.2.2 Steepest descent with golden-section search

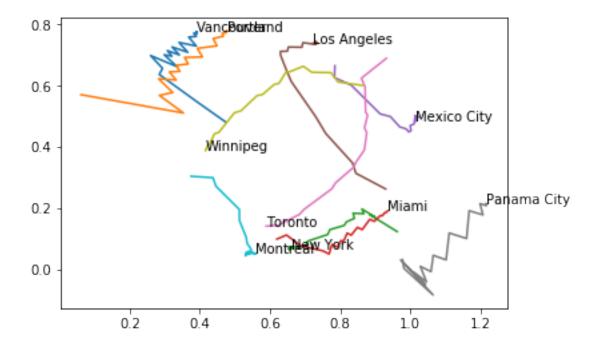
Now, let's use golden-section search again for computing the line search parameter instead of a learning rate.

Wrap the function that we are minimzing so that α is a parameter.

Rewrite your steepest descent function so that it uses scipy.optimize.golden.

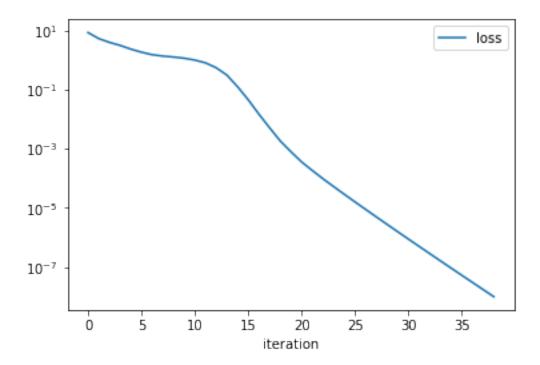
Use your new function for steepest descent with line search to find the location of the cities and plot the result. You can use the code snippets for plotting that we provided above.

```
for i in range(num_cities):
    plt.plot(city_hist3[i,0,:], city_hist3[i,1,:])
    plt.text(city_hist3[i,0,-1], city_hist3[i,1,-1], city_names[i])
plt.show()
```



What do you notice about how the solution evolves? Do you expect using a line search method that the solution will converge faster or slower? Will using a line search method increase the cost per iteration of steepest descent?

Plot the loss function at each iteration to see if it converges in fewer number of iterations.



1.2.3 Using scipy function

We can now compare the functions you defined above with the minimize function from scipy

```
In [39]: import scipy.optimize as sopt
         num\_cities = 6
         tol = 1e-5
         city_data_small = city_data[:num_cities,:num_cities]/np.max(city_data[:num_cities,:num_
         x0 = np.random.rand(2*city_data_small.shape[0])
In [40]: # Providing only the function to the optimization algorithm
         # Note that it takes a lot more function evaluations for the optimization, since
         # gradient and Hessians are approximated in the backend
         res1 = sopt.minimize(loss, x0, args=(city_data_small), tol=tol )
         xopt1 = res1.x.reshape(num_cities,2)
         print(xopt1)
         print('Optimized loss value is ', res1.fun)
         print('converged in', res1.nit, 'iteration with', res1.nfev, 'function evaluations')
[[ 0.99727467  0.19577814]
 [ 0.93997053  0.28885891]
 [ 0.07359406 -0.01680459]
 [ 0.01025728  0.35639055]
```

```
[ 0.26011486  0.64108988]
 [ 0.72842223  0.51556442]]
Optimized loss value is 4.914436537619181e-12
converged in 25 iteration with 420 function evaluations
In [41]: # Providing function and gradient to the optimization algorithm
         # Note that the number of function evaluations are reduced, since only Hessian are now
         res2 = sopt.minimize(loss, x0, args=(city_data_small) , jac=gradientLoss, tol = tol )
         xopt2 = res2.x.reshape(num_cities,2)
         print(xopt2)
         print('Optimized loss value is ', res2.fun)
         print('converged in', res2.nit, 'iteration with', res2.nfev, 'function evaluations')
[[ 0.99727878  0.19577931]
 [ 0.93997462  0.28886007]
 [ 0.07359823 -0.01680365]
 [ 0.01026136  0.35639146]
 [ 0.26011886  0.64109087]
 [ 0.72842626  0.51556553]]
Optimized loss value is 4.891271920960368e-12
converged in 25 iteration with 30 function evaluations
In [42]: xhist,loss_hist = sd_line(x0, city_data_small, 400, tol)
         xopt3 = xhist[-1]
         print(xopt3)
         print('Optimized loss value is ', loss_hist[-1])
         print('convergend in ', len(loss_hist), 'iterations')
[[ 1.00869074  0.24834242]
 [ 0.94198693  0.33441859]
 [ 0.11179536 -0.05898141]
 [ 0.01031788  0.30363077]
 [ 0.22918813  0.61473137]
 [ 0.70767907  0.53874186]]
Optimized loss value is 1.5088095356543901e-05
convergend in 30 iterations
In [43]: xhist,loss_hist = steepest_descent(x0, 0.01, city_data_small, 400, tol)
         xopt3 = xhist[-1]
         print(xopt3)
         print('Optimized loss value is ', loss_hist[-1])
         print('convergend in ', len(loss_hist), 'iterations')
[[ 0.76503197  0.77043717]
 [ 0.78305132  0.66878356]
 [-0.04714062 0.2788438]
```

