Project 1 MA 493

Authored: Sarah Bird (The Do-er), Nicholas Gawron (Group Parent), Jamie Loring (The Facilitator), Andrea Stancescu (The Caffeinated)

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Part I: K++ Initalization

Concept

k++ initialization can be summarized as follows: To begin with, the first representative vector $\vec{c_1}$ should be chosen randomly from the data. The next vector $\vec{c_2}$ should be chosen such that it's the furthest data point value away from $\vec{c_1}$. This process should be repeated until all vectors $\vec{c_i}$ are assigned, such that the inital value of the next representative vector c_l is the data point that is furthest away from the nearest vector among $\vec{c_1}$, ..., $\vec{c_{l-1}}$.

Clear the workspace and close all figure windows

```
clear;
close all
clc
```

Load the data for this question

```
load Q1data.mat
```

a) Random Initialization

We will be sampling components using a uniform distribution for each component on the interval [-1.2, 1.2]

Set the number of data vectors (n) and the dimension of the data space (m)

```
[n,m] = size(XData);
```

Set the number of clusters (k)

```
k=5;
```

Assign each data vector, randomly to one of the k clusters

```
IndexSeti = randi(k,n,1);
```

Plot the data

```
scatter(XData(:,1),XData(:,2),64,IndexSeti,'filled');
hold on
```

Create data structures to store the weight vectors for cluster (c), and the weight vectors from the previous iteration (cPrev)

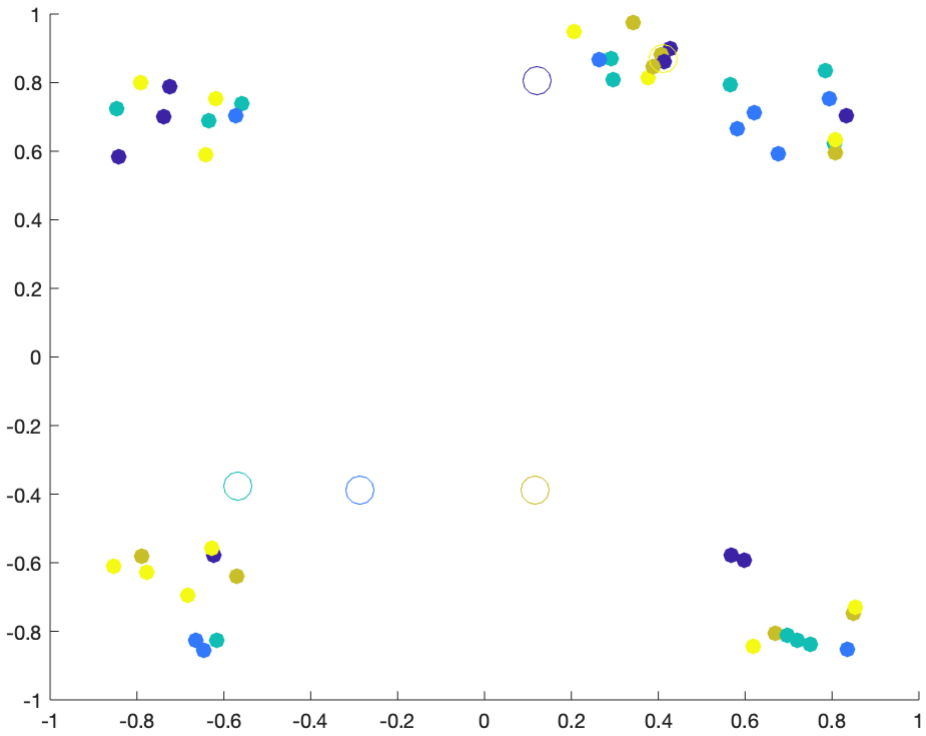
```
ci = zeros(k,m);
cPrev = zeros(k,m);
```

Randomly initialize the weight vectors so that each component is sampled from the interval [-1.2,1.2]

```
ci = -1.2 + 2.4*rand(k,m);
```

Plot the initial weight vectors

```
scatter(ci(:,1),ci(:,2),200,linspace(1,k,k))
hold off
```



The Alternating Minimization Scheme

Calls the function that will perform the Alternating Minimization Scheme.

```
[IndexSetf,cf] = kmeans493(XData,k,IndexSeti,ci);
```

b) the k++ initialization outlined in the project instructions

Calls the function that will perform the *k*++ initialization.

```
[ci,IndexSeti] = KPlusPlusInit(XData,k);
```

10 Realizations of K-Means

This first section runs 10 realizations of the clustering for the random initialization

```
OvCO_forkPP = zeros(1,10);
OvCO_forRand = zeros(1,10);
k=5;

for realz = 1:10
    [n,m]= size(XData);
```

```
    IndexSeti = randi(k,n,1);
    ci = -1.2 + 2.4*rand(k,m);

    % scatter(XData(:,1),XData(:,2),64,IndexSeti,'filled')
    % hold on
    % scatter(ci(:,1),ci(:,2),200,linspace(1,k,k))
    % hold off
    % pause

    [IndexSetf,cf]= kmeans493(XData,k,IndexSeti,ci);
    OvCo=oaco(XData,IndexSetf,cf);
    OvCO_forRand(:,realz) = OvCo ;

    % scatter(XData(:,1),XData(:,2),64,IndexSetf,'filled')
    % hold on
    % scatter(cf(:,1),cf(:,2),200,linspace(1,k,k))
    % hold off

end
```

This next section runs 10 realizations of the clustering for the k++ initialization

```
for realz = 1:10
    [ci,IndexSeti]=KPlusPlusInit(XData,k);

% scatter(XData(:,1),XData(:,2),64,IndexSeti,'filled')
% hold on
% scatter(ci(:,1),ci(:,2),200,linspace(1,k,k))
% hold off
% pause

    [IndexSetf,cf]= kmeans493(XData,k,IndexSeti,ci);

    OvCo=oaco(XData,IndexSetf,cf);
    OvCO_forkPP(:,realz) = OvCo ;

% scatter(XData(:,1),XData(:,2),64,IndexSetf,'filled')
% hold on
% scatter(cf(:,1),cf(:,2),200,linspace(1,k,k))
% hold off

end
```

To make a conclusion about which initialization yields better performance, we decided to look at the means of the overall coherences for each one

```
mean(OvCO_forkPP)
```

```
ans = 0.7737
```

```
mean(OvCO_forRand)
```

```
ans = 5.4794
```

Conclusions

We set a seed for this problem for inter-group consistency. After running through the 20 different realizations of the k-means algorithm, we computed means for the overall coherence of each initialization structure. The mean for the random initialization was found to be 6.4022 while the mean for the k++ initialization is 0.7737. The data from these 10 observations points to k++ leading to a better performance as it minimizes the overall coherence value more effectively. A potential explanation for this is that k++ uses the data vectors themselves, not just a random number generated.

Part II: Elbow Method

Concept

The Elbow Method can be summarized as follows: To being with, a set of successive values should be picked to represent the possible number of clusters. For each value of k, the k-means clustering algorithm should be run and then the overall coherence should be calculated. These overall coherence values, for each value of k, should be graphed (on the same plot), and the "elbow" in this graph is the point where there is a sharp change in slope. The "elbow" corresponds to the best value of k.

Generalized Code

Setting intialization values and vectors, where rows represents the number of initializations used, and columns are the values of k for each initialization scheme

```
suck = 8;
initalz = 5;

mat2PlotKPP = zeros(initalz,suck);
mat2PlotRand = zeros(initalz,suck);
```

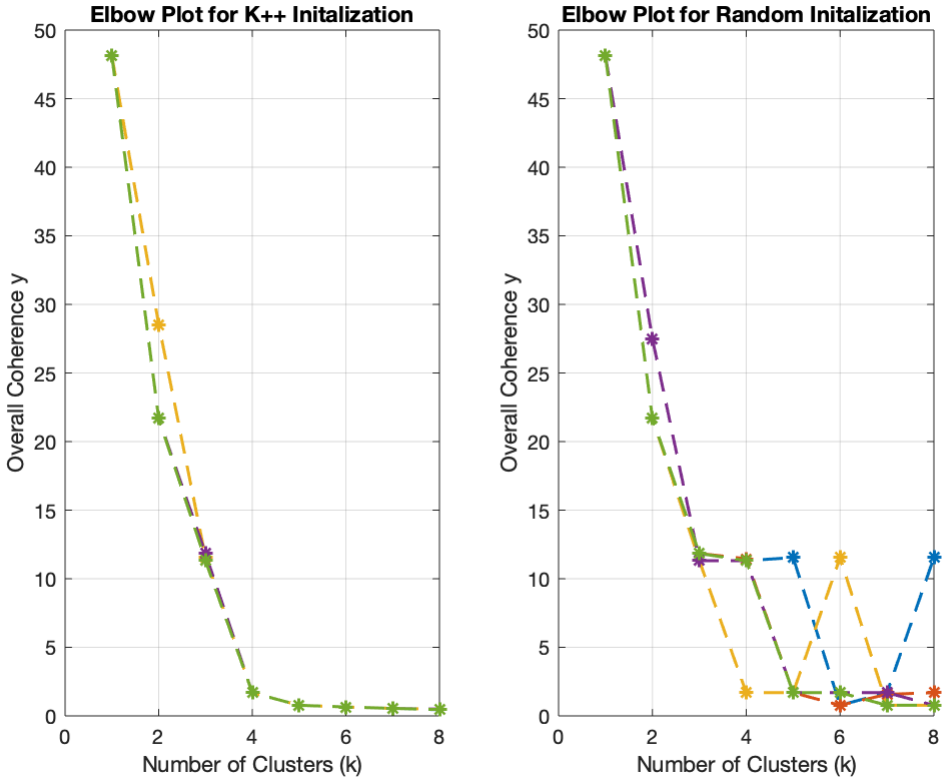
Getting the data values needed for graphing the Elbow Method -- k++ initialization first, then random initialization

```
for k=1:suck

    for realz = 1:initalz

        [ci,IndexSeti]=KPlusPlusInit(XData,k);
        [IndexSetf,cf]= kmeans493(XData,k,IndexSeti,ci);

        OvCo = oaco(XData,IndexSetf,cf);
        mat2PlotKPP(realz,k) = OvCo;
    end

    for realz = 1:initalz

        [n,m]= size(XData);
        IndexSeti = randi(k,n,1);
        ci = -1.2 + 2.4*rand(k,m);
        [IndexSetf,cf]= kmeans493(XData,k,IndexSeti,ci);
```

```
        OvCo=oaco(XData,IndexSetf,cf);
        mat2PlotRand(realz,k) = OvCo;
    end

end
```

Creates the Elbow Method plots for *k*++ initialization and random initialization, respectively

```
subplot(1,2,1)
for iter = 1:5
    plot(1:suck, mat2PlotKPP(iter,:),'LineWidth',1.5,'Marker',"*",'LineStyle','--')
    hold on
    title('Elbow Plot for K++ Initalization')
    xlabel('Number of Clusters (k)')
    ylabel('Overall Coherence y')
    %rectangle('Position',[4-1 7-1 1 1],'Curvature',[.5 .5])
    %legend('Realiz 1','Realiz 4','Realiz 3','Realiz 4','Realiz 5')
    grid on
end



hold on

subplot(1,2,2)
for iter = 1:5
    plot(1:suck, mat2PlotRand(iter,:),'LineWidth',1.5,'Marker',"*",'LineStyle','--')
    hold on
    title('Elbow Plot for Random Initalization')
    xlabel('Number of Clusters (k)')
    ylabel('Overall Coherence y')
    %legend('Realiz 1','Realiz 4','Realiz 3','Realiz 4','Realiz 5')
    grid on
end

hold off
```



Discussion on Optimal k per Initialization

Looking at the two plots that are created from the Elbow Method code, we can see that the results definitely vary between the two different types of initalizations. It appears that k++ initialization has less variability between the different realizations of the data. Utilizing the Elbow Method, our group determined that k++ initalization minimized the overall coherency most accurately around k=4 clusters. Random initalization had more variablility between the realizations of the data. From the plot we obtained, our group determined that either 3 or 4 clusters minimized overall coherency. However, the overall coherency was much higher on average than the k++ initalization scheme.

Keeping in mind the discussion of variability in the previous paragraph, we can see that when using the k++ initalization scheme, we can be more certain about the number of clusters needed to minimize the coherence, which leads to a better clustering process.

Part III: MNIST Application

Primer code needed for this application

```
NImages = 100;

[imgs, labels] = readMNIST('testImages','testLabels', NImages, 0);

% Example of how to convert the first 10 images into vectors for input into
% the clustering algorithm
```

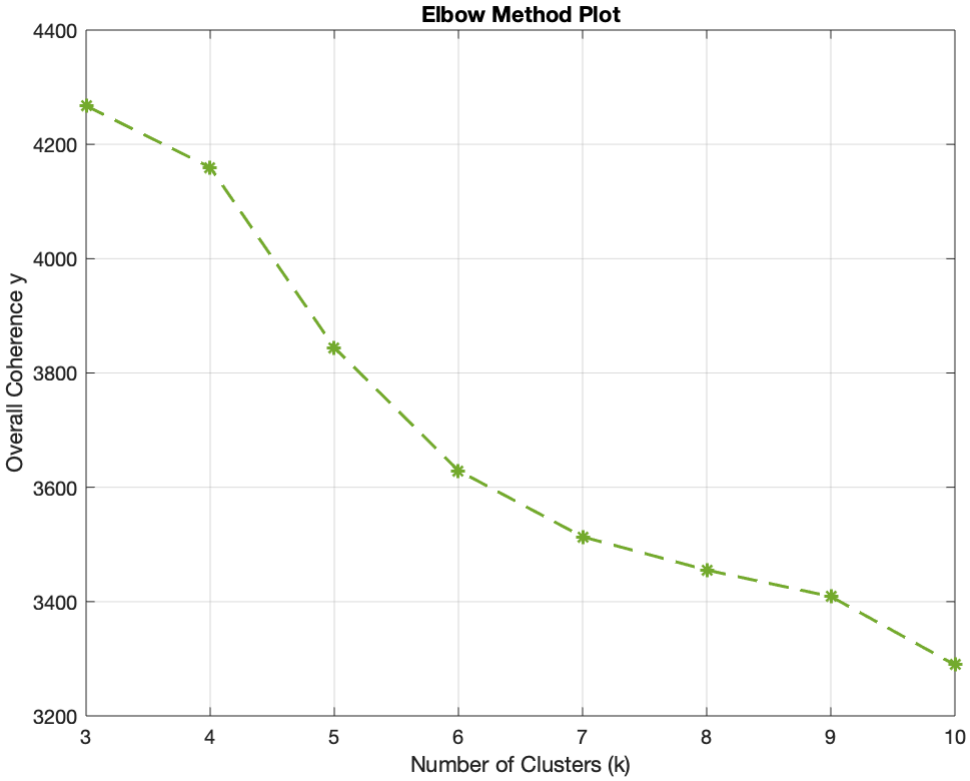
```
m = 20*20;
v = zeros(1,m);
XData3 = zeros(NImages,m);

for i=1:NImages
    XData3(i,:) = reshape(imgs(:,:,i),[1,m]);
end
```

Performs k-means clustering with *k*++ initialization on the first 100 images from the MNIST data set with k equals 3 through 10

```
k_vec = 3:10;
initial_z = 5;
plot3_kpp = zeros(initial_z,length(k_vec));

figure;

for j=1:length(k_vec)
    for realz = 1:initial_z
        [ci,IndexSeti]=KPlusPlusInit(XData3,k_vec(j),42);
        [IndexSetf,cf]= kmeans493(XData3,k_vec(j),IndexSeti,ci);

        OvCo = oaco(XData3,IndexSetf,cf);
        plot3_kpp(realz,j) = OvCo;
    end
end
```

Creating the plot using the Elbow Method for k equals 3 through 10

```
for i = 1:5
    plot(k_vec, plot3_kpp(i,:),'LineWidth',1.5,'Marker',"*",'LineStyle','--')
    hold on
    title('Elbow Method Plot')
    xlabel('Number of Clusters (k)')
    ylabel('Overall Coherence y')
    %rectangle('Position',[4-1 7-1 1 1],'Curvature',[.5 .5])
    %legend('Realiz 1','Realiz 4','Realiz 3','Realiz 4','Realiz 5')
    grid on
end
```

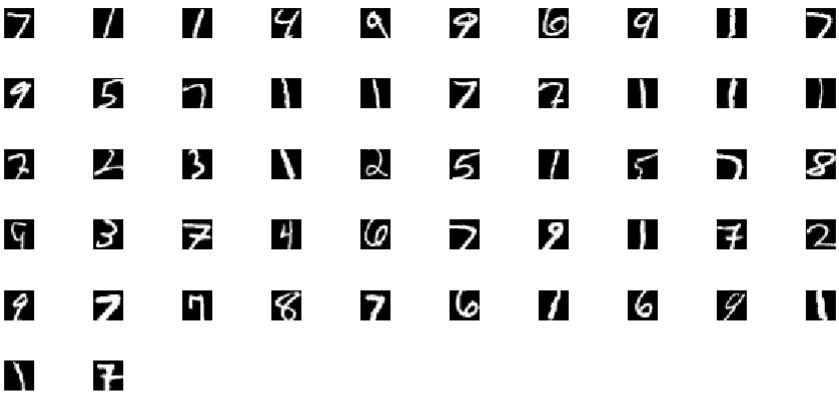


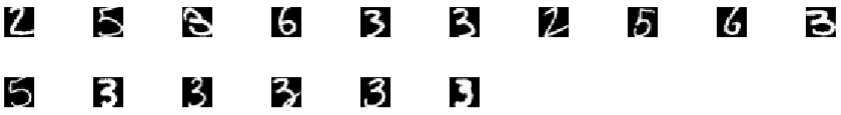
Based on the Elbow Method graph produced, the "best" value for the number of clusters k is k=6

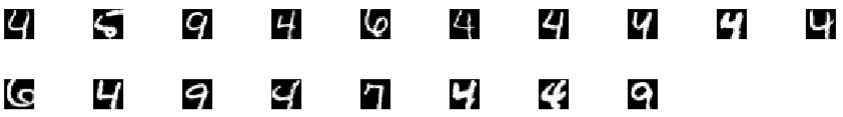
"Primer code" for determining a success score using k=6

```
numim = 100; % number of images
% use parts of Haider Code to extract data frame from 100 images
% 400 cols for 20 x 20 pixels

[XDataM ,labels2test]= DatHaider(numim);

% use k = 6 from previous elbow graph!
k_fromelbow=6;


% initalizes and does kmeans
[c,IndexSeti]=KPlusPlusInit(XDataM,k_fromelbow,42);
[IndexSetf, cf] = kmeans493(XDataM,k_fromelbow,IndexSeti,c);

% for the  cluster we...
for val_k= 1:k_fromelbow

    figure(val_k)

    str = sprintf('Images associated with Cluster %d', val_k);
```

```
% look at all the points in this cluster from k means
    for i=1:sum(IndexSetf==val_k)
       % creates the rows and coloumns for images in a cluster
        rows_img = round(numim/10);
        cols_img = round(numim/10);
       %creates a subplot for a certain cluster k
       subplot(rows_img,cols_img,i)
       title(str)
       %and shows all the images associated with that cluster
       Cluster_image = XDataM(IndexSetf==val_k,:);
       currImg = reshape(Cluster_image(i,:),[20,20]);
       imshow(currImg,'InitialMagnification',1000)
    end

end
```







```
% cluster 1 is 1
% cluster 2 is 0
% cluster 3 is 3
% cluster 4 is 2
% cluster 5 is 4
% cluster 6 is 0
```

Looking at the clusters generated above, the following states the number/image occurring most frequently (from top to bottom): 1, 0, 3, 2, 4, 0

Calculating the actual success score (using k=6)

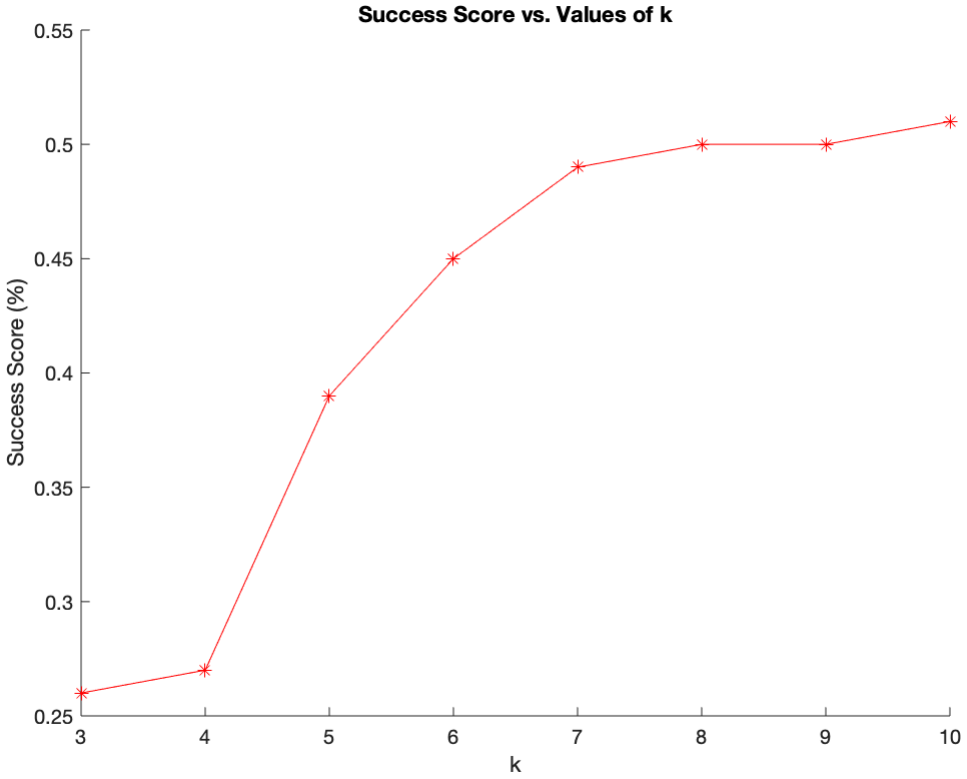
```
ClusterMostOccurNum = [1 0 3 2 4 0];

expLabs = zeros(100,1);

for val_k = 1:k_fromelbow
    WhereImagesR=IndexSetf==val_k;
    expLabs = ClusterMostOccurNum(val_k).*(WhereImagesR)+expLabs ;
end

SucScore = sum(expLabs == labels2test)/100;

pct = SucScore*100
```

```
pct = 45
```

From the code above, we see that clustering of the digits in the MNIST data set with k=6 clusters gives us a 45% accuracy.

Part IV: Bonus

```
BonusSuck = 10;

numim = 100; % number of images
% use parts of Haider Code to extract data frame from 100 images
% 400 cols for 20 x 20 pixels

[XDataM ,labels2test]= DatHaider(numim);

SucScoresforAll = zeros(1,8);

% calc success score for each k
for k_to_test =3:BonusSuck

    %initalizes and does kmeans
    [c,IndexSeti]=KPlusPlusInit(XDataM,k_to_test,42);
    [IndexSetf, cf] = kmeans493(XDataM,k_to_test,IndexSeti,c);

    MostOccurNum = zeros(1,k_to_test);
    expLabs = zeros(100,1);

    % for the  cluster we...
    for val_k= 1:k_to_test
        % computes the number that occurs most in the label
        MostOccurNum(val_k)  =  mode(labels2test(IndexSetf==val_k));
        %find location of image
        WhereImagesR=IndexSetf==val_k;
        %update expiermental labels with mode of image number
        expLabs = MostOccurNum(val_k).*(WhereImagesR)+expLabs ;
    end

        % computes the success score!
        SucScore = sum(expLabs == labels2test)/100;

        SucScoresforAll(val_k-2)= SucScore;

end

figure;

hold on
plot(3:BonusSuck,SucScoresforAll,'r*-')
title('Success Score vs. Values of k')
xlabel('k')
ylabel('Success Score (%)')
hold off
```



Looking at the graph output here, we see that the highest success score occurs at k=10 (51%), while the elbow method yields a success score of 45% (at k=6). It makes sense that the highest success score occurs at a larger value of k than the elbow method shows because having more clusters allows for more differences in images to be separated, therefore resulting in higher accuracy.

Functions

KPlusPlusInIt: This function establishes the k++ initalization for k-means clustering algorithm. It takes in a parameter of x and y values called XData. It also takes in a parameter, k, which is the number of clusters.

```
function [c,IndexSeti]= KPlusPlusInit(XData,k,varargin)


% returns the k num of clusters in the matrix c
% IndexSeti  is the inital clustering for k means

% XData  is input data n by m for m dimensional
% k - num of clusters
 %varargin{1} - set the inital centriod value!

[n,m]=size(XData);

% Establishes Index Set
% first is theinital index set
IndexSeti = randi(k,n,1);
IndexSet = IndexSeti;
```

```
%haider likes zero initalization!
c = zeros(k,m);

%%%%%% Gets C_1

if nargin == 2
    % first step of k++
    randIndex = randi(n);

    % first cluster rep vector!
    c(1,:)= XData(randIndex,:);
else
     SetInit42 = varargin{1};
     c(1,:) = XData(SetInit42,:);
end


%%
% Create a data structure to store closest weight vector for each data
% point
closestCluster=zeros(n,1);


for l = 2:k

    % Reassign each data vector to the new, closest cluster
    for d=1:n

        % Store the coordinates of the current data vector
        xD = XData(d,:);

        % Set the minimum distance tracker to be a very large number
        sqDistMin=1e16;

        % Find the closest weight vector (cluster) to the current data
        % vector
        for i=1:l-1
            sqDist = norm(c(i,:)-xD,2);

            % If the distance is less than the current min, assign the
            % current data vector to this cluster
            if sqDist<sqDistMin
                closestCluster(d)=i;
                sqDistMin=sqDist;
            end

        end
    end



    % Update the assignments of the data vectors to their new clusters
    IndexSet = closestCluster;
```

```
    % sets up a matrix [distance , data point] for each max dist point per
    % cluster initalizes values to zero!
    % note we use 1+m dimensions since we need m dimensions to store the
    % cluster value
    % AND the additional one is used to store the distnace
    DistanceANDClusterCani = zeros(l-1,1+m);


    % we have l-1 clusters looking for the l th cluster
    for y = 1:l-1
        % fetches points closest to y-th cluster
        PointsClosest2y = XData(IndexSet ==y,:);
        % computes the distance from closest points to the y-th cluster
        % gets the max!
        % 2 in the sum lets us sum by row!
        [Max_dist_forClosestClus,IndexInClosest] = max (sum( (PointsClosest2y -c(y,:)).^2,2));
        DistanceANDClusterCani(y,:)= [Max_dist_forClosestClus,PointsClosest2y(IndexInClosest,:)
    end
    [~, NextCentriodLoc]= max(DistanceANDClusterCani(:,1));
    c(l,:) = DistanceANDClusterCani(NextCentriodLoc,2:end);
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%REMOVE EVERYTHING BELOW BEFORE THE END IF WE NEED TO USE A TOTALLY
%%%%%RANDOM CLUSTERING  BEFOREHAND


   for d=1:n

        % Store the coordinates of the current data vector
        xD = XData(d,:);

        % Set the minimum distance tracker to be a very large number
        sqDistMin=1e16;

        % Find the closest weight vector (cluster) to the current data
        % vector
        for i=1:k
            sqDist = norm(c(i,:)-xD,2);

            % If the distance is less than the current min, assign the
            % current data vector to this cluster
            if sqDist<sqDistMin
                closestCluster(d)=i;
                sqDistMin=sqDist;
            end

        end
   end

   IndexSeti = closestCluster;

end
```

kmeans493: This function carries out the alternating minimization scheme. This function takes in 4 parameters. XData is a matrix of x and y values. k is the number of clusters, IndexSet is the index set for initalization. C is the vector of cluster points.

```
function [IndexSetf,cf]=kmeans493(XData,k,IndexSet,c)

[n,m]=size(XData);

% intialized C_prev
cPrev = zeros(k,m);

doneFlag=0;

% Keep alternating updates to weight vectors and cluster assignments until weight
% vectors no longer change their locations

while (~doneFlag)

    % Update the weight vectors in each cluster via the centroid formula
    for i=1:k

        % Find the indices for all data vectors currently in cluster i
        ClusterIndices = find(IndexSet==i);

        % Find the number of data vectors currently in cluster i
        NumVecsInCluster = size(ClusterIndices,1);

        % Create a data structure to store weight vector for the current
        % cluster
        c(i,:)=0;

        % Update cluster vector using the centroid formula
        for j=1:NumVecsInCluster
            for l=1:m
                c(i,l) = c(i,l) + XData(ClusterIndices(j,1),l)/NumVecsInCluster;
            end
        end

    end


    % Now reassign all data vectors to the closest weight vector (cluster)

    % Create a data structure to store closest weight vector for each data
    % point
    closestCluster=zeros(n,1);

    % Reassign each data vector to the new, closest cluster
    for d=1:n

        % Store the coordinates of the current data vector
        xD = XData(d,:);
```

```
        % Set the minimum distance tracker to be a very large number
        sqDistMin=1e16;

        % Find the closest weight vector (cluster) to the current data
        % vector
        for i=1:k
            sqDist = norm(c(i,:)-xD,2);

            % If the distance is less than the current min, assign the
            % current data vector to this cluster
            if sqDist<sqDistMin
                closestCluster(d)=i;
                sqDistMin=sqDist;
            end

        end
    end

    % Update the assignments of the data vectors to their new clusters
    IndexSet = closestCluster;


    % Terminate the alternating scheme if the weight vectors are unaltered
    % relative to the previous iteration
    if c==cPrev
        doneFlag=1;
    else
        cPrev=c;
    end
end


cf = c ;
IndexSetf = IndexSet;
end
```

oaco: This function computes the overall coherence value. It takes in a matrix called XDataf, which is a matrix of x and y values of the data. It also takes in a column vector called IndexSetf which is the final index set. It also takes in a matrix named c which are the final centroid points.

```
function OvCo=oaco(XDataf,IndexSetf,c)
    % output overall coherence
        % calculated by summing the coherence from each
        %cluster sum_{1 to k } ||x_i-c_i||
    % input final indexSet after K-Means is run!
    % input final set of clusters
    % input orginal data of form nxm for n rows of m dimensional data
    OvCo = 0;
    for i=1:size(c,1) % number of k clusters
        % gets the i-th final cluster points
        Dist_i =sum(sum((XDataf(IndexSetf==i,:)-c(i,:)).^2,2));
        OvCo = Dist_i + OvCo;
    end
```

```
end
```

readMNIST: Reads digits and labels from raw MNIST data files

```
function [imgs, labels] = readMNIST(imgFile, labelFile, readDigits, offset)

    % Read digits
    fid = fopen(imgFile, 'r', 'b');
    header = fread(fid, 1, 'int32');
    if header ~= 2051
        error('Invalid image file header');
    end
    count = fread(fid, 1, 'int32');
    if count < readDigits+offset
        error('Trying to read too many digits');
    end

    h = fread(fid, 1, 'int32');
    w = fread(fid, 1, 'int32');

    if offset > 0
        fseek(fid, w*h*offset, 'cof');
    end

    imgs = zeros([h w readDigits]);

    for i=1:readDigits
        for y=1:h
            imgs(y,:,i) = fread(fid, w, 'uint8');
        end
    end

    fclose(fid);
    % Read digit labels
    fid = fopen(labelFile, 'r', 'b');
    header = fread(fid, 1, 'int32');
    if header ~= 2049
        error('Invalid label file header');
    end
    count = fread(fid, 1, 'int32');
    if count < readDigits+offset
        error('Trying to read too many digits');
    end

    if offset > 0
        fseek(fid, offset, 'cof');
    end

    labels = fread(fid, readDigits, 'uint8');
    fclose(fid);

    % Calc avg digit and count
    imgs = trimDigits(imgs, 4);
```

```
    imgs = normalizePixValue(imgs);
    %[avg num stddev] = getDigitStats(imgs, labels);

end
```

trimDigits: This function will trim the 4 pixel padding around the digits

```
function digits = trimDigits(digitsIn, border)
    dSize = size(digitsIn);
    digits = zeros([dSize(1)-(border*2) dSize(2)-(border*2) dSize(3)]);
    for i=1:dSize(3)
        digits(:,:,i) = digitsIn(border+1:dSize(1)-border, border+1:dSize(2)-border, i);
    end
end
```

normalizePixValue: This function will normalize pixel values to the [0...1] range

```
function digits = normalizePixValue(digits)
    digits = double(digits);
    for i=1:size(digits, 3)
        digits(:,:,i) = digits(:,:,i)./255.0;
    end
end
```