

Project 1 MA 493

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Part I: k++ Initialization

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 initial value of the next representative vector \vec{c}_i is the data point that is furthest away from the nearest vector among $\vec{c}_1, \dots, \vec{c}_{i-1}$.

Clear the workspace and close all figure windows

```
clear;  
close all  
clc
```

Load the data for this question

```
load Q1data.mat
```

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);
```

Create data structures to store the weight vectors for cluster c_i 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);
```

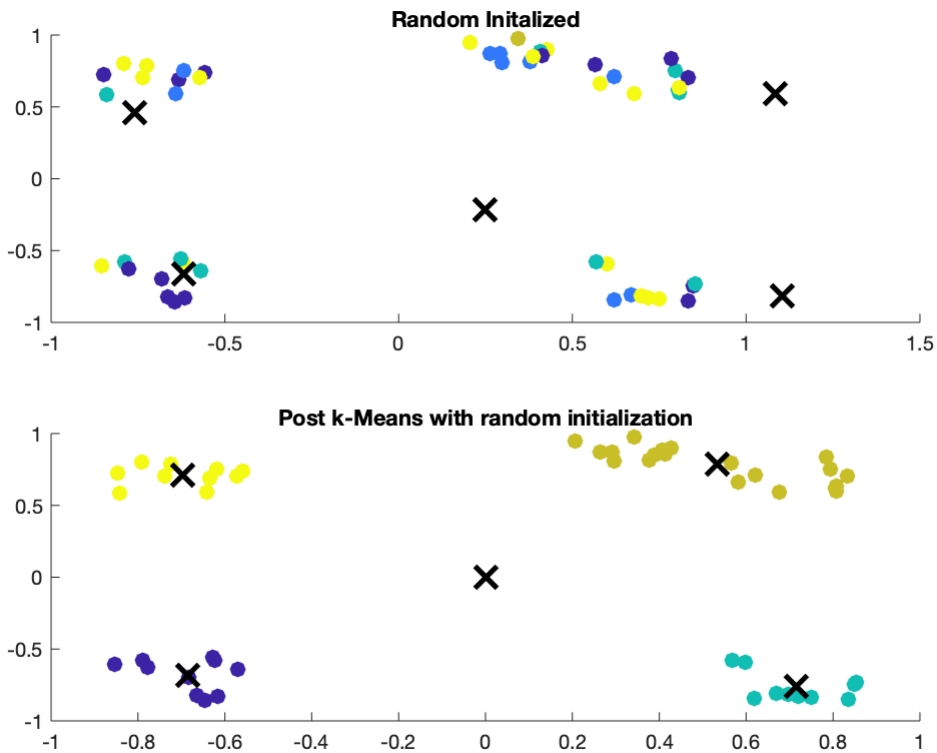
The Alternating Minimization Scheme

Calls the function that will perform the Alternating Minimization Scheme

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

The first panel below shows the random initialization prior to any k-means clustering. Then, the second panel shows the clustering after performing the k-means alternating minimization scheme.

```
figure;  
subplot(2,1,1)  
    scatter(XData(:,1),XData(:,2),64,IndexSeti,'filled')  
    hold on;  
    plot(ci(:,1),ci(:,2),'kx','MarkerSize',15,'LineWidth',3)  
    title('Random Initalized')  
  
subplot(2,1,2)  
  
    scatter(XData(:,1),XData(:,2),64,IndexSetf,'filled')  
    hold on;  
    plot(cf(:,1),cf(:,2),'kx','MarkerSize',15,'LineWidth',3)  
    title('Post k-Means with random initialization')
```



The k++ Initialization

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

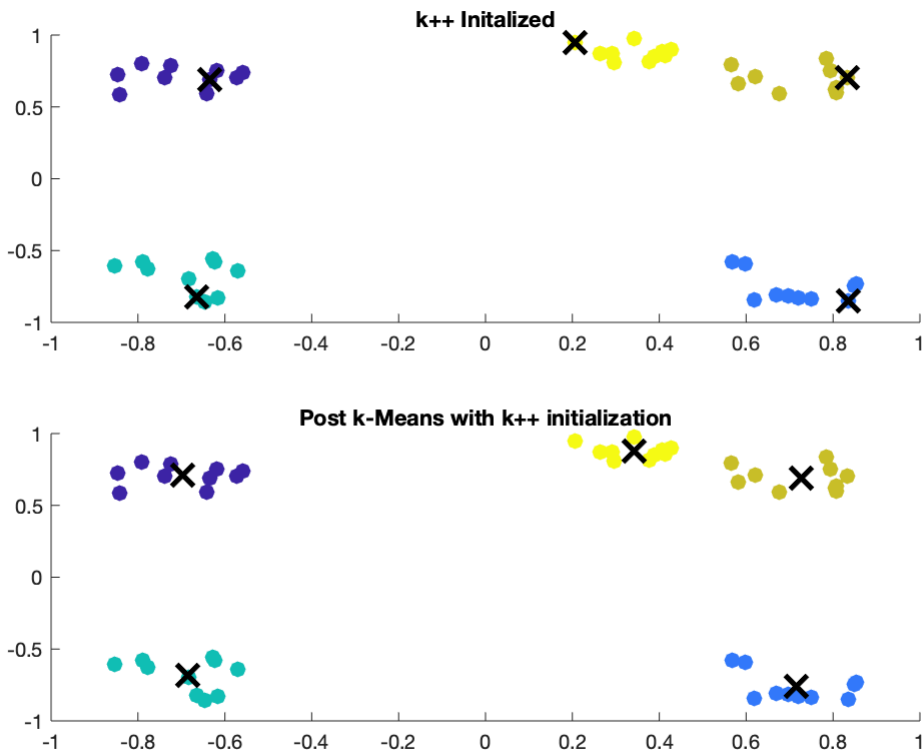
```
[ci, IndexSeti] = KPlusPlusInit(XData, k);
[IndexSetf, cf] = kmeans493(XData, k, IndexSeti, ci);
```

The first panel below shows the *k++* initialization prior to any k-means clustering. Then, the second panel shows the clustering after performing the k-means alternating minimization scheme.

```
figure;
subplot(2,1,1)
    scatter(XData(:,1),XData(:,2),64,IndexSeti,'filled')
    hold on;
    plot(ci(:,1),ci(:,2),'kx','MarkerSize',15,'LineWidth',3)
    title('k++ Initalized')

subplot(2,1,2)

    scatter(XData(:,1),XData(:,2),64,IndexSetf,'filled')
    hold on;
    plot(cf(:,1),cf(:,2),'kx','MarkerSize',15,'LineWidth',3)
    title('Post k-Means with k++ initialization')
```



10 Realizations of K-Means

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

```
% initializes the vectors to store overall coherence
OvCO_forkPP = zeros(1,10);
OvCO_forRand = zeros(1,10);

% sets k clusters to be 5
k=5;

% runs 10 realizations
for realz = 1:10

    [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);
    OvCO_forRand(:,realz) = OvCo ;

end
```

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

```

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

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

    OvCo=oaco(XData,IndexSetf,cf);

    OvCO_forkPP(:,realz) = OvCo ;

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.

```

% prints out the mean overall coherence for each method!
% first for k++ followed by random initialization
mean(OvCO_forkPP)

```

```
ans = 0.7737
```

```
mean(OvCO_forRand)
```

```
ans = 7.1063
```

Conclusions

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 begin 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. This "elbow" corresponds to the best value of k .

Generalized Code

Setting initialization 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(italz,suck);
mat2PlotRand = zeros(italz,suck);
```

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

```
for k=1:suck

    for realz = 1:italz

        [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:italz

        [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')
    grid on
end
legend('Realiz 1','Realiz 4','Realiz 3','Realiz 4','Realiz 5')

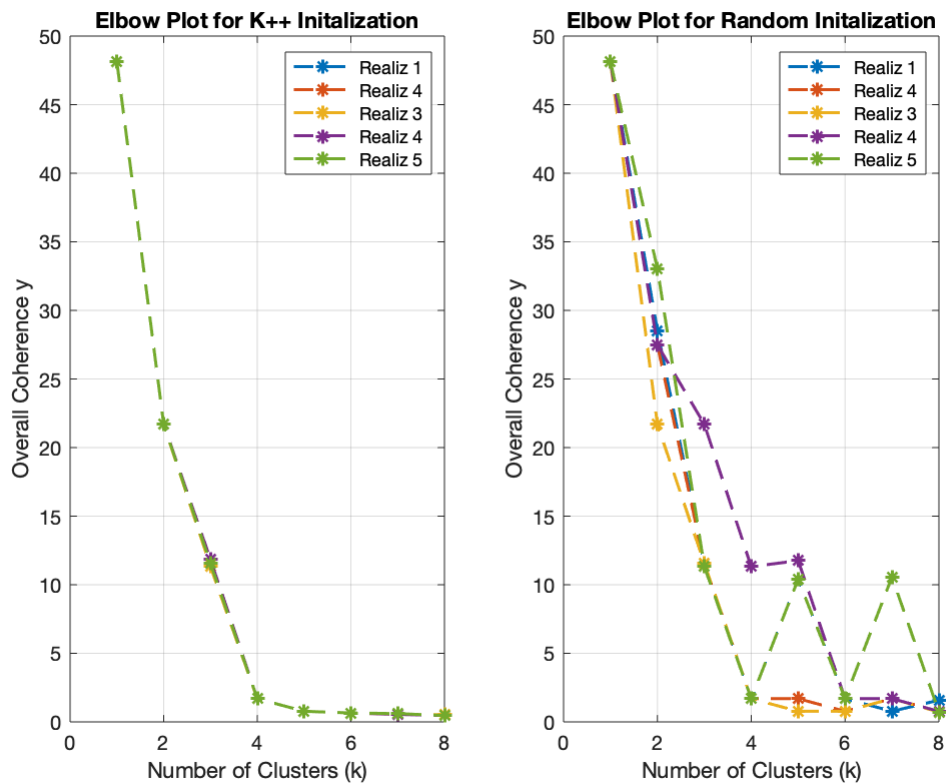
hold on

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')
grid on
end
legend('Realiz 1','Realiz 4','Realiz 3','Realiz 4','Realiz 5')
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 initializations. It appears that $k++$ initialization has less variability between the different realizations of the data. Utilizing the Elbow Method, our group determined that $k++$ initialization minimized the overall coherence most accurately around $k = 4$ clusters. Random initialization had more variability between the realizations of the data. From the plot we obtained, our group determined that either 3 or 4 clusters minimized overall coherence. However, the overall coherence was much higher on average than the $k++$ initialization scheme.

Keeping in mind the discussion of variability in the previous paragraph, we can see that when using the $k++$ initialization 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 $k = 3$ through $k = 10$,

```

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

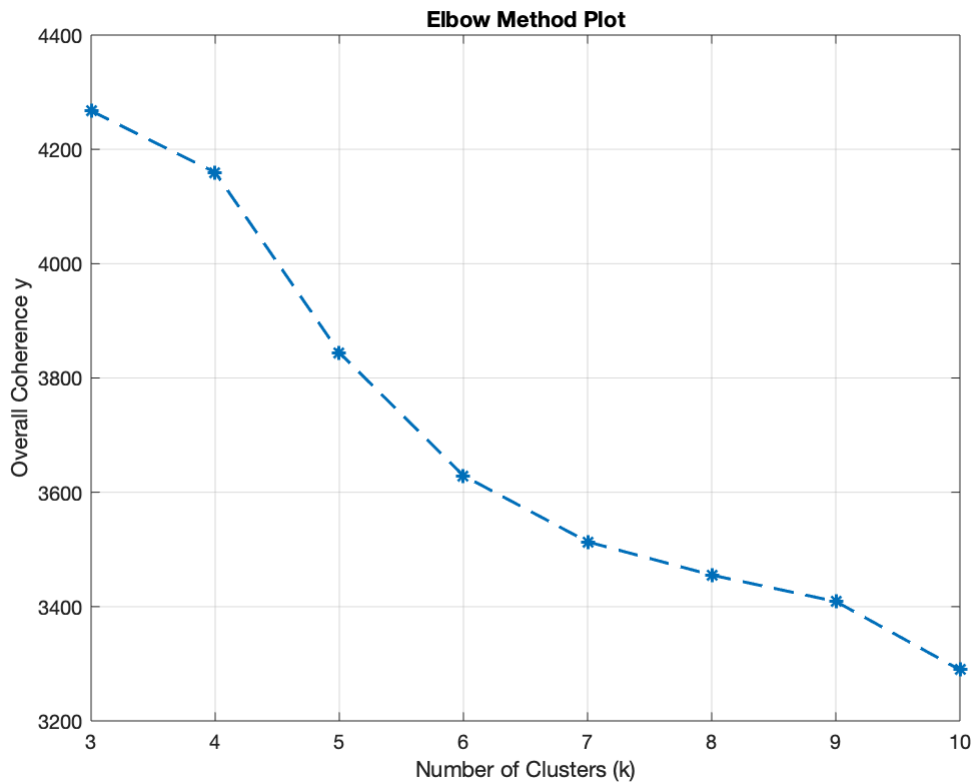
```

Creating the plot using the Elbow Method for $k = 3$ through $k = 10$,

```

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')
    grid on
    hold off
end

```

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

All Images from Each Cluster

"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;

% initializes 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;
    modeNum=mode(labels2test(IndexSetf==val_k));
    fprintf(['The images below are associated with cluster %d.\n ' ...
            'We note that the most common number that has appeared in this cluster' ...
            ' is %d.'], val_k,modeNum);
```

```

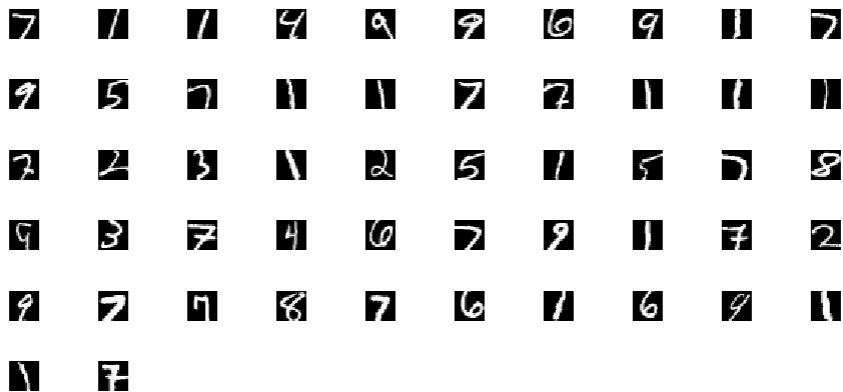
% look at all the points in this cluster from k means
for i=1:sum(IndexSetf==val_k)
    % creates the rows and coloumns for images in a cluster
    rows_img = round(numim/10);
    cols_img = round(numim/10);
    %creates a subplot for a certain cluster k
    subplot(rows_img,cols_img,i)
    %and shows 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

```

The images below are associated with cluster 1.

We note that the most common number that has appeared in this cluster is 1.



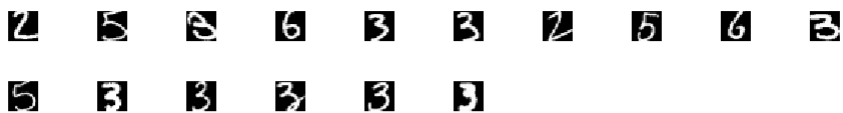
The images below are associated with cluster 2.

We note that the most common number that has appeared in this cluster is 0.



The images below are associated with cluster 3.

We note that the most common number that has appeared in this cluster is 3.



The images below are associated with cluster 4.

We note that the most common number that has appeared in this cluster is 2.



The images below are associated with cluster 5.

We note that the most common number that has appeared in this cluster is 4.



The images below are associated with cluster 6.

We note that the most common number that has appeared in this cluster is 0.

0 0 0 4 0 6 6

Success Score

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.

Discussion of Clusters

Provide examples of two clusters, including images, that performed well in detecting similar patterns and an example of one cluster that performed less well. Use these examples to discuss the strengths and limitations of this overall approach in the context of this application.

Above, we included several clusters that the clustering method produced. As you can see, there were some clusters that performed very well. Examples of those include cluster 2 and cluster 4. Both of those clusters have less than 5 observations in them. We can hypothesize that clusters that have a smaller number of observations in them have a, generally, higher success rate than those that have larger numbers of observations. Thus, we can make the claim that a higher number of clusters has a higher coherence value than lower number of clusters (which aligns with intuition). When you aim to have a high number of clusters, this technique is ideal.

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

    %initializes 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 experimental labels with mode of image number
        expLabs = MostOccurNum(val_k).*(WhereImagesR)+expLabs ;
    end

    % computes the success score!
    SucScore = sum(expLabs == labels2test)/100;
    % success score stored as a matrix
    SucScoresforAll(val_k-2)= SucScore;

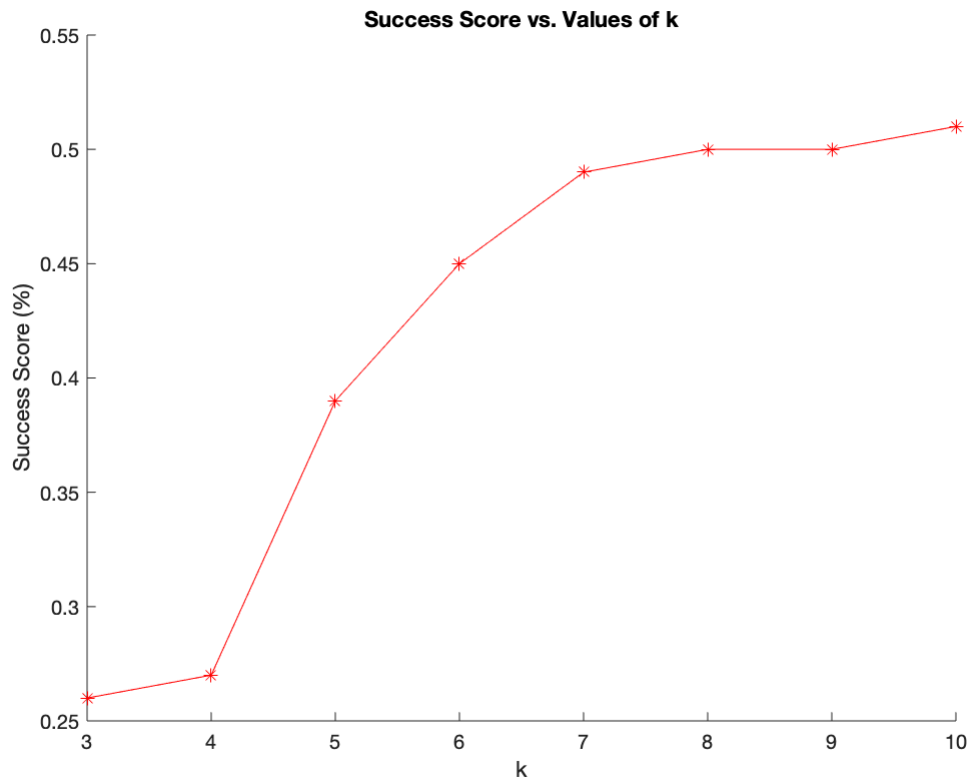
end
```

```

%plots the images
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. We found it interesting that the success score seemed to start leveling off after reaching $k = 7$.

Functions

KPlusPlusInit: This function establishes the $k++$ initialization 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 initial clustering for k means

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

[n,m]=size(XData);

% Establishes Index Set
% first is the initial index set
IndexSeti = randi(k,n,1);
IndexSet = IndexSeti;
%haider likes zero initialization!
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 initializes values to zero!
% note we use l+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,:)).
    DistanceANDClusterCani(y,:)= [Max_dist_forClosestClus,PointsClosest2y(IndexInCl
end
[~, NextCentriodLoc]= max(DistanceANDClusterCani(:,1));
c(1,:) = DistanceANDClusterCani(NextCentriodLoc,2:end);
end

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

```

```

        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 initialization. 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,l),l)/NumVecsInCluster;
            end
        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 original 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

```