University of Maryland-College Park

Advance Scientific Computing I,II

Spectral Clustering on Handwritten Digits Database

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Abstract

Spectral Clustering is a technique used to group together data points of similar behavior in order to analyze the overall data. The goal of this project will be to implement a spectral clustering algorithm on the MNIST handwritten digits database in which we will be able to cluster similar images using a similarity matrix derived from the dataset. We will develop code in order to implement each step of the algorithm and optimize to efficiently obtain a reasonable clustering of the dataset.

Contents

1 Introduction

Spectral clustering is clustering technique based on the spectral analysis of a similarity matrix derived from a given data set. The main goal of spectral clustering or any clustering algorithm is to implement a procedure that groups objects in a data set to other objects with ones that have a similar behavior. For this project, we would like to use the MNIST Handwritten digits database in order to implement a clustering algorithm that will cluster together same digits and be in a different cluster from different digits. Spectral clustering implements a clustering algorithm such a k-means clustering on a reduced dimension which allows the formation of tight clusters. Thus given some data point $X_i \in \mathbb{R}^d$, spectral clustering performs a clustering in $\mathbb{R}^k$ where $k << d$. The advantage of spectral clustering is the simplicity of the algorithm to implement where only the use of standard linear algebra methods are needed in order to solve the problem efficiently. It also has many application areas such as machine learning, exploratory data analysis, computer vision and speech processing.

1.1 Definitions

The motivation behind spectral clustering is given from ideas in graph theory. In this section we define some notation that will be used throughout this report. Define a graph $G = (V, E)$ as a set of vertices together with a set of edges. We assume G is an undirected graph with vertex set $V = \{v_1, ..., v_n\}$. We also assume G is unweighted or in other words each edge has the same weight of 1. Thus the adjacency matrix W is defined to be

$$W = w_{ij} = \begin{cases} 1, & \text{if } v_i, v_j \text{ are connected by an edge} \\ 0, & \text{otherwise} \end{cases}.$$

Since G is undirected we require that $w_{ij} = w_{ji}$ and hence gives a symmetric adjacency matrix. The degree of a vertex $v_i \in V$ is defined as

$$d_i = \sum_{j=1}^{n} w_{ij}.$$

This can also be viewed as just the number of edges connected to that vertex. The degree matrix denoted D is a diagonal matrix where each $d_1, ..., d_n$ lies on the diagonal. We denote a subset of vertices $A \subset V$ and its complement as $\bar{A} = V \setminus A$. For simplicity, we define $i \in A$, as the set of indices i of vertices $v_i \in A$. We also define two ways of measuring the size of a subset A of V.

$$|A| = \text{ number of vertices in } A.$$

and

$$vol(A) = \sum_{i \in A} d_i.$$

$|A|$ measures the size of the subset by the number of vertices, while $vol(A)$ measures the size by the number of edges. Finally we define the weight between two subsets $A, B \in V$ as

$$W(A, B) = \sum_{i \in A, j \in B} w_{ij}.$$

This counts the number of edges connecting the two subsets. One final definition we would like to introduce is the unnormalized laplacian matrix which is defined as $L = D - W$.

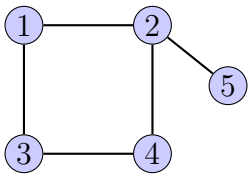
1.2 Motivation

Clustering is a way to separate data points such that similar points are grouped together, and are in a different group from ones that are dissimilar. Another way to think about this is from the viewpoint of graph cuts. Given a graph, we want to partition the vertices such that those connected by edges with high weights are grouped together and separate from the ones connected by low weights. Spectral clustering is motivated by approximating a graph partitioning and in particular approximating the RatioCut or NCut on a given graph.

One of the most direct ways to partition a graph is to solve the min cut problem. That is, given a similarity graph, we want to partition the graph into k subsets and hence solve the optimization problem of minimizing

$$cut(A_1, ..., A_k) := \frac{1}{2} \sum_{1}^{k} W(A_i, \bar{A}_i) \tag{1}$$

over all partitions where $W(A_i, \bar{A}_i)$ defines the weight between a subset and its complement. In other words, we want to minimize the number of edges cut in order to partition the graph. This is very straightforward and easy to solve, in particular for the case when $k = 2$ by using Karger's algorithm which provides an efficient randomized method for finding this cut. However in some cases it may lead to an unhelpful partition. Consider the example graph below:



The min cut problem would cut through the edge connecting 2 to 5 and give one partition to be relatively smaller than the other. This is not helpful in clustering since we want each cluster to be relatively large. To account for this, modifications known as the RatioCut and the normalized cut or NCut can be introduced. For the RatioCut, we want the size of each partition to be measured by the number of vertices in it. For the NCut, we would like the size of each partition to be measured

by the number of edges. Thus we define the RatioCut and NCut as follows:

$$RatioCut(A_1, ..., A_k) := \frac{1}{2}\sum_{i=1}^{k}\frac{W(A_i, \bar{A}_i)}{|A_i|} \tag{2}$$

$$NCut(A_1, ..., A_k) := \frac{1}{2}\sum_{i=1}^{k}\frac{W(A_i, \bar{A}_i)}{vol(A_i)} \tag{3}$$

In both cases, the objective functions try to balance out each partition. This makes solving these versions of the min cut problem NP hard. Spectral clustering allows us to solve relaxed versions of these problems. For this project, we will be focusing on the relaxed version of the NCut problem to solve the clustering problem.

We will start with approximating the NCut problem for the case where $k = 2$. Relaxing the min NCut problem will derive the motivation behind normalized spectral clustering which we will define later in this section. For the case $k = 2$, we want to solve the optimization problem of minimizing

$$NCut(A, \bar{A}) = \frac{W(A, \bar{A})}{vol(A)} + \frac{W(A, \bar{A})}{vol(\bar{A})} = \frac{W(A, \bar{A})(vol(\bar{A}) + vol(A))}{vol(A)vol(\bar{A})} \tag{4}$$

over both partitions. We define a cluster indicator vector f by

$$f(v_i) = f_i = \begin{cases} \sqrt{\frac{vol(\bar{A})}{vol(A)}}, & \text{if } \ v_i \in A \\ -\sqrt{\frac{vol(A)}{vol(\bar{A})}}, & \text{if } \ v_i \in \bar{A} \end{cases} \tag{5}$$

The cluster indicator vector is giving some value depending on whether the vertex lies in A or $\bar{A}$. Thus we compute $f^T Lf$ and $f^T Df$ which gives the following:

$$f^T Lf = \sum w_{ij}(f_i - f_j)^2 = W(A, \bar{A})\left(\sqrt{\frac{vol(\bar{A})}{vol(A)}} + \sqrt{\frac{vol(A)}{vol(\bar{A})}}\right)^2 = W(A, \bar{A})\frac{(vol(\bar{A}) + vol(A))^2}{vol(A)vol(\bar{A})} \tag{6}$$

$$f^T Df = \sum d_i f_i^2 = \sum_{i\in A} d_i\left(\sqrt{\frac{vol(\bar{A})}{vol(A)}}\right)^2 + \sum_{j\in\bar{A}} d_j\left(\sqrt{\frac{vol(A)}{vol(\bar{A})}}\right)^2 = vol(\bar{A}) + vol(A) \tag{7}$$

Note that the ratio of the two gives us the NCut problem we want to minimize. Thus minimizing the NCut problem is equivalent to

$$\begin{aligned} &\text{minimize} \quad NCut(A, B) = \frac{f^T Lf}{f^T Df} \\ &\text{subject to} \quad f_i = \begin{cases} \sqrt{\frac{vol(\bar{A})}{vol(A)}}, & \text{if } \ v_i \in A \\ -\sqrt{\frac{vol(A)}{vol(\bar{A})}}, & \text{if } \ v_i \in \bar{A} \end{cases} \end{aligned} \tag{8}$$

The relaxation problem is given by

$$\begin{aligned} \underset{f\in\mathbb{R}^n}{\text{minimize}} \quad & \frac{f^T L f}{f^T D f} \\ \text{subject to} \quad & f^T D\mathbf{1} = 0 \end{aligned} \tag{9}$$

where f is allowed to take on real values. It can be shown the relaxation problem is a form of the Rayleigh-Ritz quotient. Since we have the constraint that $f^T D\mathbf{1} = 0$ we want a solution that will not be the constant one vector $\mathbf{1}$ which is the eigenvector of the smallest eigenvalue of 0. Thus we want to find the eigenvector corresponding the the second smallest eigenvalue. Substituting $g = D^{1/2} f$ the problem becomes

$$\begin{aligned} \underset{g\in\mathbb{R}^n}{\text{minimize}} \quad & \frac{g^T (D^{-1/2} L D^{-1/2}) g}{g^T g} \\ \text{subject to} \quad & g \perp D^{1/2}\mathbf{1} \end{aligned} \tag{10}$$

where $D^{1/2}\mathbf{1}$ is the first eigenvector of $L_{sym} = D^{-1/2} L D^{-1/2}$ which corresponds to the lowest eigenvalue of 0. Letting $U = [u_1 u_2 \dots u_n]$ be the matrix whose columns are the orthonormal eigenvectors of L_{sym}. If we only consider vectors g that are orthogonal to u_1 and since L is non negative, then

$$g^T L_{sym} g = \sum_{i=1}^{n} \lambda_i |(U^T x)_i|^2 = \sum_{i=1}^{n} \lambda_i |u_i^T x|^2 = \sum_{i=2}^{n} \lambda_i |u_i^T x|^2$$

This gives a non negative linear combination of $\lambda_2, \lambda_3 \dots, \lambda_n$, thus

$$g^T L_{sym} g = \sum_{i=2}^{n} \lambda_i |u_i^T x|^2 \geq \lambda_2 \sum_{i=2}^{n} |u_i^T x|^2 = \lambda_2 \sum_{i=2}^{n} |(U^T x)_i|^2 = \lambda_2 g^T g$$

provided that g is orthogonal to the first column of U. This inequality becomes equality if we choose $g = u_2$. Therefore

$$\min_{\substack{g\neq 0 \\ g\perp D^{1/2}\mathbf{1}}} \frac{g^T L_{sym} g}{g^T g} = \min_{\substack{g^T g = 1 \\ g\perp D^{1/2}\mathbf{1}}} g^T L_{sym} g = \lambda_2$$

which gives the second smallest eigenvalue and g is the corresponding eigenvector. In general applying the Courant-Fisher theorem, we can find the k smallest eigenvalues and their corresponding eigenvectors.

Theorem 1 (Courant-Fischer Theorem)**.** *Given A a Hermitian matrix with eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{n-1} \leq \lambda_n$, let k be a given integer with $1 \leq k \leq n$, and let $w_i \in \mathbb{C}^n$, then*

$$\max_{w_1, w_2, \dots, w_{k-1}} \min_{\substack{x\neq 0, x\in\mathbb{C}^n \\ x\perp w_1, w_2, \dots, w_{k-1}}} \frac{x^T A x}{x^T x} = \lambda_k$$

We only included part of the theorem which finds the smallest eigenvalue and corresponding eigenvector under some given constraints. For the complete statement and proof of the Courant-Fischer theorem, see appendix A.

This can be extended to the general case for $k > 2$. The outline for this proof comes from the paper by Von Luxberg [1]. In this case, we define a cluster indicator vector f_k by

$$f_j(v_i) = f_j(i) = \begin{cases} \frac{1}{\sqrt{vol(A_j)}}, & \text{if } v_i \in A_j \\ 0, & \text{otherwise} \end{cases} \tag{11}$$

We define the matrix F as the matrix whose columns are the k indicator vectors. Then, $f_i^T f_j = 0$, $f_i^T D f_i = 1$ and $f_i^T L f_i = \frac{cut(A_i, \bar{A}_i)}{vol(A_i)}$. Thus the NCut optimization problem becomes

$$\begin{aligned} \underset{A_1,\ldots,A_k}{\text{minimize}} \quad & Tr(F^T L F) \\ \text{subject to} \quad & F^T D F = I \\ & F \text{ defined in (10)} \end{aligned} \tag{12}$$

Relaxing the second constraint and substituting $T = D^{1/2} F$ gives of the relaxation problem of

$$\begin{aligned} \underset{T \in \mathbb{R}^{n \times k}}{\text{minimize}} \quad & Tr(T^T D^{-1/2} L D^{-1/2} T) \\ \text{subject to} \quad & T^T T = I \end{aligned} \tag{13}$$

This is a standard trace minimization problem in which the solution T which is a matrix whose columns are the first k eigenvectors of L_{sym}. The proof of the standard trace minimization problem will be provided in appendix A. L_{sym} is the normalized laplacian matrix defined as

$$L_{sym} = D^{-1/2} L D^{-1/2}. \tag{14}$$

Thus the first k eigenvectors will solve the relaxed version of the min NCut problem.

2 Approach

The following subsections outline the various steps of the project. We will start by developing code to produce a similarity graph from our database. Given the similarity graph we will compute the normalized laplacian matrix. From there we will compute the first k eigenvectors of the laplacian and place in a matrix, perform a dimension reduction on the matrix of eigenvectors and use a clustering algorithm on the reduced dimension in order to cluster the data points.

2.1 Similarity Graph

Given the data set $X_1, ..., X_n$ and a notion of "similar", a similarity graph is a graph where X_i and X_j have an edge between them if they are considered "similar".The Gaussian similarity function is

defined as $s(X_i, X_j) = e^{\frac{-||X_i - X_j||^2}{2\sigma^2}}$ where σ is a parameter. to be determined which varies depending on the dataset used. We use the Gaussian similarity function to define the distance between any two data points. We must then define some threshold ϵ that will determine if two data points are similar enough. If $s(X_i, X_j) > \epsilon$ we will consider them similar and connect an edge between X_i and X_j. For our project, choosing the best ϵ is not immediately apparent so we need to be careful in choosing this correctly. Note that since each $X_i \in \mathbb{R}^{28\times 28}$, to compute the distance between any two points we use the ℓ^2 norm for matrixes in this case given as

$$||X_i - X_j||_2^2 = \sum_{k=1}^{28}\sum_{l=1}^{28}(X_i(k,l) - X_j(k,l))^2$$

2.2 Laplacian Matrix

Recall that the unnormalized laplacian matrix is defined as $L = D - W$. The normalized laplacian is

$$L_{sym} = D^{-1/2}LD^{-1/2} = I - D^{-1/2}WD^{-1/2}. \tag{15}$$

The eigenvectors of the normalized laplacian is directly related to the indicator vectors in the NCut problem. Thus finding the k first eigenvectors of the normalized laplacian will give a clustering into k partitions. Recall W is the adjacency matrix. Given the Gaussian similarity function, W and D are defined as

$$W = (w_{ij})_{1\le i,j\le n}, w_{ij} = \begin{cases} 1, & \text{if } \ s(X_i, X_j) > \epsilon \\ 0, & \text{otherwise} \end{cases} \tag{16}$$

$$D = (d_{ij})_{1\le i,j\le n}, d_{ij} = \sum_{j=1}^{n} w_{ij} \tag{17}$$

which will be used in computing the normalized laplacian. Our computation of the normalized laplacian matrix was validated by verification of one of the known eigenvectors. As described above in the motivation section of this report, $L\mathbf{1} = 0$ gives an eigenvalue of 0 corresponding to the eigenvector $\mathbf{1}$. This is equivalent to $L_{sym}D^{1/2}\mathbf{1} = 0$ or the normalized laplacian having an eigenvector of $D^{1/2}\mathbf{1}$. Thus after computing the normalized laplacian in Matlab, it was verified by multiplying L_{sym} by its eigenvector of $D^{1/2}\mathbf{1}$ to obtain a value of zero (its corresponding eigenvalue). ✓

2.3 Computing the first k eigenvectors

We then computed the first k eigenvectors of the normalized laplacian matrix. We used an iterative method called the Power Method to find them. Let $B = D^{-1/2}WD^{-1/2}$.

Power Method Algorithm on Matrix B
Start with an initial nonzero vector, v_0.Set tolerance, max iteration and iteration= 1
Repeat
$v_0 = B * v_0$;
$v_0 = v_0/norm(v_0, 2)$;
lambda= $v_0' * B * v_0$;
converged = (norm($B * v_0$− lambda∗v_0,2) < tol);
iter=iter+1;
if iter > maxiter
warning('Did Not Converge')
Until Converged

The largest eigenvalue of B will correspond to the smallest eigenvalue of L_{sym}. Hence this will give us our first eigenvector we are looking for. To find the next eigenvalues we need to implement the power method with deflation. But when using the power method on any symmetric matrix, the eigenvalues found are the largest ones in magnitude. Since we only want the first largest we modify our B matrix into to make B positive semidefinite which will shift all the eigenvalues to being positive and we can find the first k of them. To make B a positive semidefinite matrix, we create a new B, denoted B_{mod}, such that

$$B_{mod} = B + \mu I$$

This makes B_{mod} diagonally dominant and hence positive semidefinite. Letting μ = the largest row sum of B, this gave us B_{mod} which is now positive semidefinite and we found its largest k eigenvalues.

So we actually run the power method on B_{mod} and use the following deflation algorithm in order to find the first k of eigenpairs.

Deflation Algorithm for finding the first K eigenvalues
Initialize d = length(B_{mod}); V = zeros(d,K); lambda=zeros(K,1);
for j from $1, \ldots, K$
[lambda(j), V(:,j)] = power-method(B_{mod},v_0);
$B_{mod} = B_{mod}$− lambda(j)∗$V(:, j) * V(:, j)'$;
$v_0 = v_0 - \frac{v_0 \cdot V(:,j)}{v_0 \cdot v_0} * v_0$
end

where λ_j, v_j are the previous eigenvalues and eigenvectors found respectively. Initially v_0 is a randomize vector to approximate the first eigenvector. Then in the deflation algorithm, the j^{th} eigenvector is approximated using the previous initial vector v_0 with the projection of the previous eigenvectors subtracted from it to obtain the new v_0. This removes the orthogonal components of the previous eigenvectors found.

The speed of convergence of this method depends on the size of the eigengap $\gamma_k = |\lambda_k - \lambda_{k+1}|$.

[1]. The larger the eigengap, the faster the convergence of the algorithm in computing the first k eigenvectors.

We will then put these first k eigenvectors into a matrix and normalize the rows. Let $T \in \mathbb{R}^{n \times k}$ be the eigenvector matrix with rows having norm 1. Set

$$t_{i,j} = \frac{v_{i,j}}{(\sum_s v_{i,s}^2)^{1/2}}$$

This will transforms our matrix V consisting of the first k eigenvector as columns to a new matrix T.

$$\begin{bmatrix} v_{11} & v_{12} & v_{13} & \dots & v_{1k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ v_{i1} & v_{i2} & v_{i3} & \dots & v_{ik} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ v_{n1} & v_{n2} & v_{n3} & \dots & v_{nk} \end{bmatrix} \Rightarrow \begin{bmatrix} t_{11} & t_{12} & t_{13} & \dots & t_{1k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ t_{i1} & t_{i2} & t_{i3} & \dots & t_{ik} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ t_{n1} & t_{n2} & t_{n3} & \dots & t_{nk} \end{bmatrix}$$

We will then project the eigenvectors onto new space. Let $y_i \in \mathbb{R}^k$ be a vector from the i^{th} row of T. This will form the new matrix $Y = T^T$ where each y_i vector is a column of Y.

$$\begin{bmatrix} t_{11} & t_{12} & t_{13} & \dots & t_{1k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ t_{i1} & t_{i2} & t_{i3} & \dots & t_{ik} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ t_{n1} & t_{n2} & t_{n3} & \dots & t_{nk} \end{bmatrix} \Rightarrow y_i = \begin{bmatrix} t_{i1} \\ t_{i2} \\ \vdots \\ t_{ik} \end{bmatrix}$$

We will then preform a clustering algorithm on our new matrix Y of a reduced dimension.

2.4 Clustering

We can perform a k-means algorithm on the new set of vectors of reduced dimension.

- Randomly select k cluster centroids, z_j.
- Calculate the distance between each y_i and z_j.
- Assign the data point to the closest centroid.
- Recalculate centroids and distances from data points to new centroids.
- If no data point was reassigned then stop, else reassign data points and repeat.

Finally, assign the original point X_i to cluster j if and only if row i of the matrix Y was assigned to cluster j. This is the final step in the algorithm. If the algorithm was implement correctly, similar handwritten digits should be clustered together.

3 Implementation

The spectral clustering algorithm outlined above is planned to be implemented in the programming language MatLab R2014b. This is the programming language that we are most comfortable with using with the most prior knowledge of this language. This will be run on a personal laptop, a Macbook Pro which is a 2.5 GHz Intel Core processor and has 4 GB of Memory. If needed we may be able to upgrade to a more power computer but as of right now that does not seem necessary.

4 Databases

The database used will be the MNIST Handwritten digits database. The database includes a training set of 60,000 images and a testing set of 10000 images. We will first consider the testing set which has 1000 of each digit 0-9. Each image is of size 28×28 pixels. We denote an image $X_i \in \mathbb{R}^{28\times 28}$. A variety of methods have been tested using this database. For this project, we want to use these images for testing the spectral clustering algorithm to see if we can cluster the images such that same digits are cluster together despite the different handwritings. In our code, each image reads into a 4 array called $X(n1, n2, d, p)$ where n1,n2 represents the size of the image, d is its corresponding digit (0-9) and p represents the number of its corresponding digit (for the test set p ranges from 1 to 1000). The link below can be used to view this database.

http://yann.lecun.com/exdb/mnist/

5 Validation

There are various phases in which we can validate various steps of the algorithm.

5.1 Validation of Computation of Eigenvectors

Validate the computation of the eigenvectors.
We can compare our results from the power method algorithm with the eigenvectors computed by using the Matlab command eigs(L_{sym}). The graphs on page 12 shows the first 5 eigenvalues found and a comparison to the ones found using the built in Matlab function eigs. The residual between the first 5 eigenvectors found from the power method and the eigs function were also computed. Both the graph and tables are shown for first the set of 5,000 images and then the entire test set of 10,000 images.

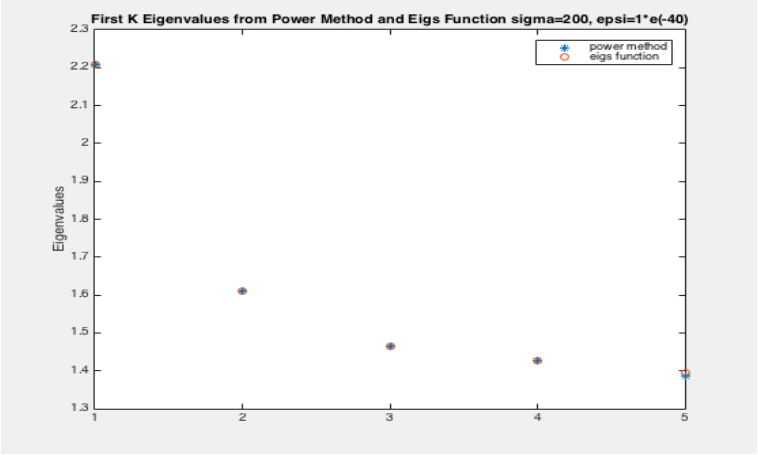


Figure 1: Comparison of eigenvalues found on sample of 5,000 images

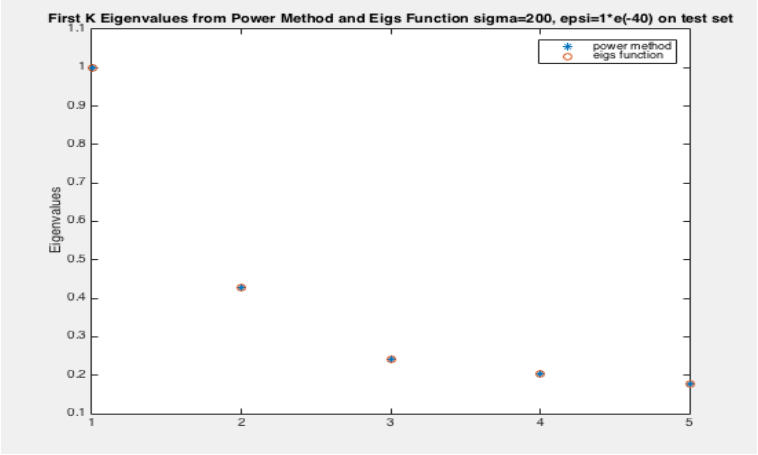


Figure 2: Comparison of eigenvalues found on sample of 10,000 images

	λ_1	λ_2	λ_3	λ_4	λ_5
r	1.05E-10	9.54E-7	4.11E-1	7.30E-1	6.83E-1

	λ_1	λ_2	λ_3	λ_4	λ_5
r	4.62E-11	6.30E-10	1.59E-8	1.58E-1	2.61E-1

$r = ||v_i - \hat{v}_i||_2$ where v_i comes from using the power method and $\hat{v}_i$ comes from the eigs function and $1 \leq i \leq 5$ corresponding to the first 5 eigenvalues. In both cases the first few eigenvalues found from the power method give a reasonable approximation to the ones found from the Matlab command. After the third eigenvector and so on, the residuals found were larger than the first two found mostly because of rounding errors. The deflation algorithm relies on available eigenvalues and eigenvectors. Since the previous eigenvalues and eigenvectors were estimates that came from the power method, the new approximated matrix is subject to round off errors and thus the error increases as more eigenvectors are found. This may also have to do with the size of the eigengaps found. In the 5,000 set the eigengaps were 0.6, 0.2, 0.01, and 0.04 respectively. However, with pretty good confident the power method can still be applied to the entire training set of 60,000 images and a good approximation to only the first few eigenvalues and eigenvectors can be used.

5.2 Validation of k-means clustering

We can validate the k-means clustering algorithm on a well known clustered set. Since we are able to repeat the initial randomize starting centroids, we can repeat the algorithm on say the Swiss Role dataset to obtain a "good" clustering.

5.3 Validation of Final solution

We can visually validate the solution of the algorithm by displaying the clusters and seeing if similar images are grouped together as predicted.

6 Testing

For testing purposes we can implement the spectral clustering algorithm on another database such as a database of face images. One that could be testing on is the public database supplied by Yale University called "The Extended Yale Face Database B". This database contains 16128 images of 28 different subjects, each under 9 poses and 64 different viewing conditions. If testing on this database, one would expect the algorithm to give similar results. Ultimately the algorithm would cluster similar faces together and put in different clusters of faces that were dissimilar. If time allows we may be able to test on this database.

7 Project Schedule/ Milestones

We have split the project into different phases and allocated time to complete each phase.

- End of October/ Early November
  Develop code to generate a Similarity Graph and Normalized Laplacian matrix from the MNIST database. This will include testing for the correct parameter σ in the Gaussian Similarity function as described previously. ✓
- End of November/ Early December
  Compute first k eigenvectors of the Normalized Laplacian matrix as well as validate this. Also prepare for the mid-year presentation and report. ✓
- February
  Normalize the rows of matrix of eigenvectors and perform dimension reduction.
- March/April
  Cluster the points using k-means clustering algorithm and validate this step.
- End of Spring semester: Implement entire algorithm, optimize and obtain final results as well as prepare for the final presentation and final report.

8 Deliverables

The deliverables for this project are the MNIST database and code that delivers this. We will deliver code that implements the spectral clustering algorithm and code that was use for testing and validations at various steps. If time allows this code will be optimized for effective performance. We will also deliver reports at the various periods throughout the course as requested which covers the approach, implementation, validation, testing and milestones of the project. Finally we will give the various presentations throughout the course that introduce the project, give a mid-year update and a final presentation of results found.

A Appendix

Theorem (Courant-Fischer Theorem). *Given A a Hermitian matrix with eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{n-1} \leq \lambda_n$, let k be a given integer with $1 \leq k \leq n$, and let $w_i \in \mathbb{C}^n$, then*

$$\max_{w_1,w_2,\ldots,w_{k-1}} \min_{\substack{x\neq 0, x\in\mathbb{C}^n \\ x\perp w_1,w_2,\ldots,w_{k-1}}} \frac{x^TAx}{x^Tx} = \lambda_k$$

and

$$\min_{w_1,w_2,\ldots,w_{n-k}} \max_{\substack{x\neq 0, x\in\mathbb{C}^n \\ x\perp w_1,w_2,\ldots,w_{n-k}}} \frac{x^TAx}{x^Tx} = \lambda_k$$

[5.]

Proof. Since A is Hermitian, there exist a unitary matrix $U \in M_n$ such that $A = U\Lambda U^T$ with $\Lambda = diag(\lambda_1, \lambda_2, ..., \lambda_n)$. Let $1 \leq k \leq n$. If $x \neq 0$ then

$$\frac{x^TAx}{x^Tx} = \frac{(U^Tx)^T\Lambda(U^Tx)}{x^Tx} = \frac{(U^Tx)^T\Lambda(U^Tx)}{(U^Tx)^T(U^Tx)}$$

and $\{U^Tx | x \in \mathbb{C}^n \text{ and } x \neq 0\} = \{y \in \mathbb{C}^n | y \neq 0\}$. Thus if $w_1, w_2, ..., w_{k-1} \in \mathbb{C}^n$ are given, then

$$\begin{aligned}
\inf_{\substack{x\neq 0 \\ x\perp w_1,w_2,\ldots,w_{k-1}}} \frac{x^TAx}{x^Tx} &= \inf_{\substack{y\neq 0 \\ y\perp U^Tw_1,U^Tw_2,\ldots,U^Tw_{k-1}}} \frac{y^T\Lambda y}{y^Ty} \\
&= \inf_{\substack{y^Ty=1 \\ y\perp U^Tw_1,U^Tw_2,\ldots,U^Tw_{k-1}}} \sum_{i=1}^{n} \lambda_i|y_i|^2 \\
&\geq \inf_{\substack{y^y=1 \\ y\perp U^Tw_1,U^Tw_2,\ldots,U^Tw_{k-1} \\ y_k=y_{k+1}=\ldots=y_n=0}} \sum_{i=1}^{n} \lambda_i|y_i|^2 \\
&= \inf_{\substack{|y_1|^2+|y_2|^2+\ldots+|y_{k-1}|^2=1 \\ y\perp U^Tw_1,U^Tw_2,\ldots,U^Tw_{k-1}}} \sum_{i=1}^{k} \lambda_i|y_i|^2 \geq \lambda_k
\end{aligned}$$

This shows that

$$\inf_{\substack{x\neq 0 \\ x\perp w_1,w_2,\ldots,w_{k-1}}} \frac{x^TAx}{x^Tx} \geq \lambda_k$$

for any $k-1$ vectors. But equality will hold for one choice of the vectors which is $w_i = u_{n-i+k}$, where $U = [u_1 \ldots u_n]$. Thus,

$$\sup_{w_1,\ldots,w_{k-1}} \inf_{\substack{x\neq 0 \\ x\perp w_1,w_2,\ldots,w_{k-1}}} \frac{x^TAx}{x^Tx} = \lambda_k$$

and we can replace inf and sup with min and max, respectfully, since the extremum is achieved. The proof for the second case is similar. □

Theorem (Min Trace Problem)**.** *Let A be Hermitian matrix with eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{n-1} \leq \lambda_n$, then*

$$\begin{aligned} &\underset{X \in \mathbb{R}^{n \times k}}{minimize} \quad Tr(X^T A X) = \sum_1^k \lambda_i \\ &subject\ to \quad X^T X = I \end{aligned} \tag{18}$$

and the columns of X contain the corresponding eigenvectors of the k smallest eigenvalues of A.[1.]

Proof. Let $h(X) = tr(X^T A X)$. Then

$$\begin{aligned} h(X+Y) - h(X) &= tr((X^T + Y^T)A(X+Y)) - tr(X^T A X) \\ &= tr(X^T A X) + tr(X^T A Y) + tr(Y^T A X) + tr(Y^T A Y) - tr(X^T A X) \\ &= 2tr(X^T A Y) + tr(Y^T A Y) \end{aligned}$$

Since

$$\lim_{||Y|| \to 0} \frac{tr(Y^T A Y)}{||Y||} = 0$$

and

$$\lim_{||Y|| \to 0} \frac{h(X+Y) - h(X) - tr(Y^T A Y)}{||Y||} = 0$$

then

$$D_X h(Y) = 2tr(X^T A Y)$$

So the lagrange problem to be solved is

$$D_X h(Y) = X^T \Lambda$$

hence

$$\begin{aligned} 2X^T A &= 2X^T \Lambda \\ \Rightarrow AX &= \Lambda X \end{aligned}$$

which gives

$$\begin{aligned} Ax_1 &= \lambda_1 x_1 \\ Ax_2 &= \lambda_2 x_2 \\ &\vdots \\ Ax_k &= \lambda_k x_k \end{aligned}$$

Thus the solution X of the eigenvalue problem is the matrix whose columns are the eigenvectors of the corresponding eigenvalues of A. □

Theorem (Diagonally dominant matrix)**.** *A Hermitian diagonally dominant matrix A with real non-negative diagonal entries is positive semidefinite. [5.]*

Proof. Let A be a Hermitian diagonally dominant matrix with real nonnegative diagonal entries; then its eigenvalues are real and, by Gershgorin's circle theorem, for each eigenvalue an index i exists such that:

$$\lambda \in \left[a_{ii} - \sum_{j \neq i} |a_{ij}|, a_{ii} + \sum_{j \neq i} |a_{ij}|\right]$$

which implies, by definition of diagonally dominance, $\lambda \geq 0$ and thus A is positive semidefinite. □

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