Research Report - Spectral Clustering

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Clustering Algorithms

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  - PCA Based clustering [Zhang et al. 2018]

Spectral Clustering

Graph Laplacian - Construction

- Given an undirected graph, $\mathbf{G} = (\mathbf{V}, \mathbf{E})$ with set of vertices $\mathbf{V} = \{\mathbf{v_1}, \ldots, \mathbf{v_n}\}$ and $\mathbf{E}$ set of weighted edges. The weight of the edge between v_i and v_j, denoted by w_{ij} is assigned based on the 'similarity' between the data-points v_i and v_j. For example, if the similarity function chosen is a Gaussian kernel and the data that these vertices represent are scalars x_i and x_j, then $w_{ij} = e^{-|x_i - x_j|^2/2}$

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- Construct the Weighted adjacency matrix $\mathbf{W} = (\mathbf{w_{ij}})_{\mathbf{i,j=1,\ldots,n}}$ and Degree matrix $\mathbf{D} = diag(d_1, \ldots, d_n)$ where $\mathbf{d_i} = \sum_{\mathbf{j=1}}^{\mathbf{n}} \mathbf{w_{ij}}$ is called Degree of a vertex v_i.

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- Graph Laplacian is defined as $L = D - W$
- A fully connected graph can be made sparse by converting it into a k-nearest neighbor or an ϵ-neighborhood graph.

- Unnormalized Graph Laplacian [Mohar, 1991], [Mohar, 1997]
    - $L = D - W$ (Symmetric)

Spectral Clustering

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- All Laplacians are Positive-semidefinte, hence have non-Negative Real-Valued Eigenvalues
- 0 is an eigenvalue with multiplicity equal to number of connected components

Spectral Clustering

Graph Cuts

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- Minimizing the between cluster similarity equals to minimizing the objective function

$$\text{cut}(A_1, \ldots, A_k) := \frac{1}{2} \sum_{i-1}^{k} W(A_i, \bar{A}_i), \quad \text{where } W(A, B) = \sum_{i \in A, j \in B} w_{ij}, \bar{A} = V \backslash A$$

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- To maximize the within-cluster similarity, we define two objective functions

$$RatioCut(A_1, \ldots, A_k) = \frac{1}{2} \sum_{i=1}^{k} \frac{W(A_i, \bar{A}_i)}{|A_i|} = \sum_{i=1}^{k} \frac{cut(A_i, \bar{A}_i)}{|A_i|} [Hagen, Kahng, 1992]$$

$$Ncut(A_1, \ldots, A_k) = \frac{1}{2} \sum_{i=1}^{k} \frac{W(A_i, \bar{A}_i)}{vol(A_i)} = \sum_{i=1}^{k} \frac{cut(A_i, \bar{A}_i)}{vol(A_i)} [Shi, Malik, 2000]$$

Spectral Clustering

Algorithms - Unnormalized Spectral Clustering - Hagen & Kahng (1992)

Input: Similarity matrix $S \in \mathbb{R}^{n \times n}$, number k of clusters to construct.
begin

Construct a similarity graph and its weighted adjacency matrix W according to the chosen similarity function
Compute the unnormalized Laplacian L
Compute the first k eigenvectors $u_1, \ldots, u_k$ of L
Let $U \in \mathbb{R}^{n \times k}$ be the matrix containing the vectors $u_1, \ldots, u_k$ as columns
For $i = 1, \ldots, n$, let $y_i \in \mathbb{R}^k$ be the vector corresponding to the i^{th} row of U
Cluster the points $(y_i), i = 1, \ldots, n$ in $\mathbb{R}^k$ with the k-means algorithm into clusters $C_1, \ldots, C_k$

end
Output: Clusters $A_1, \ldots, A_k$ with $A_i = \{x_j | y_j \in C_i\}$

Spectral Clustering

Algorithms - Normalized Spectral Clustering - Shi & Malik (2000)

This algorithm uses generalized eigenvectors of L, which are the eigenvectors of normalized random-walk Laplacian $L_{rw} = D^{-1}L$

Input: Similarity matrix $S \in \mathbb{R}^{n \times n}$, number k of clusters to construct

begin

- Construct a similarity graph and its weighted adjacency matrix W according to the chosen similarity function
- Compute the unnormalized Laplacian L.
- Compute the first k generalized eigenvectors $u_1, \ldots, u_k$ of generalized eigenproblem $Lu = \lambda Du$.
- Let $U \in \mathbb{R}^{n \times k}$ be the matrix containing the vectors $u_1, \ldots, u_k$ as columns.
- For $i = 1, \ldots, n$, let $y_i \in \mathbb{R}^k$ be the vector corresponding to the i^{th} row of U.
- Cluster the points $(y_i), i = 1, \ldots, n$ in $\mathbb{R}^k$ with the k-means algorithm into clusters $C_1, \ldots, C_k$.

end

Output: Clusters $A_1, \ldots, A_k$ with $A_i = \{x_j | y_j \in C_i\}$

Spectral Clustering

Algorithms - Normalized Spectral Clustering - Ng, Jordan & Weiss (2002)

This algorithm uses the eigenvectors of normalized symmetric Laplacian $L_{sym} = D^{-1/2}LD^{-1/2}$. Note that if $D^{1/2}u$ is an eigenvector of L_{sym} if u is an eigenvector of L hence an additional normalization step is needed.

Input: Similarity matrix $S \in \mathbb{R}^{n\times n}$, number k of clusters to construct.
begin

- Construct a similarity graph and its weighted adjacency matrix W according to the chosen similarity function
- Compute the normalized Laplacian L_{sym}
- Compute the first k eigenvectors $u_1, \ldots, u_k$ of L_{sym}
- Let $U \in \mathbb{R}^{n\times k}$ be the matrix containing the vectors $u_1, \ldots, u_k$ as columns
- Form the matrix $T \in \mathbb{R}^{n\times k}$ from U by normalizing the norm to 1, $t_{ij} = u_{ij}/(\sum_k u_{ik}^2)^{1/2}$
- For $i = 1, \ldots, n$, let $y_i \in \mathbb{R}^k$ be the vector corresponding to the i^{th} row of U
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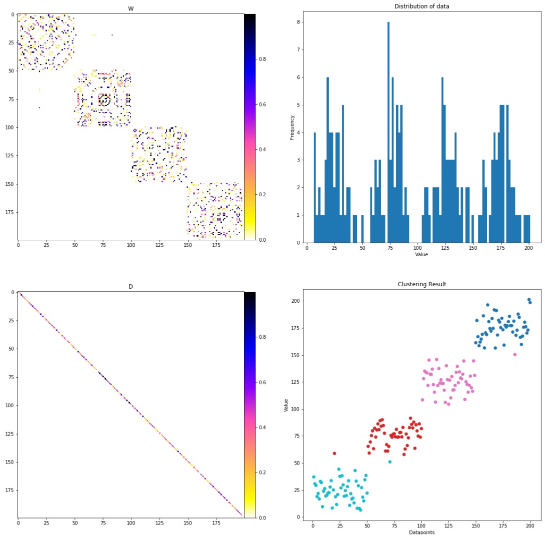
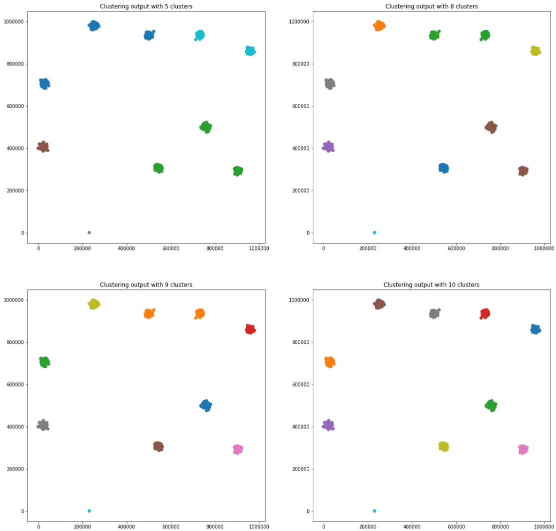
Numerical Experiments

Mixture of 4 Gaussians in $\mathbb{R}^1$. Similarity function: $e^{-|x_i - x_j|^2/2}$



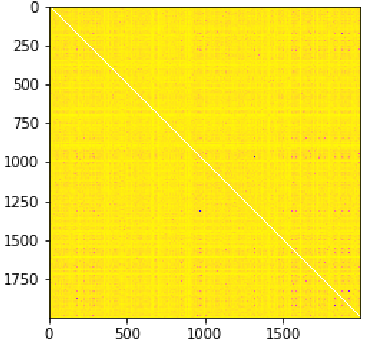
Numerical Experiments

1351 Points in $\mathbb{R}^2$. Similarity function: $||x - y||_2^{-1}$

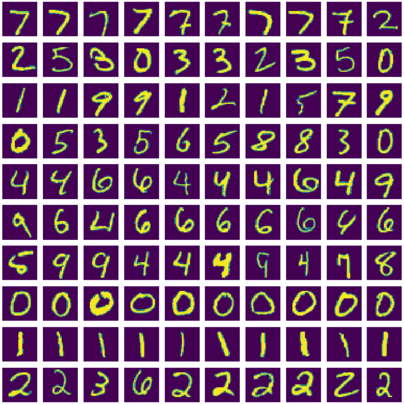


Numerical Experiments

Image Classification. Similarity function: $||\mathbf{v_i} \circ \mathbf{v_j}||_1$



(a) Weighted Adjacency Matrix

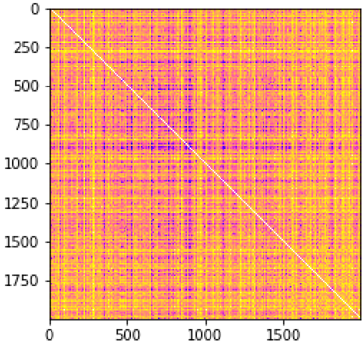


(b) Clustering Result

Figure: 2000 images from MNIST data-set were clustered into 10 clusters. (b) shows first 10 images in each cluster with one row per cluster

Numerical Experiments

Image Classification. Similarity function: $||\mathbf{v_i} - \mathbf{v_j}||_2^{-1}$



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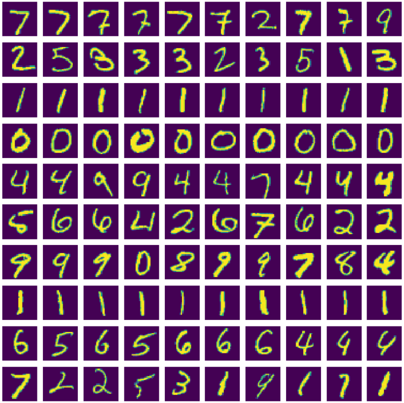

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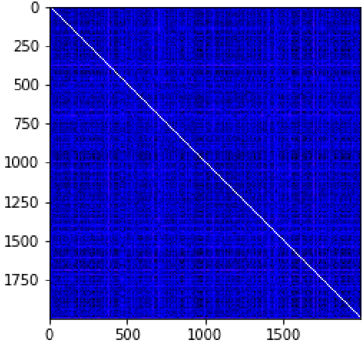
Numerical Experiments

Image Classification. Similarity function: number of pixels that either 0 or non-zero in both $\mathbf{v_i}$ & $\mathbf{v_j}$



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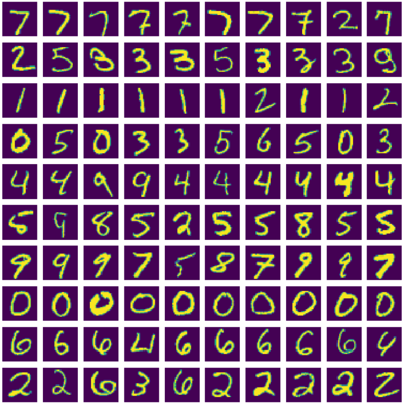

(b) Clustering Result

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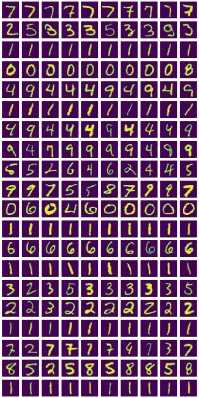
Numerical Experiments

Image Classification. Doubling the number of clusters to capture handwriting style differences

(a) Similarity function: $||\mathbf{v_i} \circ \mathbf{v_j}||_1$



(b) Similarity function: $||\mathbf{v_i} - \mathbf{v_j}||_2^{-1}$

Figure: 2000 images from MNIST data-set were clustered into 20 clusters, showing first 10 images in each cluster with one row per cluster.

Compressive Spectral Clustering

[Tremblay et al. 2016]

Challenges with Spectral Clustering: Eigenvector computation, Cold-restart, expensive k-means due to high dimensionality.

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Challenges with Spectral Clustering: Eigenvector computation, Cold-restart, expensive k-means due to high dimensionality.

- Sample $\mathcal{O}(\log(k))$ randomly filtered signals on the graph to serve as feature vectors instead of eigenvectors
  - Estimate k^{th} eigenvalue per [Napoli 2013]
  - Approximate the action of a low-pass filter H that selects the first k eigenvectors on the graph Laplacian
  - Generate $\mathcal{O}(\log(k))$ Gaussian signals, filtered by H to generate feature vectors $\mathbf{f_i}$

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- Infer the cluster label of all N nodes by interpolating.

Future Work

- Accelerated Eigensolvers
  - Accelerating Lanczos
  - Chebyshev-Davidson Methods [Zhou & Saad 2007] [Z. Wang, 2015]
  - Taking advantage of structure
- Detecting number of clusters adaptively.
- Hot-restart information from the pass with k clusters to bootstrap clustering process with $k + l$ clusters
- Dimensionality reduction for k-means

Thank You!