[WORK IN PROGRESS] Research Report - Spectral Clustering

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Clustering Algorithms

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- **Partitions** of a graph :Non-empty sets $A_1, \ldots, A_k$ form partition of graph if $A_i \cap A_j = \emptyset$ and $A_1 \cup \cdots \cup A_k = V$

Unnormalized	Normalized (Symmetric)	Normalized (Random Walk)
$L = D - W$	$L_{sym} = D^{-1/2} L D^{-1/2}$ $= I - D^{-1/2} W D^{-1/2}$	$L_{rw} = D^{-1} L$ $= I - D^{-1} W$
Symmetric	Symmetric	Not-Symmetric
u - eigenvector	$D^{1/2} u$ - eigenvector	u - eigenvector
Positive-semidefinte, Non-Negative Real-Valued Eigenvalues		
0 is an eigenvalue with multiplicity equal to no. of connected components		

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Graph Cuts

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

$$\mathrm{cut}(A_1, \ldots, A_k) := \frac{1}{2}\sum_{i-1}^{k} W(A_i, \bar{A}_i)$$

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

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

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

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
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) [10]

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

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

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- Construct a similarity graph and its weighted adjacency matrix W
- 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 $C_1, \ldots, C_k$.

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Algorithms - Normalized Spectral Clustering - Ng, Jordan & Weiss (2002) [11]

This algorithm uses the eigenvectors of normalized symmetric Laplacian L_{sym}. 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

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

Cluster the points $(y_i), i = 1, \ldots, n$ in $\mathbb{R}^k$ with the k-means algorithm into clusters $C_1, \ldots, C_k$

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Numerical Experiments

Mixture of 4 Gaussians in $\mathbb{R}^1$ with a Gaussian kernel $e^{-|x_i - x_j|^2/(2\sigma^2)}$ with $\sigma = 1$ as similarity function.

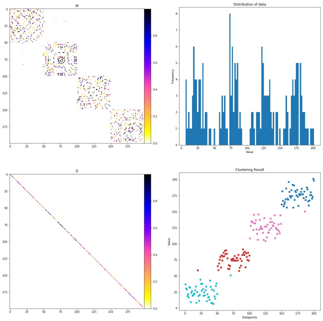


Figure: Clustering results for 200 points in $\mathbb{R}^1$

Spectral Clustering

Numerical Experiments

Points in $\mathbb{R}^2$ with $||x - y||_2$ as similarity function

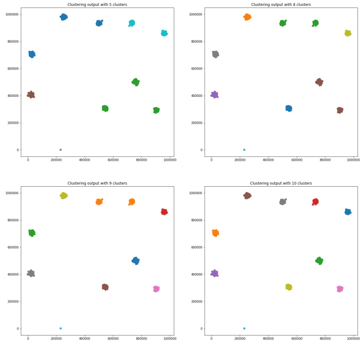
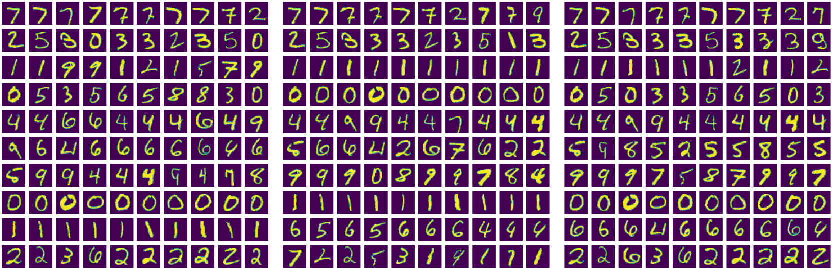


Figure: Clustering results for 1351 points in $\mathbb{R}^2$

Spectral Clustering

Numerical Experiments

Unsupervised Image Classification



(a) Count of pixels that are non-zero in both images as similarity measure

(b) Inverse of 2-norm of the difference vector between two images as similarity measure

(c) Count of pixels that are zero or non-zero in both images as similarity measure

Figure: 2000 images from MNIST data-set were clustered into 10 clusters. In the above figure, each row of images represent a cluster and show the first 10 images in that cluster

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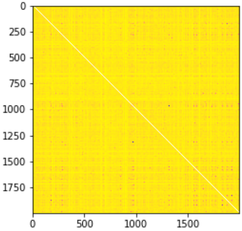

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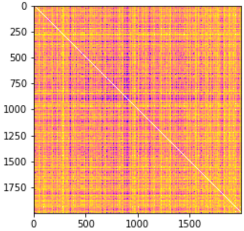

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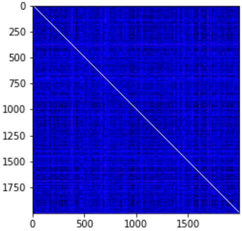

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Figure: Weighted adjecency matrix for 2000 images from MNIST data-set with similarity functions described under the images

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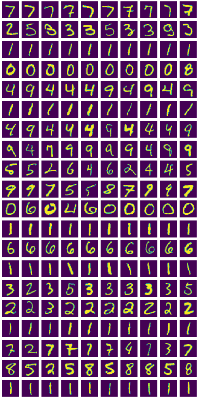

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