DDA4210/MAIR6002 Advanced Machine Learning
Lecture 05-I Graph Cut and Spectral Clustering

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Overview

Unsupervised Learning

- Supervised learning
  - Use labeled data pairs $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^{N}$ to learn a function $\mathbf{y} = f(\mathbf{x})$.
- Unsupervised learning
  - Learn something useful from unlabeled data $\{\mathbf{x}_i\}_{i=1}^{N}$.

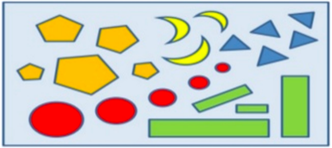
Clustering

- Clustering

  $$\boxed{\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_5, \mathbf{x}_6, \mathbf{x}_7, \mathbf{x}_8, \mathbf{x}_9, \mathbf{x}_{10}\}}$$

  $$\{\mathbf{x}_1, \mathbf{x}_3, \mathbf{x}_8\} \quad \{\mathbf{x}_2, \mathbf{x}_4, \mathbf{x}_5, \mathbf{x}_{10}\} \quad \{\mathbf{x}_6, \mathbf{x}_7, \mathbf{x}_9\}$$

  - Unsupervised grouping of datapoints.
  - Knowledge discovery.
  - Useful when don't know what you're looking for.
- Basic idea of clustering
  - Group together similar instances.



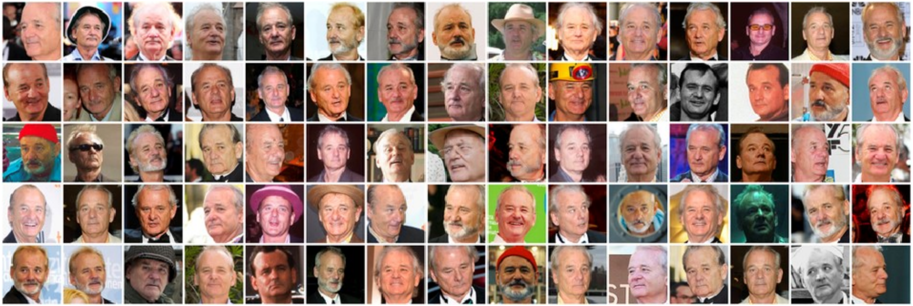
Clustering Algorithms

- Hierarchical clustering (intuitive, not included in this course)
- K-means clustering (learned in basic ML courses)
- Mixture of Gaussians (learned in basic ML courses)
- **Spectral clustering**
- Subspace clustering (not included in this course)
- Deep learning based clustering (not included in this course)

- Image segmentation
  - Break up image into meaningful or perceptually similar regions.

Applications of Clustering

- Image clustering



Difficult!

Applications of Clustering

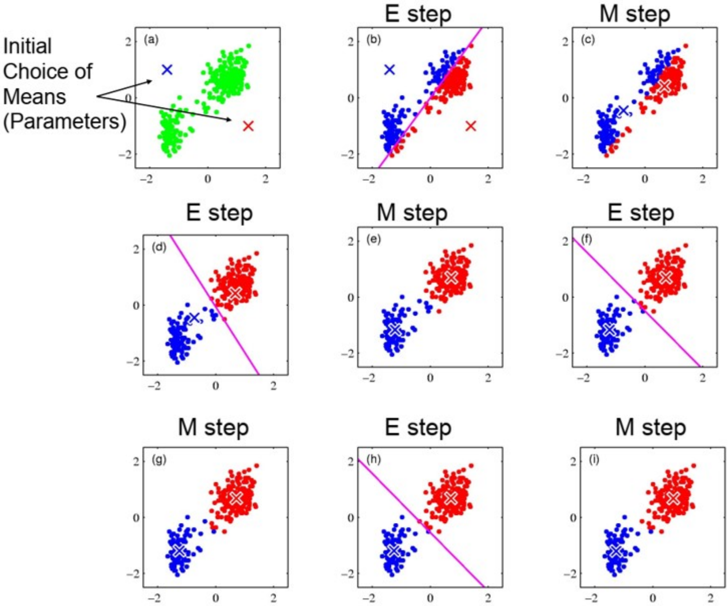
- Image clustering

Very difficult!

Applications of Clustering

- Gene and cell clustering
- Document clustering
- Recommendation system (How to do?)
- Social network analysis
- Community detection

K-Means Clustering: Example

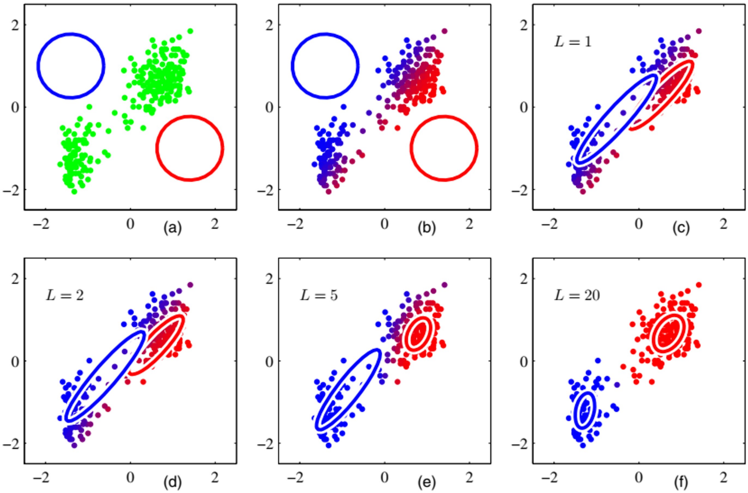


E step:
parameters are fixed
Distributions are optimized

M step:
distributions are fixed
Parameters are optimized

Final Clusters And Means

GMM: Example

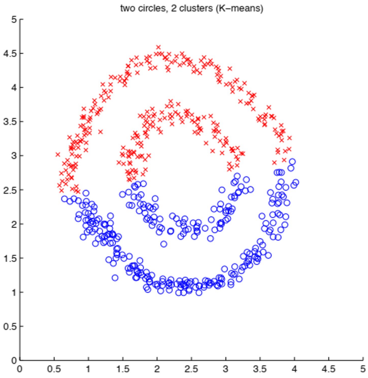


L: cycles of EM

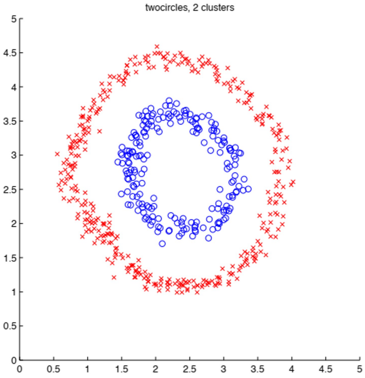
This is the Old Faithful Geyser dataset [PRML, Bishop]

Main Limitation of K-means

K-means

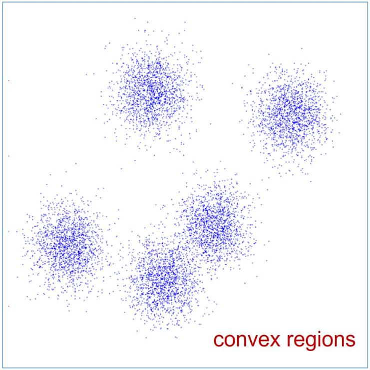


Spectral clustering

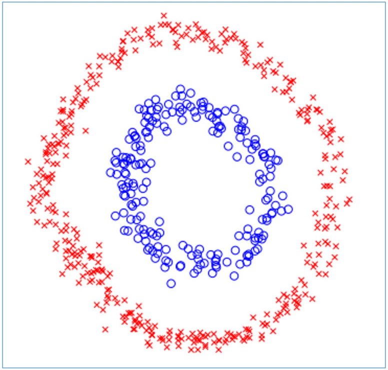


Clustering Criterion

- Two different clustering criteria
  - Compactness, e.g., k-means, Gaussian mixture models
  - Connectivity, e.g., spectral clustering



Compactness



Connectivity

Graph Partition

Similarity Graph: G(V,E,W)

$G = (N, \mathcal{E})$

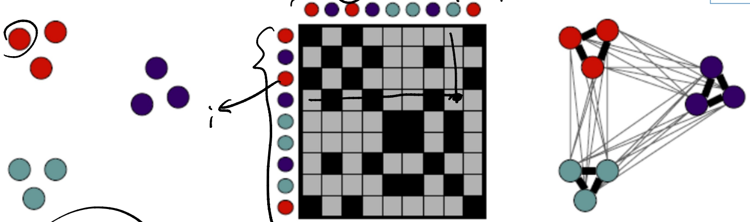
V – Vertices (Data points)
E – Edge if similarity > 0
W - Edge weights (similarities)

$|V| = n$

affinity matrix

j

i



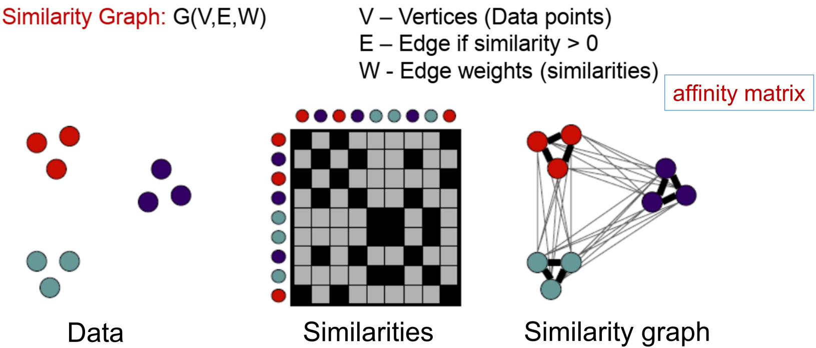
Data | Similarities | Similarity graph

$n \times n$

$$V = \{v_1, v_2, \ldots, v_N\}, \quad E = \{e_1, e_2, \ldots, e_l\}, \quad W = \begin{bmatrix} & \vdots & \\ \cdots & w_{ij} & \cdots \\ & \vdots & \end{bmatrix}$$

W is usually nonnegative and symmetric, and $w_{ii} = 0$.

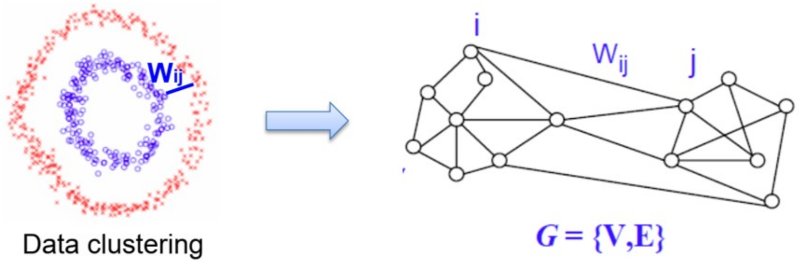
Graph Partition



- Similarity graph
  - Model local neighborhood relations between data points
  - Exist naturally or need to be constructed
- Graph partition: Partition the graph so that edges within a group have large weights and edges across groups have small weights.

Similarity Graph Construction

Given $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$, construct a similarity graph.



Similarity Graph Construction

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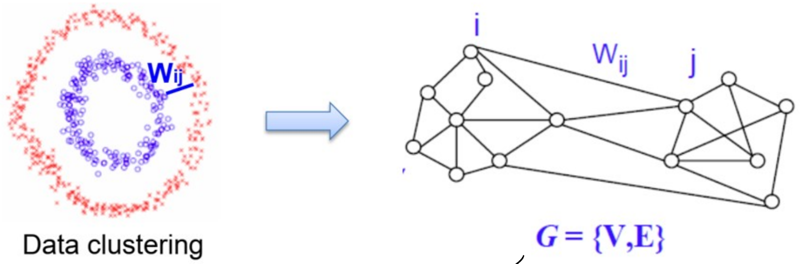


- k-nearest neighbor graph
- ϵ-neighborhood graph
- Gaussian kernel similarity function

$$k(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2}\right)$$

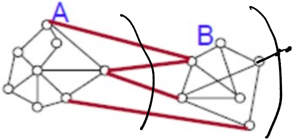
w_{ij}

Minimum Cut

Minimum cut: Partition graph into two sets A and B such that weight of edges connecting vertices in A to vertices in B is minimum.

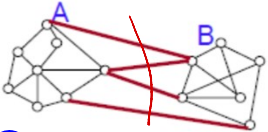
$(K = 2)$ $A \cup B = V$ $G = (V, \mathcal{E}, W)$.

$$\mathrm{cut}(A, B) := \sum_{i \in A, j \in B} w_{ij}$$



Minimum Cut

Minimum cut: Partition graph into two sets A and B such that weight of edges connecting vertices in A to vertices in B is minimum.



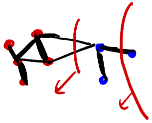
$$\text{cut}(A, B) := \sum_{i \in A, j \in B} w_{ij}$$

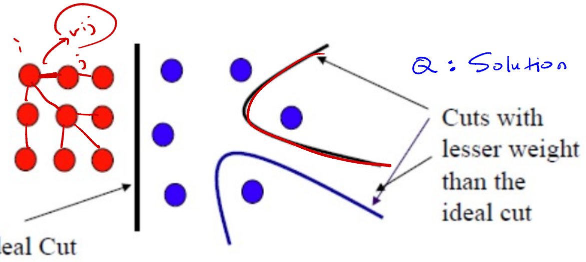
$$\boxed{\min_{A,B} \ \text{cut}(A,B) \quad \text{s.t.} \ A \cup B = V} \qquad A, B \neq \emptyset$$

LP.

- Easy to solve $O(|V||E|)$ algorithm
- Not satisfactory partition? Often isolates vertices

Q: Solution to fix ?





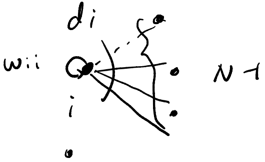
Normalized Cut

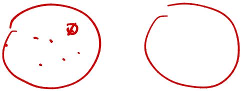
k=2

Normalized cut: Partition graph into two sets A and B such that weight of edges connecting vertices in A to vertices in B is minimum & sizes of A and B are very similar.

Let $\mathrm{vol}(A) = \sum_{i \in A} d_i$, where $d_i = \sum_{j=1}^{N} w_{ij}$. Define the objective function as

$$\mathrm{Ncut}(A, B) := \mathrm{cut}(A, B)\left[\left(\frac{1}{\mathrm{vol}(A)} + \frac{1}{\mathrm{vol}(B)}\right)\right]$$





Normalized Cut

Normalized cut: Partition graph into two sets A and B such that weight of edges connecting vertices in A to vertices in B is minimum & sizes of A and B are very similar.

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$$\mathrm{Ncut}(A, B) := \mathrm{cut}(A, B) \left(\frac{1}{\mathrm{vol}(A)} + \frac{1}{\mathrm{vol}(B)} \right)$$

- Ncut is NP-hard to solve
- Spectral clustering is a relaxation

Degree Matrix and Graph Laplacian

- Given a graph with similarity matrix

$$\mathbf{W} = \begin{bmatrix} w_{11} & w_{12} & \cdots & w_{1N} \\ w_{21} & w_{22} & \cdots & w_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ w_{N1} & w_{N2} & \cdots & w_{NN} \end{bmatrix}$$

$N \times N$.

$d_1 \quad d_2 \quad d_N$

- The degree matrix of the graph is defined as

$d_j = \sum_{i=1}^{N} w_{ij}$.

$$\mathbf{D} = \begin{bmatrix} d_1 & 0 & \cdots & 0 \\ 0 & d_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & d_N \end{bmatrix}$$

where $d_j = \sum_{i=1}^{N} w_{ij}$. d_j is the degree of vertex j of the graph.

- The graph Laplacian matrix is defined as $\mathbf{L} = \mathbf{D} - \mathbf{W}$

Normalized Cut and Graph Laplacian (optional)

Recall $\mathbf{L} = \mathbf{D} - \mathbf{W}$ and $\mathbf{D} = \mathrm{diag}(d_1, \ldots, d_N)$

$A \cup B = V$

$$\text{Let } \mathbf{u} = [u_1, u_2, \ldots, u_N]^\top \quad \text{with } u_i = \begin{cases} \frac{1}{\mathrm{vol}(A)}, & \text{if } i \in A \\ -\frac{1}{\mathrm{vol}(B)}, & \text{if } i \in B \end{cases}$$

TBD

why ?

$$\mathbf{u}^\top \mathbf{L} \mathbf{u} = \frac{1}{2} \sum_{ij} w_{ij} (u_i - u_j)^2 = \sum_{i \in A, j \in B} w_{ij} \left(\frac{1}{\mathrm{vol}(A)} + \frac{1}{\mathrm{vol}(B)} \right)^2$$

$$\mathbf{u}^\top \mathbf{D} \mathbf{u} = \sum_i d_i u_i^2 = \sum_{i \in A} \frac{d_i}{\mathrm{vol}(A)^2} + \sum_{j \in B} \frac{d_j}{\mathrm{vol}(B)^2} = \frac{1}{\mathrm{vol}(A)} + \frac{1}{\mathrm{vol}(B)}$$

why ?

Normalized Cut and Graph Laplacian (optional)

Recall $\mathbf{L} = \mathbf{D} - \mathbf{W}$ and $\mathbf{D} = \mathrm{diag}(d_1, \ldots, d_N)$ $\quad A \cup B = V \quad G = (V, E)$

$$\text{Let } \mathbf{u} = [u_1, u_2, \ldots, u_N]^\top \quad \text{with} \quad u_i = \begin{cases} \frac{1}{\mathrm{vol}(A)}, & \text{if } i \in A \\ -\frac{1}{\mathrm{vol}(B)}, & \text{if } i \in B \end{cases} \quad \text{TBD}$$

$$\mathbf{u}^\top \mathbf{L} \mathbf{u} \overbrace{= \frac{1}{2} \sum_{ij} w_{ij} (u_i - u_j)^2}^{\text{why ?}} = \sum_{i \in A, j \in B} w_{ij} \left(\frac{1}{\mathrm{vol}(A)} + \frac{1}{\mathrm{vol}(B)} \right)^2$$

$$\mathbf{u}^\top \mathbf{D} \mathbf{u} = \sum_i d_i u_i^2 = \sum_{i \in A} \frac{d_i}{\mathrm{vol}(A)^2} + \sum_{j \in B} \frac{d_j}{\mathrm{vol}(B)^2} = \frac{1}{\mathrm{vol}(A)} + \frac{1}{\mathrm{vol}(B)}$$

$$u^T L u = u^T (D - W) u = u^T D u - u^T W u$$

$$= \sum_{i=1}^N d_i u_i^2 - \sum_{i=1}^N \sum_{j=1}^N w_{ij} u_i u_j$$

$$\left(d_i = \sum_{j=1}^N w_{ij} \right)$$

$$= \frac{1}{2} \left(\sum_{i=1}^N \sum_{j=1}^N w_{ij} u_i^2 + \sum_{i=1}^N \sum_{j=1}^N w_{ij} u_j^2 - 2 \sum_{i=1}^N \sum_{j=1}^N w_{ij} u_i u_j \right)$$

Normalized Cut and Graph Laplacian (optional)

Recall $\mathbf{L} = \mathbf{D} - \mathbf{W}$ and $\mathbf{D} = \mathrm{diag}(d_1, \ldots, d_N)$

$$\text{Let } \mathbf{u} = [u_1, u_2, \ldots, u_N]^\top \quad \text{with} \quad u_i = \begin{cases} \frac{1}{\mathrm{vol}(A)}, & \text{if } i \in A \\ -\frac{1}{\mathrm{vol}(B)}, & \text{if } i \in B \end{cases}$$

$$\mathbf{u}^\top \mathbf{L} \mathbf{u} = \frac{1}{2} \sum_{ij} w_{ij} (u_i - u_j)^2 = \sum_{i \in A, j \in B} w_{ij} \left(\frac{1}{\mathrm{vol}(A)} + \frac{1}{\mathrm{vol}(B)} \right)^2$$

$$\mathbf{u}^\top \mathbf{D} \mathbf{u} = \sum_i d_i u_i^2 = \sum_{i \in A} \frac{d_i}{\mathrm{vol}(A)^2} + \sum_{j \in B} \frac{d_j}{\mathrm{vol}(B)^2} = \frac{1}{\mathrm{vol}(A)} + \frac{1}{\mathrm{vol}(B)}$$

Get the Normalized Cut Objective!

Then we have

$$\frac{\mathbf{u}^\top \mathbf{L} \mathbf{u}}{\mathbf{u}^\top \mathbf{D} \mathbf{u}} = \sum_{i \in A, j \in B} w_{ij} \left(\frac{1}{\mathrm{vol}(A)} + \frac{1}{\mathrm{vol}(B)} \right) = \mathrm{Ncut}(A, B)$$

Normalized Cut and Graph Laplacian

Ncut is equivalent to the minimization of $\frac{\mathbf{u}^\top \mathbf{L}\mathbf{u}}{\mathbf{u}^\top \mathbf{D}\mathbf{u}}$, i.e.,

$$\min_{A,B} \mathrm{Ncut}(A,B) \Longleftrightarrow \min_{\mathbf{u}} \frac{\mathbf{u}^\top \mathbf{L}\mathbf{u}}{\mathbf{u}^\top \mathbf{D}\mathbf{u}}, \quad \mathbf{u} \in \mathbb{R}^N,\ u_i = \begin{cases} \frac{1}{\mathrm{vol}(A)}, & \text{if } i \in A \\ -\frac{1}{\mathrm{vol}(B)}, & \text{if } i \in B \end{cases}$$

[1] Detailed derivation can be found in: *Shi and Malik. Normalized Cuts and Image Segmentation. 2000.*

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Ncut is equivalent to the minimization of $\frac{\mathbf{u}^\top \mathbf{L}\mathbf{u}}{\mathbf{u}^\top \mathbf{D}\mathbf{u}}$, i.e.,

$$\min_{A,B} \mathrm{Ncut}(A,B) \iff \min_{\mathbf{u}} \frac{\mathbf{u}^\top \mathbf{L}\mathbf{u}}{\mathbf{u}^\top \mathbf{D}\mathbf{u}}, \quad \mathbf{u} \in \mathbb{R}^N,\ u_i = \begin{cases} \frac{1}{\mathrm{vol}(A)}, & \text{if } i \in A \\ -\frac{1}{\mathrm{vol}(B)}, & \text{if } i \in B \end{cases}$$

Equivalent to[1]: $\min_{\mathbf{u}} \frac{\mathbf{u}^\top \mathbf{L}\mathbf{u}}{\mathbf{u}^\top \mathbf{D}\mathbf{u}}$ s.t. $\mathbf{u}^\top \mathbf{D}\mathbf{1} = \mathbf{0}$, $u_i \in \{1, -b\}$

$\{2, -2b\}$

* b is some positive constant.

"connectivity", >0 iff G is connected.

Relaxation: $\mathbf{u}$ – second eigenvector of generalized eigenvalue problem

relax the integer programming constraints.

$$\mathbf{L}\mathbf{u} = \lambda \mathbf{D}\mathbf{u}$$

Obtain cluster assignments by thresholding $\mathbf{u}$ at 0

[1] Detailed derivation can be found in: *Shi and Malik. Normalized Cuts and Image Segmentation. 2000.*

Normalized Cut and Graph Laplacian

$$\min_{A,B} \text{Ncut}(A,B) \iff \min_{\mathbf{u}} \frac{\mathbf{u}^\top \mathbf{L}\mathbf{u}}{\mathbf{u}^\top \mathbf{D}\mathbf{u}} \quad \text{s.t. } \mathbf{u}^\top \mathbf{D}\mathbf{1} = \mathbf{0},\ u_i \in \{1, -b\}$$

- Relaxation: Let $\mathbf{u}$ be the eigenvector corresponding to the second smallest eigenvalue of the generalized eigenvalue problem $\mathbf{L}\mathbf{u} = \lambda \mathbf{D}\mathbf{u}$
- Equivalent to eigenvector corresponding to the second smallest eigenvalue of the normalized Laplacian

$$\widetilde{\mathbf{L}} = \mathbf{D}^{-1}\mathbf{L} = \mathbf{I} - \mathbf{D}^{-1}\mathbf{W}$$

Normalized Cut and Graph Laplacian

$$\min_{A,B} \ \mathrm{Ncut}(A,B) \iff \min_{\mathbf{u}} \frac{\mathbf{u}^\top \mathbf{L}\mathbf{u}}{\mathbf{u}^\top \mathbf{D}\mathbf{u}} \quad \text{s.t.} \ \ \mathbf{u}^\top \mathbf{D}\mathbf{1} = \mathbf{0}, \ u_i \in \{1, -b\}$$

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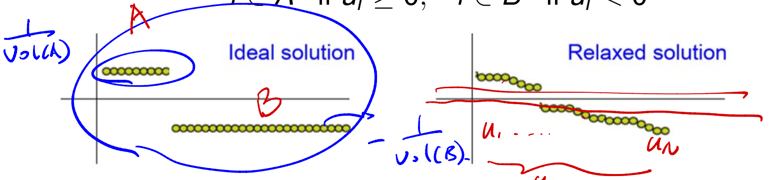
threshold-based partition

- Obtain binary partition as follows:

$$i \in A \quad \text{if } u_i \geq 0, \qquad i \in B \quad \text{if } u_i < 0$$



- It can be extended to multiple clusters $\xrightarrow{u}$ Spectral Clustering

Spectral Clustering Algorithm

Input: data $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}$, number K of clusters

- Step 1. Construct a similarity matrix $\mathbf{W}$

  e.g. use $w_{ij} = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2}\right)$

  k-nearest neighbor graph, or ϵ-neighborhood graph

- Step 2. Compute the Laplacian matrix $\mathbf{L}$ (or normalized $\mathbf{L}$)
  - $\mathbf{L} = \mathbf{D} - \mathbf{W}$
  - $\widetilde{\mathbf{L}} = \mathbf{I} - \mathbf{D}^{-1}\mathbf{W}$ (normalized)
  - $\widehat{\mathbf{L}} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{W}\mathbf{D}^{-1/2}$ (symmetric normalized, recommended)

Spectral Clustering Algorithm

- Step 3. Perform eigenvalue decomposition on **L** (or normalized **L**) and use the first K eigenvectors to form a matrix **Z**

# of nodes

$$\widehat{\mathbf{L}} = \mathbf{V}\Sigma\mathbf{V}^\top, \quad \mathbf{Z} = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_K]^\top \in \mathbb{R}^{K \times N}$$

often, $K << N$

# of clusters

- Step 4. Normalize the columns of **Z** to unit L_2 norm, i.e.,

$$\mathbb{R}^K \ni \mathbf{z}_i \leftarrow \mathbf{z}_i / \|\mathbf{z}_i\|, \quad i = 1, \ldots, N$$

Q: Can we always do $\hat{L} = V\Sigma V^T$?

A: Yes! $\hat{L}$ is symmetric!

Spectral Clustering Algorithm

$\lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_{N-1} \longrightarrow$ spectrum.

- Step 3. Perform eigenvalue decomposition on **L** (or normalized **L**) and use the first K eigenvectors to form a matrix **Z**

$$\widehat{\mathbf{L}} = \mathbf{V}\Sigma\mathbf{V}^\top, \quad \mathbf{Z} = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_K]^\top \in \mathbb{R}^{K \times N}$$

K

- Step 4. Normalize the columns of **Z** to unit L_2 norm , i.e.,

z_1

$$\mathbb{R}^K \ni \mathbf{z}_i \leftarrow \mathbf{z}_i / \|\mathbf{z}_i\|, \quad i = 1, \ldots, N$$

generalize to "K clusters" case

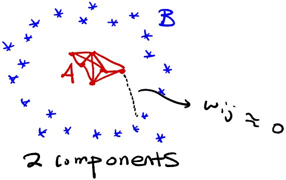
- Step 5. Perform K-means on $\{\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_N\}$

Output: K of clusters of **Z** or **X**

Property of Graph Laplacian Matrix

Revisit:

$$\mathbf{L} = \mathbf{D} - \mathbf{W} \quad \text{or} \quad \widehat{\mathbf{L}} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{W}\mathbf{D}^{-1/2}$$



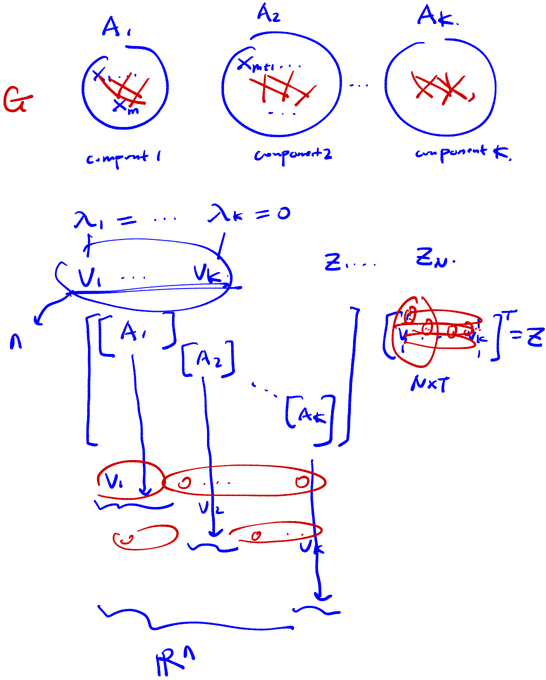
- Symmetric and positive semi-definite
- The eigenvalues satisfy

$$0 = \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \cdots \leq \lambda_{N-1} \leq \lambda_N \qquad \{A_i\}_{i=1}^{K}$$

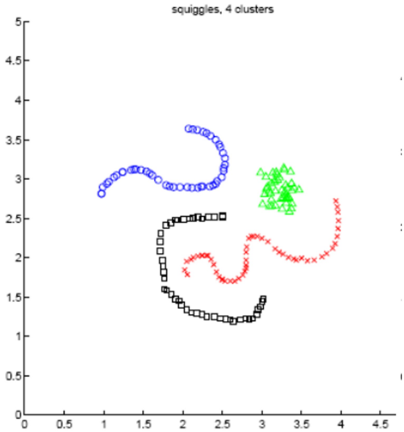
- If the number of zero eigenvalues is K, the graph has K connected components, corresponding to K clusters.

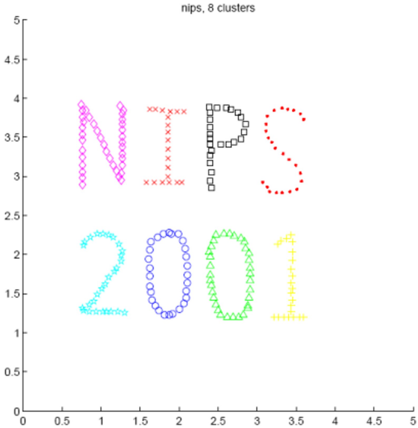
. Linear Algebra. Basics.

If a Laplacian $L \in \mathbb{R}^{N\times N}$ corresponds to a graph G that has K components, $\lambda_1 = \cdots = \lambda_K = 0$. $\lambda_{K+1}, \ldots \lambda_N > 0$. $\{\mathbb{1}_{\{A_i\}}\}$ spans the space $\mathbb{R}^N$..


G
A1
A2
Ak.
xm
xm+1
component 1
component 2
component k.
λ1 = ... λk = 0
v1 ... vk
n
z1 ... zN.
N×T
= Z
A1
A2
Ak
v1
v2
vk
ℝn

Examples of Spectral Clustering





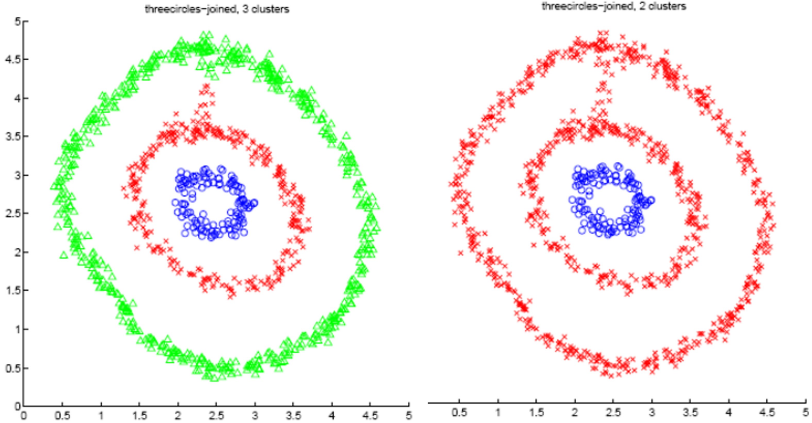
Images from Ng et al. 2001

Examples of Spectral Clustering

- Influence of K

k=3

k=2

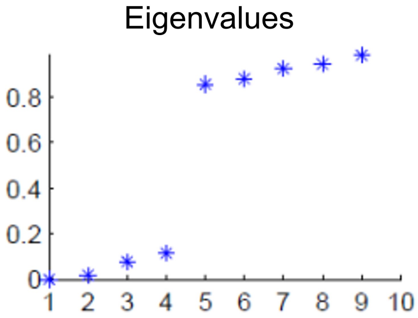


Images from Ng et al. 2001

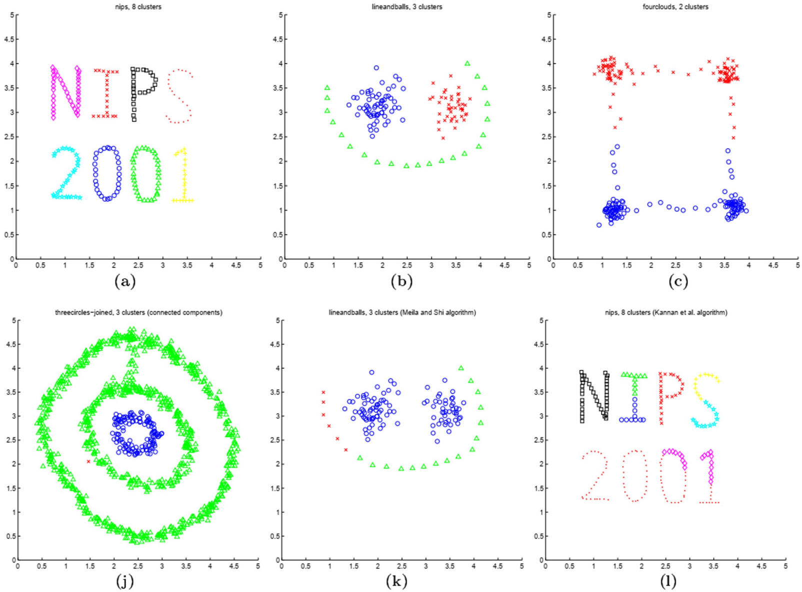
Determine K in Spectral Clustering

- Use the k that maximizes the eigengap (difference between consecutive eigenvalues)

$$\Delta_j = \left|\lambda_{j+1} - \lambda_j\right|, \qquad K^* = \arg\max_j \Delta_j$$



More Examples of Spectral Clustering



Images from Ng et al. 2001

Characteristics of Spectral Clustering[2]

- High clustering accuracy in real applications
  - Often outperform k-means
- High computational cost, not applicable to big data
  - Space complexity: $O(N^2)$
  - Time complexity: $O(N^3)$

[2] More about spectral clustering can be found in: *A Tutorial on Spectral Clustering. Ulrike von Luxburg. 2007.*

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  - Often outperform k-means
- High computational cost, not applicable to big data
  - Space complexity: $O(N^2)$
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- Not easy to determine the similarity matrix
  - *kNN*, ϵ-neighborhood, Gaussian kernel, etc
  - Which method and what hyperparameter?

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Learning Outcomes

- Know the definitions of cut and Ncut
- Know the main steps of spectral clustering
- Know the property of graph Laplacian matrix
- Know the advantage and disadvantage of spectral clustering