Spectral Clustering
Introduction

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Objective

Objective

Illustrate the key idea of spectral clustering

Objective

Define basic graph notations useful for spectral clustering

Revisiting k-means & Mixture Models

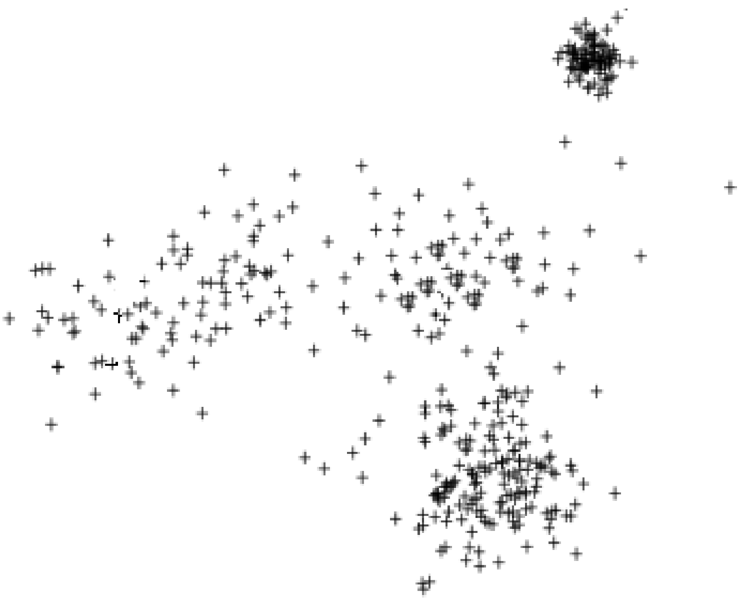
- **K-means use “hard” membership while mixture models allow “soft” membership**

- **Both use feature/vector representation of the data as input ➔ E.g., Euclidean distance is one natural (dis)similarity measure.**
  - What if the input data is NOT represented in feature/vector, format?
    - E.g., graph data.
    - E.g., objects with only pair-wise similarities (like individuals on a social network ➔ community detection)

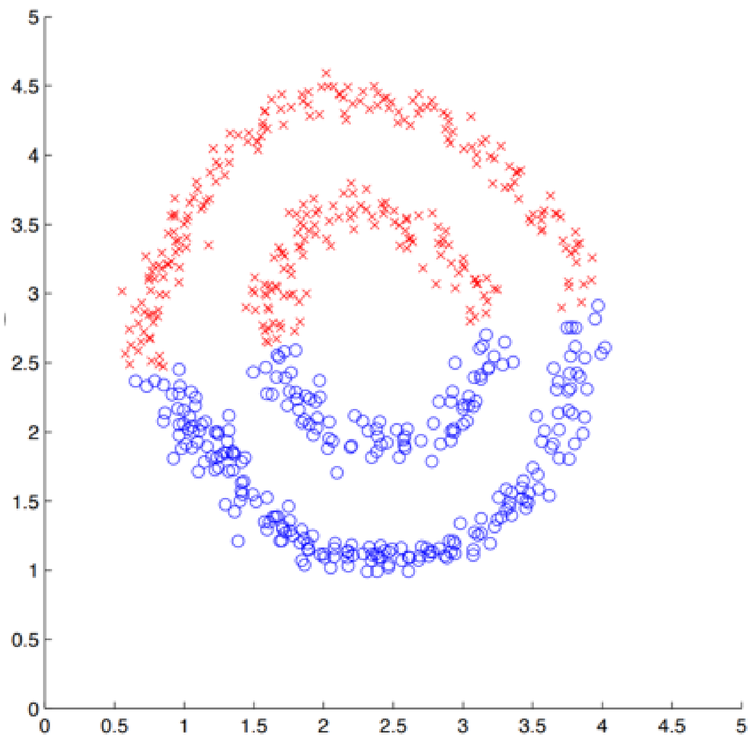
Revisiting k-means & Mixture Models

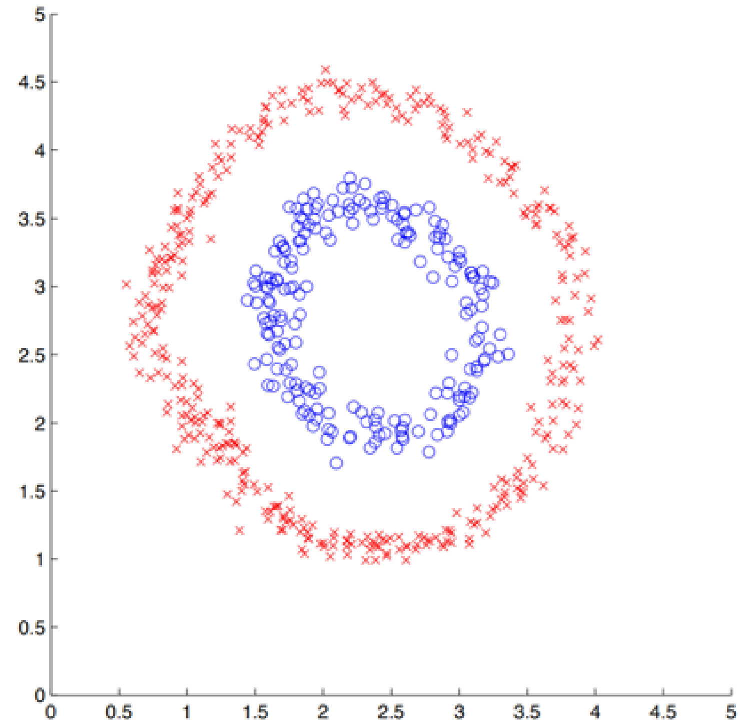
- In both k-means and mixture models, we look for compact clustering structures.

- In some cases, connected-component structures may be more desirable.



Example





Source: Ng, A.Y., Michael I.J., and Yair, W. "On spectral clustering: Analysis and an algorithm." *Advances in neural information processing systems*. 2002.

Spectral Clustering

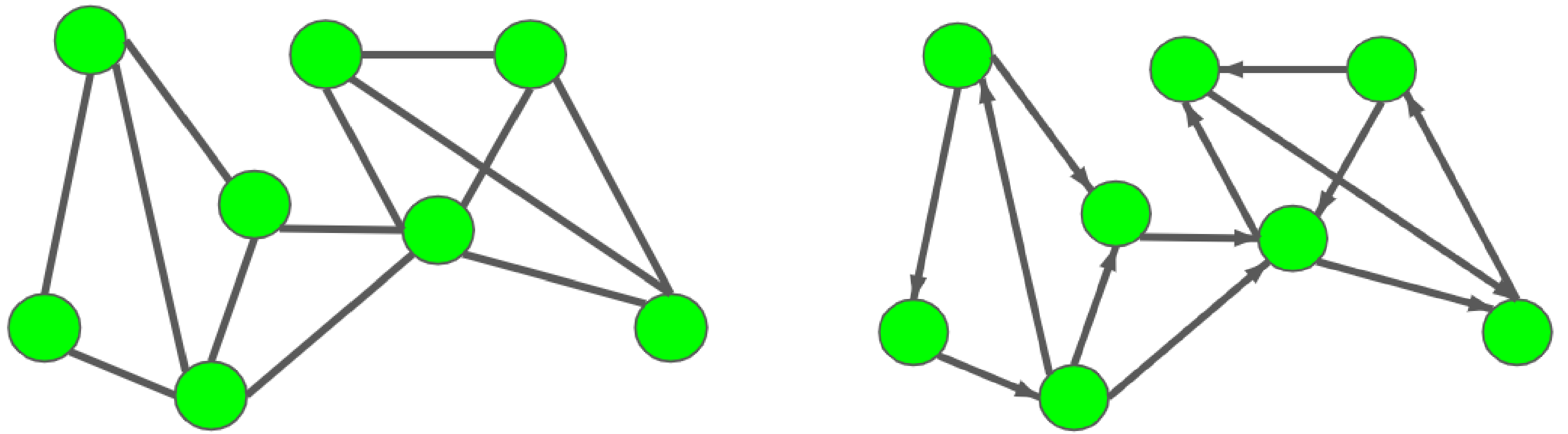
- **A family of methods for finding such similarity-based clusters**
  - “Spectral”: for using the eigenvalues (spectrum) of the *similarity matrix* of the data.
  - Graph clustering, similarity-based clustering

- **The objects to be clustered are not in a vector space.**
  - The primary feature is the similarity between objects.
  - For any pair of objects *i* and *j*, we have a value *s*(*i*,*j*) measuring their similarity; all such values form the similarity matrix.

➔ **Graphs** are intuitive for representing/visualizing such data.

Graph Representation

- **Definition: A graph *G* = (*V*, *E*) is defined by *V*, a set of N *vertices*, and *E*, a set of *edges*.**



Undirected graph Directed graph

- **In spectral clustering, we consider undirected graphs.**

Graph Representation (1/4)

Adjacency matrix W of undirected graph

- $\mathrm{N} \times N$ symmetric binary matrix
- The row and columns are indexed by the vertices and the entries represent the edges of the graph

$$\begin{cases} w_{i,j} = 0 \quad if\ vertices\ i,j\ are\ not\ connected \\ w_{i,j} = 1 \quad \quad if\ vertices\ i,j\ are\ connected \end{cases}$$

- Simple graph = zero diagonal

Graph Representation (2/4)

- **Weighted adjacency matrix (sometimes called affinity matrix)**
  - Allow values other than 0 or 1
  - Each edge is weighted by pairwise similarity

$$\begin{cases} w_{i,j} = 0 & if\ i,j\ are\ not\ connected \\ w_{i,j} = s(i,j) & if\ i,j\ are\ connected \end{cases}$$

- **$w_{i,j}$ may be defined through some kernel functions.**

Graph Representation (3/4)

Degree matrix D of undirected graph

- $N \times N$ diagonal matrix that contains information about the degree of each vertex.
- Degree $d(v_i)$ of a vertex v_i: # of edges incident to the vertex.
  - Extended to sum of weights from edges incident to the vertex.
- So, we have:

$$\mathbf{D} = \begin{bmatrix} d(v_1) & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & d(v_N) \end{bmatrix}$$

Graph Representation (4/4)

Laplacian matrix L of undirected graph

- $\mathbf{L} = \mathbf{D} - \mathbf{W}$ (Degree-Affinity) (Unnormalized)
- $\mathbf{L}$ is symmetric and positive semi-definite
- N non-negative real-valued eigenvalues
- The smallest eigen-value is 0, the corresponding eigenvector is the 1-vector (all elements being 1).
- The smallest non-zero eigenvalue of **L** is called the spectral gap.

Spectral Clustering

A Graph Cut Formulation

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Objective

Objective

Define the graph partition formulation

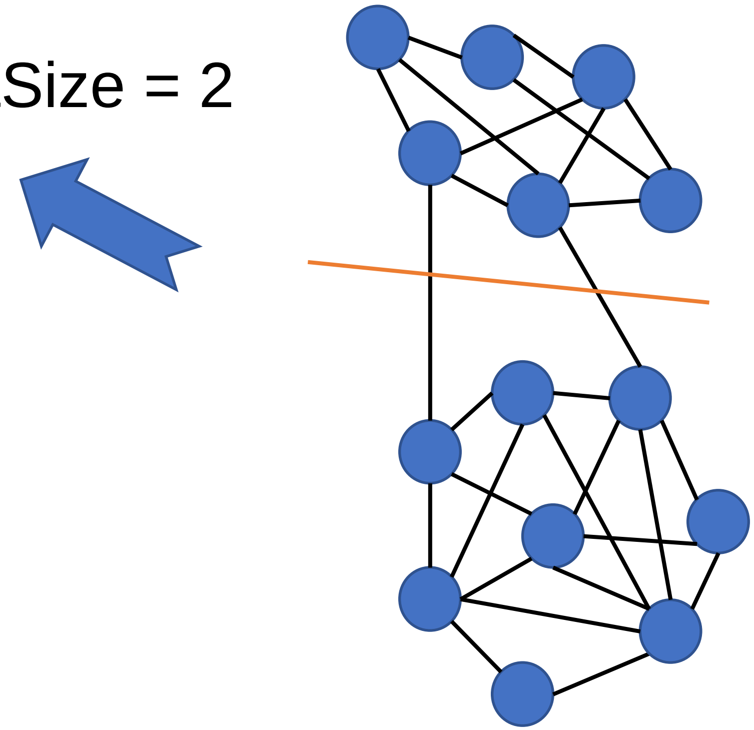
Objective

Learn how to solve simple graph partition

Clustering as Graph Partition/Cut

- Find a partition of a graph such that the edges between different groups have a very low weight while the edges within a group have high weight.
- E.g., minimum cut
- More general, consider weighted edges.

CutSize = 2



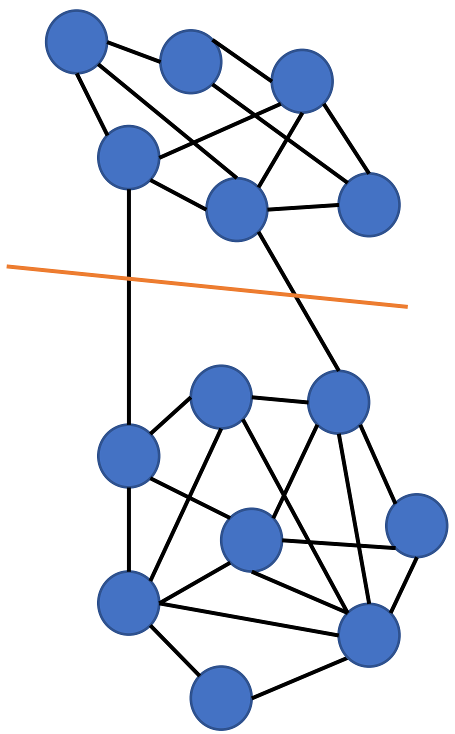
2-way Spectral Graph Partitioning

- **Weighted adjacency matrix W**
  - $w_{i,j}$: the weight between two vertices *i* and *j*
- **(Cluster) Membership vector q**

$$q_i = \begin{cases} 1 & i \in Cluster\ A \\ -1 & i \in Cluster\ B \end{cases}$$

$$\mathbf{q} = \underset{\mathbf{q} \in [-1,\ \ 1]^n}{\operatorname{argmin}}\ CutSize\,,$$

$$CutSize = \mathrm{J} = \frac{1}{4}\sum_{i,j}(q_i - q_j)^2 w_{i,j}$$



Solving the Optimization Problem

$$\mathbf{q} = \underset{\mathbf{q}\in[-1,\quad 1]^n}{\operatorname{argmin}} \frac{1}{4}\sum_{i,j}(q_i - q_j)^2 w_{i,j}\ ,$$

- Directly solving the above problem requires combinatorial search → exponential complexity
- How to reduce the computational complexity?

Relaxation Approach

- **Key difficulty: $\mathbf{q_i}$ has to be either -1,1.**
  - Relax q_i to be any real number.
  - Impose Constraint: $\sum_{i=1}^{n} q_i^2 = n$

$$J = \frac{1}{4}\sum_{i,j}(q_i - q_j)^2 w_{i,j} = \frac{1}{4}\sum_{i,j}(q_i^2 - 2q_i q_j + q_j^2) w_{i,j}$$

$$= \frac{1}{4}\sum_i 2q_i^2\left(\sum_j w_{i,j}\right) - \frac{1}{4}\sum_{i,j} 2q_i q_j w_{i,j}$$

$$= \frac{1}{2}\sum_i q_i^2 d_i - \frac{1}{2}\sum_{i,j} q_i (d_i \delta_{i,j} - w_{i,j}) q_j$$

where $d_i = \sum_j w_{i,j}$ and $D \equiv [d_i \delta_{i,j}]$

$$\Rightarrow \; J = \frac{1}{2}\mathbf{q}^T(\mathbf{D} - \mathbf{W})\mathbf{q}$$

Relaxation Approach (cont'd)

The final problem formulation:

$$\mathbf{q} = \underset{\mathbf{q}}{\operatorname{argmin}}\ J = \underset{\mathbf{q}}{\operatorname{argmin}}\, \mathbf{q}^T(\mathbf{D} - \mathbf{W})\mathbf{q}\ ,$$

subject to $\sum_{i=1}^{n} q_i^2 = n$

Solution: the second minimum eigenvector for D-W

$$(\mathbf{D} - \mathbf{W})\mathbf{q} = \lambda_2\ \mathbf{q}$$

Graph Laplacian

- $L = D - W$
- **L is semi-positive definitive matrix.**
  - For any $\mathbf{x}$, we have $\mathbf{x}^T \mathbf{L} \mathbf{x} \geq 0$. (Why?)
- **Minimum eigenvalue $\lambda_1 = 0$ (what is the eigenvector?)**

$$0 = \lambda_1 < \lambda_2 < \lambda_3 \ldots < \lambda_k$$

- **The eigenvector that corresponds to the second minimum eigenvalue λ_2 gives the best bipartite graph partition.**

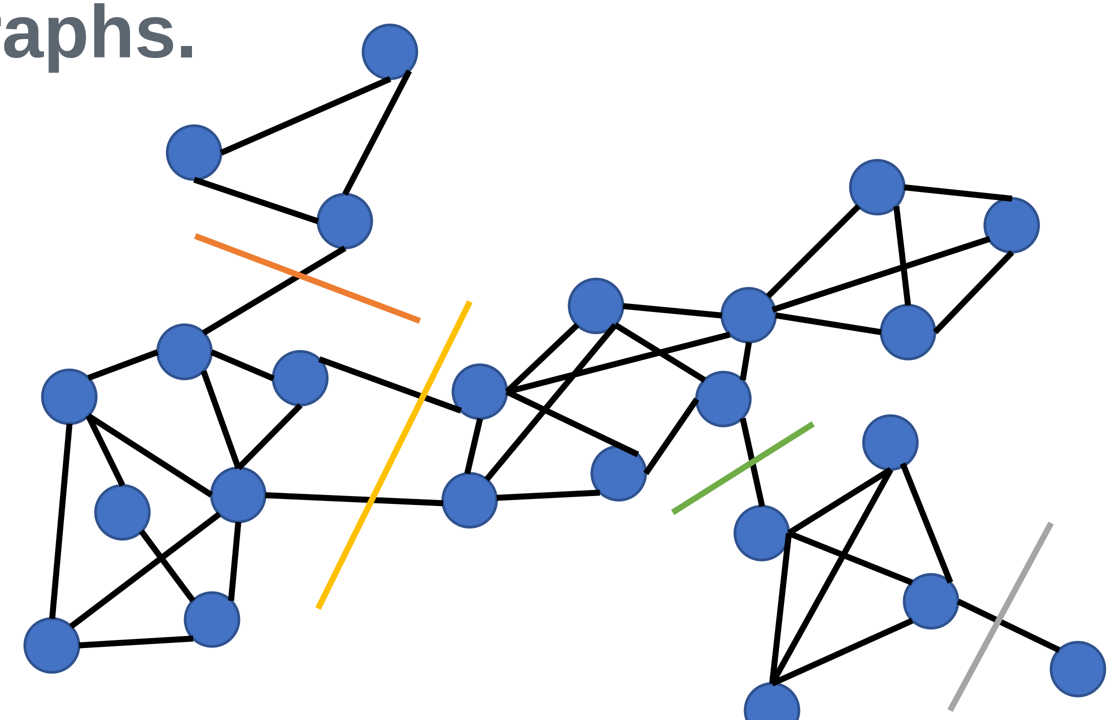
Recovering the Partitions

- Due to the relaxation, q can be any number (not just -1 and 1)
- How to construct the partition based on the eigenvector?
- A simple strategy :

$$A = \{i | q_i < 0\}, \quad B = \{i | q_i \geq 0\}$$

One Obvious Drawback

- **Minimum cut does not balance the size of bipartite graphs.**



- **How should we consider other factors like the sizes of the partitions?**

Spectral Clustering

Going Beyond MinCut

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Objective

Objective

Discuss several graph cut approaches

Objective

Illustrate the algorithm through an example

MinCut

- In MinCut, we used the following objective function:

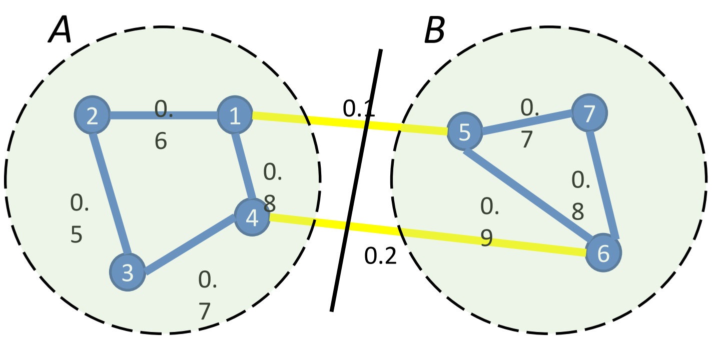
$$J_{MinCut} = Cut(A, B)$$

- We noted one drawback of MinCut: the sizes of the partitions are not considered.

- A few extensions exist.

Characterizing Graph Cut

- $Cut(A,B) = \sum_{i\in A, j\in B} w_{ij}$ $e.g., Cut(A,B) = 0.3$
- $Cut(A,A) = \sum_{i\in A, j\in A} w_{ij}$ $e.g., Cut(A,A) = 2.6$
- $Cut(B,B) = \sum_{i\in B, j\in B} w_{ij}$ $e.g., Cut(B,B) = 2.4$
- $Vol(A) = \sum_{i\in A} \sum_{i=1}^{n} w_{ij}$ $e.g., Vol(A) = 5.5$
- $Vol(B) = \sum_{i\in B} \sum_{i=1}^{n} w_{ij}$ $e.g., Vol(B) = 5.1$
- $|A| = 4, |B| = 3$



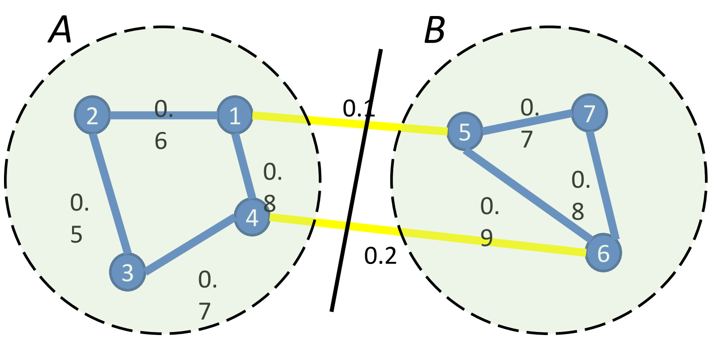
The Ratio Cut Method

The Objective function:

$$J_{RatioCut}(A,B) = Cut(A,B)\left(\frac{1}{|A|} + \frac{1}{|B|}\right)$$

Attempts to produce balanced clusters.

Example: $J_{RatioCut}(A,B) = \frac{7}{40}$



The Ratio Cut Method (cont'd)

- Similar to MinCut, the solution can be found by the following generalized eigenvalue problem:

$$(\mathbf{D} - \mathbf{W})\mathbf{q} = \lambda \mathbf{D}\mathbf{q}$$

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

Normalized Cut (NCut)

- In Ratio Cut, the balance of the partitions is defined based on the number of vertices.
- We may consider the “size” of a set based on weights of its edges ➔ Ncut
- The objective function is:

$$J_{NCut}(A,B) = Cut(A,B)\left(\frac{1}{Vol(A)} + \frac{1}{Vol(B)}\right)$$

Example: $J_{NCut}(A,B) = 0.1134$

Additional Considerations

- **In clustering, we should also consider within-cluster connections.**
- **A good partition should consider**
  - Inter-cluster connections, and
  - Intra-cluster connections.

MinMaxCut

- 1st constrant: inter-connection should be minimized: $MinCut(A, B)$

- 2nd constraint: intra-connection should be maximized : $MaxCut(A, A)$ and $MaxCut(B, B)$

- These requirements may be simultaneously satisfied by minimizing the objective function:

$$J_{MinMaxCut}(A, B) = Cut(A, B)\left(\frac{1}{Cut(A,A)} + \frac{1}{Cut(B,B)}\right)$$

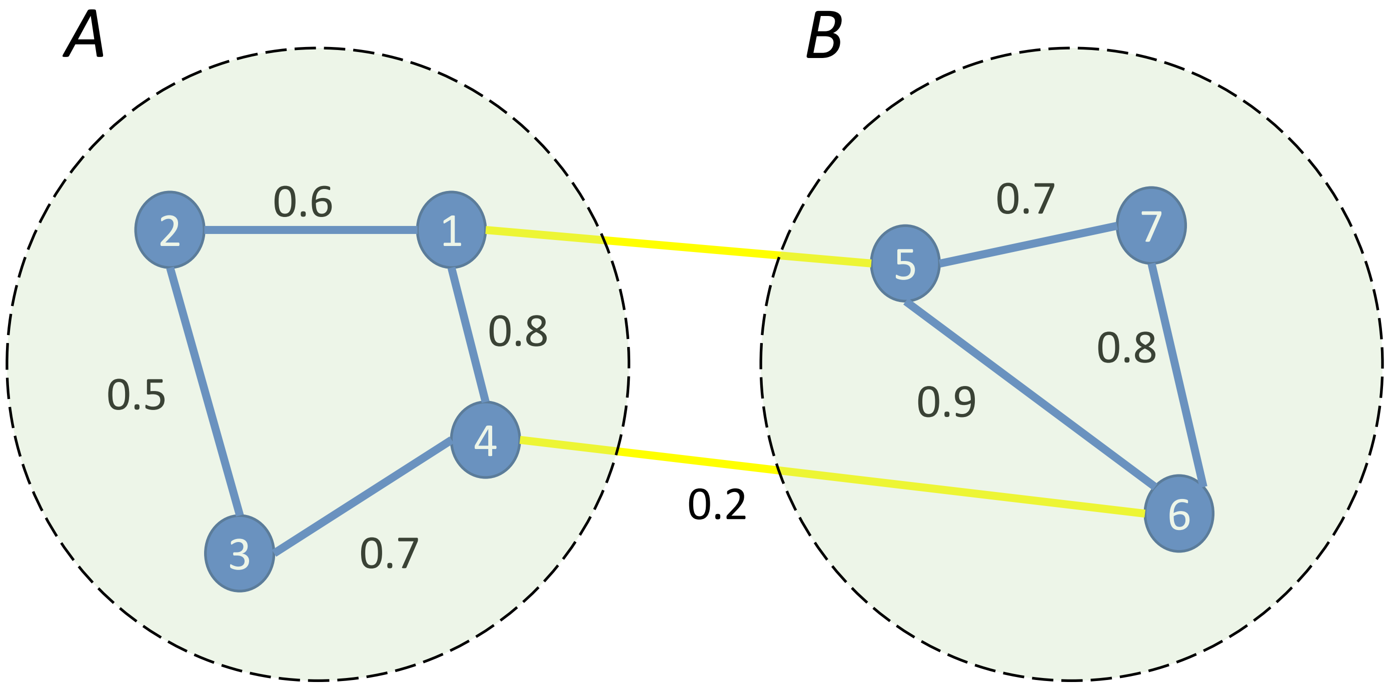
Example: $J_{MinMaxCut}(A, B) = 0.240$

Normalized and MinMaxCut Methods

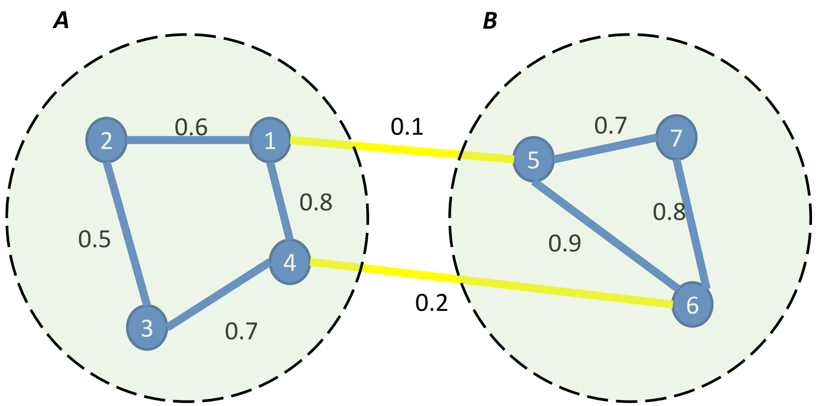
- Similar to before, we may relax the indicator vector q to real values.

- For both NCut and MinMaxCut, the solution may be found by solving generalized eigenvalue problems.

An Illustrative Example

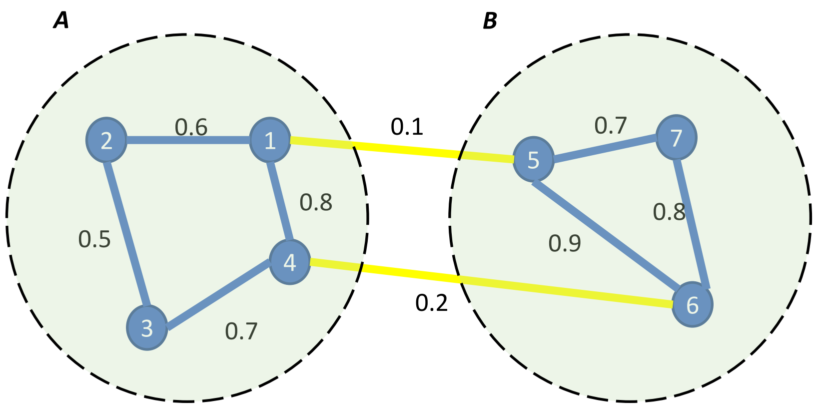


Graph and Similarity Matrix



	x1	x2	x3	x4	x5	x6	x7
x1	0	0.6	0	0.8	0.1	0	0
x2	0.6	0	0.5	0	0	0	0
x3	0	0.5	0	0.7	0	0	0
x4	0.8	0	0.7	0	0	0.2	0
x5	0.1	0	0	0	0	0.9	0.7
x6	0	0	0	0.2	0.9	0	0.8
x7	0	0	0	0	0.7	0.8	0

Graph and Laplacian Matrix

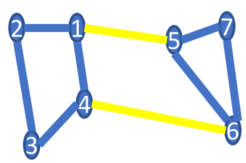


	x1	x2	x3	x4	x5	x6	x7
x1	1.5	-0.6	0	-0.8	-0.1	0	0
x2	-0.6	1.1	-0.5	0	0	0	0
x3	0	-0.5	1.2	-0.7	0	0	0
x4	-0.8	0	-0.7	1.7	0	-0.2	0
x5	-0.1	0	0	0	1.7	-0.9	-0.7
x6	0	0	0	-0.2	-0.9	1.9	-0.8
x7	0	0	0	0	-0.7	-0.8	1.5

Solve Eigen Problem

Pre-processing

- Build Laplacian matrix L of the graph.



Λ =

0
0.1588
1.2705
1.3692
2.2751
2.6238
2.9027

X =

0.378	-0.2962	0.3027	-0.6041	0.0429	0.3638	-0.4226
0.378	-0.3805	0.6392	0.4487	-0.0125	-0.233	0.2192
0.378	-0.3608	-0.5812	0.4834	-0.0221	0.2736	-0.2832
0.378	-0.2649	-0.398	-0.4373	0.0429	-0.3899	0.5323
0.378	0.4298	0.0443	0.0159	-0.6004	0.4291	0.3544
0.378	0.406	-0.0317	0.0012	-0.2174	-0.6116	-0.5196
0.378	0.4665	0.0247	0.0923	0.7667	0.1681	0.1195

Find

- Eigenvalues Λ and eigenvectors **x** of matrix **L**.
- Map vertices to the corresponding components of the 2nd eigenvector.

x1	-0.2962
x2	-0.3805
x3	-0.3608
x4	-0.2649
x5	0.4298
x6	0.406
x7	0.4665

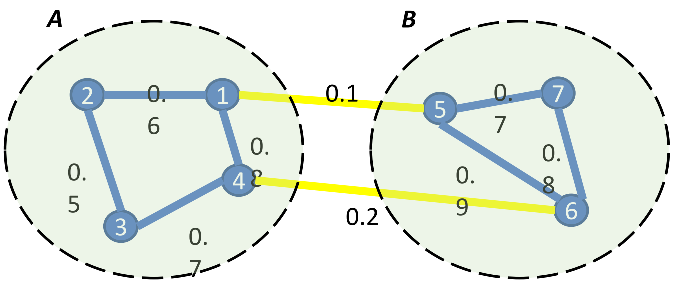
Spectral Clustering

x1	-0.2962
x2	-0.3805
x3	-0.3608
x4	-0.2649
x5	0.4298
x6	0.406
x7	0.4665

Split at value 0
Cluster A: Negative points
Cluster B: Positive Points

x1	-0.2962
x2	-0.3805
x3	-0.3608
x4	-0.2649

X5	0.4298
X6	0.406
X7	0.4665



Spectral Clustering

Practical Considerations in Implementation

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Objective

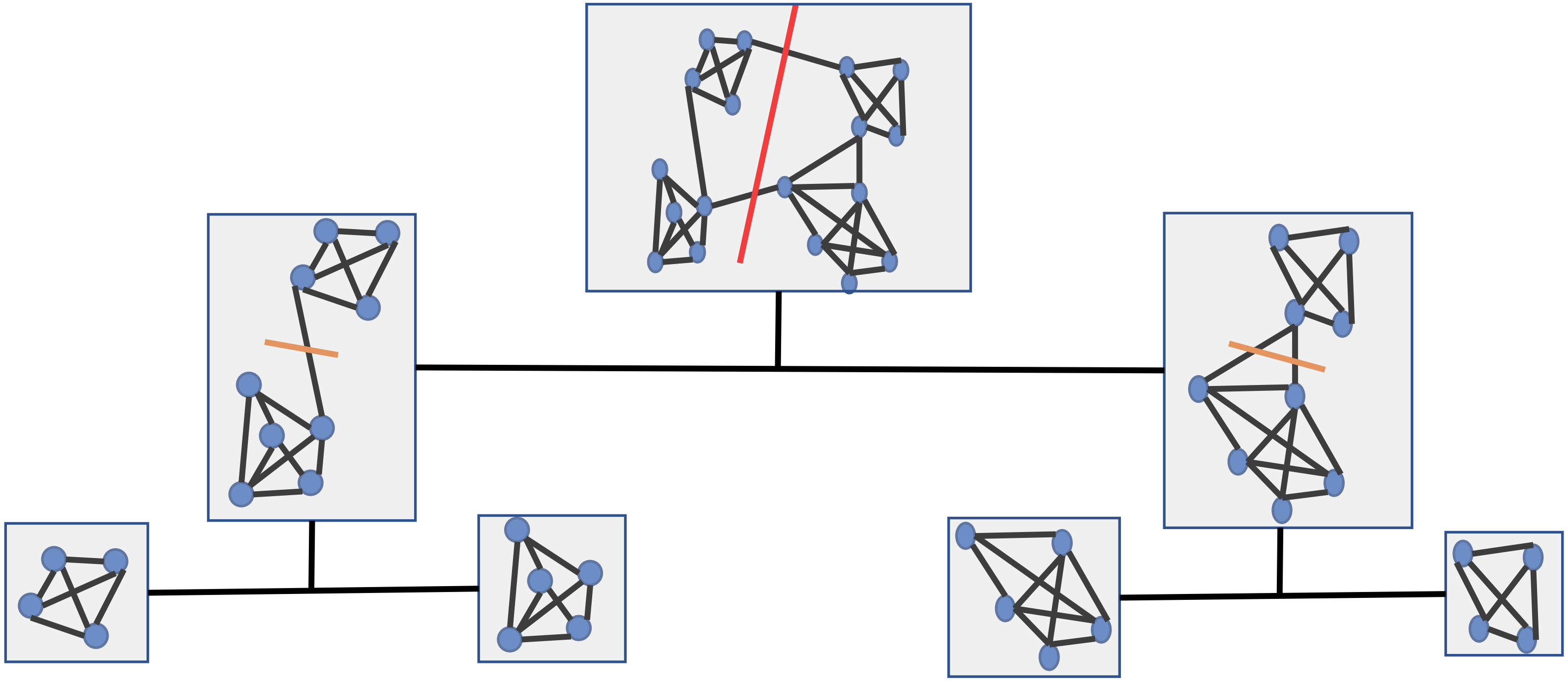
Objective

Discuss several practical implementation issues

Recursive Bi-partitioning

- Recursively apply bi-partitioning algorithm in a hierarchical divisive manner.

- Disadvantages: inefficient, stability issues.



K-way Graph Cuts

Generalizing the 2-way objective functions :

$$J_{RatioCut}(A_1, \dots, A_k) = \sum_{i=1}^{k} \frac{Cut(A_i, \overline{A_i})}{|A_i|}$$

$$J_{NCut}(A_1, \dots, A_k) = \sum_{i=1}^{k} \frac{Cut(A_i, \overline{A_i})}{Vol(A_i)}$$

$$J_{MinMaxCut}(A_1, \dots, A_k) = \sum_{i=1}^{k} \frac{Cut(A_i, \overline{A_i})}{Cut(A_i, A_i)}$$

Implementation Considerations (1/4)

- **Preprocessing: spectral clustering methods can be interpreted as tools for analysis of the block structure of the similarity matrix.**
  - Building such matrices may certainly ameliorate the results.

- **When building graphs from real data**
  - Calculation of the similarity matrix is not evident.
  - Choosing the similarity function can highly affect the results of the following steps.
  - A Gaussian kernel is often chosen, but other similarities like cosine similarity might be proper for specific applications.

Implementation Considerations (2/4)

Graph and similarity matrix construction: Laplacian matrices are generally chosen to be positive and semi-definite thus their eigenvalues will be non-negatives.

- A few variants

Unnormalized	$\boldsymbol{L} = \boldsymbol{D} - \boldsymbol{W}$
symmetric	$\boldsymbol{L}_{Sy} = \boldsymbol{D}^{-1/2}\boldsymbol{L}\boldsymbol{D}^{-1/2} = \boldsymbol{I} - \boldsymbol{D}^{-1/2}\boldsymbol{W}\boldsymbol{D}^{-1/2}$
Asymmetric	$\boldsymbol{L}_{As} = \boldsymbol{D}^{-1}\boldsymbol{L} = \boldsymbol{I} - \boldsymbol{D}^{-1}\boldsymbol{W}$

Implementation Considerations (3/4)

Computing the eigenvectors.

- Efficient methods exist for sparse matrices.

Different ways of building the similarity graphs

- ε-neighborhood graph.
- k-nearest neighbor graph.
- fully connected graph.

Implementation Considerations (4/4)

Choosing *k*:

- Similar to k-means, there are many heuristics to use.
- The eigengap heuristic: to choose a k such that first k eigenvalues are very small but the (k+1)th one is relatively large.

Clustering: simple algorithms other than k-means can be used in the last stage, such as simple linkage, k-lines, elongated k-means, mixture model, etc.

Recap: Pros and Cons of Spectral Clustering

Advantages:

- Does not make strong assumptions on the forms of the clusters.
- Easy to implement, and can be implemented efficiently even for large data sets as long as the similarity graph is sparse.
- Good clustering results.
- Reasonably fast for sparse data sets of several thousand elements.

Disadvantages:

- May be sensitive to choice of parameters for neighborhood graph.
- Computationally expensive for large datasets.