CPSC 8420 Advanced Machine Learning
Week 8: Spectral Clustering and Manifold Learning

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Motivation

All we algorithms have learnt by so far is based on (Euclidean) distance, such as Least Squares, PCA, LDA, *etc*.

- In some cases, distance based method can't achieve the result as we expect.
- Graph based algorithm may provide a different perspective and offer better results.

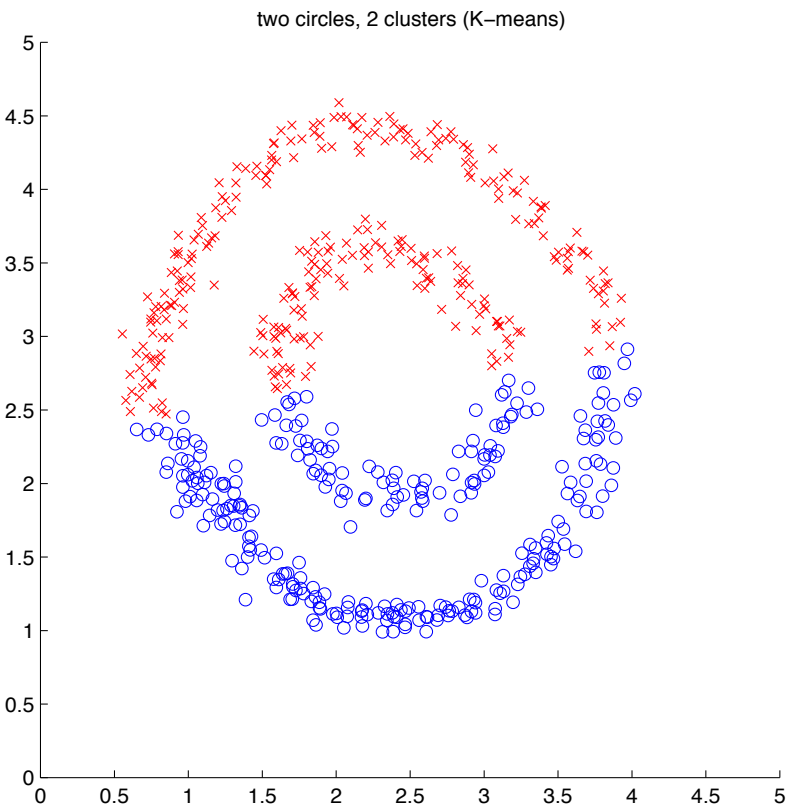
Learning Outcomes

Our goal for today's lecture is to understand:

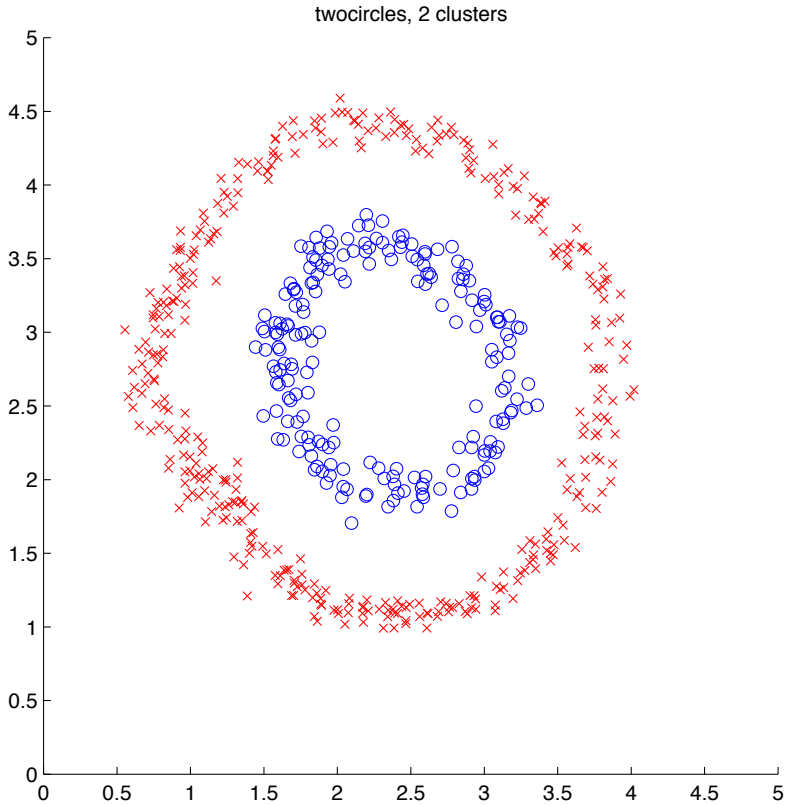
- Basic concept in graph such as Adjacency Matrix, Degree Matrix, Laplacian Matrix, *etc*.
- How to utilize RatioCut idea for clustering
- How to obtain the optimal solution

A Gentle Start

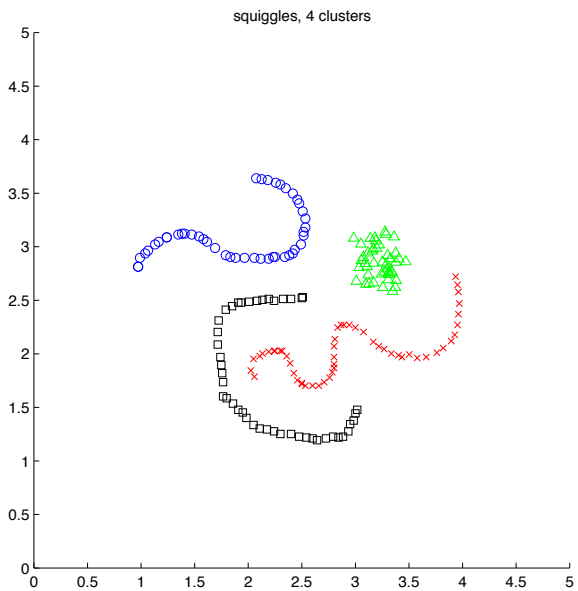
K-means

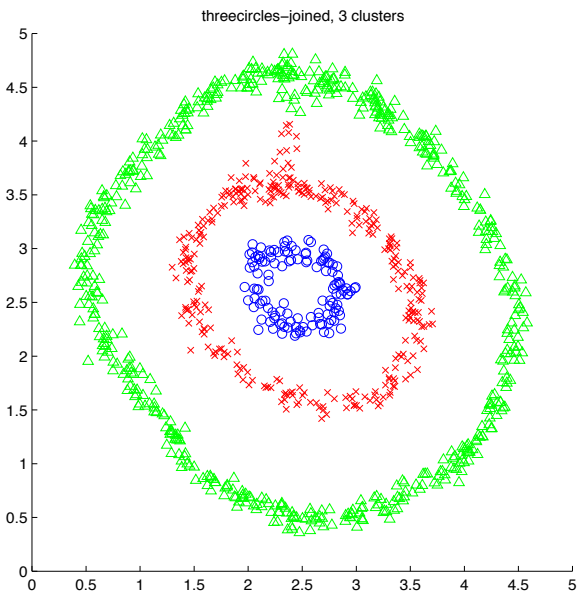


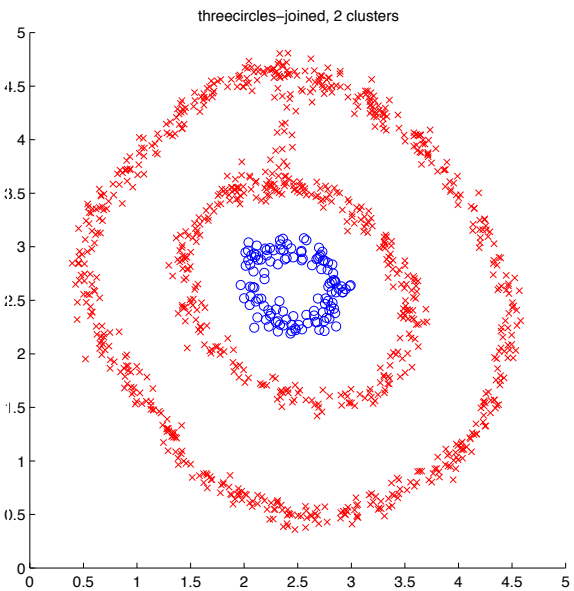
Spectral clustering



A Gentle Start

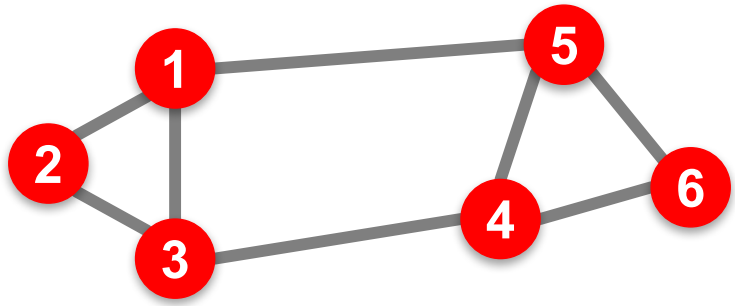




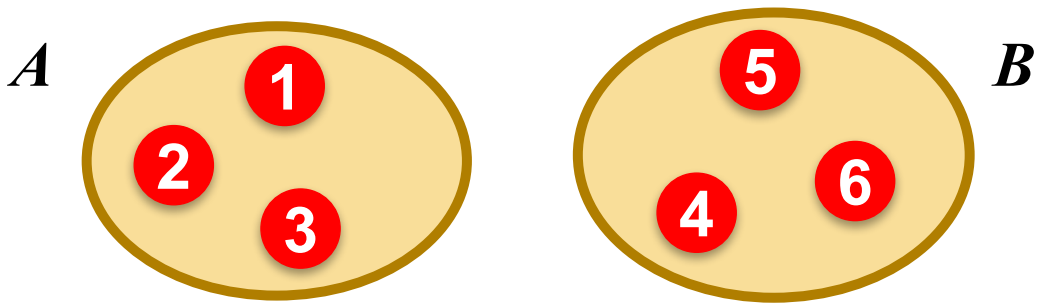


Basic Concept

- **Undirected graph $G(V, E)$:**



- **Bi-partitioning task:**
  - Divide vertices into two disjoint groups A, B

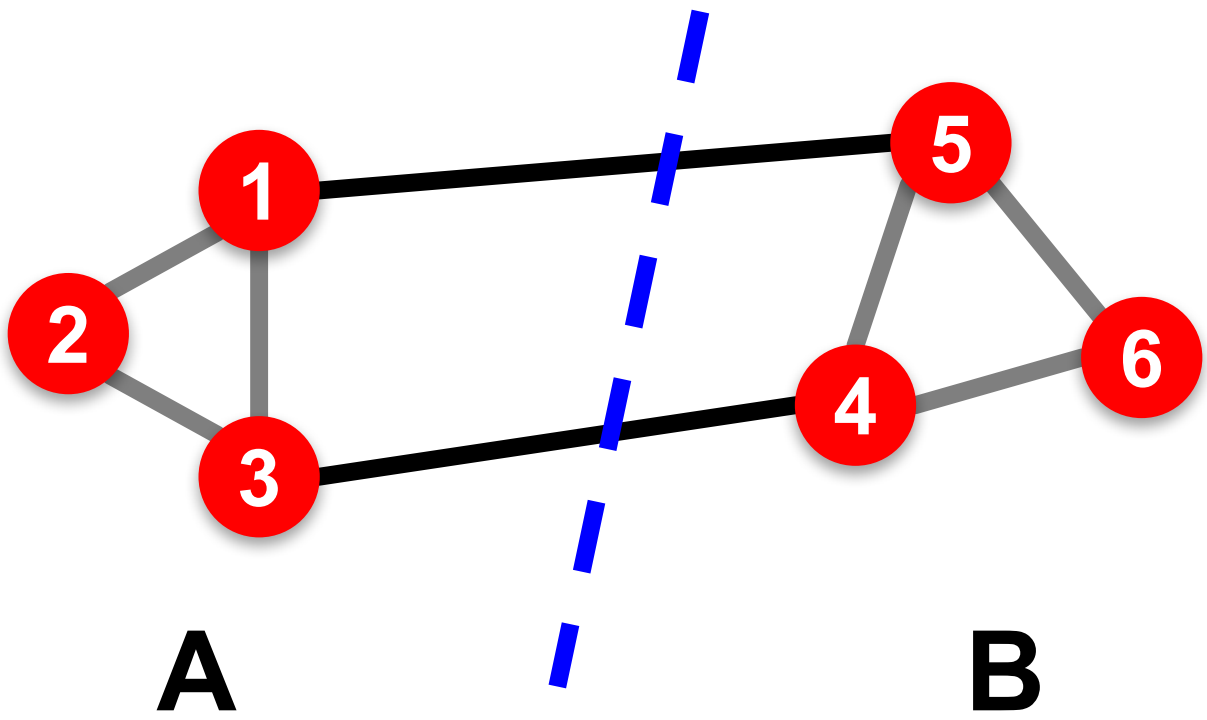


- **Questions:**
  - How can we define a "good" partition of G?
  - How can we efficiently identify such a partition?

Graph Partitioning

What makes a good partition?

1. Maximize the number of within-group connections
2. Minimize the number of between-group connections



Definition

Express partitioning objectives as a function of the 'edge cut' of the partition. For two not necessarily disjoint sets $A, B \subset V$, we define $W(A, B) = \sum_{i \in A, j \in B} w_{ij}$ and Cut as set of edges with only one vertex in a group $cut(A, B) = \sum_{i \in A, j \in B} w_{ij}$, and when there are k subsets, then

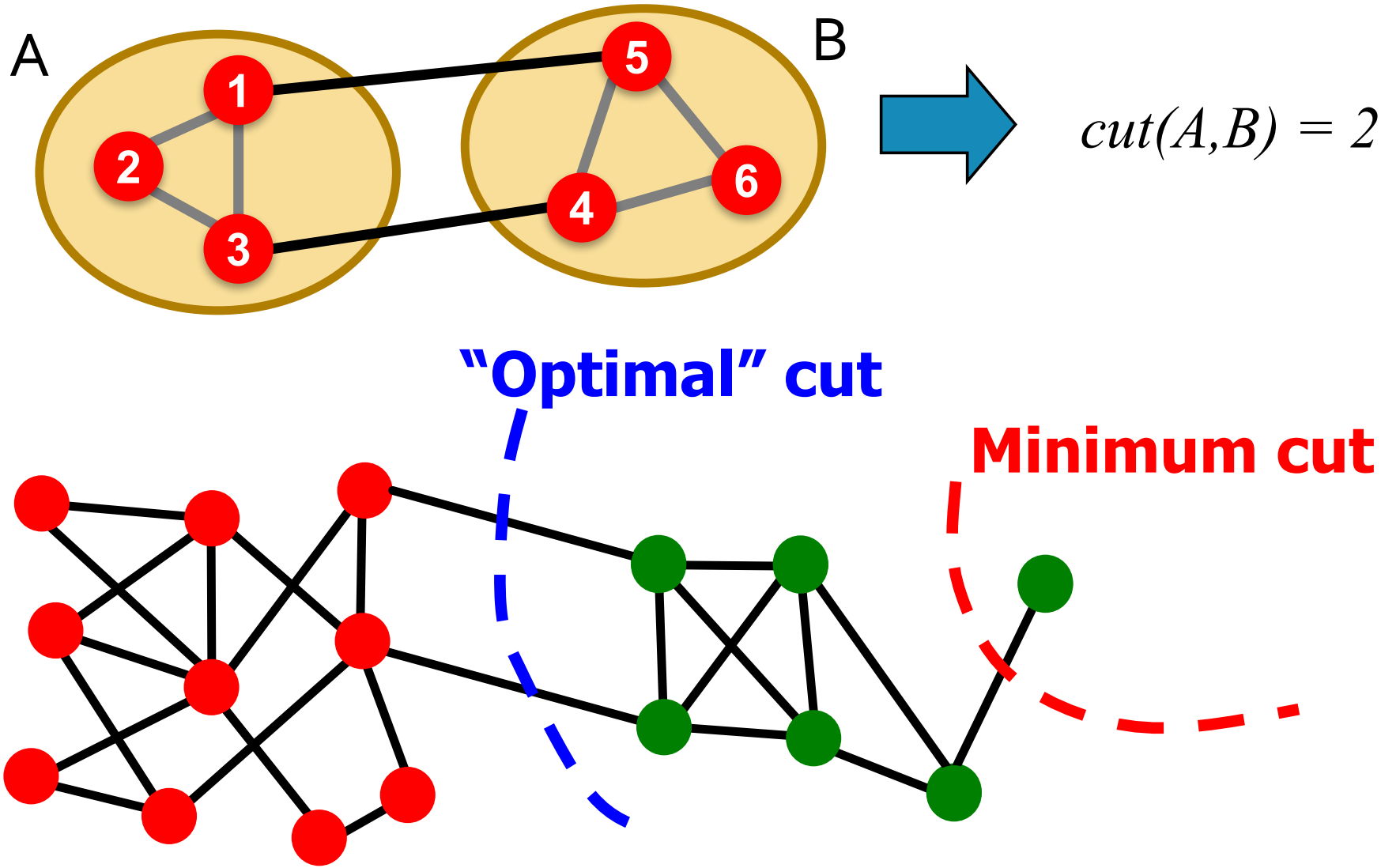
$cut(A_1, A_2, ...A_k) = \frac{1}{2} \sum_{i=1}^{k} W(A_i, \overline{A}_i)$.

The degree of a vertex $v_i \in V$ is defined as: $d_i = \sum_{j=1}^{n} w_{ij}$. We consider two different ways of measuring the 'size' of a subset $A \subset V$:

$$|A| := \textit{the number of vertices in } A$$

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

Example



Adjacency Matrix

	1	2	3	4	5	6
1	0	1	1	0	1	0
2	1	0	1	0	0	0
3	1	1	0	1	0	0
4	0	0	1	0	1	1
5	1	0	0	1	0	1
6	0	0	0	1	1	0

Adjacency Matrix

There are several popular constructions to transform a given set $x_1, \ldots, x_n$ of data points with pairwise similarities s_{ij} into a graph.

- The ϵ-neighborhood graph: Here we connect all points whose pairwise distances are smaller than ϵ: $w_{ij} = \begin{cases} 0 & s_{ij} > \epsilon \\ \epsilon & s_{ij} \leq \epsilon \end{cases}$.

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- k-nearest neighbor graphs: Here the goal is to connect vertex v_i with vertex v_j if v_j is among the k-nearest neighbors of v_i: $w_{ij} = w_{ji} = \begin{cases} 0 & x_i \notin KNN(x_j) \text{ or } x_j \notin KNN(x_i) \\ exp(-\frac{||x_i - x_j||_2^2}{2\sigma^2}) & x_i \in KNN(x_j) \text{ and } x_j \in KNN(x_i) \end{cases}$.

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- The fully connected graph: Here we simply connect all points with positive similarity with each other, and we weight all edges by s_{ij}. An example for such a similarity function is the Gaussian similarity function: $w_{ij} = s_{ij} = exp(-\frac{||x_i - x_j||_2^2}{2\sigma^2})$, where the parameter σ controls the width of the neighborhoods.

Degree Matrix

	1	2	3	4	5	6
1	3	0	0	0	0	0
2	0	2	0	0	0	0
3	0	0	3	0	0	0
4	0	0	0	3	0	0
5	0	0	0	0	3	0
6	0	0	0	0	0	2

Laplacian Matrix

	1	2	3	4	5	6
1	3	-1	-1	0	-1	0
2	-1	2	-1	0	0	0
3	-1	-1	3	-1	0	0
4	0	0	-1	3	-1	-1
5	-1	0	0	-1	3	-1
6	0	0	0	-1	-1	2

$$L = D - A$$

Property of Laplacian Matrix

L is always symmetric and SPD. For arbitary vector f, we have:

$$f^T Lf = f^T Df - f^T Wf = \sum_{i=1}^{n} d_i f_i^2 - \sum_{i,j=1}^{n} w_{ij} f_i f_j$$

$$= \frac{1}{2}(\sum_{i=1}^{n} d_i f_i^2 - 2\sum_{i,j=1}^{n} w_{ij} f_i f_j + \sum_{j=1}^{n} d_j f_j^2) = \frac{1}{2}\sum_{i,j=1}^{n} w_{ij}(f_i - f_j)^2 \tag{1}$$

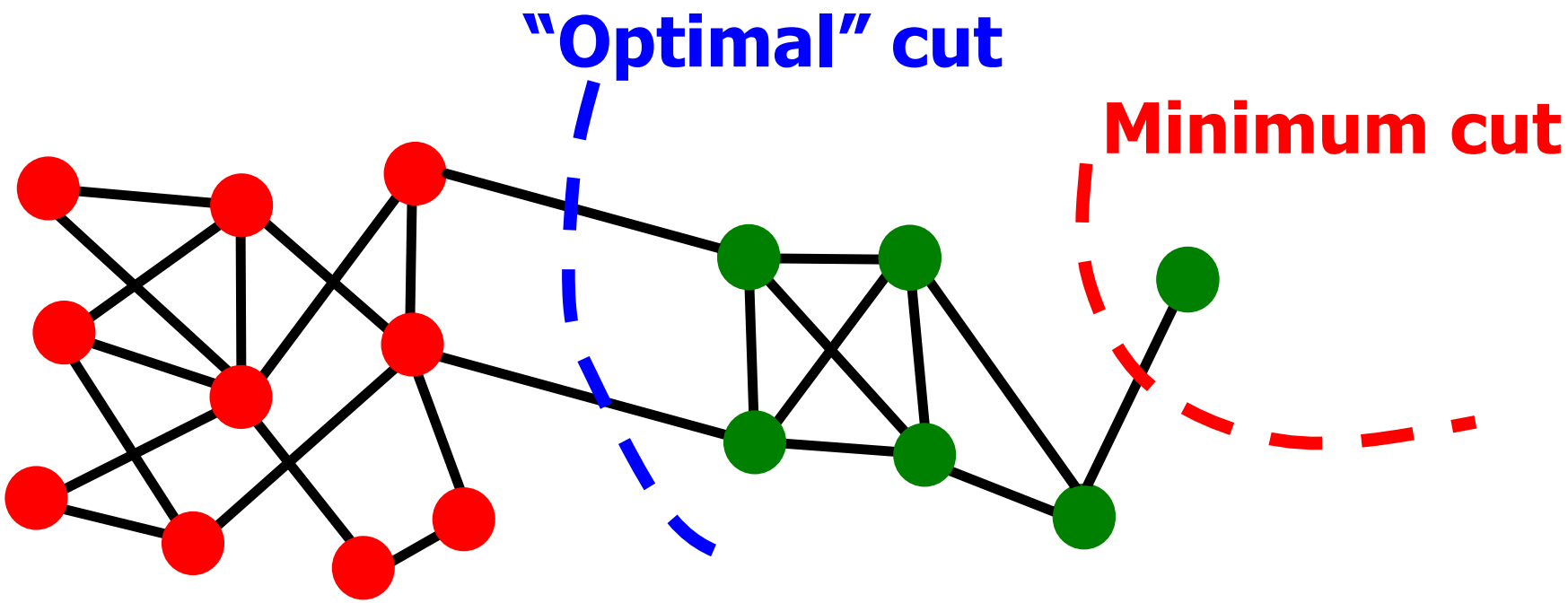
Then the multiplicity k of the eigenvalue 0 of L equals the number of connected components $A_1, \ldots, A_k$ in the graph.

$$\mathrm{L} = \begin{pmatrix} L_1 & \cdots & \cdots & \cdots \\ \cdots & L_2 & \cdots & \cdots \\ \vdots & \vdots & \ddots & \vdots \\ \cdots & \cdots & \cdots & L_n \end{pmatrix}$$

RatioCut

$$RatioCut(A_1, A_2, ...A_k) = \frac{1}{2} \sum_{i=1}^{k} \frac{W(A_i, \overline{A}_i)}{|A_i|}$$

$$Cut(A_1, A_2, ...A_k) = \frac{1}{2} \sum_{i=1}^{k} W(A_i, \overline{A}_i)$$



RatioCut

If we introduce indicator vector: $h_j \in \{h_1, h_2, ..h_k\}, j \in [1, k]$, for any vector $h_j \in R^n$, we define: $h_{ij} = \begin{cases} 0 & v_i \notin A_j \\ \frac{1}{\sqrt{|A_j|}} & v_i \in A_j \end{cases}$, then:

$$
\begin{aligned}
h_i^T L h_i &= \frac{1}{2} \sum_{m=1} \sum_{n=1} w_{mn} (h_{im} - h_{in})^2 \\
&= \frac{1}{2} (\sum_{m \in A_i, n \notin A_i} w_{mn} (\frac{1}{\sqrt{|A_i|}} - 0)^2 + \sum_{m \notin A_i, n \in A_i} w_{mn} (0 - \frac{1}{\sqrt{|A_i|}})^2 \\
&= \frac{1}{2} (\sum_{m \in A_i, n \notin A_i} w_{mn} \frac{1}{|A_i|} + \sum_{m \notin A_i, n \in A_i} w_{mn} \frac{1}{|A_i|} \\
&= \frac{1}{2} (cut(A_i, \overline{A}_i) \frac{1}{|A_i|} + cut(\overline{A}_i, A_i) \frac{1}{|A_i|}) \\
&= \frac{cut(A_i, \overline{A}_i)}{|A_i|}
\end{aligned}
$$

RatioCut

For a subset, its RatioCut is $h_i^T L h_i$, then for k subsets we have:

$$RatioCut(A_1, A_2, ...A_k) = \sum_{i=1}^{k} h_i^T L h_i = \sum_{i=1}^{k} (H^T LH)_{ii} = tr(H^T LH) \tag{2}$$

Unfortunately, this is an integer programming problem which we cannot solve efficiently. Instead, we relax the latter requirement and simply search an orthonormal matrix $H \in \mathbb{R}^{n \times k}$. By observing $H^T H = I$, we have the objective as:

$$\underbrace{arg\ min}_{H}\ tr(H^T LH)\ \ s.t.\ H^T H = I \tag{3}$$

RatioCut

Unnormalized spectral clustering

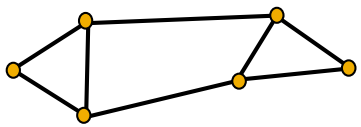
Input: Similarity matrix $S \in \mathbb{R}^{n \times n}$, number k of clusters to construct.

- Construct a similarity graph by one of the ways described in Section 2. Let W be its weighted adjacency matrix.
- 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 $C_1, \ldots, C_k$.

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

RatioCut

- **1) Pre-processing:**
  - Build Laplacian matrix L of the graph



	1	2	3	4	5	6
1	3	-1	-1	0	-1	0
2	-1	2	-1	0	0	0
3	-1	-1	3	-1	0	0
4	0	0	-1	3	-1	-1
5	-1	0	0	-1	3	-1
6	0	0	0	-1	-1	2

- **2) Decomposition:**
  - Find eigenvalues λ and eigenvectors x of the matrix L

$\lambda =$

0.0
1.0
3.0
3.0
4.0
5.0

$X =$

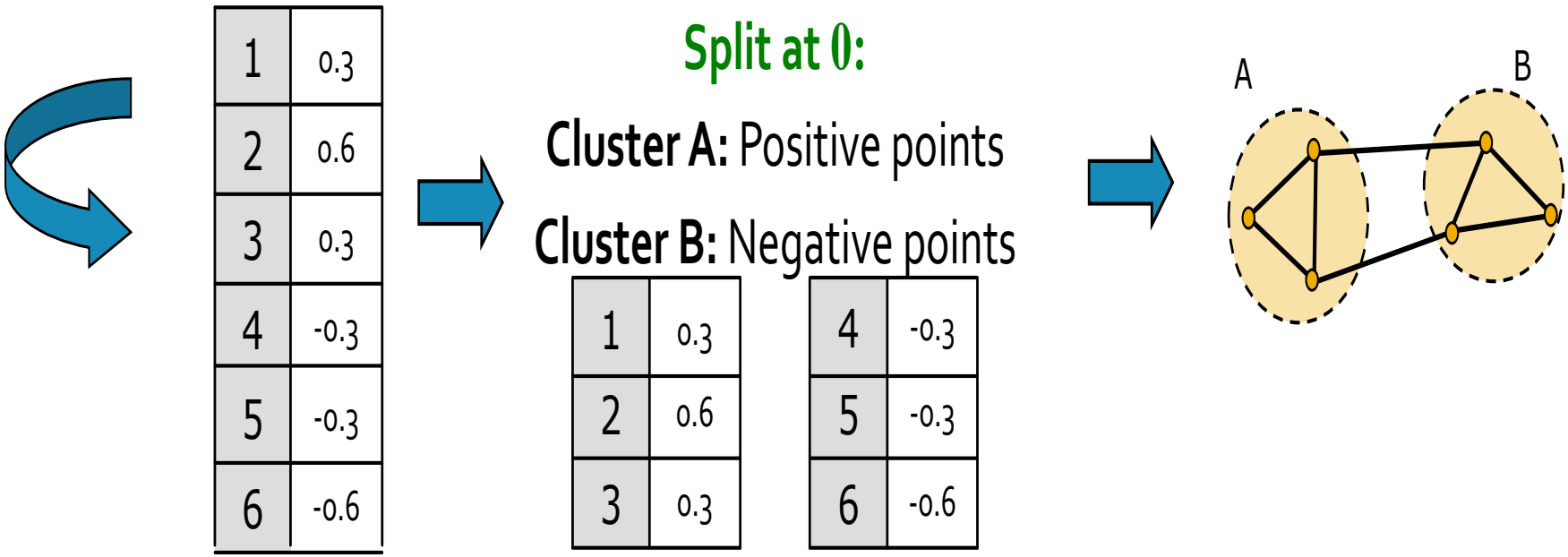
0.4	0.3	-0.5	-0.2	-0.4	-0.5
0.4	0.6	0.4	-0.4	0.4	0.0
0.4	0.3	0.1	0.6	-0.4	0.5
0.4	-0.3	0.1	0.6	0.4	-0.5
0.4	-0.3	-0.5	-0.2	0.4	0.5
0.4	-0.6	0.4	-0.4	-0.4	0.0

  - Map vertices to corresponding components of λ_2

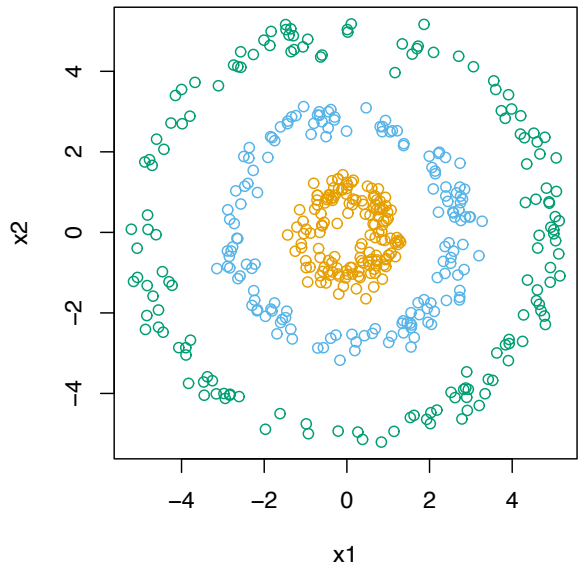
1	0.3
2	0.6
3	0.3
4	-0.3
5	-0.3
6	-0.6

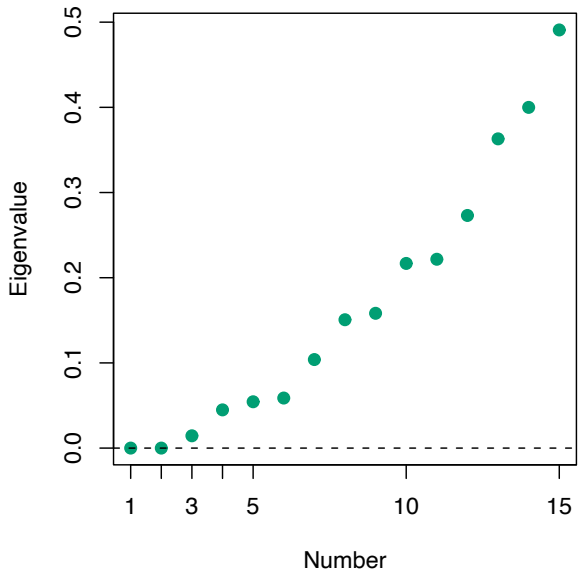
How do we now find the clusters?

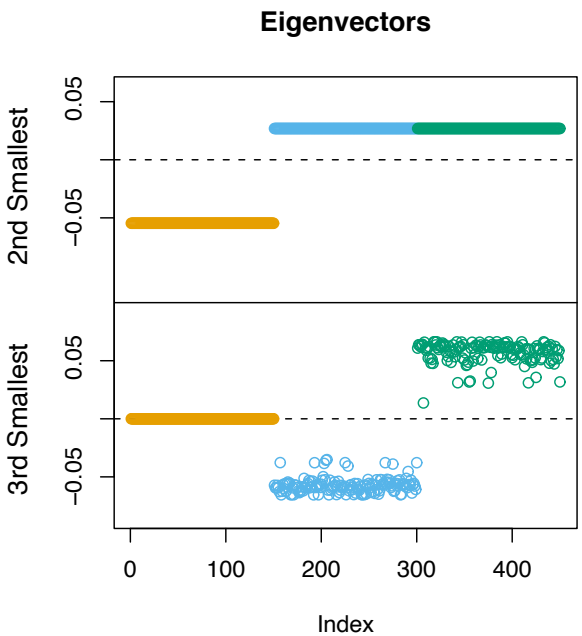
RatioCut


1 0.3
2 0.6
3 0.3
4 -0.3
5 -0.3
6 -0.6
Split at 0:
Cluster A: Positive points
Cluster B: Negative points
1 0.3
2 0.6
3 0.3
4 -0.3
5 -0.3
6 -0.6
A
B

RatioCut


x2
x1
−4
−2
0
2
4


Eigenvalue
Number
0.0
0.1
0.2
0.3
0.4
0.5
1
3
5
10
15


Eigenvectors
2nd Smallest
3rd Smallest
Index
0.05
−0.05
0
100
200
300
400

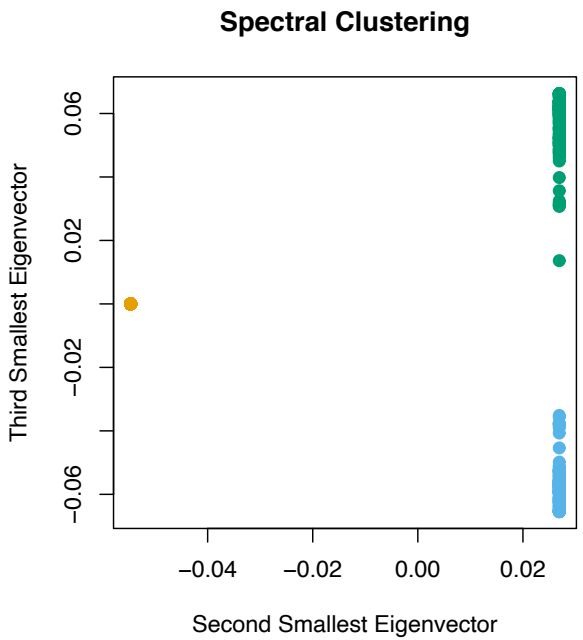
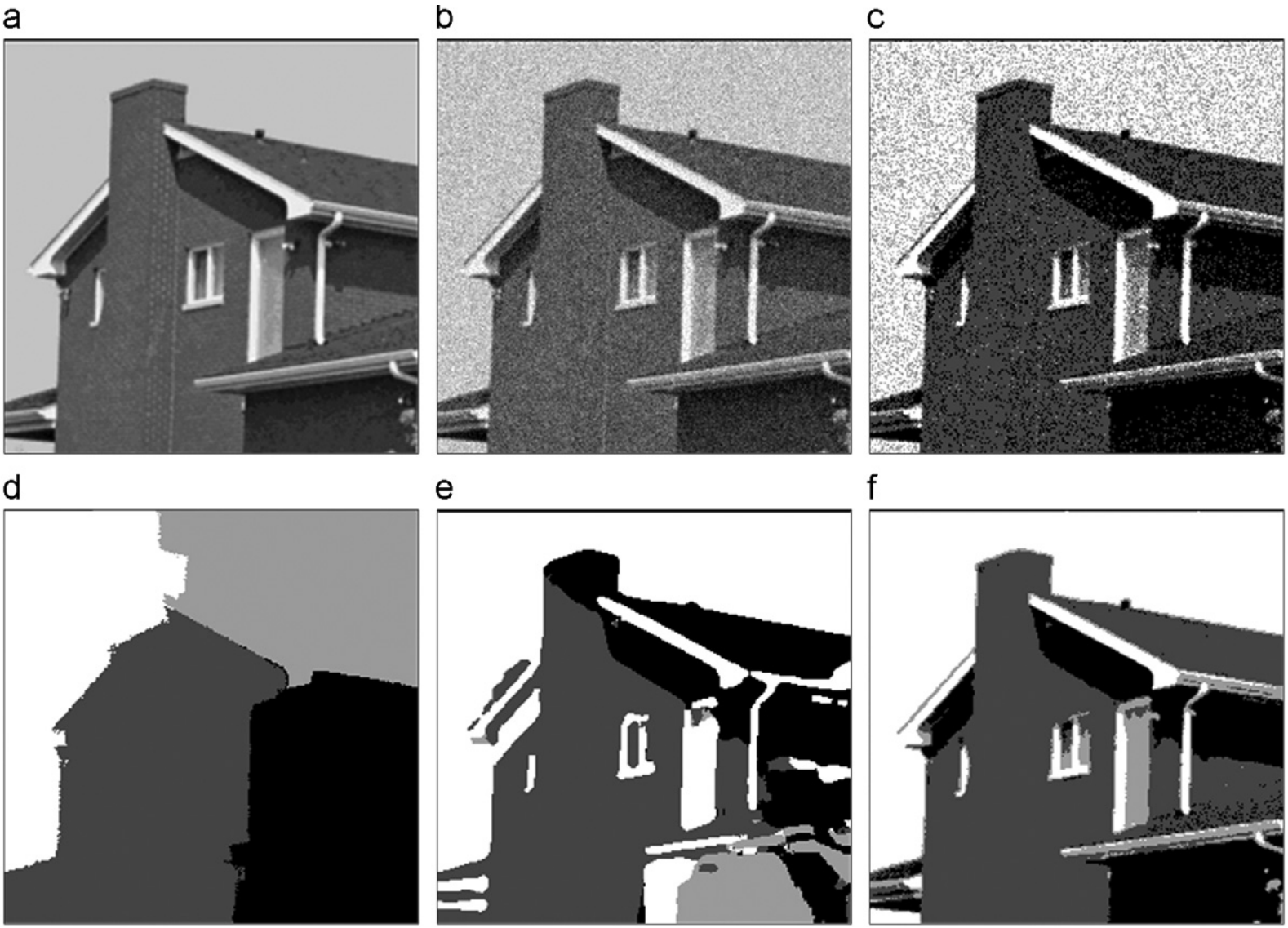

Spectral Clustering
Third Smallest Eigenvector
Second Smallest Eigenvector
0.06
0.02
−0.02
−0.06
−0.04
0.00

Image Segmentation

Image Segmentation



Clustering Results VS. K-means

k	TDT2		Reuters-21578	
	K-means	SC	K-means	SC
2	0.989	0.998	0.871	0.923
3	0.974	0.996	0.775	0.816
4	0.959	0.996	0.732	0.793
...				
9	0.852	0.984	0.553	0.625
10	0.835	0.979	0.545	0.615