Spectral Clustering

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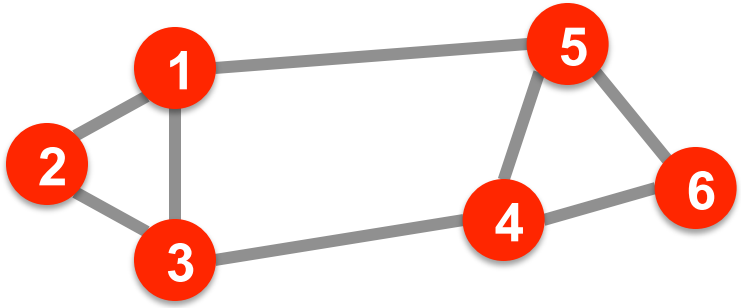
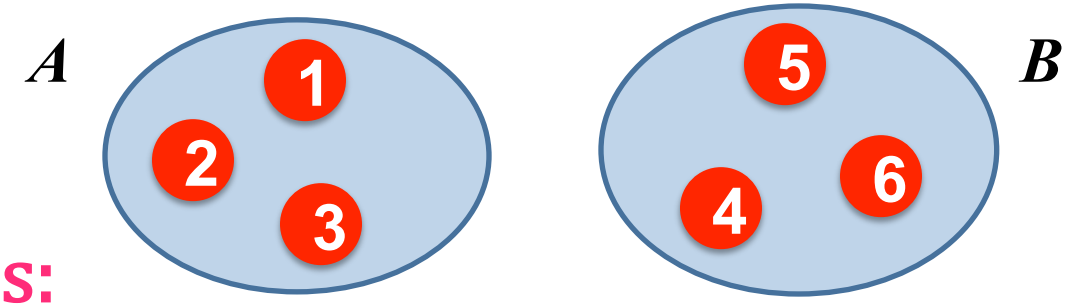
(with thanks to William Cohen of Carnegie Mellon University, and J. Leskovec, A. Rajaraman, and J. Ullman of Stanford University)

Graph Partitioning

- Undirected graph



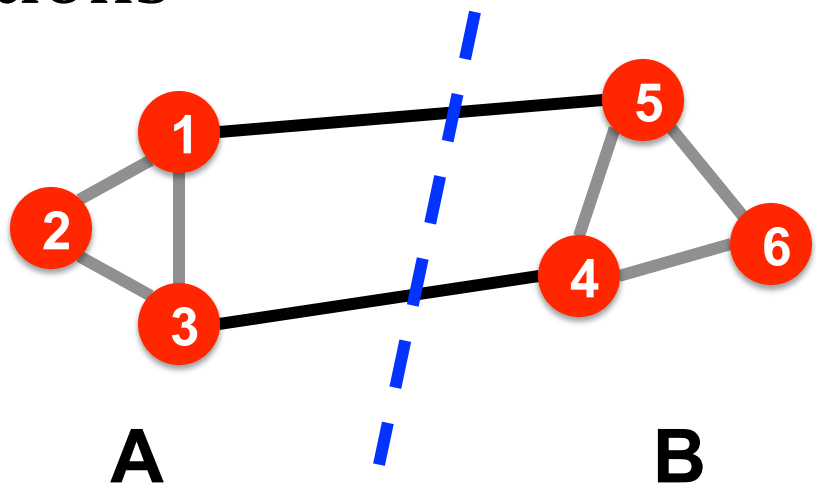
- Bi-partitioning task:
  - Divide vertices into two disjoint groups



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

Graph Partitioning

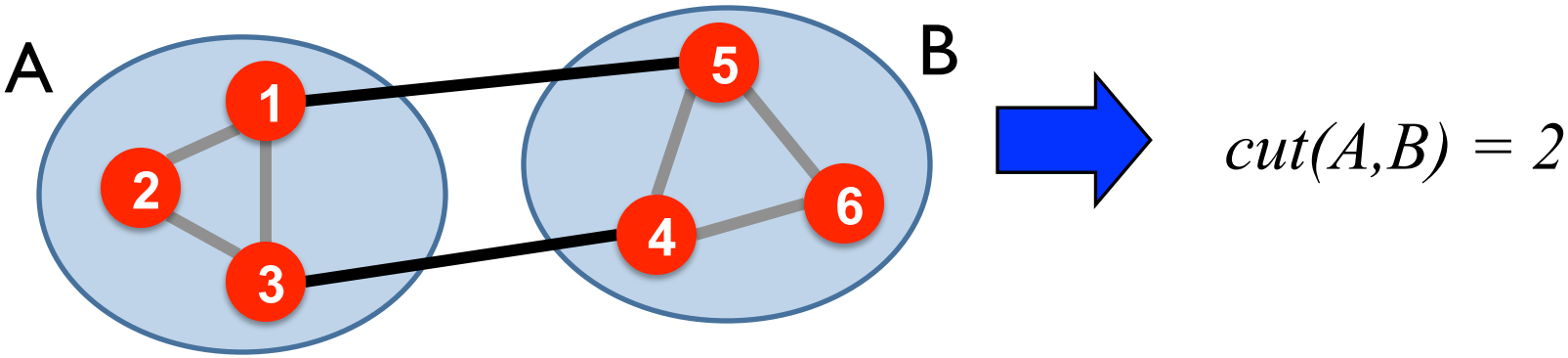
- What makes a good partition?
  - Maximize the number of within-group connections
  - Minimize the number of between-group connections



Graph Cuts

- **Express partitioning objectives as a function of the "edge cut" of the partition**
- **Cut:** Set of edges with only one vertex in a group:

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

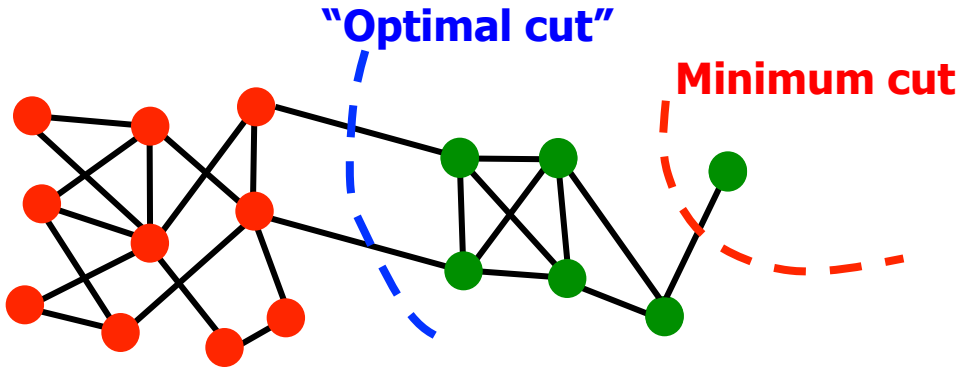


Graph Cut Criterion

- **Criterion: Minimum-cut**
  - Minimize weight of connections between groups

$$\arg\min_{A,B} cut(A,B)$$

- **Degenerate case:**



- **Problem:**
  - Only considers external cluster connections
  - Does not consider internal cluster connectivity

Graph Cut Criteria

- **Criterion:** Normalized-cut [Shi-Malik, '97]
  - Connectivity between groups relative to the density of each group

$$ncut(A,B) = \frac{cut(A,B)}{vol(A)} + \frac{cut(A,B)}{vol(B)}$$

: total weight of the edges with at least one endpoint in :

- Why use this criterion?
  - Produces more balanced partitions
- How do we efficiently find a good partition?
  - **Problem:** Computing optimal cut is NP-hard

Spectral Graph Partitioning

- A: adjacency matrix of undirected G
  - $A_{ij}=1$ if is an edge, else 0
- x is a vector in $\Re^n$ with components
  - Think of it as a label/value of each node of
- **What is the meaning of $A \cdot x$?**

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \vdots \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

$$y_i = \sum_{j=1}^{n} A_{ij} xj = \sum_{(i,j) \in E} x_j$$

- **Entry y_i is a sum of labels x_j of neighbors of i**

What is the meaning of *Ax*?

- j^{th} coordinate of $A \cdot x$:
  - Sum of the x-values of neighbors of j
  - Make this a new value at node j

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \vdots \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \lambda \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

$A \cdot x = \lambda \cdot x$

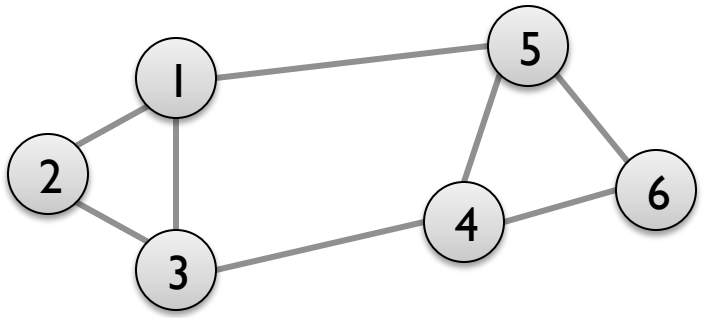
- **Spectral Graph Theory:**
  - Analyze the "spectrum" of matrix representing
  - **Spectrum:** Eigenvectors of a graph, ordered by the magnitude (strength) of their corresponding eigenvalues :

$$\Lambda = \{\lambda_1, \lambda_2, \dots, \lambda_n\}$$

$$\lambda_1 \le \lambda_2 \le \dots \le \lambda_n$$

Matrix Representations

- **Adjacency matrix (A):**
  - $n \times n$ matrix
  - $A=[a_{ij}]$, $a_{ij}=1$ if edge between node i and j

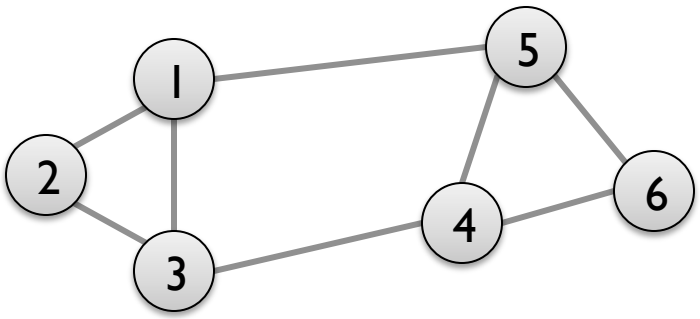


	1	2	3	4	5	6
1	0	1	1	0	1	0
2	1	0	1	0	0	0
3	1	1	0	1	0	0
4	0	0	1	0	1	1
5	1	0	0	1	0	1
6	0	0	0	1	1	0

- **Important properties:**
  - Symmetric matrix
  - Eigenvectors are real and orthogonal

Matrix Representations

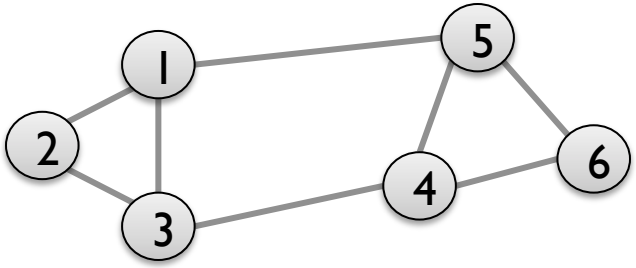
- Degree matrix (D):
  - $n \times n$ diagonal matrix
  - $D=[d_{ii}]$, d_{ii} = degree of node i



	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

Matrix Representations

- Laplacian matrix (L):
  - $n \times n$ symmetric matrix



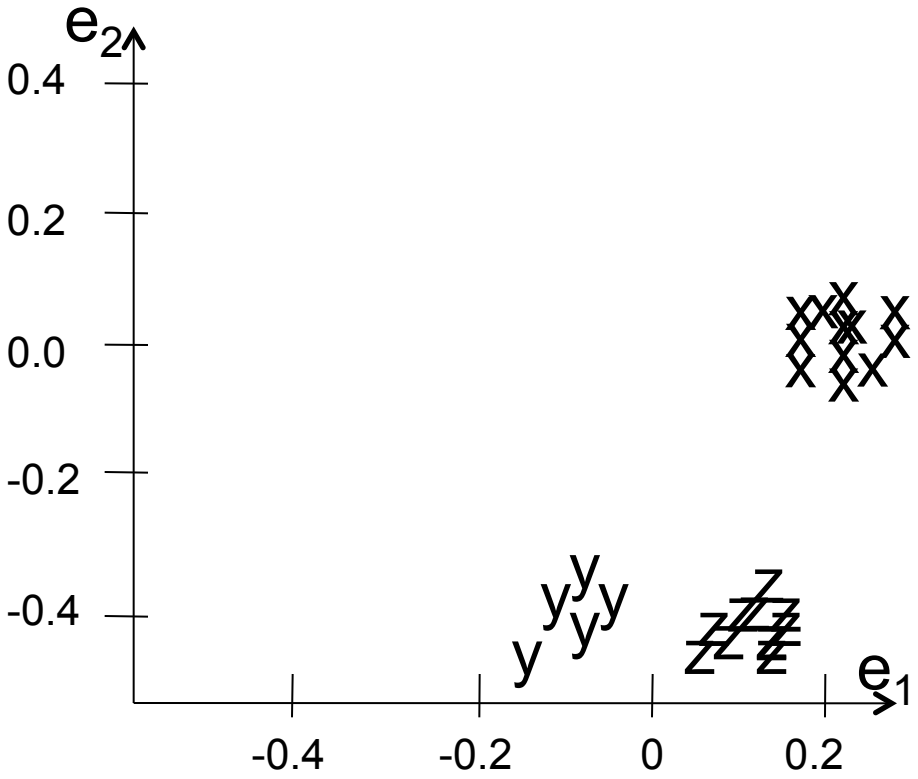
	1	2	3	4	5	6
1	3	-1	-1	0	-1	0
2	-1	2	-1	0	0	0
3	-1	-1	3	-1	0	0
4	0	0	-1	3	-1	-1
5	-1	0	0	-1	3	-1
6	0	0	0	-1	-1	2

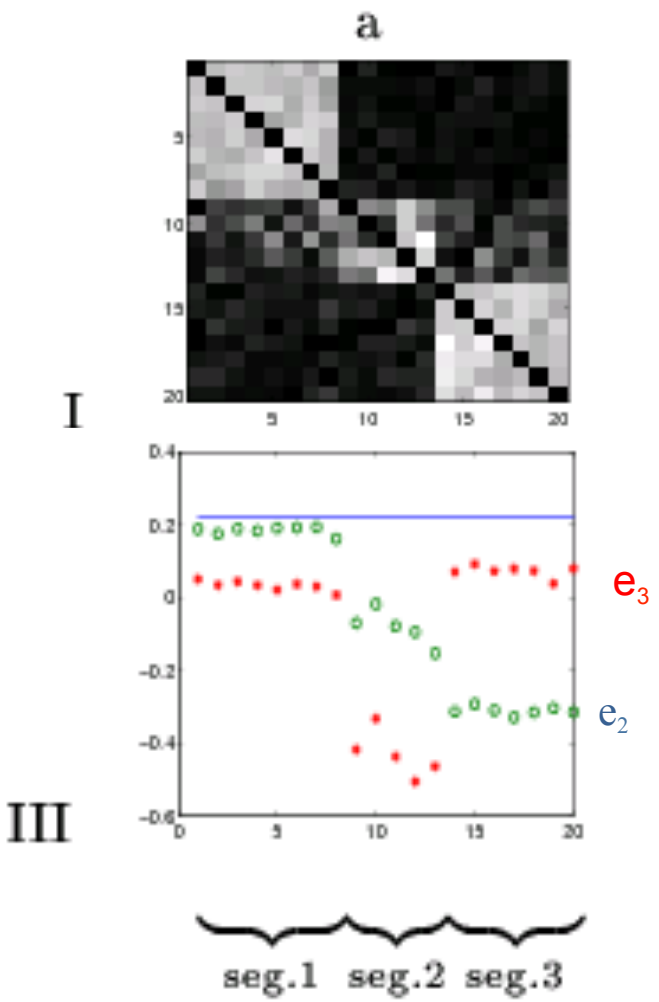
$L = D - A$

- What is trivial eigenpair?
- Important properties:
  - **Eigenvalues** are non-negative real numbers
  - **Eigenvectors** are real and orthogonal

Spectral Clustering: Graph = Matrix

$W*v_1 = v_2$ "propogates weights from neighbors"





[Shi & Meila, 2002]

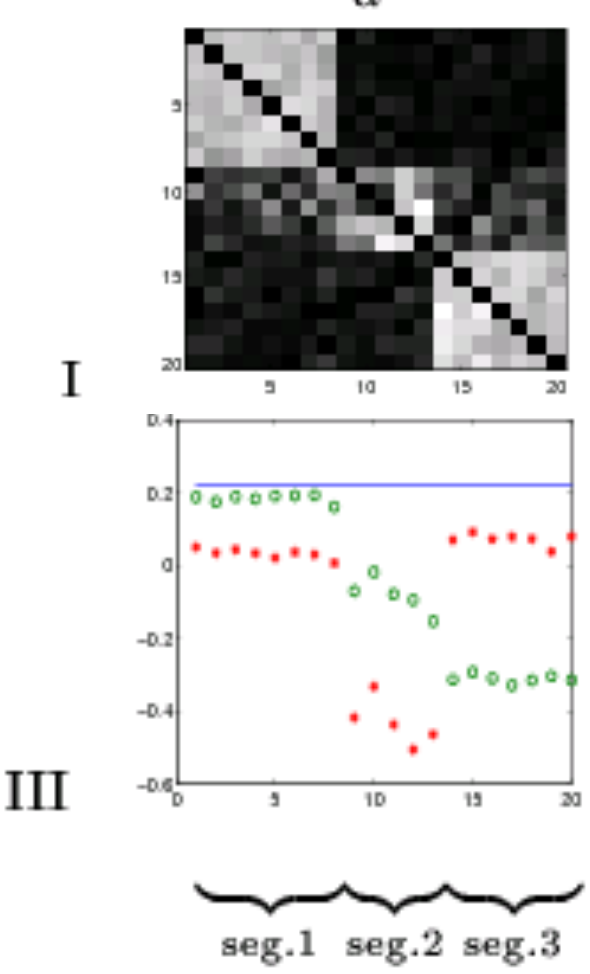
Spectral Clustering: Graph = Matrix

$W*v_1 = v_2$ "propagates weights from neighbors"

$$\mathbf{W} \cdot \mathbf{v} = \lambda \mathbf{v} : \mathbf{v} \text{ is an eigenvector with eigenvalue } \lambda$$

If Wis connected but roughly block diagonal with *k* blocks then

- the top eigenvector is a constant vector
- the next *k* eigenvectors are roughly piecewise constant with "pieces" corresponding to blocks



M

Spectral Clustering: Graph = Matrix

$W*v_1 = v_2$ "propagates weights from neighbors"

$$\mathbf{W} \cdot \mathbf{v} = \lambda \mathbf{v} : \mathbf{v} \text{ is an eigenvector with eigenvalue } \lambda$$

If **W** is connected but roughly block diagonal with *k* blocks then

- the "top" eigenvector is a constant vector
- the next *k* eigenvectors are roughly piecewise constant with "pieces" corresponding to blocks

Spectral clustering:

- Find the top *k+1* eigenvectors $\mathbf{v}_1,\ldots,\mathbf{v}_{k+1}$
- Discard the "top" one
- Replace every node *a* with *k*-dimensional vector $x_a = \langle \mathbf{v}_2(a),\ldots,\mathbf{v}_{k+1}(a) \rangle$
- Cluster with *k*-means

M

Spectral Clustering: Graph = Matrix

$W^*v_1 = v_2$ "propogates weights from neighbors"

$$\mathbf{W} \cdot \mathbf{v} = \lambda \mathbf{v} : \mathbf{v} \text{ is an eigenvector with eigenvalue } \lambda$$

- smallest eigenvecs of D-A are largest eigenvecs of A
- smallest eigenvecs of I-W are largest eigenvecs of W

Suppose each *y(i)*=+*1* or *-1*:

- Then *y* is a cluster indicator that splits the nodes into two
- what is $\mathbf{y}^T(D-A)\mathbf{y}$?

$$\mathbf{y}^T(D-A)\mathbf{y} = \mathbf{y}^T D\mathbf{y} - \mathbf{y}^T A\mathbf{y} = \sum_i d_i {y_i}^2 - \sum_{i,j} a_{i,j} y_i y_j$$

$$= \frac{1}{2}\left[2\sum_i d_i {y_i}^2 - 2\sum_{i,j} a_{i,j} y_i y_j\right]$$

$$= \frac{1}{2}\left[\sum_i \left(\sum_j a_{ij}\right) {y_i}^2 + \sum_j \left(\sum_i a_{ij}\right) {y_j}^2 - 2\sum_{i,j} a_{i,j} y_i y_j\right]$$

$$= \frac{1}{2}\left[\sum_{i,j} a_{ij} {y_i}^2 + \sum_{i,j} a_{ij} {y_j}^2 - 2\sum_{i,j} a_{i,j} y_i y_j\right]$$

$$= \frac{1}{2}\left[\sum_{i,j} a_{i,j} (y_i - y_j)^2\right] \qquad = \text{size of CUT}(\mathbf{y})$$

$$\mathbf{y}^T(I-W)\mathbf{y} = \text{size of NCUT}(\mathbf{y})$$

NCUT: roughly minimize ratio of transitions between classes vs transitions within classes

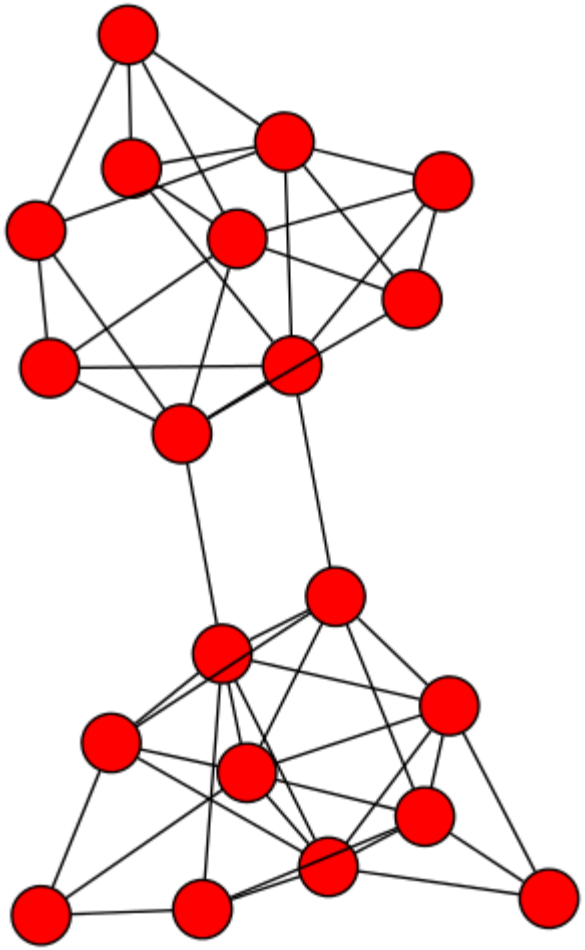
So far…

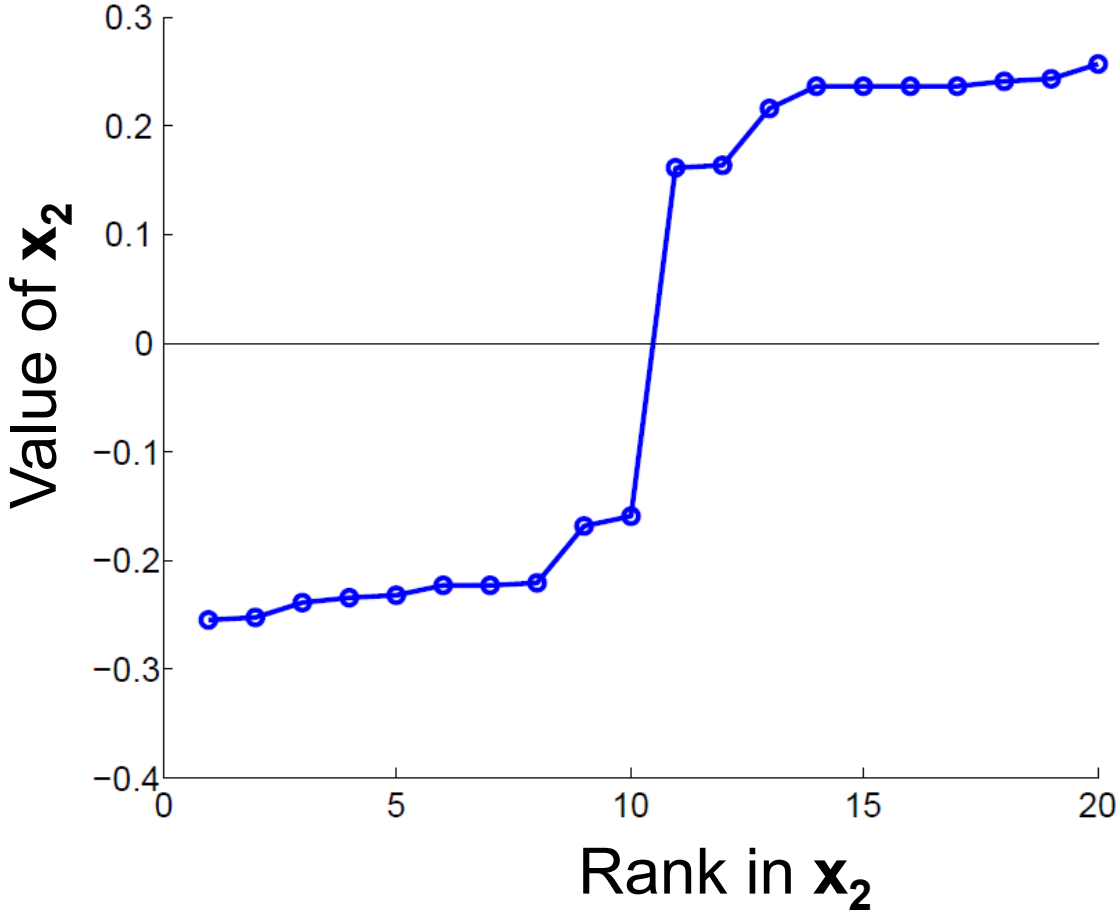
- How to define a "good" partition of a graph?
  - Minimize a given graph cut criterion
- How to efficiently identify such a partition?
  - Approximate using information provided by the eigenvalues and eigenvectors of a graph
- Spectral Clustering

Spectral Clustering Algorithms

- Three basic stages:
  - 1) Pre-processing
    - Construct a matrix representation of the graph
  - 2) Decomposition
    - Compute eigenvalues and eigenvectors of the matrix
    - Map each point to a lower-dimensional representation based on one or more eigenvectors
  - 3) Grouping
    - Assign points to two or more clusters, based on the new representation

Example: Spectral Partitioning





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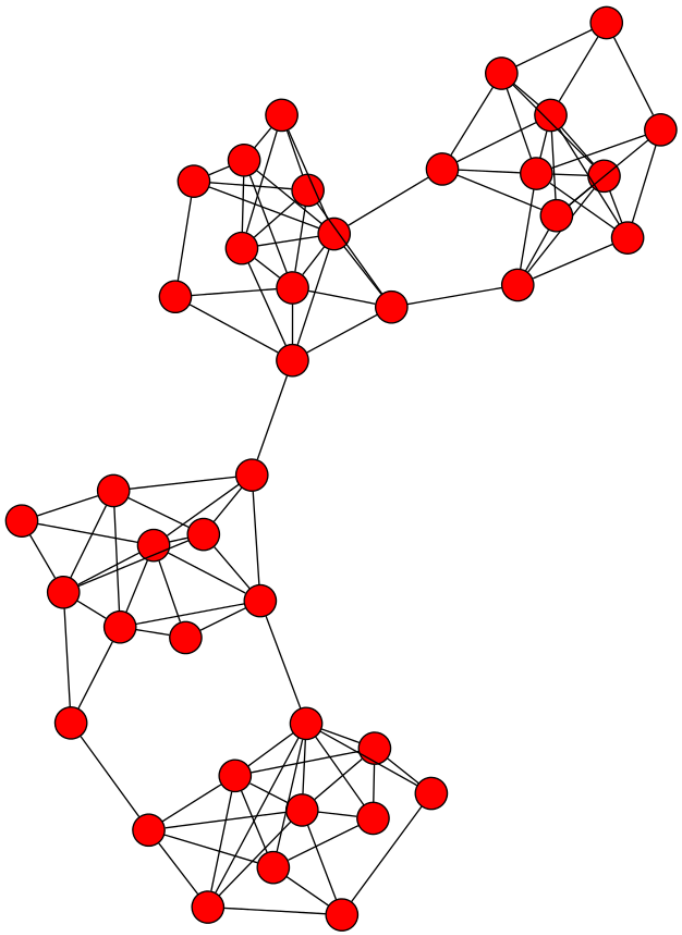
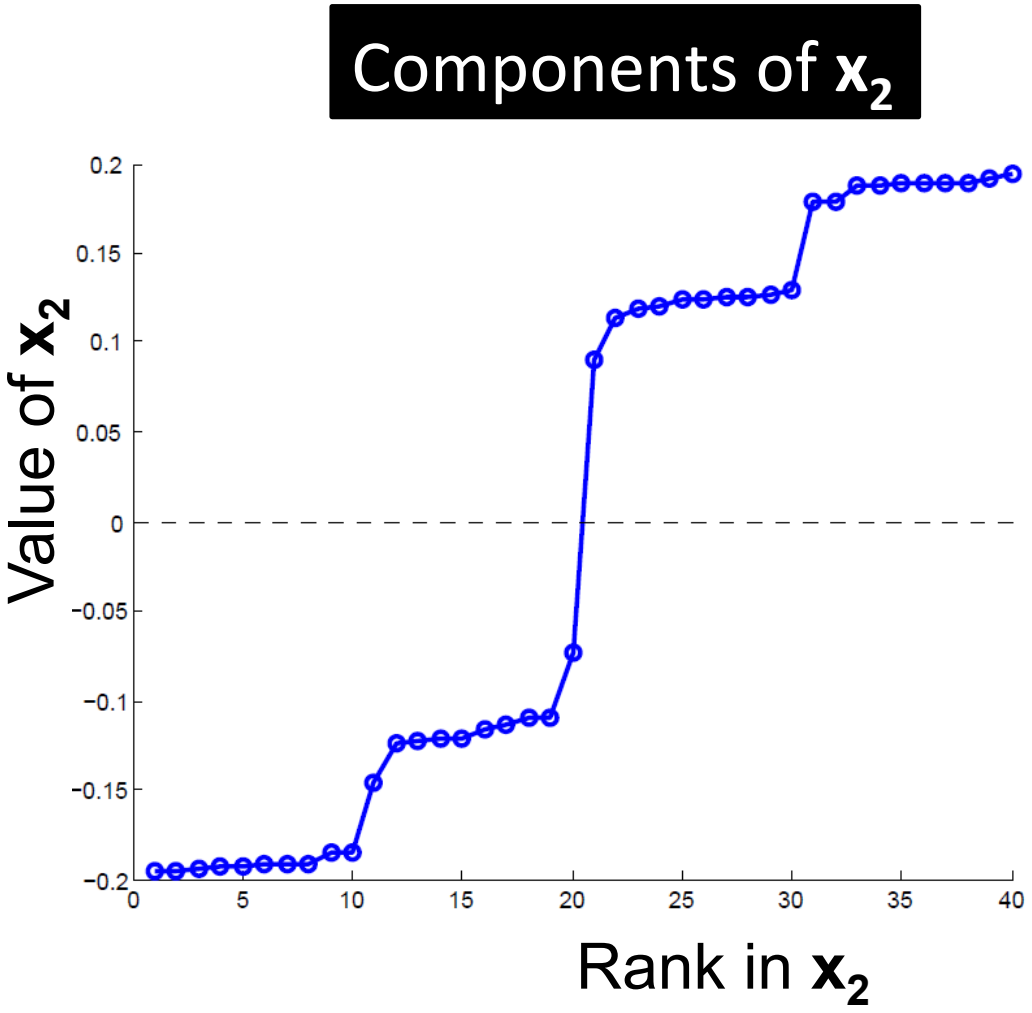
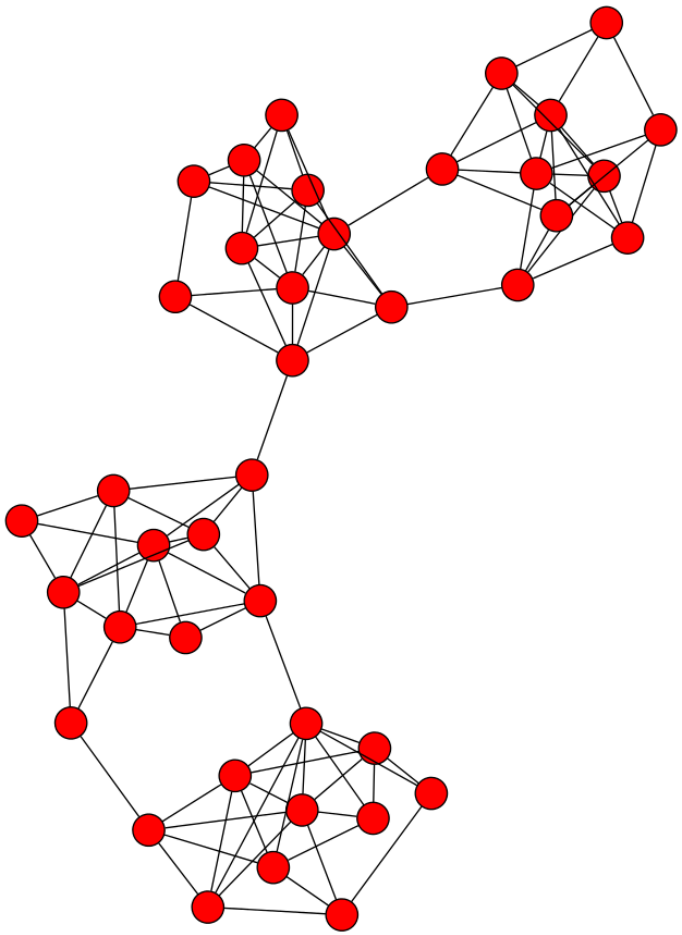
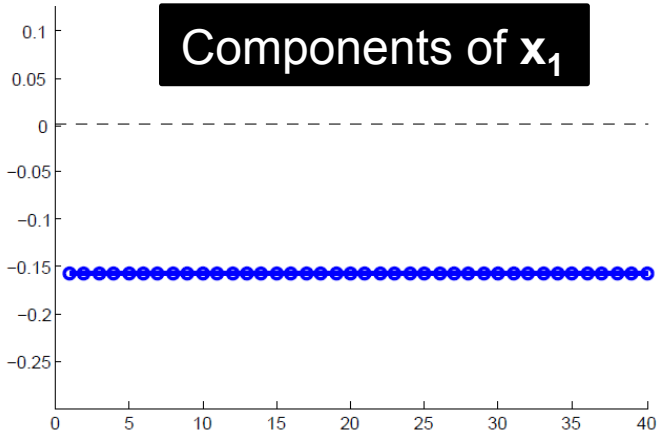


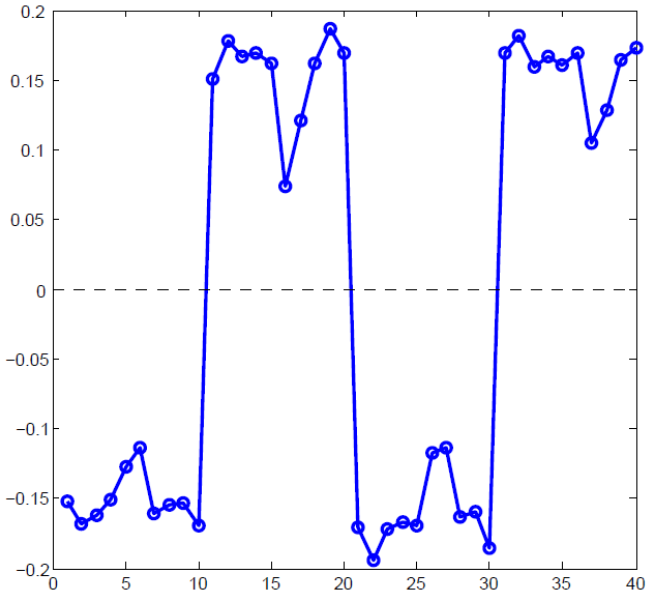


Example: Spectral partitioning



Components of x_1





Components of x_3

k-Way Spectral Clustering

- How do we partition a graph into k clusters?

- Two basic approaches:
  - **Recursive bi-partitioning** [Hagen et al., '92]
    - Recursively apply bi-partitioning algorithm in a hierarchical divisive manner
    - Disadvantages: Inefficient, unstable
  - **Cluster multiple eigenvectors** [Shi-Malik, '00]
    - Build a reduced space from multiple eigenvectors
    - Commonly used in recent papers
    - A preferable approach…

Why use multiple eigenvectors?

- **Approximates the optimal cut** [Shi-Malik, '00]
  - Can be used to approximate optimal k-way normalized cut
- **Emphasizes cohesive clusters**
  - Increases the unevenness in the distribution of the data
  - Associations between similar points are amplified, associations between dissimilar points are attenuated
  - The data begins to "approximate a clustering"
- **Well-separated space**
  - Transforms data to a new "embedded space", consisting of $\boldsymbol{k}$ orthogonal basis vectors
- Multiple eigenvectors prevent instability due to information loss

Spectral Clustering: Graph = Matrix

$W*v_1 = v_2$ "propogates weights from neighbors"

$$\mathbf{W} \cdot \mathbf{v} = \lambda \mathbf{v} : \mathbf{v} \text{ is an eigenvector with eigenvalue } \lambda$$

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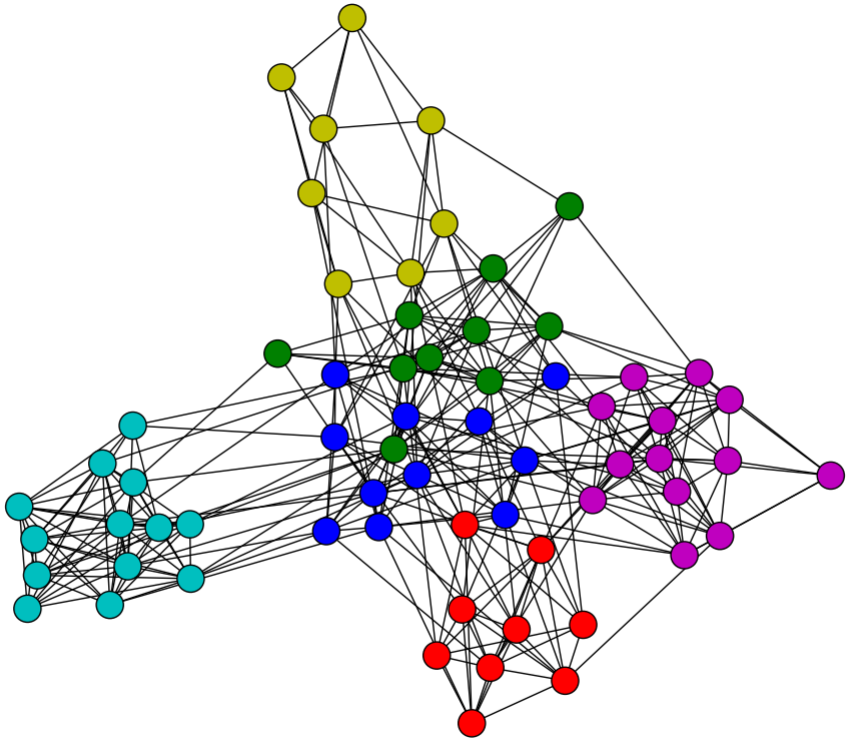
Q: How do I pick **v** to be an eigenvector for a block-stochastic matrix?



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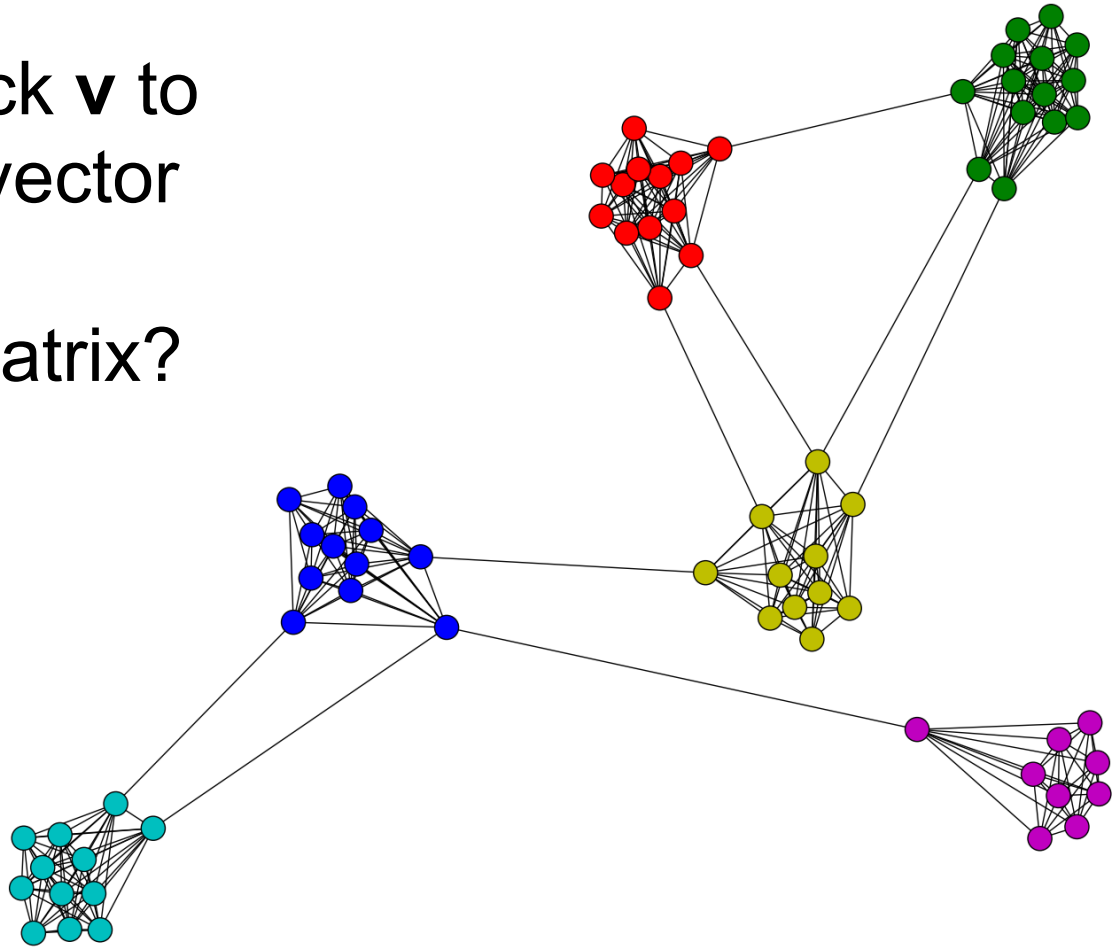

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Suppose each *y(i)=+1* or *-1*:

- Then *y* is a cluster indicator that cuts the nodes into two
- what is $\mathbf{y}^T(D-A)\mathbf{y}$? The cost of the graph cut defined by **y**
- what is $\mathbf{y}^T(I-W)\mathbf{y}$? Also a cost of a graph cut defined by **y**
- How to minimize it?
  - Turns out: to minimize $\mathbf{y}^T X \mathbf{y} / (\mathbf{y}^T\mathbf{y})$ find *smallest* eigenvector of X
  - But: this will not be +1/-1, so it's a "relaxed" solution

Spectral Clustering: Graph = Matrix

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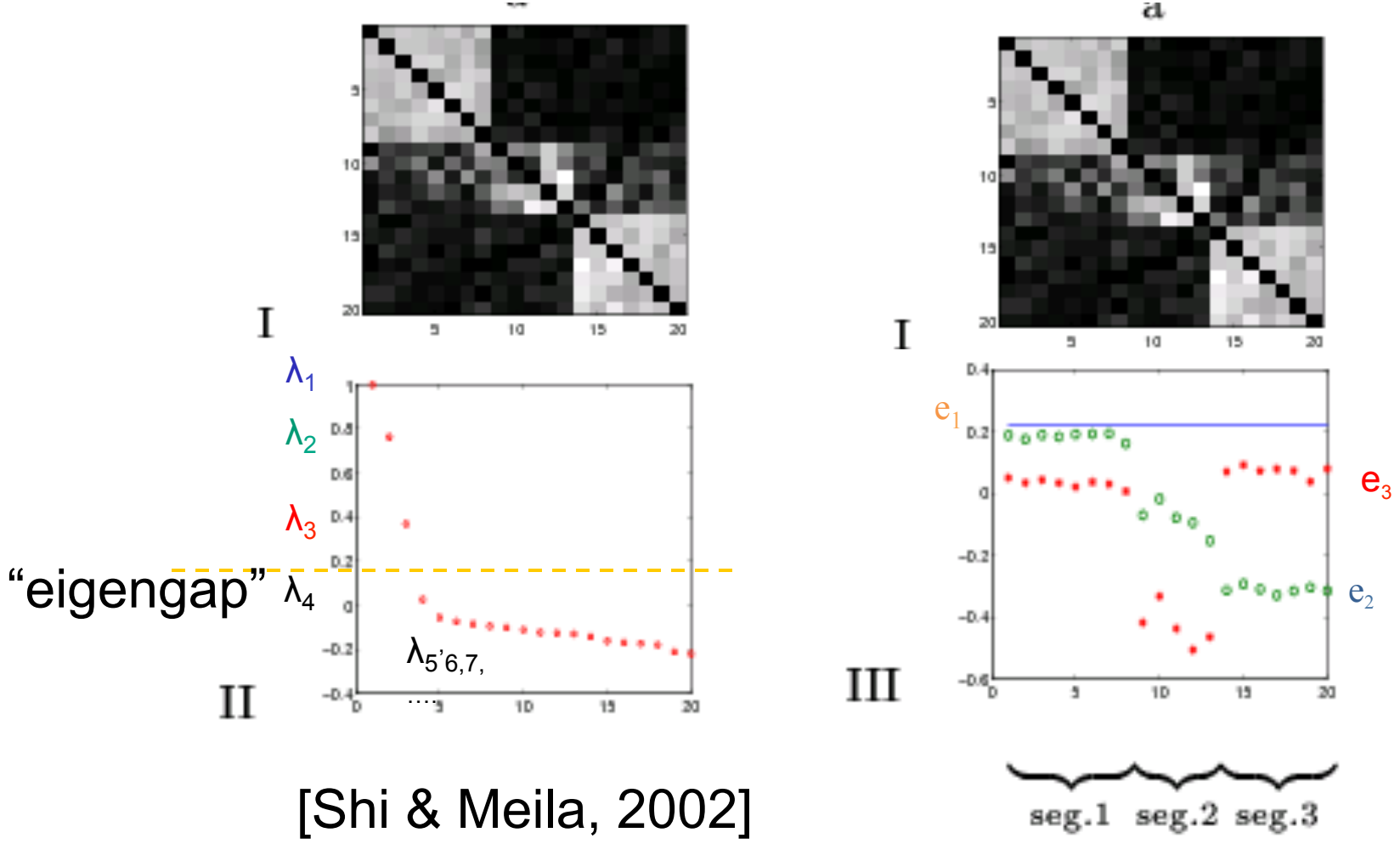


[Shi & Meila, 2002]

Some more terms

- If A is an adjacency matrix (maybe weighted) and D is a (diagonal) matrix giving the degree of each node
  - Then D-A is the *(unnormalized) Laplacian*
  - $W=AD^{-1}$ is a *probabilistic adjacency matrix*
  - I-W is the *(normalized or random-walk) Laplacian*
  - etc….
- The largest eigenvectors of W correspond to the smallest eigenvectors of I-W
  - So sometimes people talk about "*bottom eigenvectors of the Laplacian*"

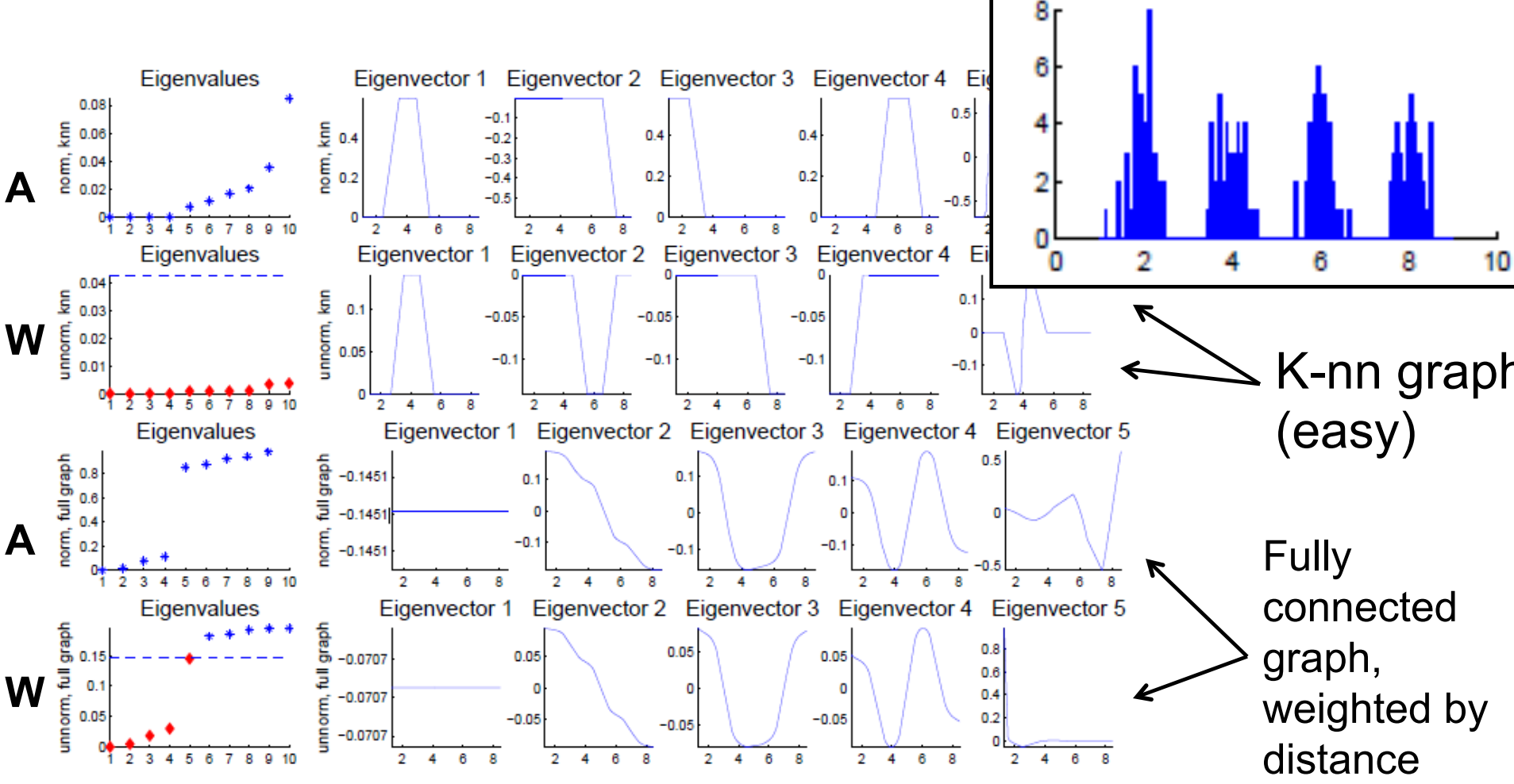


Figure 1: Toy example for spectral clustering where the data points have been drawn from a mixture of four Gaussians on $\mathbb{R}$. Left upper corner: histogram of the data. First and second row: eigenvalues and eigenvectors of L_{rw} and L based on the k-nearest neighbor graph. Third and fourth row: eigenvalues and eigenvectors of L_{rw} and L based on the fully connected graph. For all plots, we used the Gaussian kernel with $\sigma = 1$ as similarity function. See text for more details.

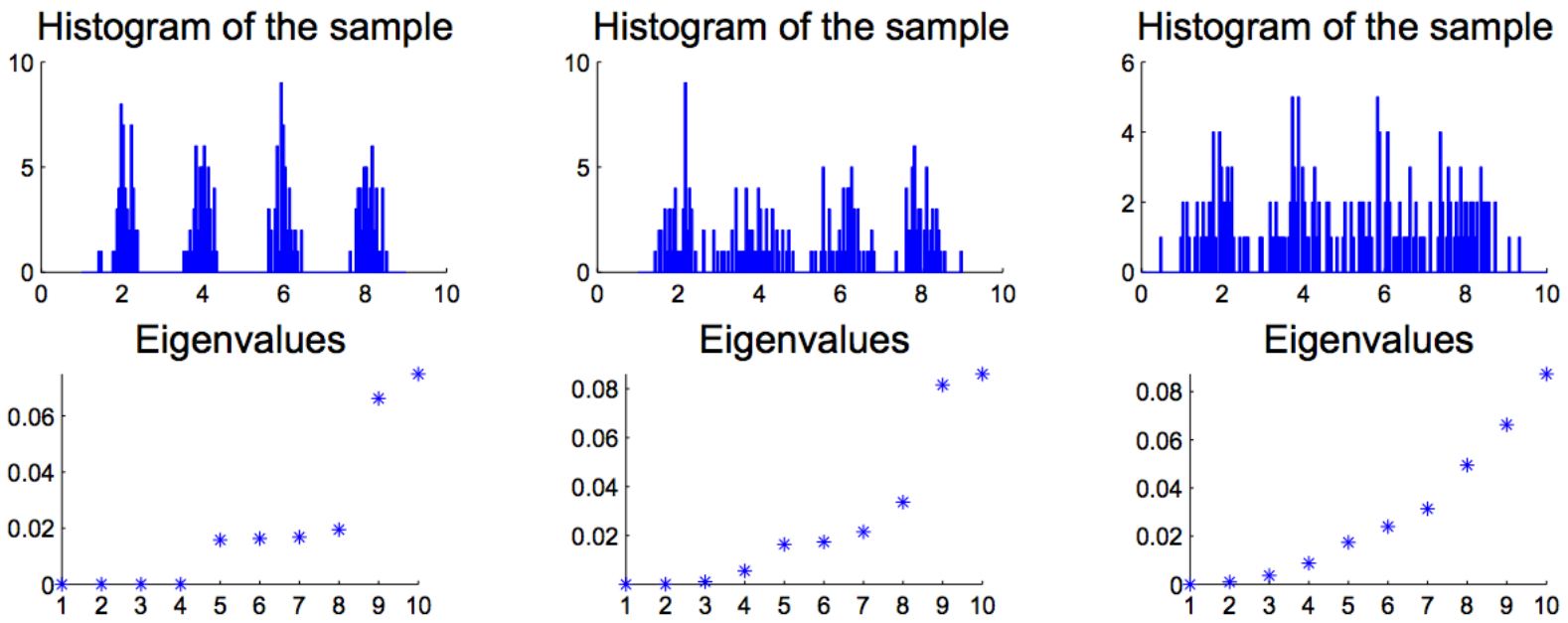


Figure 4: Three data sets, and the smallest 10 eigenvalues of L_{rw}. See text for more details.

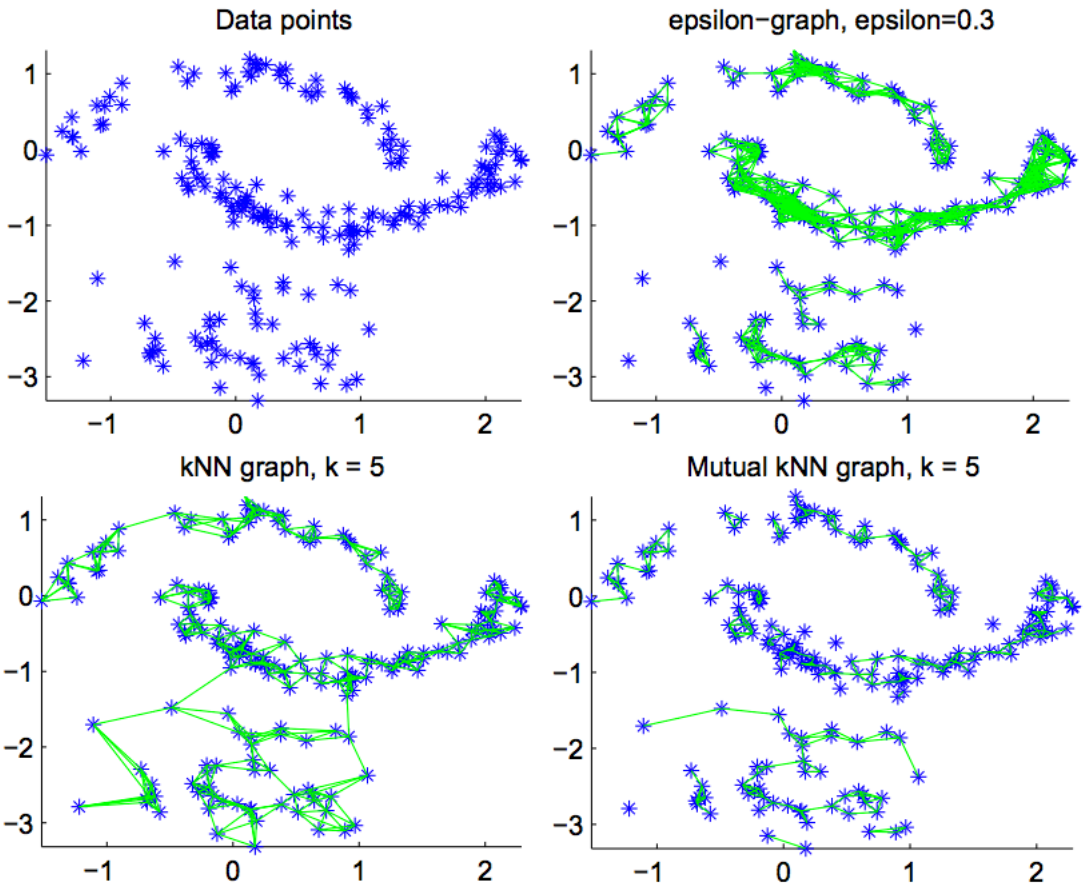


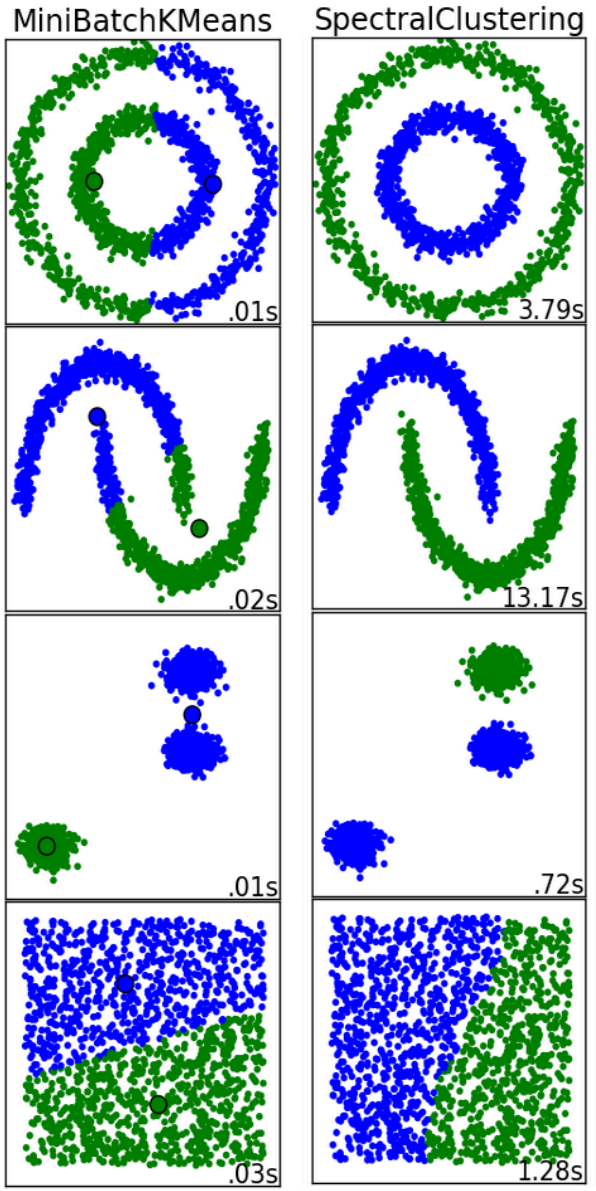
Figure 3: Different similarity graphs, see text for details.

Spectral Clustering: Pros and Cons

- Elegant, and well-founded mathematically
- Works quite well when relations are approximately transitive (like similarity)
- Very noisy datasets cause problems
  - "Informative" eigenvectors need not be in top few
  - Performance can drop suddenly from good to terrible
- Expensive for very large datasets
  - Computing eigenvectors is the bottleneck

Use cases and runtimes

- K-Means
  - FAST
  - "Embarrassingly parallel"
  - Not very useful on anisotropic data
- Spectral clustering
  - Excellent quality under many different data forms
  - Much slower than K-Means



Further Reading

- Spectral Clustering Tutorial: http://www.informatik.uni-hamburg.de/ML/contents/people/luxburg/publications/Luxburg07_tutorial.pdf