Spectral Clustering

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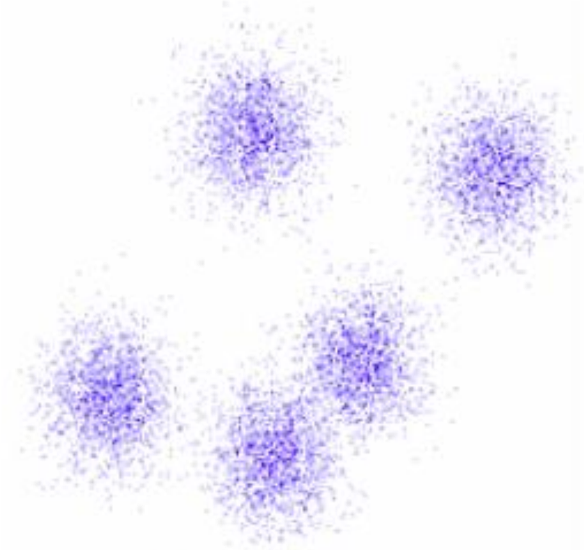
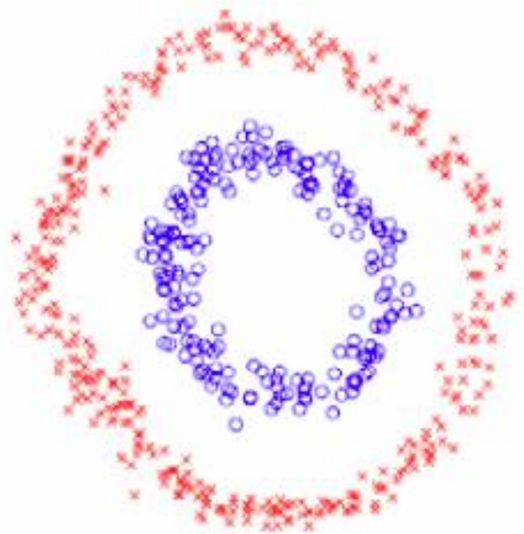
Slides Courtesy: Eric Xing, M. Hein & U.V. Luxburg

Data Clustering

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



Compactness



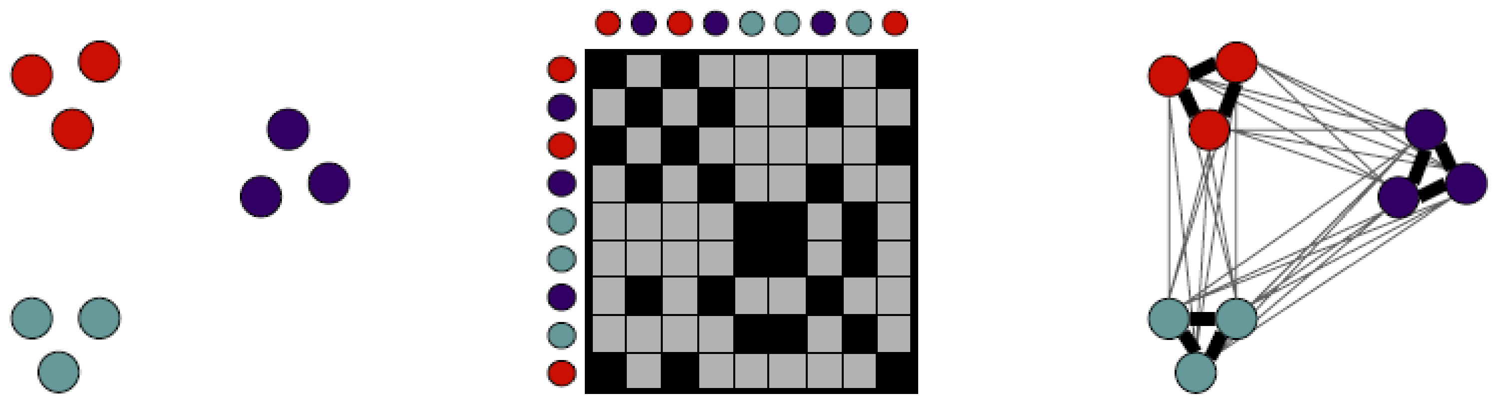
Connectivity

Graph Clustering

Goal: Given data points $X_1, \ldots, X_n$ and similarities $w(X_i,X_j)$, partition the data into groups so that points in a group are similar and points in different groups are dissimilar.

Similarity Graph: $G(V,E,W)$

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



Data | Similarities | Similarity graph

Partition the graph so that edges within a group have large weights and edges across groups have small weights.

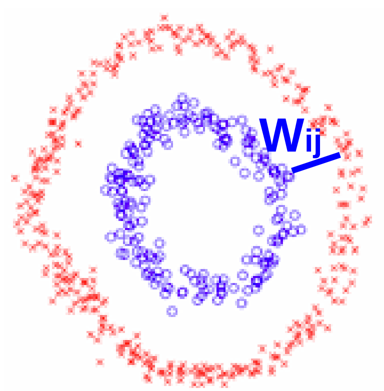
Similarity graph construction

Similarity Graphs: Model local neighborhood relations between data points

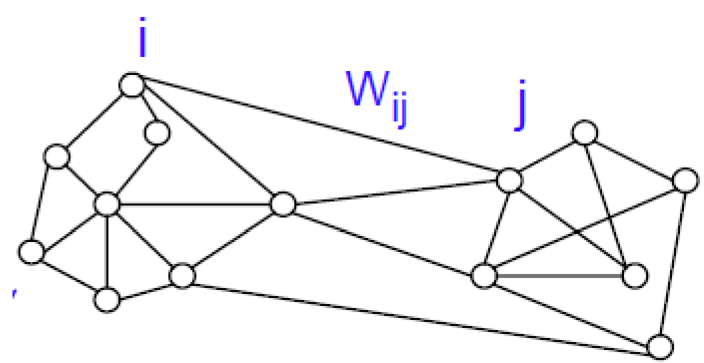
E.g. Gaussian kernel similarity function

$$W_{ij} = e^{\frac{\|x_i - x_j\|^2}{2\sigma^2}}$$

Controls size of neighborhood



Data clustering

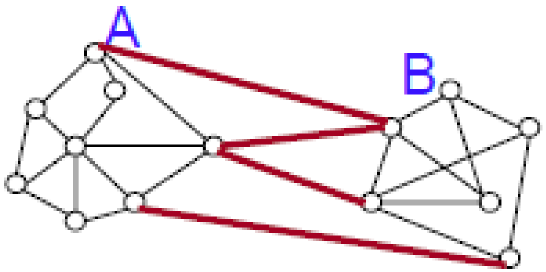


$G = \{V, E\}$

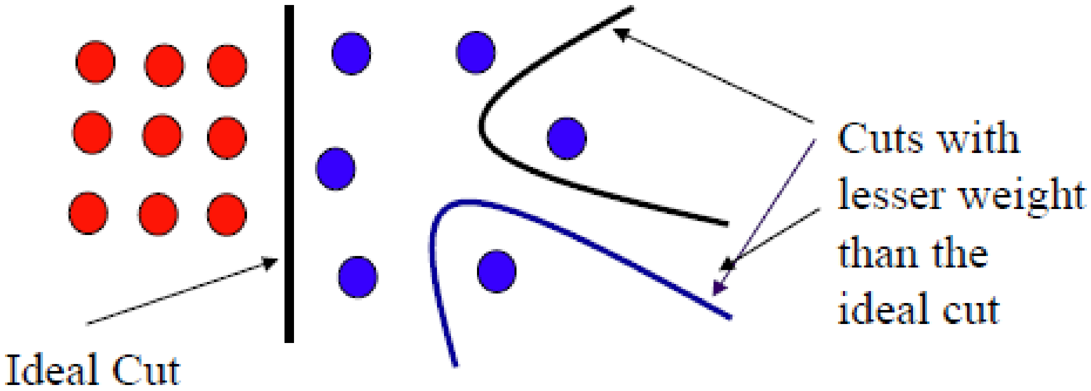
Partitioning a graph into two clusters

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

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



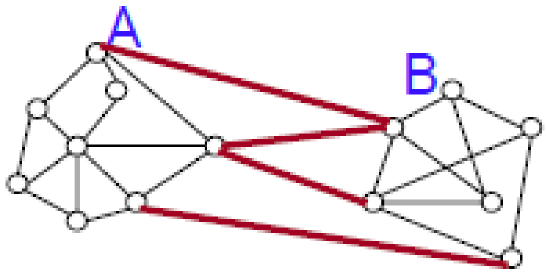
- Easy to solve O(VE) algorithm
- Not satisfactory partition – often isolates vertices



Partitioning a graph into two clusters

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

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



Normalized cut:

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

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

But NP-hard to solve!!

Spectral clustering is a relaxation of these.

Normalized Cut and Graph Laplacian

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

Let $\mathbf{f} = [f_1\ f_2\ \dots\ f_n]^T$ with $f_i = \begin{cases} \dfrac{1}{\mathrm{vol}(A)} & \text{if } i \in A \\ -\dfrac{1}{\mathrm{vol}(B)} & \text{if } i \in B \end{cases}$

$$\mathbf{f}^T\mathbf{L}\mathbf{f} = \sum_{ij} w_{ij}(\mathbf{f}_i - \mathbf{f}_j)^2 = \sum_{i\in A, j\in B} w_{ij}\left(\frac{1}{\mathrm{vol}(A)} + \frac{1}{\mathrm{vol}(B)}\right)^2$$

$$\mathbf{f}^T\mathbf{D}\mathbf{f} = \sum_j d_i\mathbf{f}_i^2 = \sum_{i\in A}\frac{d_i}{\mathrm{vol}(A)^2} + \sum_{j\in B}\frac{d_i}{\mathrm{vol}(B)^2} = \frac{1}{\mathrm{vol}(A)} + \frac{1}{\mathrm{vol}(B)}$$

$$\mathrm{Ncut}(A,B) = \frac{\mathbf{f}^T\mathbf{L}\mathbf{f}}{\mathbf{f}^T\mathbf{D}\mathbf{f}}$$

Normalized Cut and Graph Laplacian

$$\min \text{Ncut}(A, B) = \min \frac{\mathbf{f}^T \mathbf{L} \mathbf{f}}{\mathbf{f}^T \mathbf{D} \mathbf{f}}$$

where $f = [f_1\ f_2 \ldots f_n]^T$ with $f_i = \begin{cases} \frac{1}{\text{vol}(A)} & \text{if } i \in A \\ -\frac{1}{\text{vol}(B)} & \text{if } i \in B \end{cases}$

Relaxation: $\min \frac{\mathbf{f}^T \mathbf{L} \mathbf{f}}{\mathbf{f}^T \mathbf{D} \mathbf{f}}$ s.t. $f^T D 1 = 0$

Solution: f – second eigenvector of generalized eval problem

$$\boxed{\mathbf{L}\mathbf{f} = \lambda \mathbf{D}\mathbf{f}}$$

Obtain cluster assignments by thresholding f at 0

Approximation of Normalized cut

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

Let f be the eigenvector corresponding to the second smallest eval of the generalized eval problem.

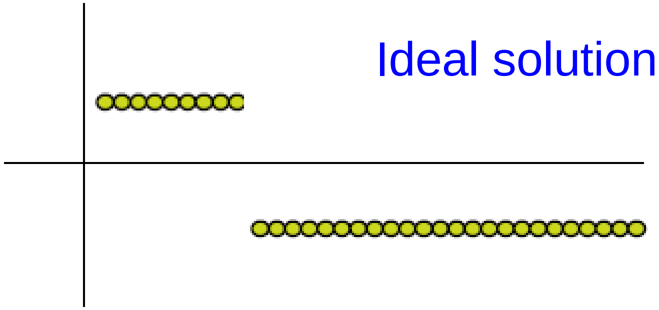
$$\boxed{\mathbf{Lf} = \lambda \mathbf{Df}}$$

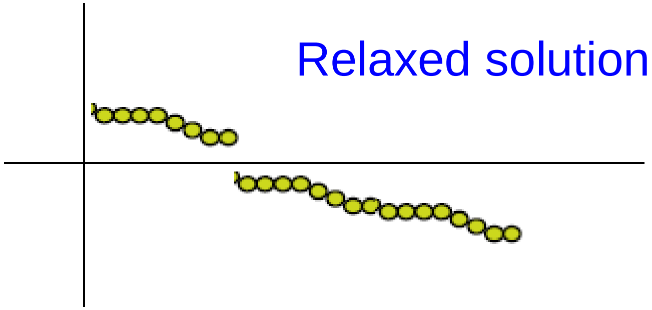
Equivalent to eigenvector corresponding to the second smallest eval of the normalized Laplacian $L' = D^{-1}L = I - D^{-1}W$

Recover binary partition as follows:

$i \in A$ if $f_i \geq 0$

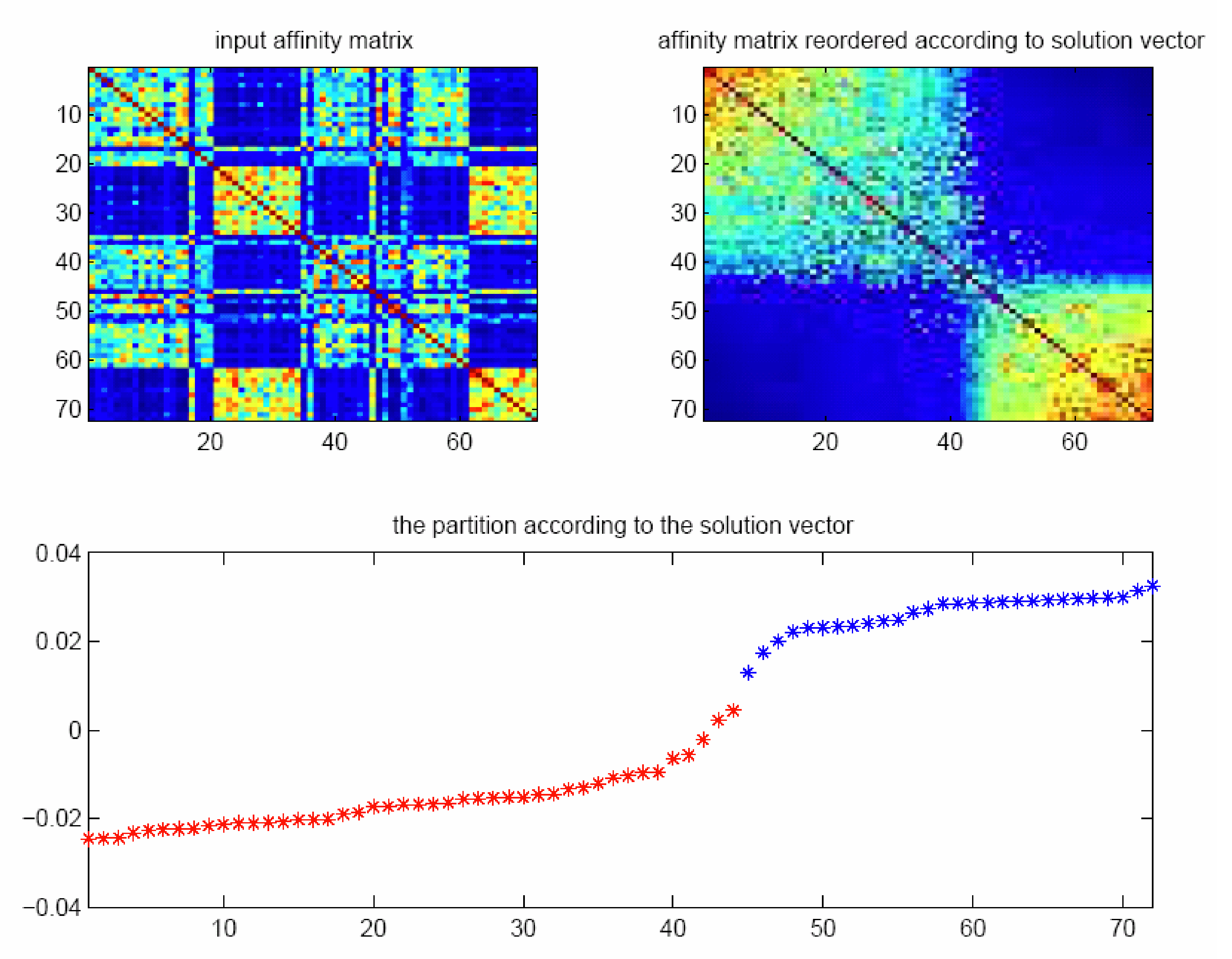
$i \in B$ if $f_i < 0$





Example

Xing et al 2001



How to partition a graph into k clusters?

Spectral Clustering Algorithm

Input: Similarity matrix W, number k of clusters to construct

- Build similarity graph
- Compute the first k eigenvectors $v_1, \ldots, v_k$ of the matrix

$$\begin{cases} L & \text{for unnormalized spectral clustering} \\ L' & \text{for normalized spectral clustering} \end{cases}$$

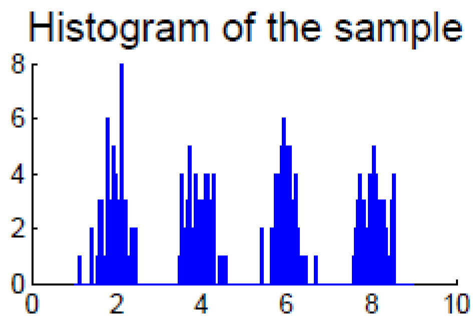
- Build the matrix $V \in \mathbb{R}^{n \times k}$ with the eigenvectors as columns
- Interpret the rows of V as new data points $Z_i \in \mathbb{R}^k$

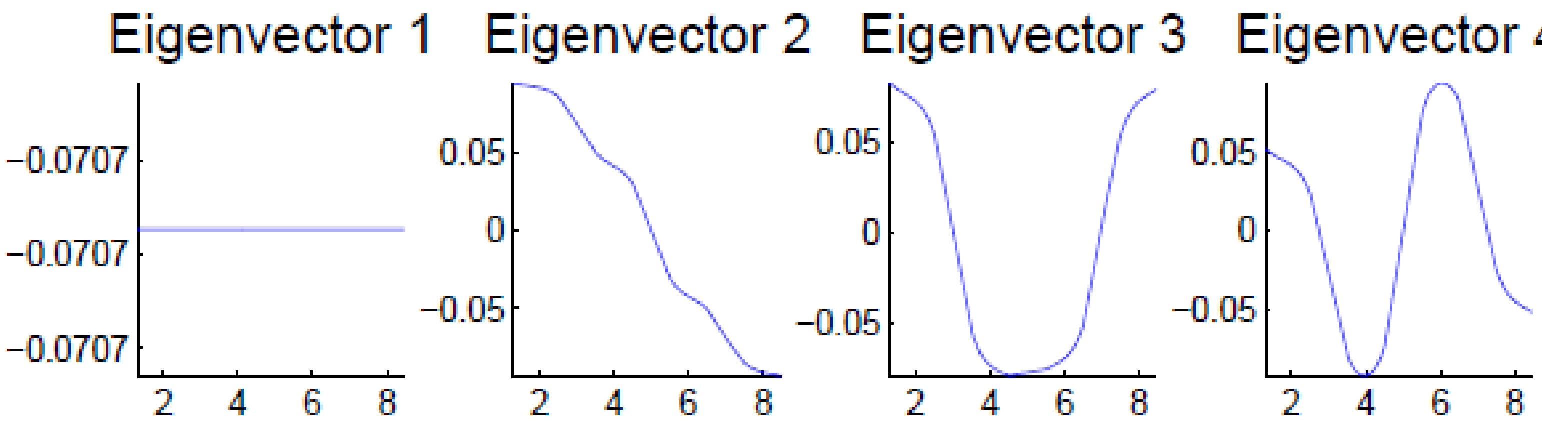
	v_1	v_2	v_3
Z_1	v_{11}	v_{12}	v_{13}
$\vdots$	$\vdots$	$\vdots$	$\vdots$
Z_n	v_{n1}	v_{n2}	v_{n3}

Dimensionality Reduction
n x n → n x k

- Cluster the points Z_i with the k-means algorithm in $\mathbb{R}^k$.

Eigenvectors of Graph Laplacian



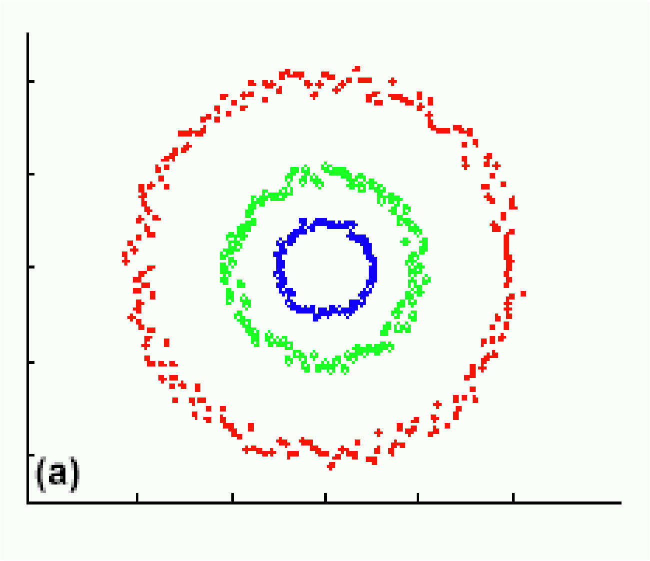


- 1st Eigenvector is the all ones vector ***1*** (if graph is connected)
- 2nd Eigenvector thresholded at 0 separates first two clusters from last two
- k-means clustering of the 4 eigenvectors identifies all clusters

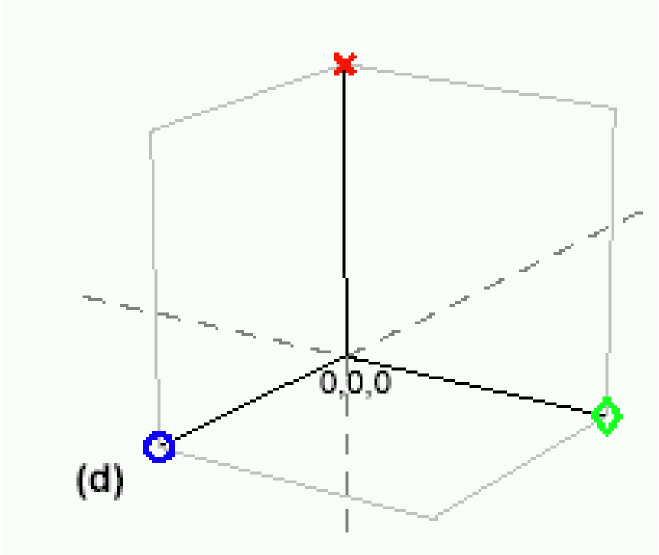
Why does it work?

Data are projected into a lower-dimensional space (the spectral/eigenvector domain) where they are easily separable, say using k-means.

Original data



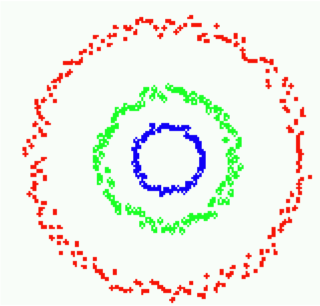
Projected data



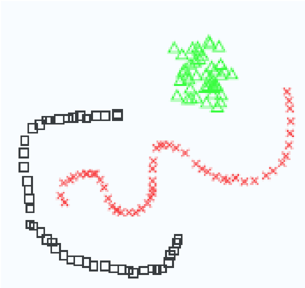
Graph has 3 connected components – first three eigenvectors are constant (all ones) on each component.

Understanding Spectral Clustering

- If graph is connected, first Laplacian evec is constant (all 1s)
- If graph is disconnected (k connected components), Laplacian is block diagonal and first k Laplacian evecs are:



OR



$$L = \begin{pmatrix} L_1 & & 0 \\ & L_2 & \\ 0 & & L_3 \end{pmatrix}$$

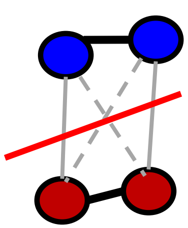
$$\begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}$$

First three eigenvectors

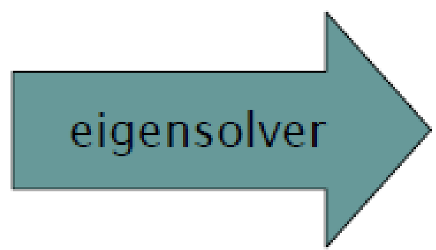
Understanding Spectral Clustering

- Is all hope lost if clusters don't correspond to connected components of graph? No!
- If clusters are connected loosely (small off-block diagonal enteries), then 1st Laplacian even is all 1s, but second evec gets first cut (min normalized cut)

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



1	1	.2	0
1	1	0	.1
.2	0	1	1
0	.1	1	1



.50
.50
.50
.50

.47
.52
-.47
-.52

1st evec is constant since graph is connected

Sign of 2nd evec indicates blocks

Why does it work?

Block weight matrix (disconnected graph) results in block eigenvectors:

$$\underbrace{\begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix}}_{W} \xrightarrow{\text{eigensolver}} \underbrace{\begin{bmatrix} .71 \\ .71 \\ 0 \\ 0 \end{bmatrix}}_{f_1} \quad \underbrace{\begin{bmatrix} 0 \\ 0 \\ .71 \\ .71 \end{bmatrix}}_{f_2}$$

Normalized to have unit norm

Slight perturbation does not change span of eigenvectors significantly:

$$\begin{bmatrix} 1 & 1 & .2 & 0 \\ 1 & 1 & 0 & .1 \\ .2 & 0 & 1 & 1 \\ 0 & .1 & 1 & 1 \end{bmatrix} \xrightarrow{\text{eigensolver}} \begin{bmatrix} .50 \\ .50 \\ .50 \\ .50 \end{bmatrix} \quad \begin{bmatrix} .47 \\ .52 \\ -.47 \\ -.52 \end{bmatrix}$$

1st evec is constant since graph is connected

Sign of 2nd evec indicates blocks

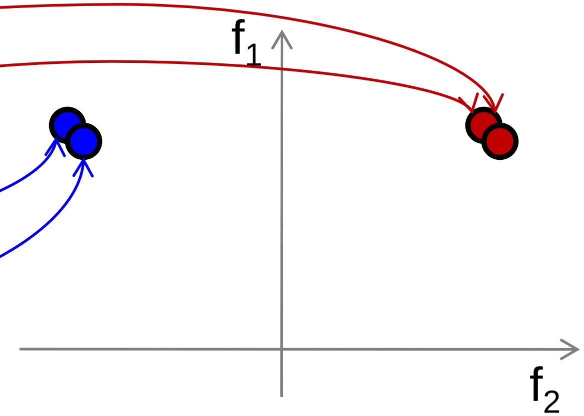
Why does it work?

Can put data points into blocks using eigenvectors:

1	1	.2	0
1	1	0	.1
.2	0	1	1
0	.1	1	1

W

f_1	f_2
.50	.47
.50	.52
.50	-.47
.50	-.52

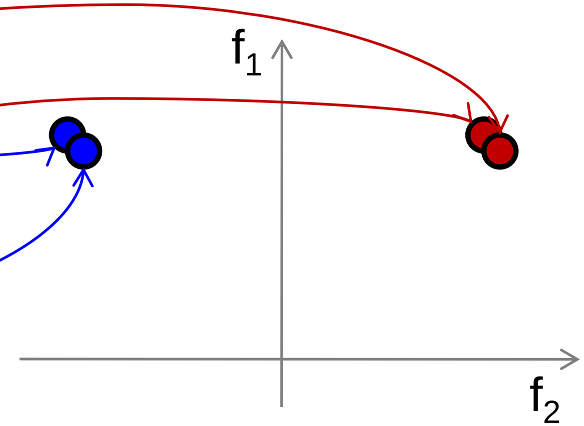


Embedding is same regardless of data ordering:

1	.2	1	0
.2	0	1	1
1	1	0	.1
0	1	.1	1

W

f_1	f_2
.50	.47
.50	-.47
.50	.52
.50	-.52



Understanding Spectral Clustering

- Is all hope lost if clusters don't correspond to connected components of graph? No!
- If clusters are connected loosely (small off-block diagonal enteries), then 1st Laplacian even is all 1s, but second evec gets first cut (min normalized cut)

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

- What about more than two clusters?

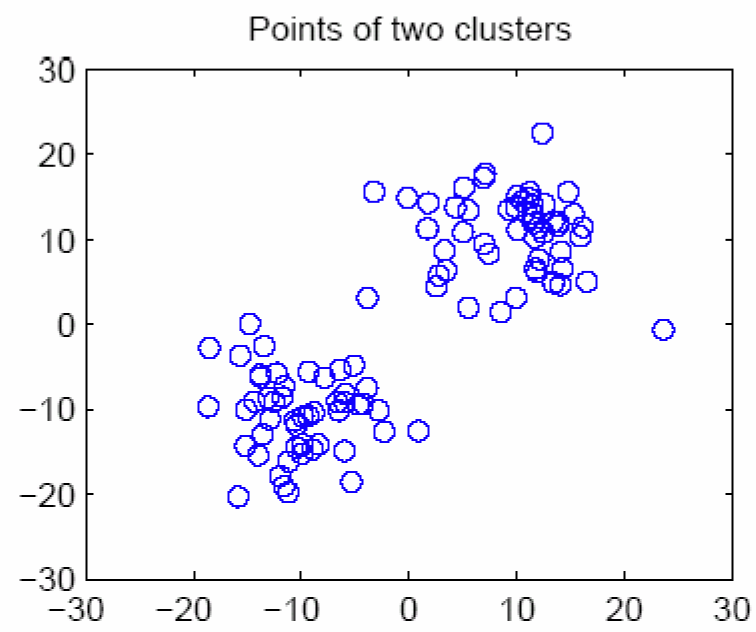
  eigenvectors $f_2, \ldots, f_{k+1}$ are solutions of following normalized cut:

$$\mathrm{Ncut}(A_1, \ldots, A_k) = \sum_{i=1}^{k} \frac{\mathrm{cut}(A_i, \overline{A}_i)}{\mathrm{vol}(A_i)}$$

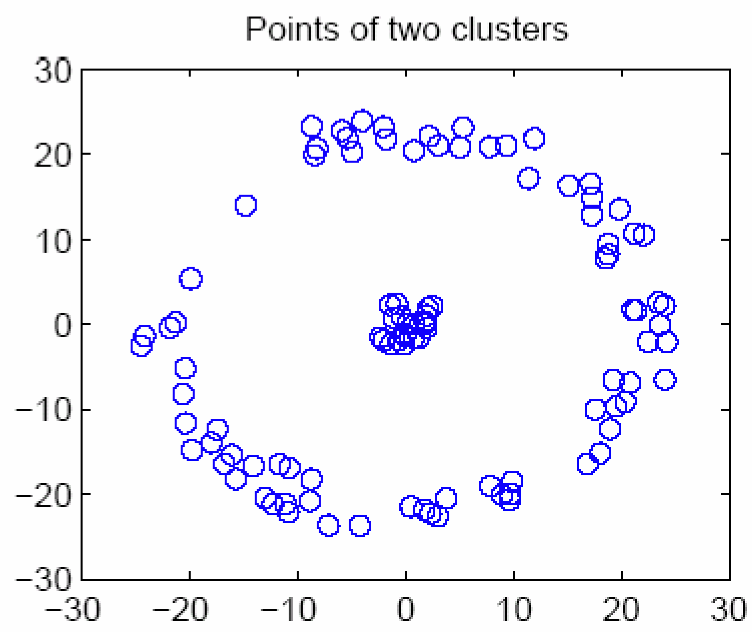
Demo: http://www.ml.uni-saarland.de/GraphDemo/DemoSpectralClustering.html

k-means vs Spectral clustering

Applying k-means to laplacian eigenvectors allows us to find cluster with non-convex boundaries.



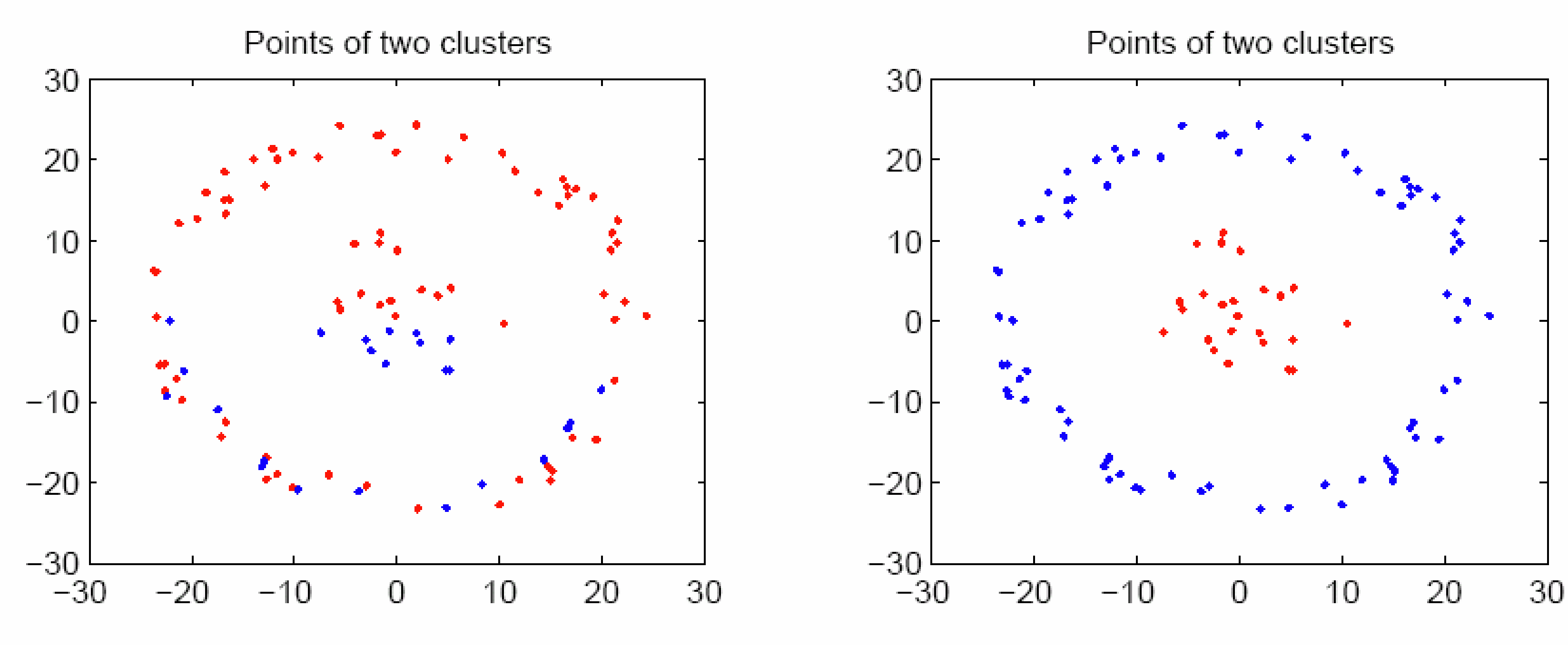
Both perform same



Spectral clustering is superior

k-means vs Spectral clustering

Applying k-means to laplacian eigenvectors allows us to find cluster with non-convex boundaries.

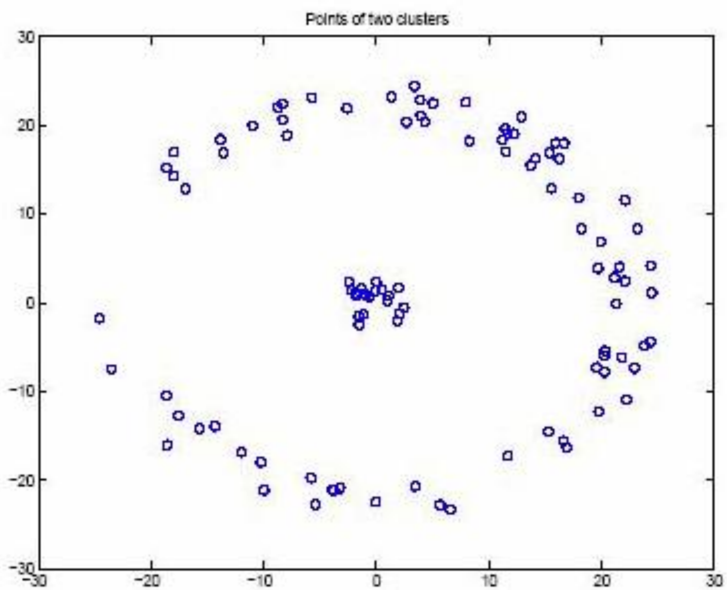


k-means output

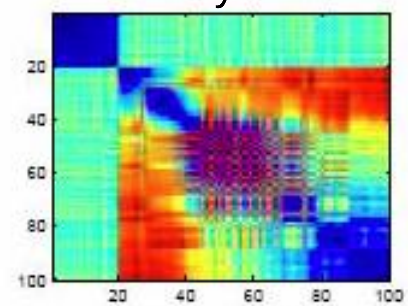
Spectral clustering output

k-means vs Spectral clustering

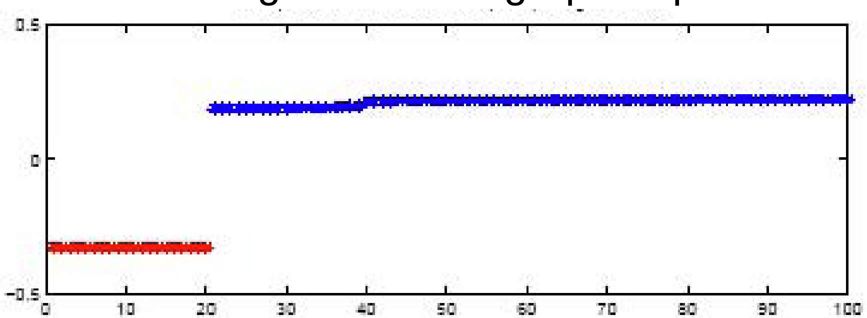
Applying k-means to laplacian eigenvectors allows us to find cluster with non-convex boundaries.



Similarity matrix

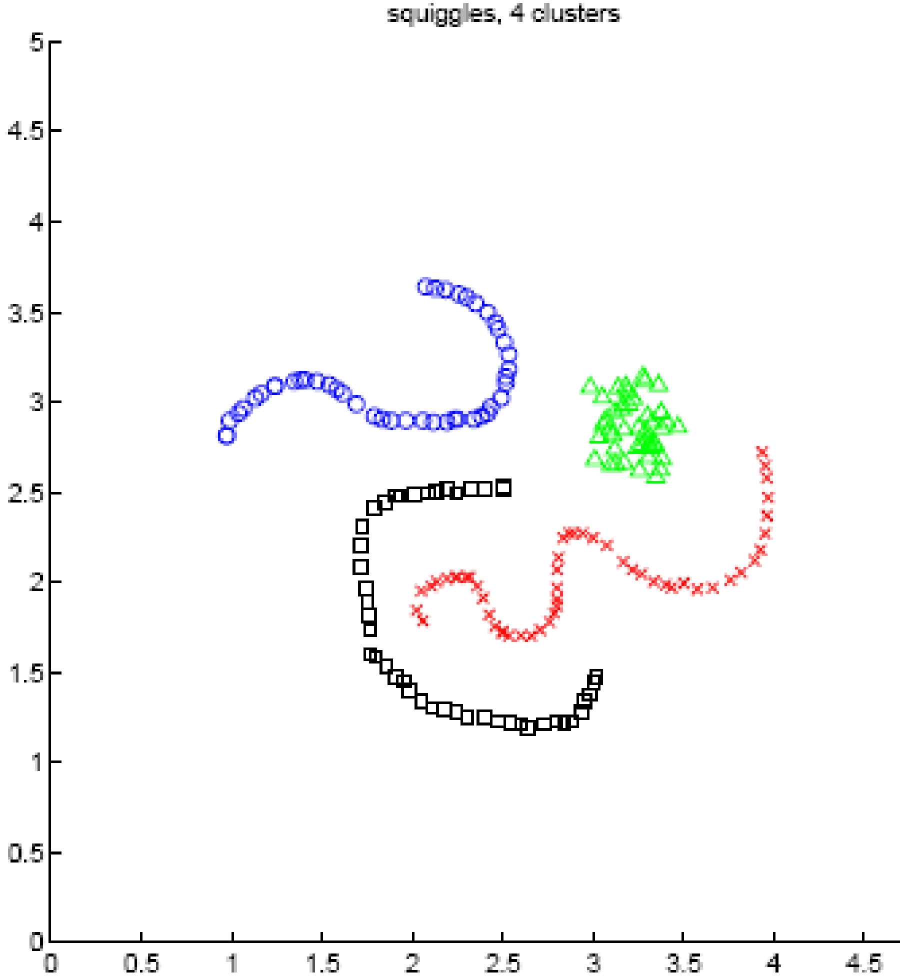


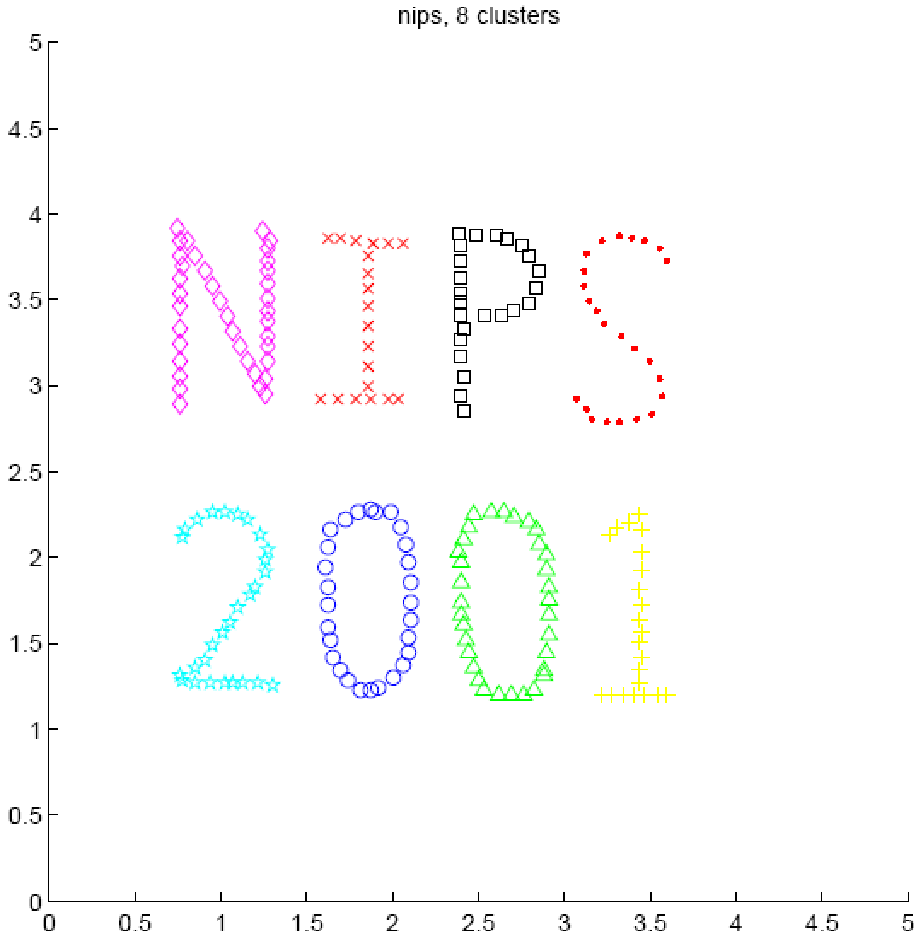
Second eigenvector of graph Laplacian



Examples

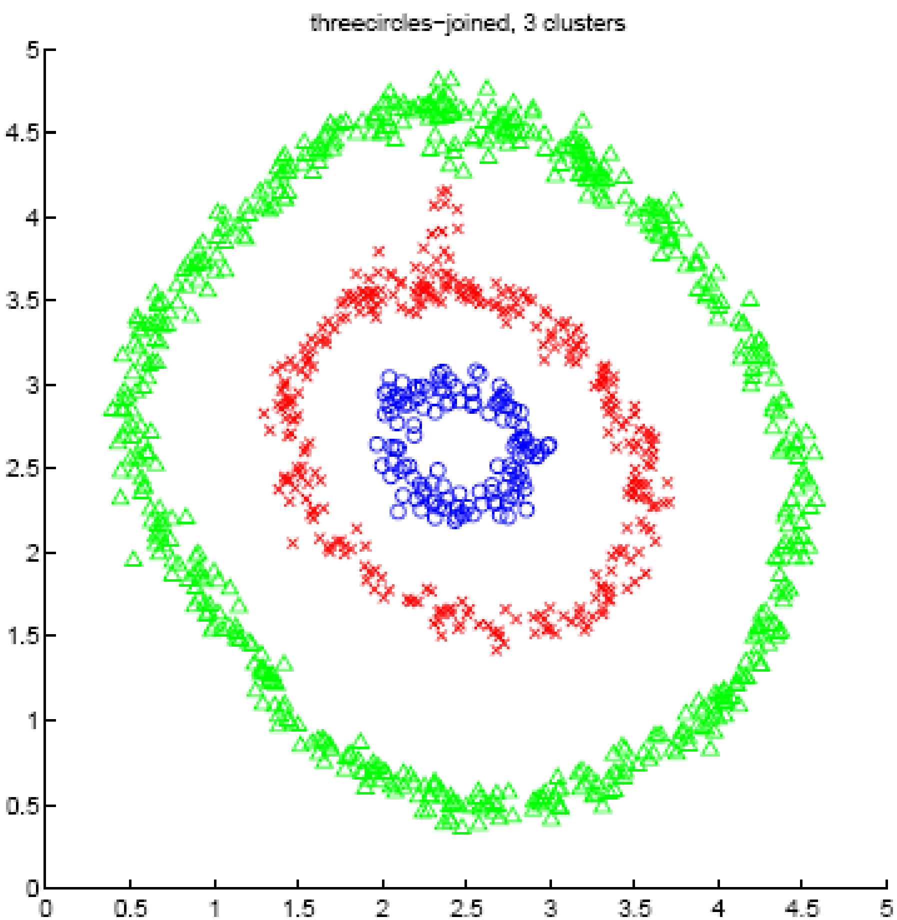
Ng et al 2001

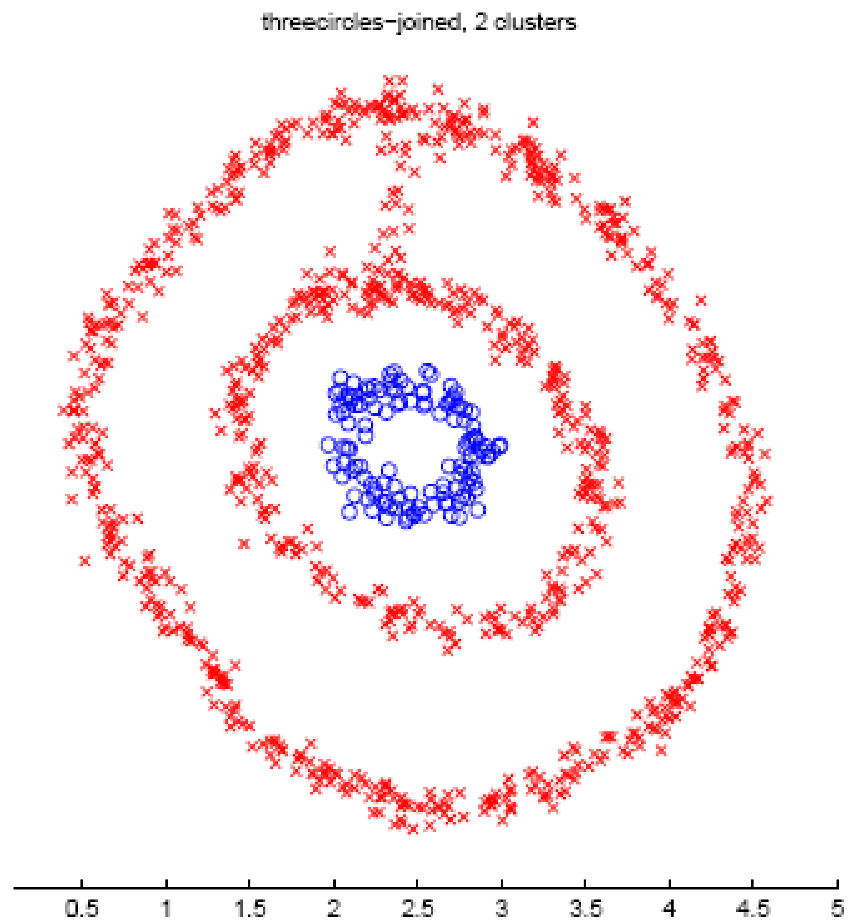




Examples (Choice of k)

Ng et al 2001



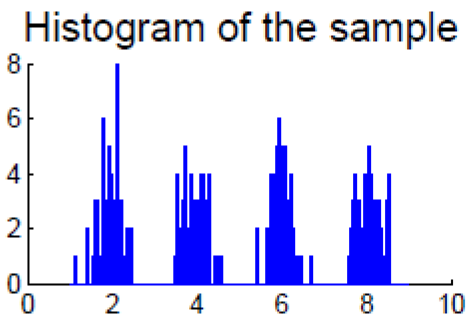


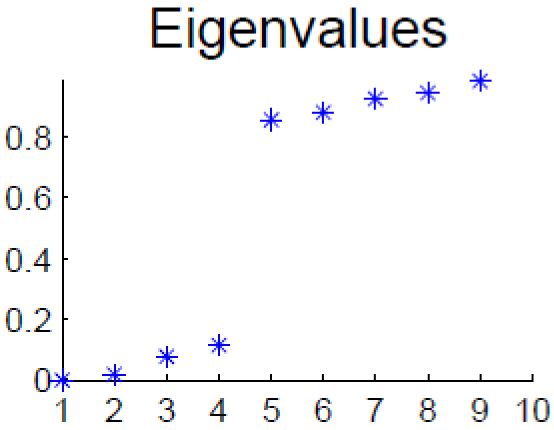
Some Issues

- Choice of number of clusters k

  Most stable clustering is usually given by the value of k that maximizes the eigengap (difference between consecutive eigenvalues)

$$\Delta_k = \left|\lambda_k - \lambda_{k-1}\right|$$

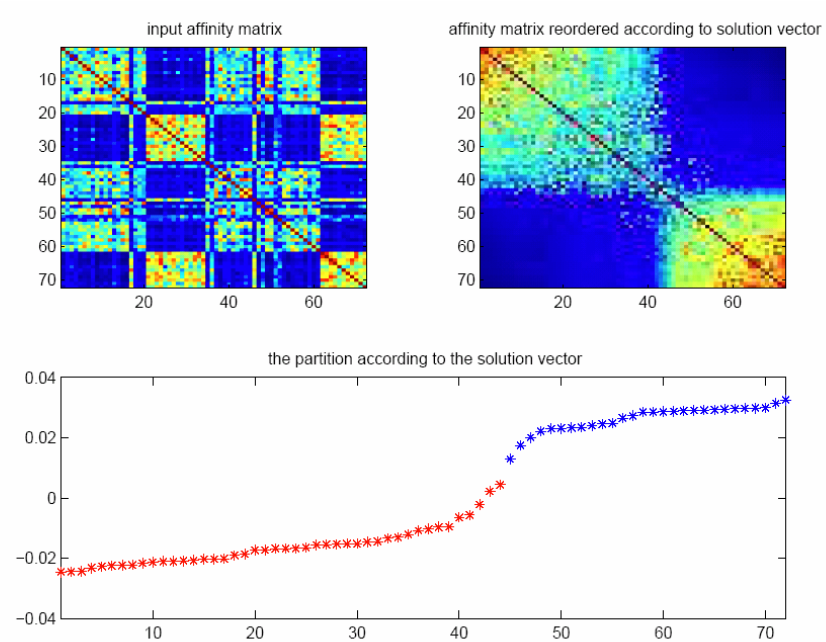




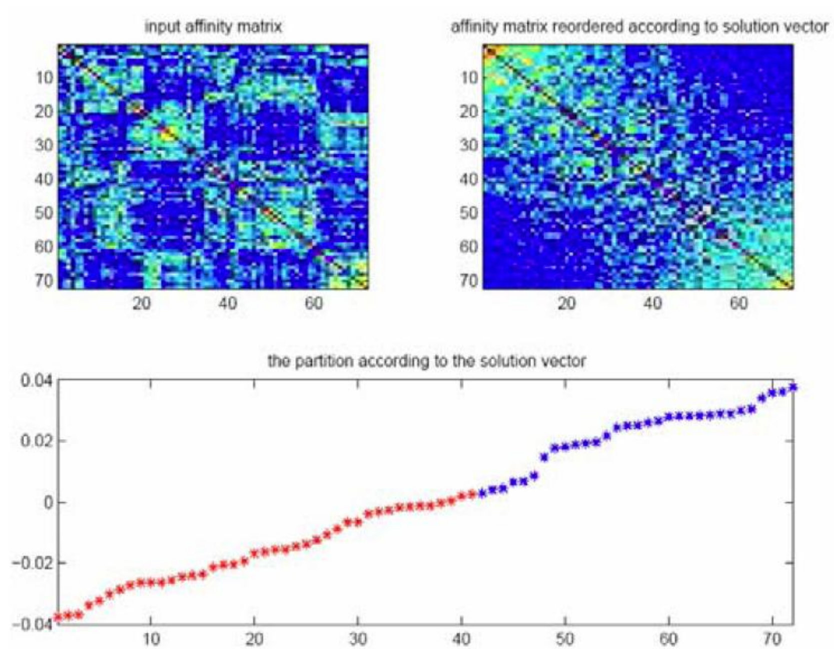
Some Issues

- Choice of number of clusters k

- Choice of similarity
  - choice of kernel
  - for Gaussian kernels, choice of σ



Good similarity measure



Poor similarity measure

Some Issues

- Choice of number of clusters k

- Choice of similarity
  choice of kernel
  for Gaussian kernels, choice of σ

- Choice of clustering method – k-way vs. recursive bipartite

Spectral clustering summary

- Algorithms that cluster points using eigenvectors of matrices derived from the data
- Useful in hard non-convex clustering problems
- Obtain data representation in the low-dimensional space that can be easily clustered
- Variety of methods that use eigenvectors of unnormalized or normalized Laplacian, differ in how to derive clusters from eigenvectors, k-way vs repeated 2-way
- Empirically very successful