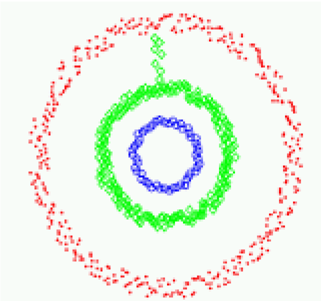
Machine Learning

10-701/15-781, Fall 2006

Spectral Clustering

Eric Xing

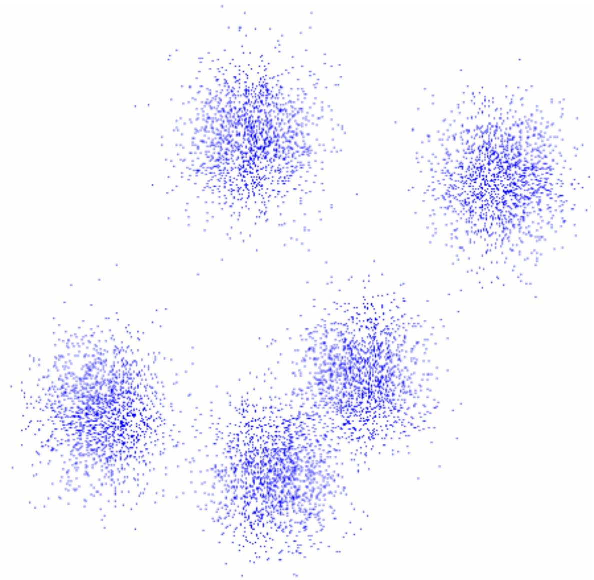
Lecture 16, November 9, 2006



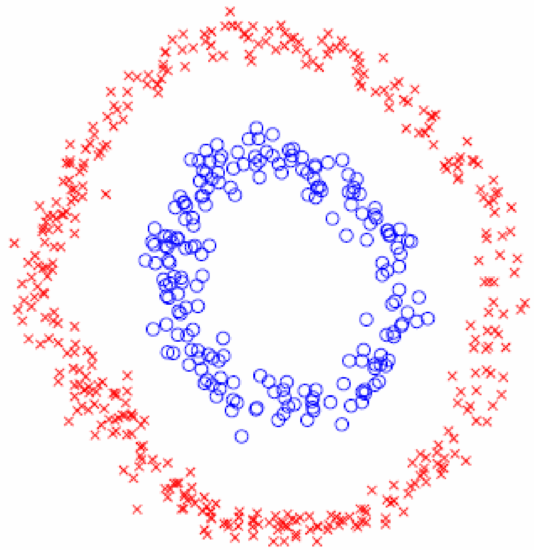
Reading: Chap. 1&2, C.B book

Data Clustering

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

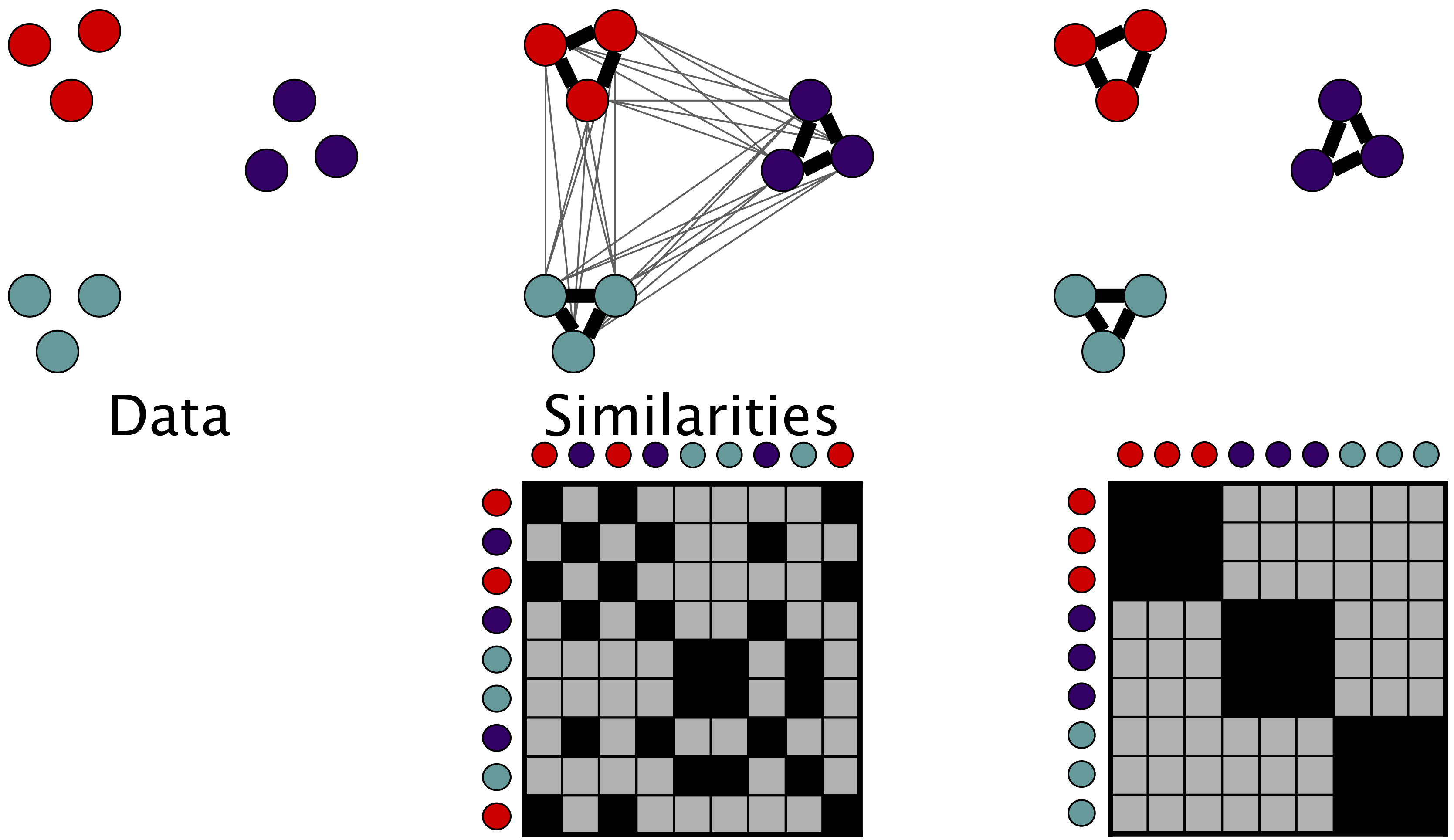


Compactness



Connectivity

Spectral Clustering



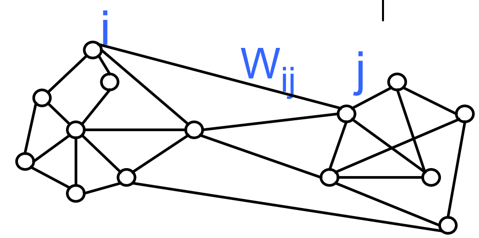
Weighted Graph Partitioning

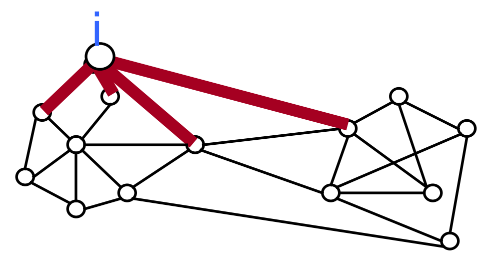
- Some graph terminology
  - Objects (e.g., pixels, data points)

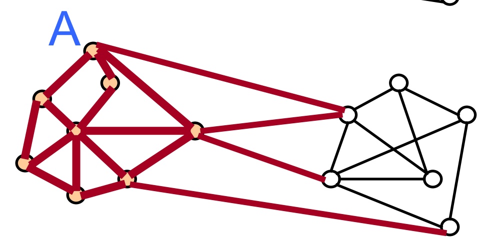
    $i \in I$ = vertices of graph G
  - Edges (ij) = pixel pairs with $W_{ij} > 0$
  - Similarity matrix $\mathbf{W} = [\ W_{ij}\ ]$
  - Degree

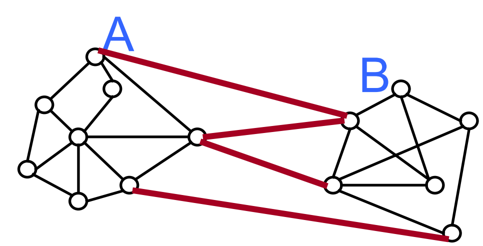
    $d_i = \Sigma_{j \in G}\, S_{ij}$

    $d_A = \Sigma_{i \in A}\, d_i$ degree of A $\subseteq$G
  - Assoc(A,B) = $\Sigma_{i \in A} \Sigma_{j \in B}\, W_{ij}$



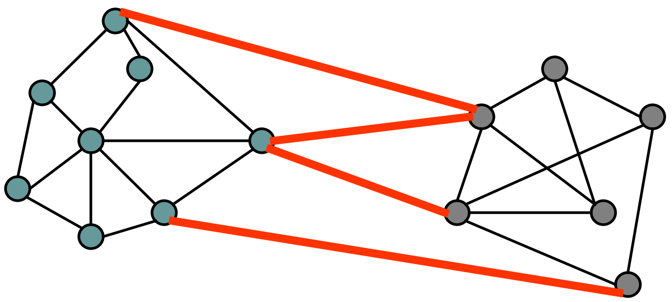






Cuts in a Graph

- (edge) cut = set of edges whose removal makes a graph disconnected



- weight of a cut:

  cut(A, B) = $\Sigma_{i\in A}\Sigma_{j\in B} W_{ij}$=Assoc(A,B)

- Normalized Cut criteria: minimum cut(A,Ā)

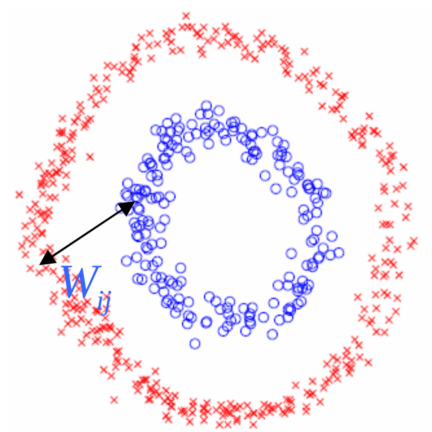
$$\mathrm{Ncut}(A,B)=\frac{\mathrm{cut}(A,B)}{d_A}+\frac{\mathrm{cut}(A,B)}{d_B}$$

More generally:

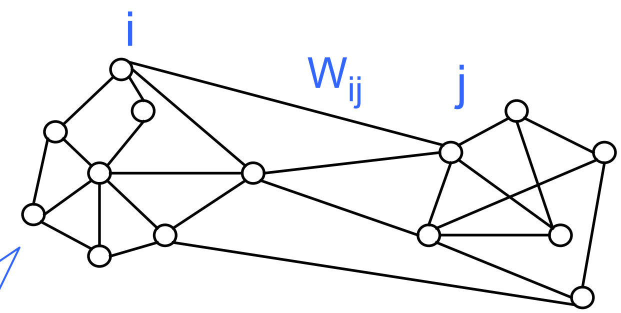
$$\mathrm{Ncut}(A_1,A_2\ldots A_k)=\sum_{r=1}^{k}\left(\frac{\sum_{i\in A_r,\, j\in V\setminus A_r} W_{ij}}{\sum_{i\in A_r,\, j\in V} W_{ij}}\right)=\sum_{r=1}^{k}\left(\frac{\mathrm{cut}(A_r,\bar{A}_r)}{d_{A_r}}\right)$$

Graph-based Clustering

- Data Grouping

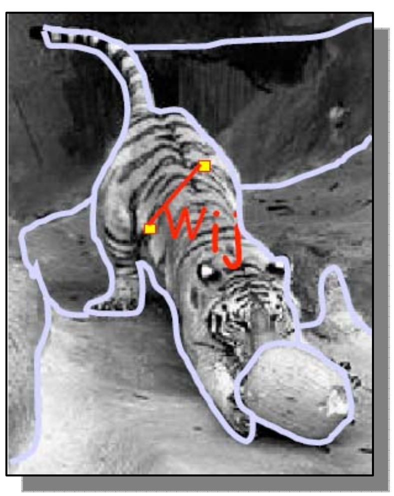


$$W_{ij} = f(d(x_i, x_j))$$



$G = \{V,E\}$

- Image sigmentation

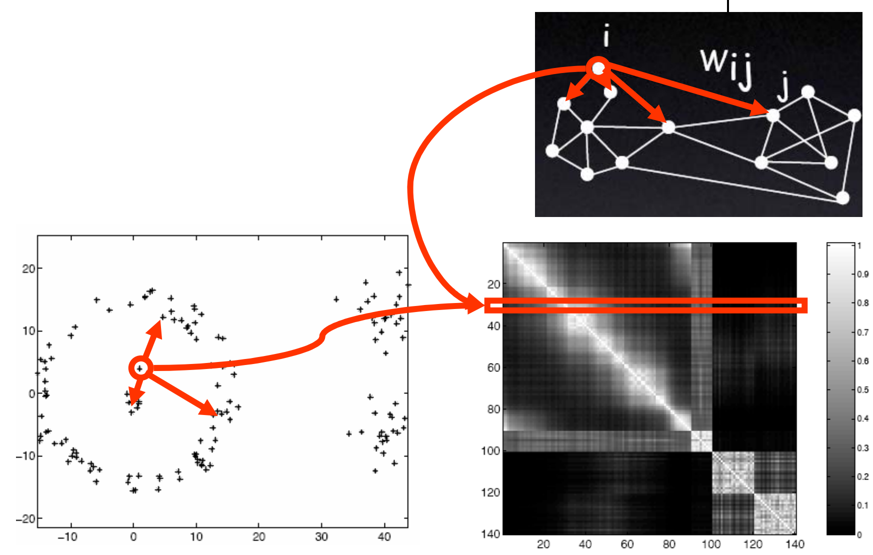


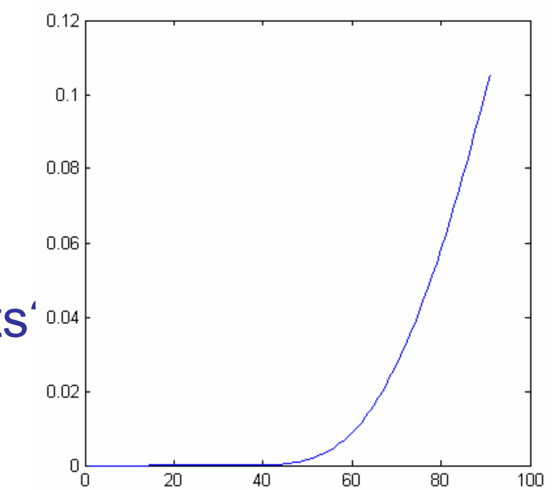
- Affinity matrix: $W = [w_{i,j}]$
- Degree matrix: $D = \mathrm{diag}(d_i)$
- Laplacian matrix: $L = D - W$
- (bipartite) partition vector:

$$x = [x_1, \ldots, x_N]$$
$$= [1, 1, \ldots 1, -1, -1, \ldots -1]$$

Affinity Function

$$W_{i,j} = e^{\frac{-\|X_i - X_j\|_2^2}{\sigma^2}}$$





- Affinities grow as σ grows →
- How the choice of σ value affects the results?
- What would be the optimal choice for σ?

Clustering via Optimizing Normalized Cut

- The normalized cut:

$$\mathrm{Ncut}(A,B) = \frac{\mathrm{cut}(A,B)}{d_A} + \frac{\mathrm{cut}(A,B)}{d_B}$$

- Computing an optimal normalized cut over all possible y (i.e., partition) is NP hard

- Transform Ncut equation to a matrix form (Shi & Malik 2000):

$$\min_x Ncut(x) = \min_y \frac{y^T(D-W)y}{y^T D y}$$

Rayleigh quotient

Subject to: $y \in \{1, -b\}^n$

$$y^T D1 = 0$$

  - Still an NP hard problem

$$\begin{aligned} Ncut(\mathrm{A},\mathrm{B}) &= \frac{cut(\mathrm{A},\mathrm{B})}{\deg(\mathrm{A})} + \frac{cut(\mathrm{A},\mathrm{B})}{\deg(\mathrm{B})} \\ &= \frac{(1+x)^T(D-S)(1+x)}{k1^T D1} + \frac{(1-x)^T(D-S)(1-x)}{(1-k)1^T D1}; \; k = \frac{\sum_{x_i>0} D(i,i)}{\sum_i D(i,i)} \\ &= \ldots \end{aligned}$$

Relaxation

$$\min_x Ncut(x) = \min_y \frac{y^T (D-W) y}{y^T D y}$$

Rayleigh quotient

Subject to: $y \in \{1, -b\}^n$

$$y^T D 1 = 0$$

- Instead, relax into the continuous domain by solving generalized eigenvalue system:

$$\min_y y^T (D-W) y, \qquad \text{s.t. } y^T D y = 1$$

  - Which gives: $(D-W) y = \lambda D y$ *Rayleigh quotient theorem*
  - Note that $(D-W)1 = 0$ so, the first eigenvector is $y_0=1$ with eigenvalue 0.
  - The second smallest eigenvector is the real valued solution to this problem!!

Algorithm

1. Define a similarity function between 2 nodes. i.e.:

$$w_{i,j} = e^{\frac{-\left\|X_{(i)} - X_{(j)}\right\|_2^2}{\sigma_X^2}}$$

2. Compute affinity matrix (W) and degree matrix (D).

3. Solve $$(D - W)y = \lambda D y$$

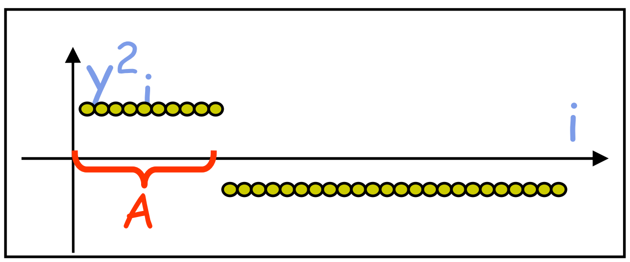
   - Do singular value decomposition (SVD) of the graph Laplacian $L = D - W$

$$L = V^T \Lambda V \quad \Rightarrow \quad y^*$$

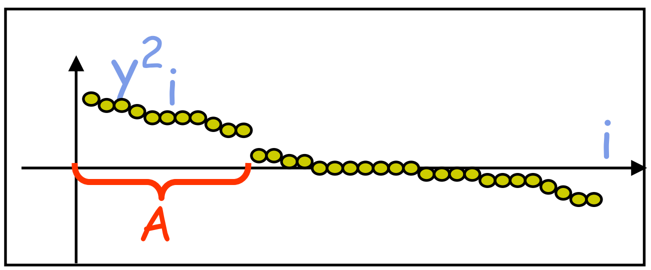
4. Use the eigenvector with the second smallest eigenvalue, y^*, to bipartition the graph.
   - For each threshold k, A_k={i | y_i among k largest element of y*}
     B_k={i | y_i among n-k smallest element of y*}
   - Compute Ncut(A_k,B_k)
   - Output $k^* = \arg\max \mathrm{Ncut}(A_k, B_k)$ and A_{k^*}, B_{k^*}

Ideally ...

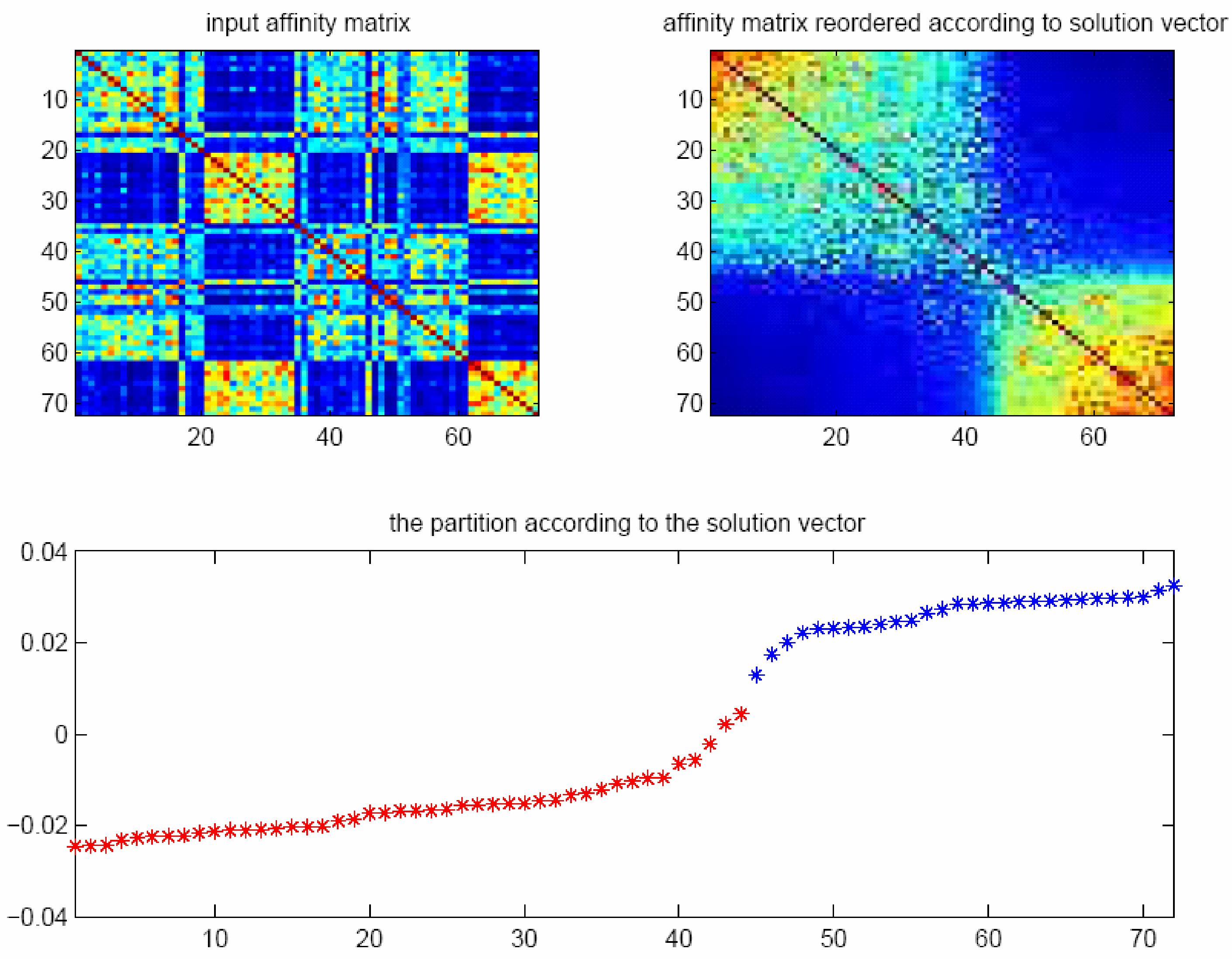
$$Ncut(A,B) = \frac{y^T(D-S)y}{y^T D y}, \quad \text{with } y_i \in \{1,-b\},\ y^T D\mathbf{1} = 0.$$



$$(D-S)y = \lambda D y$$

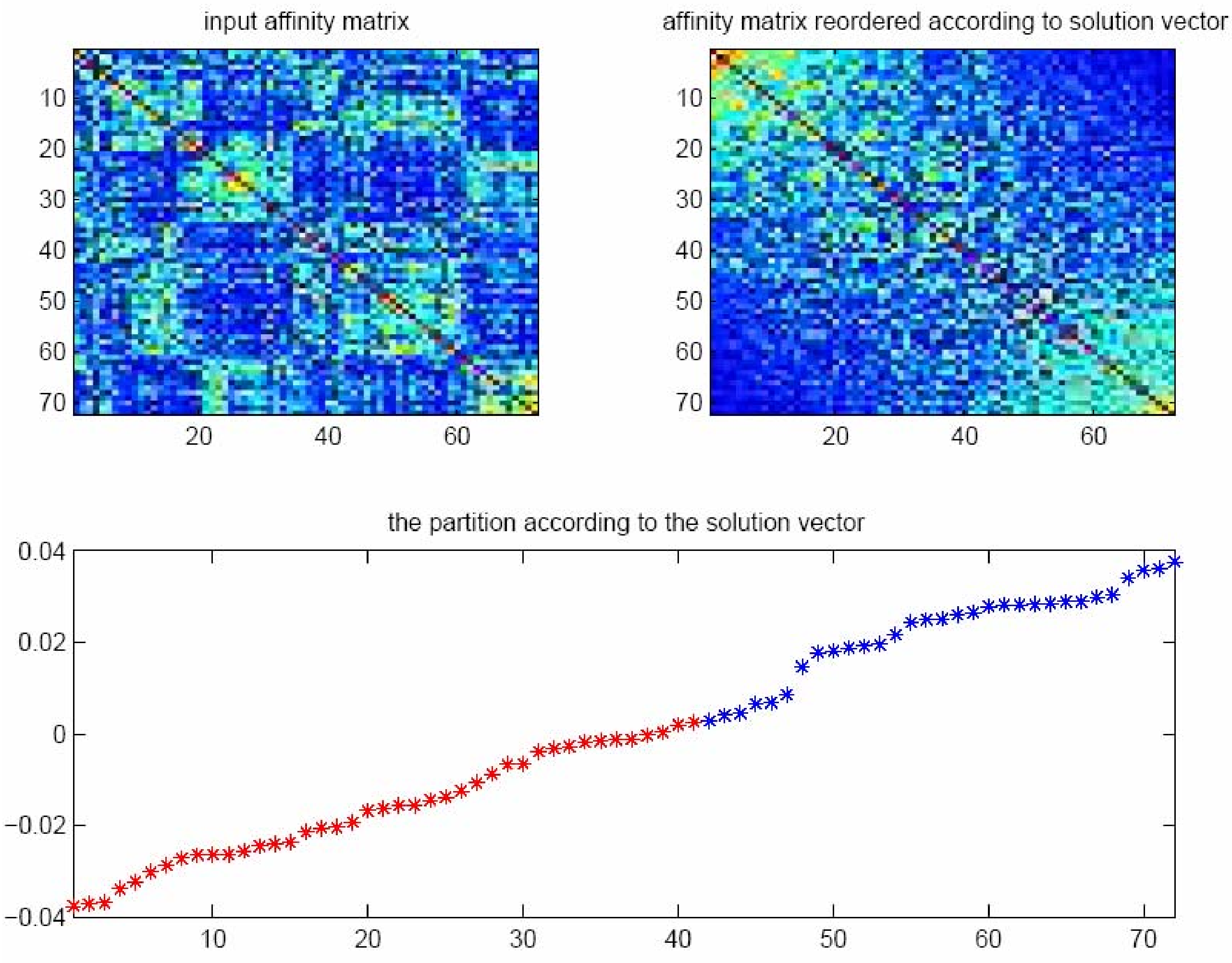


Example



input affinity matrix
10
20
30
40
50
60
70
20
40
60
affinity matrix reordered according to solution vector
10
20
30
40
50
60
70
20
40
60
the partition according to the solution vector
0.04
0.02
0
−0.02
−0.04
10
20
30
40
50
60
70

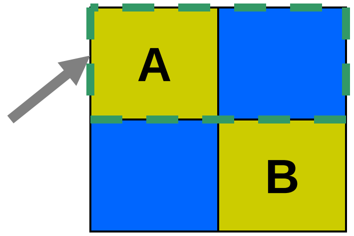
Poor features can lead to poor outcome (xing et al 2002)



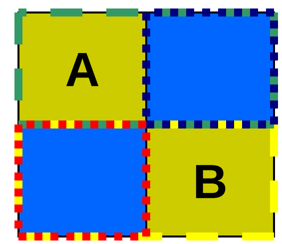
Cluster vs. block matrix

$$\mathrm{Ncut}(A,B) = \frac{\mathrm{cut}(A,B)}{d_A} + \frac{\mathrm{cut}(A,B)}{d_B}$$

$$Degree(A) = \sum_{i \in A, j \in V} W_{i,j}$$



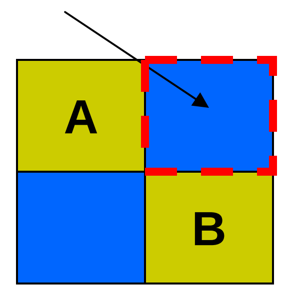
$$Ncut(A,B) = \frac{cut(A,B)}{d_A} + \frac{cut(A,B)}{d_B}$$



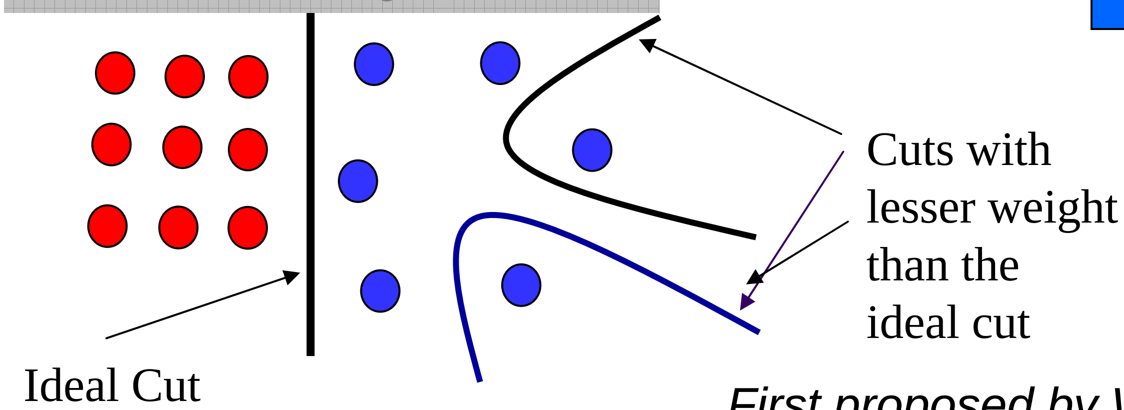
Compare to Minimum cut

- Criterion for partition:

$$\min cut(A,B) = \min_{A,B} \sum_{i \in A, j \in B} W_{i,j}$$

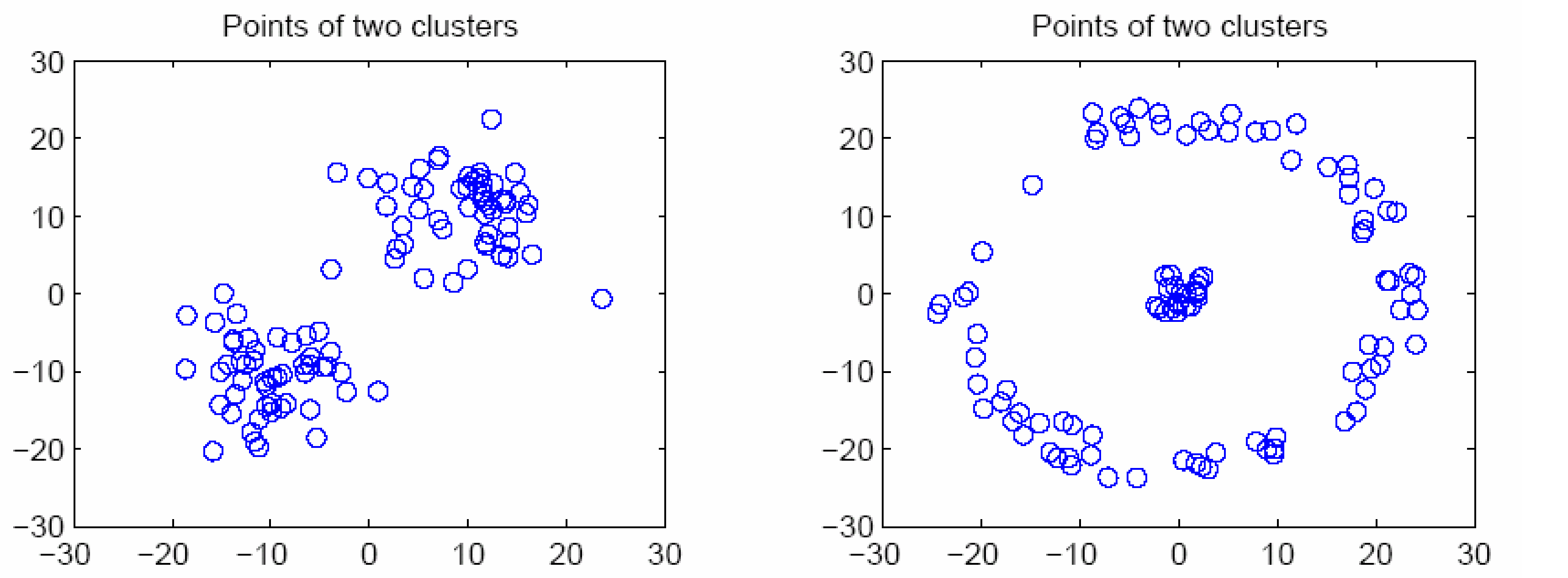


Problem!
Weight of cut is directly proportional to the number of edges in the cut.



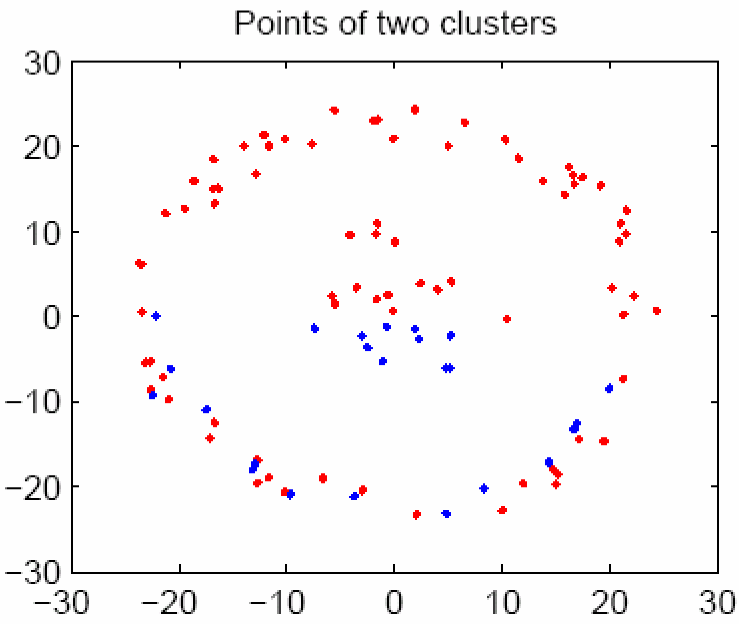
First proposed by Wu and Leahy

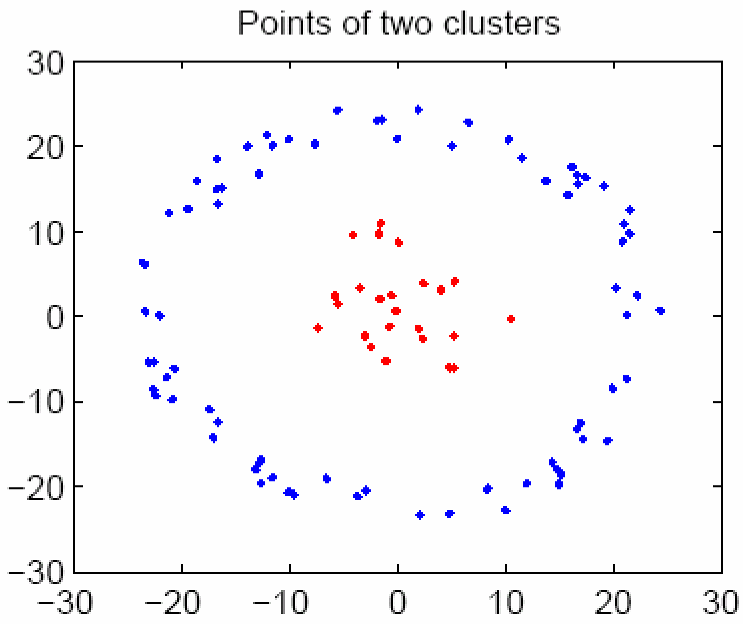
Superior performance?



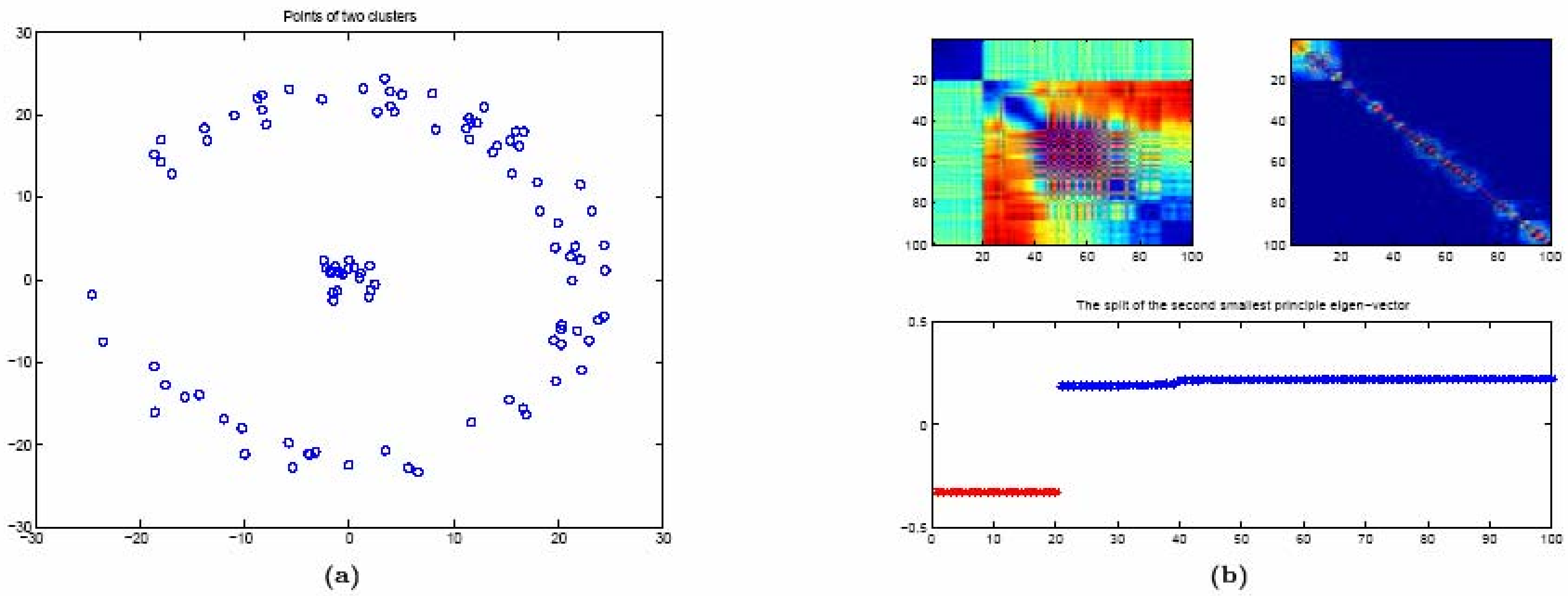
- K-means and Gaussian mixture methods are biased toward convex clusters

Ncut is superior in certain cases

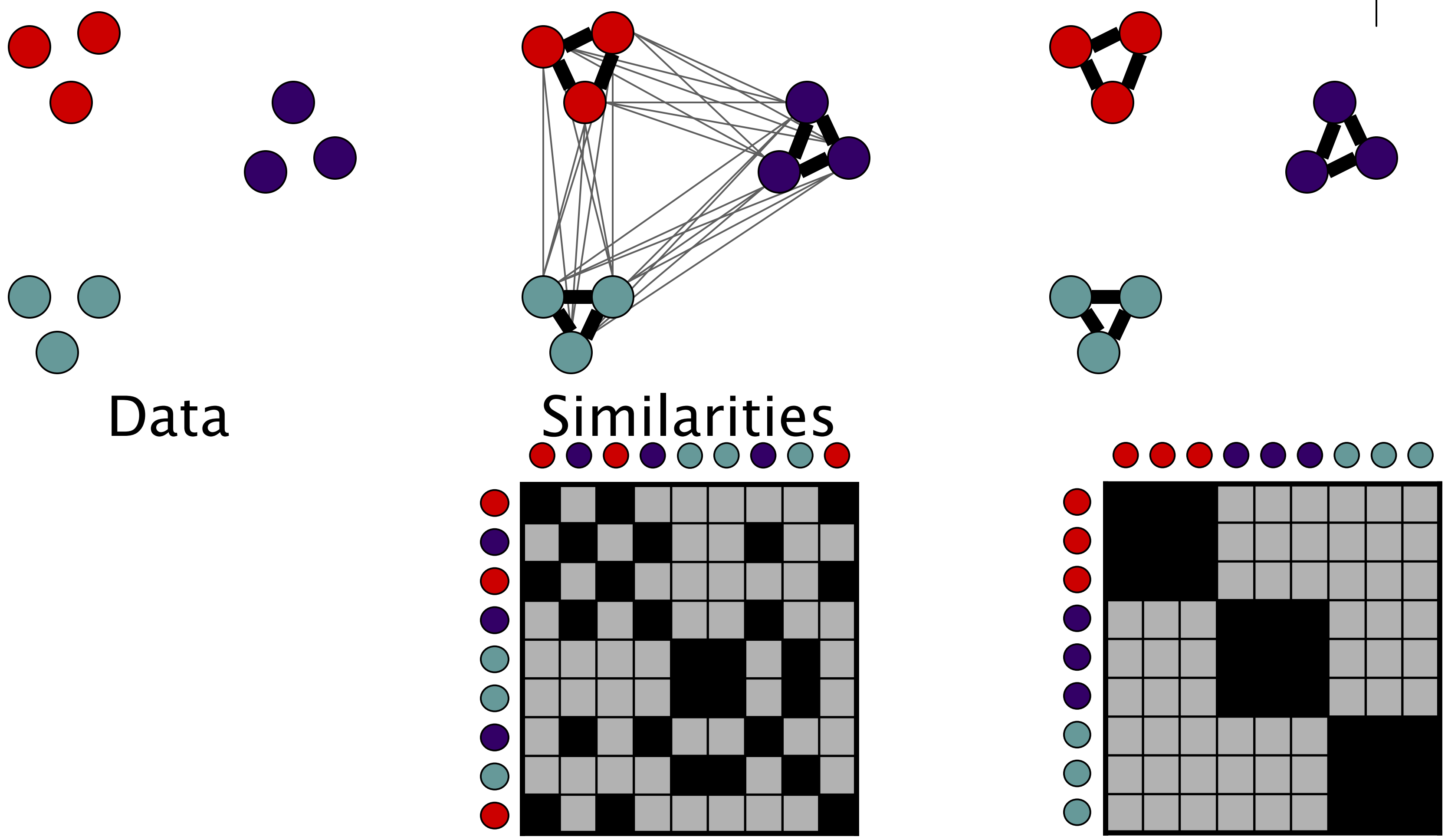




Why?


Points of two clusters
The split of the second smallest principle eigen-vector
(a)
(b)

General Spectral Clustering

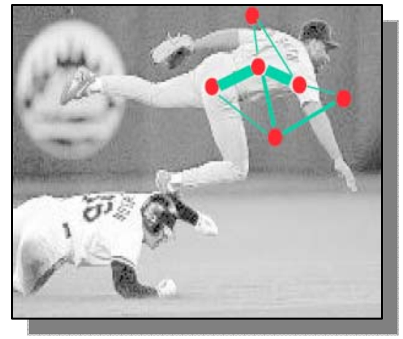


Representation

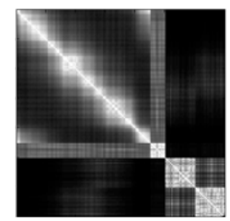
- Partition matrix X:

$$X = [X_1, \dots, X_K]$$

$$X = \begin{array}{cc} \text{segments} & \\ \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} & \text{pixels} \end{array}$$



- Pair-wise similarity matrix W: $W(i, j) = aff(i, j)$



- Degree matrix D: $D(i, i) = \sum_j w_{i,j}$

- Laplacian matrix L: $L = D - W$

Eigenvectors and blocks

- Block matrices have block eigenvectors:

1	1	0	0
1	1	0	0
0	0	1	1
0	0	1	1

$\xrightarrow{\text{eigensolver}}$

$\lambda_1= 2$ $\lambda_2= 2$ $\lambda_3= 0$ $\lambda_4= 0$

$\lambda_1= 2$	$\lambda_2= 2$
.71	0
.71	0
0	.71
0	.71

- Near-block matrices have near-block eigenvectors:

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

$\xrightarrow{\text{eigensolver}}$

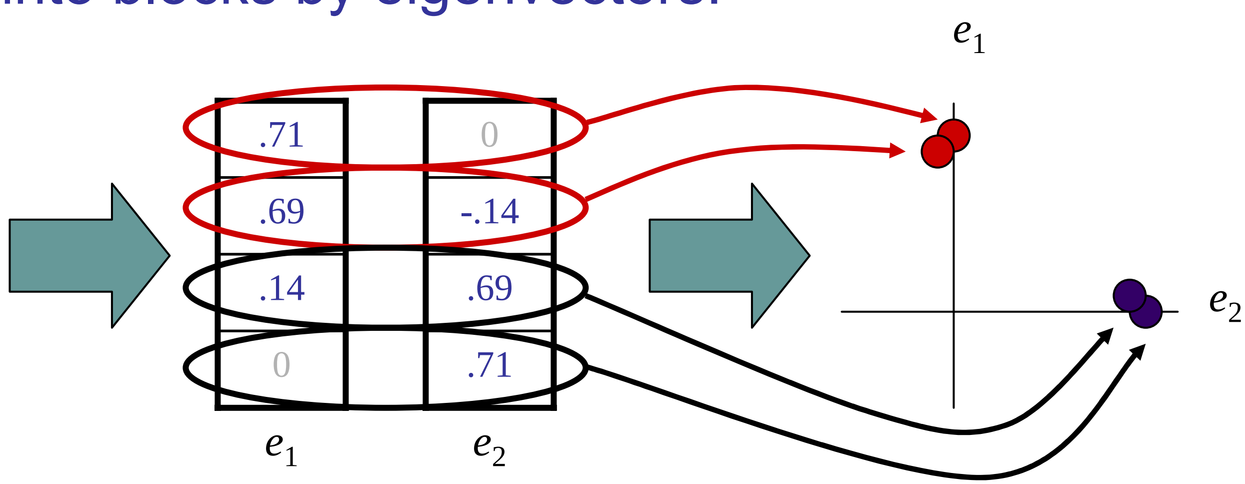
$\lambda_3= -0.02$ $\lambda_4= -0.02$

$\lambda_1= 2.02$	$\lambda_2= 2.02$
.71	0
.69	-.14
.14	.69
0	.71

Spectral Space

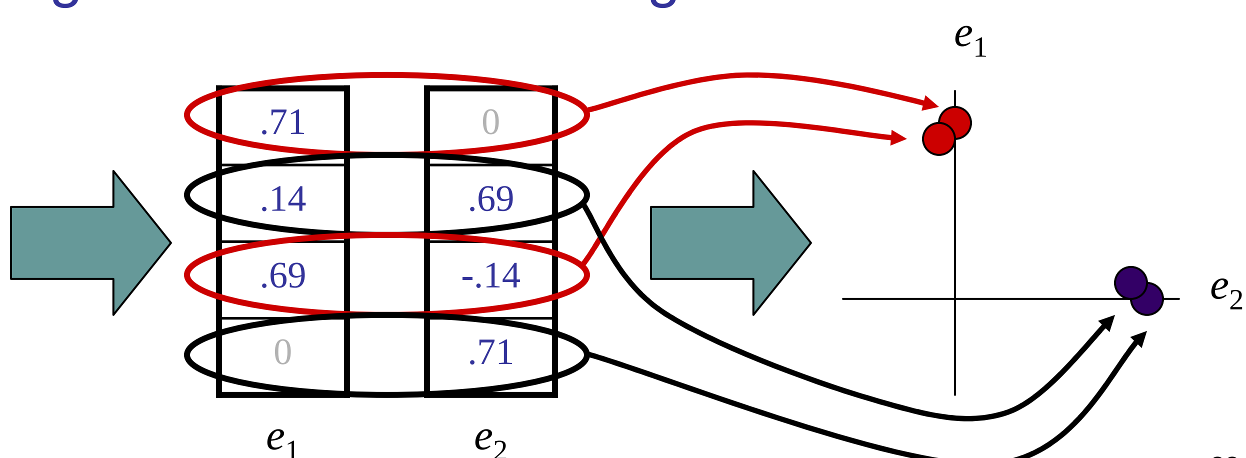
- Can put items into blocks by eigenvectors:

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



- Clusters clear regardless of row ordering:

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



Spectral Clustering

- Algorithms that cluster points using eigenvectors of matrices derived from the data
- Obtain data representation in the low-dimensional space that can be easily clustered
- Variety of methods that use the eigenvectors differently (we have seen an example)
- Empirically very successful
- Authors disagree:
  - Which eigenvectors to use
  - How to derive clusters from these eigenvectors
- Two general methods

Method #1

- Partition using only one eigenvector at a time
- Use procedure recursively
- Example: Image Segmentation
  - Uses 2^{nd} (smallest) eigenvector to define optimal cut
  - Recursively generates two clusters with each cut

Method #2

- Use k eigenvectors (k chosen by user)
- Directly compute k-way partitioning
- Experimentally has been seen to be “better”

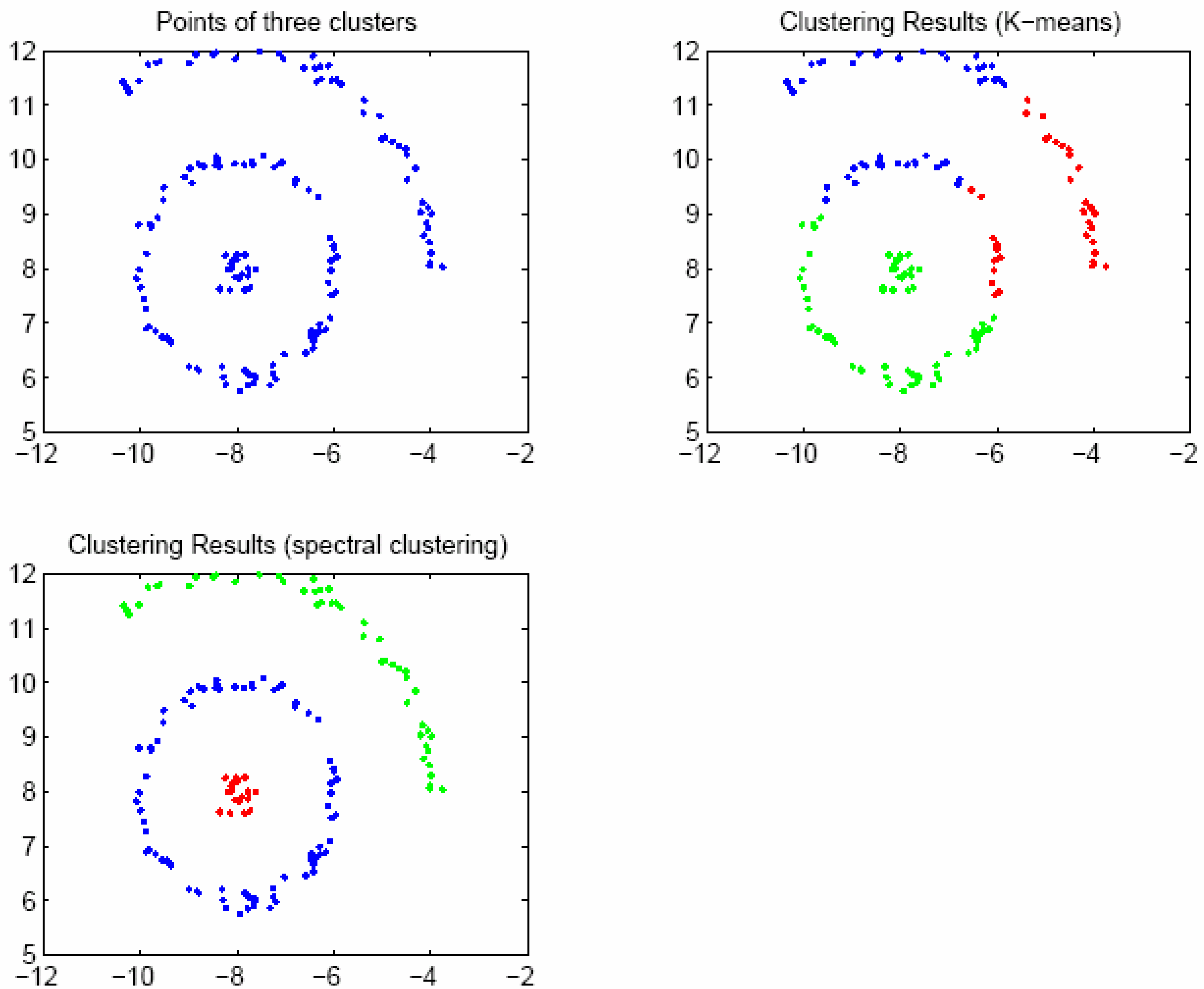
Spectral Clustering Algorithm
Ng, Jordan, and Weiss 2003

- Given a set of points $S=\{s_1,\ldots s_n\}$
- Form the affinity matrix $w_{i,j} = e^{\frac{-\|S_i - S_j\|_2^2}{\sigma^2}}, \quad \forall i \neq j, \qquad w_{i,i} = 0$
- Define diagonal matrix $D_{ii} = \Sigma_\kappa a_{ik}$
- Form the matrix $L = D^{-1/2} W D^{-1/2}$
- Stack the k largest eigenvectors of L to for the columns of the new matrix X:

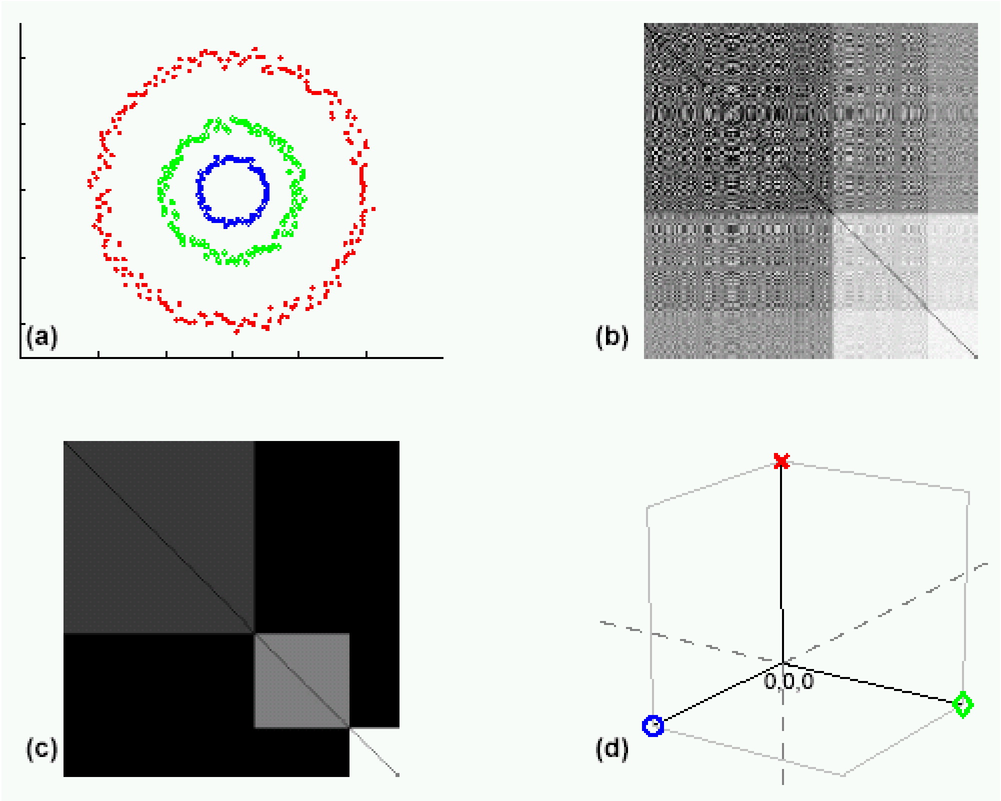
$$X = \begin{bmatrix} | & | & & | \\ x_1 & x_2 & \cdots & x_k \\ | & | & & | \end{bmatrix}$$

- Renormalize each of X's rows to have unit length and get new matrix Y. Cluster rows of Y as points in R^k

SC vs Kmeans


Points of three clusters
Clustering Results (K−means)
Clustering Results (spectral clustering)
12
11
10
9
8
7
6
5
−12
−10
−8
−6
−4
−2

Why it works?



- K-means in the spectrum space !

More formally …

- Recall generalized Ncut

$$\mathrm{Ncut}(A_1, A_2 \ldots A_k) = \sum_{r=1}^{k} \left(\frac{\sum_{i \in A_r, j \in V \setminus A_r} W_{ij}}{\sum_{i \in A_r, j \in V} W_{ij}} \right) = \sum_{r=1}^{k} \left(\frac{\mathrm{cut}(A_r, \bar{A}_r)}{d_{A_r}} \right)$$

- Minimizing this is equivalent to spectral clustering

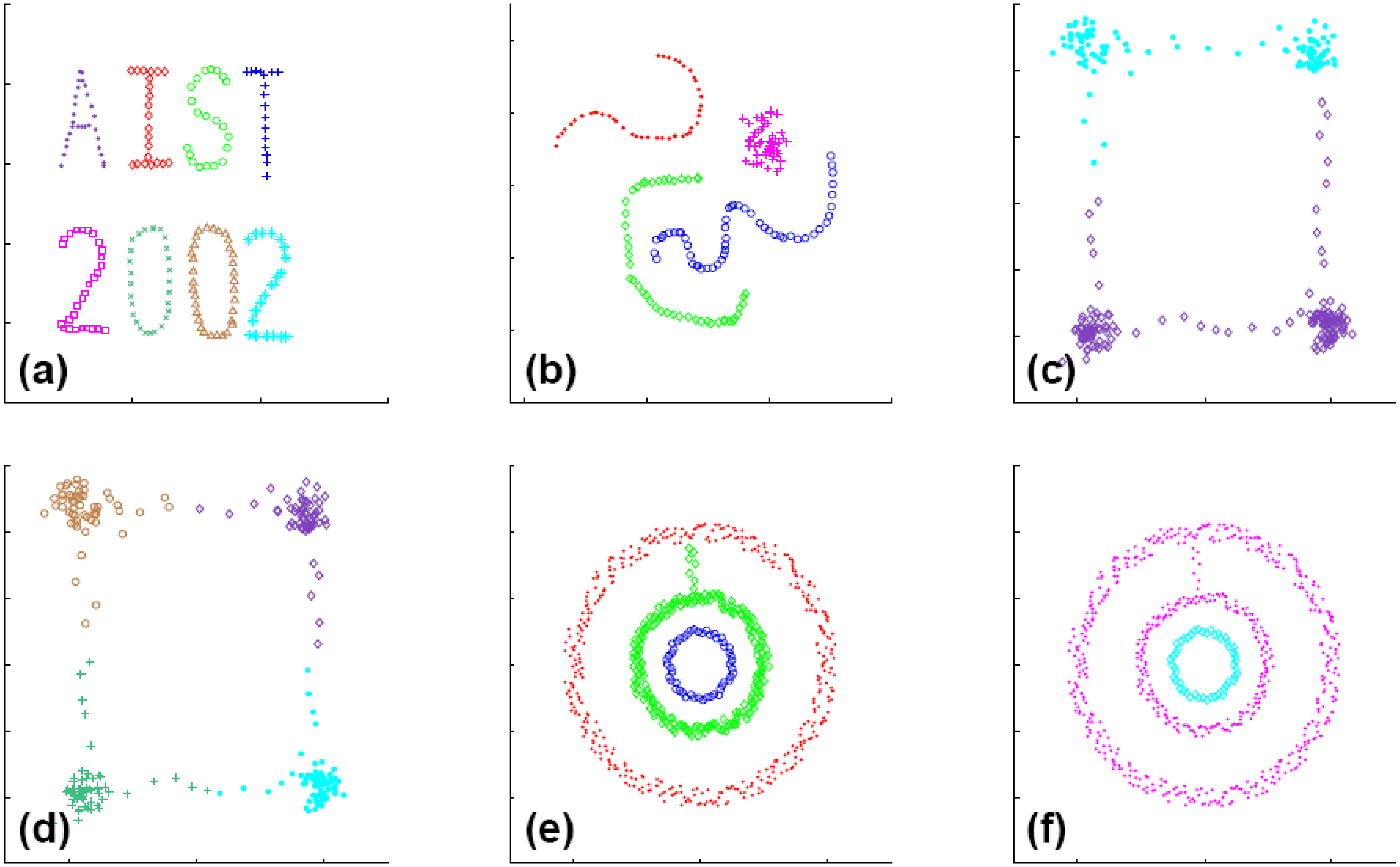
$$\min \ \mathrm{Ncut}(A_1, A_2 \ldots A_k) = \sum_{r=1}^{k} \left(\frac{\mathrm{cut}(A_r, \bar{A}_r)}{d_{A_r}} \right)$$

$$\min \ Y^{\mathrm{T}} D^{-1/2} W D^{-1/2} Y$$

$$\text{s.t.} \ \ Y^{\mathrm{T}} Y = I$$

$$Y = \begin{array}{cc} \text{segments} & \\ \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} & \text{pixels} \end{array}$$

Toy examples



Images from Matthew Brand (TR-2002-42)

User's Prerogative

- Choice of k, the number of clusters

- Choice of scaling factor
  - Realistically, search over σ^2 and pick value that gives the tightest clusters

- Choice of clustering method: k-way or recursive bipartite

- Kernel affinity matrix

$$w_{i,j} = K(S_i, S_j)$$

Conclusions

- Good news:
  - Simple and powerful methods to segment images.
  - Flexible and easy to apply to other clustering problems.
- Bad news:
  - High memory requirements (use sparse matrices).
  - Very dependant on the scale factor for a specific problem.

$$W(i, j) = e^{\frac{-\left\| X_{(i)} - X_{(j)} \right\|_2^2}{\sigma_X^2}}$$