Normalized Cuts and Spectral Clustering

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- Graph cuts
- Ncuts formulation
- Graph cuts methods comparison
- Practical issues
  - Constructing similarity graph
  - Continuous vs. discrete solutions
  - Multi-scale
- Other interpretations
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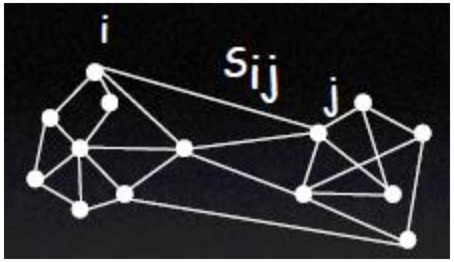
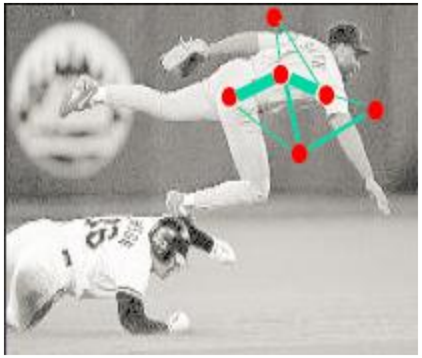
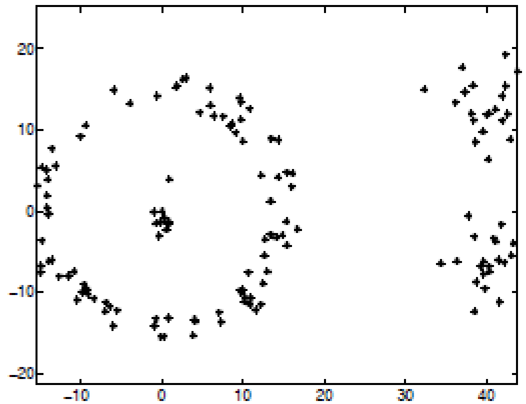
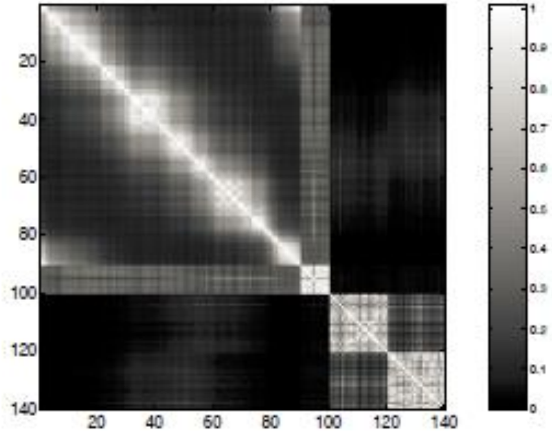
Graph cuts

- Similarity graph



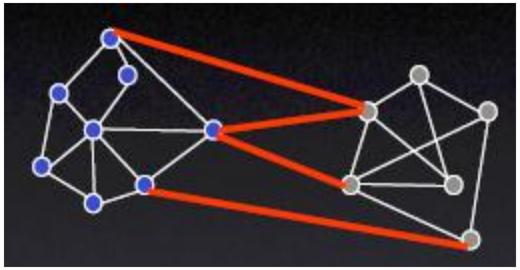


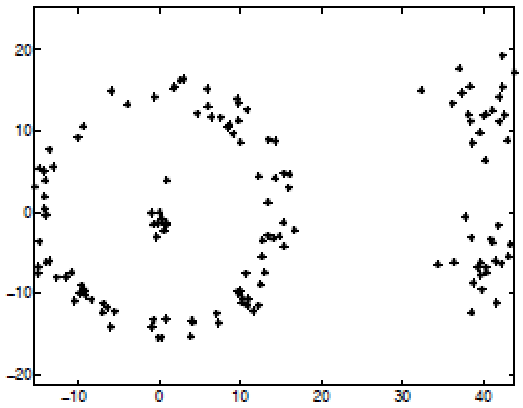


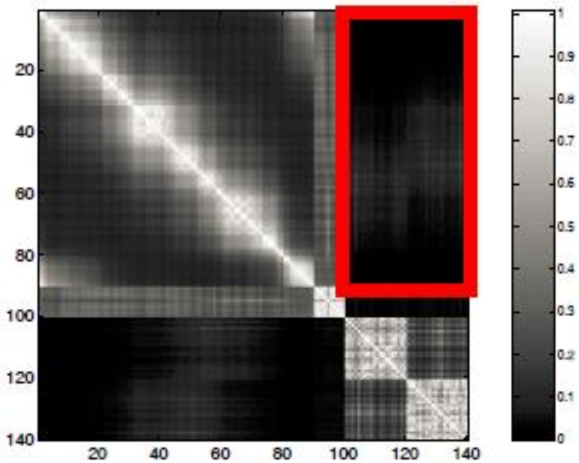


Graph cuts

- $cut(A,B) = \sum_{i \in A, j \in \bar{A}} s_{ij}$
- Objective: Find the cuts that best groups the vertices according to similarity.
- Two major concerns of Graph cuts:
  - A good optimization criterion
  - Computational tractability







Graph cuts

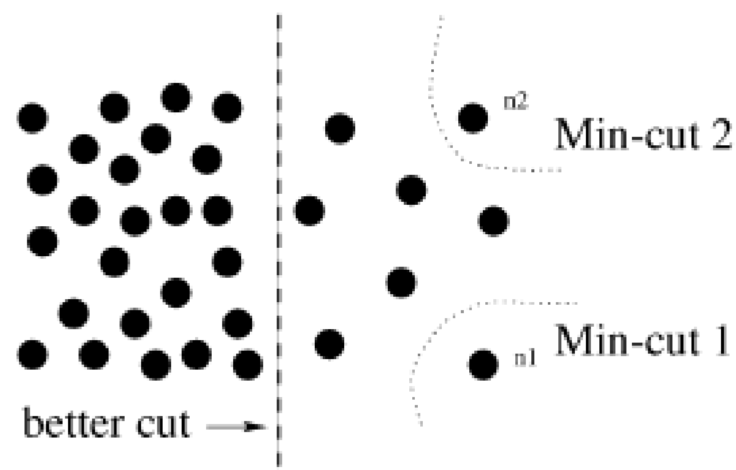
- Min cut

$$\min cut(\mathrm{A}, \overline{\mathrm{A}})$$

- Have efficient algorithm for exact discrete solution

- Problem: Tend to cut small sets of isolated nodes

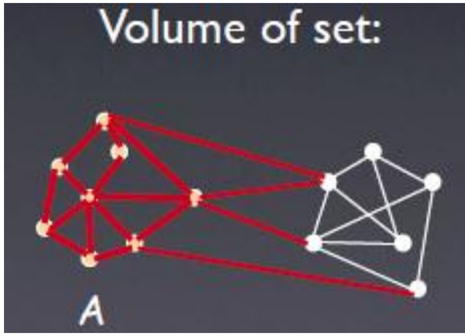
- Solution: Normalize the cuts in terms of subsets volumes(Ncuts)



Normalized cuts

- Objective

$$\min Ncut(A, \overline{A}) = \frac{cut(A, \overline{A})}{vol(A)} + \frac{cut(A, \overline{A})}{vol(\overline{A})}$$



- Graph Laplacian

$$L = D - W$$

 where $D = diag(d_1, d_2, \dots, d_N)$ and $W_{ij} = s_{ij}$

- Define cluster indicator vector

$$f_i = \begin{cases} \sqrt{\dfrac{vol(\overline{A})}{vol(A)}} & if\ v_i \in A \\ \sqrt{\dfrac{vol(A)}{vol(\overline{A})}} & if\ v_i \in \overline{A} \end{cases}$$

- We have

$$f'Lf = vol(V)Ncut(A, \overline{A})$$

Normalized cuts

- The Ncuts equivalent problem

$$\begin{aligned} &\min f'Lf\ , \\ \text{s.t.}\quad & f \text{ discrete as defined above;} \\ &(Df)'\mathbf{1} = 0; f'Df\ = vol(V). \end{aligned}$$

- Relax

$$\begin{aligned} &\min f'Lf\ , \\ \text{s.t.}\quad &(Df)'\mathbf{1} = 0; f'Df\ = vol(V). \end{aligned}$$

- Substitute $g \coloneqq D^{1/2}f$

$$\begin{aligned} &\min_{g\in\mathbb{R}^N} g'D^{-1/2}LD^{-1/2}g\ \ , \\ \text{s.t.}\quad &(g)'D^{1/2}\mathbf{1} = 0;\ \|g\|^2 = vol(V). \end{aligned}$$

- According to Rayleigh-Ritz theorem, the solution is given by second eigenvector of $D^{-1/2}LD^{-1/2}$, and thus f is second generalized eigenvector of

$$Lu = \lambda Du$$

Normalized cuts

- Generalized to $k > 2$ clusters:

$$H_{ij} = \begin{cases} \dfrac{1}{\sqrt{vol(A_j)}} & if\ v_i \in A_j \\ 0 & otherwise \end{cases}$$

$$\min tr(H'LH) \quad s.t.\ H'DH = I$$

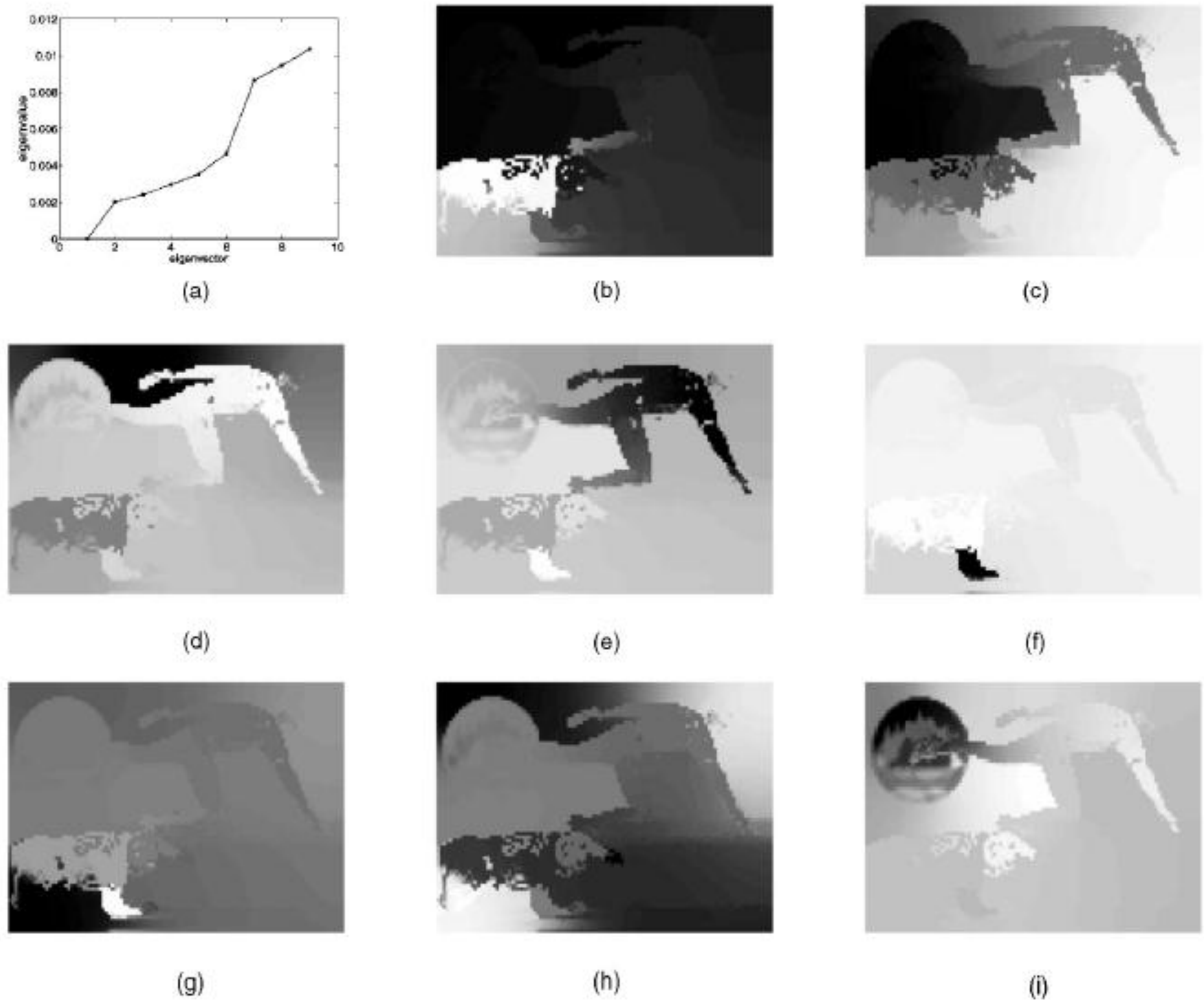
- or let $H = D^{-1/2}T$,

$$\min_{T \in \mathbb{R}^{n \times k}} tr\left(D^{-1/2} L D^{-1/2}\right) \ \ s.t. T'T = I$$

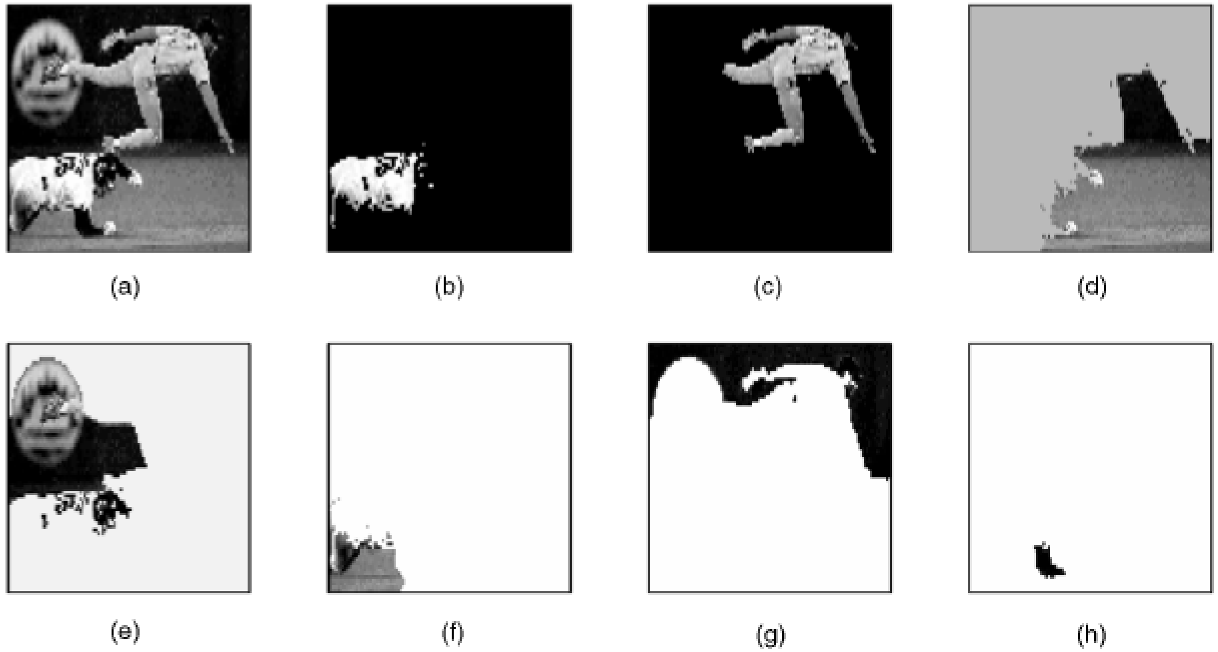
- T is given by first k eigenvectors of $D^{-1/2} L D^{-1/2}$

Normalized cuts

- Computation of eigenvector: Lanczos method
- Post processing: From relaxed to discrete
  - For 2-way cut, simply threshold. View k-way cut as recursive 2-way cut.
  - Simultaneous k-way cut, apply k-means to the relaxed solution
  - Other theories related with the approximation(Yu and Shi, ICCV'03; Bach and Jordan, NIPS'04)



0.012
0.01
0.008
0.006
0.004
0.002
0
eigenvalue
0
2
4
6
8
10
eigenvector
(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)
(i)


(a)
(b)
(c)
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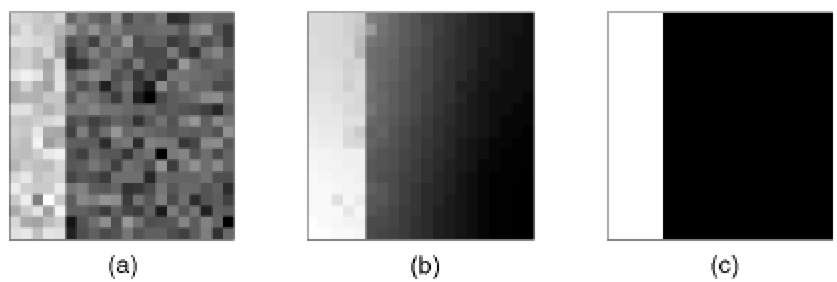
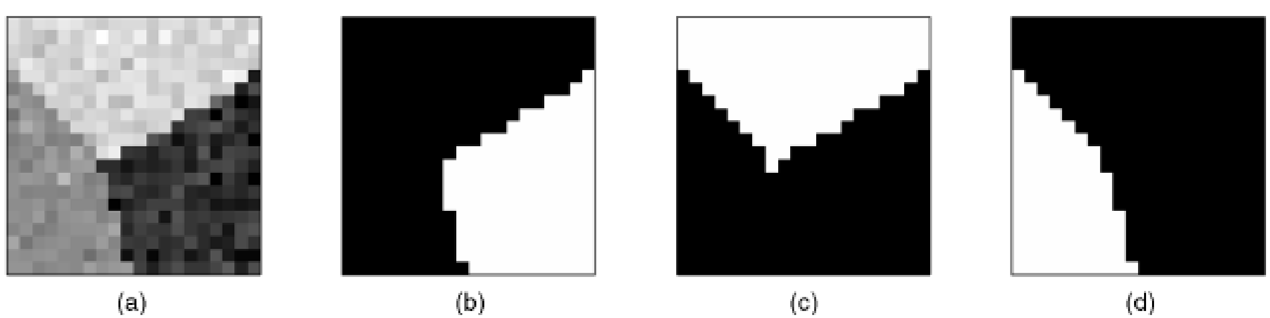
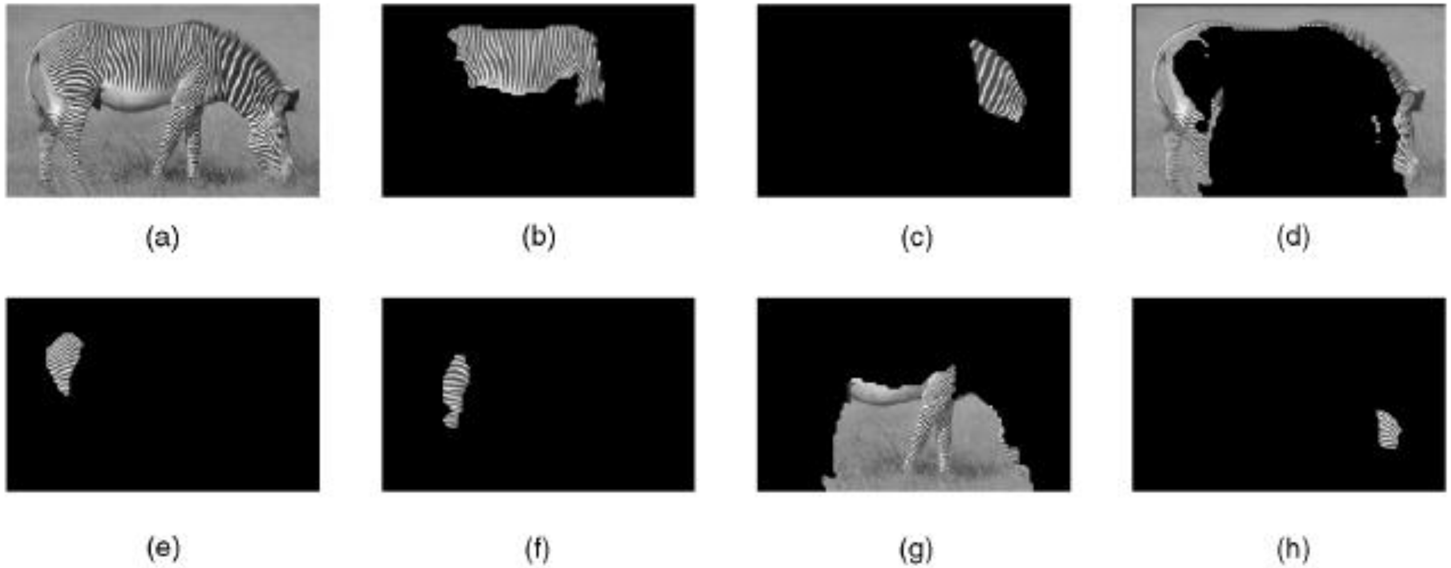
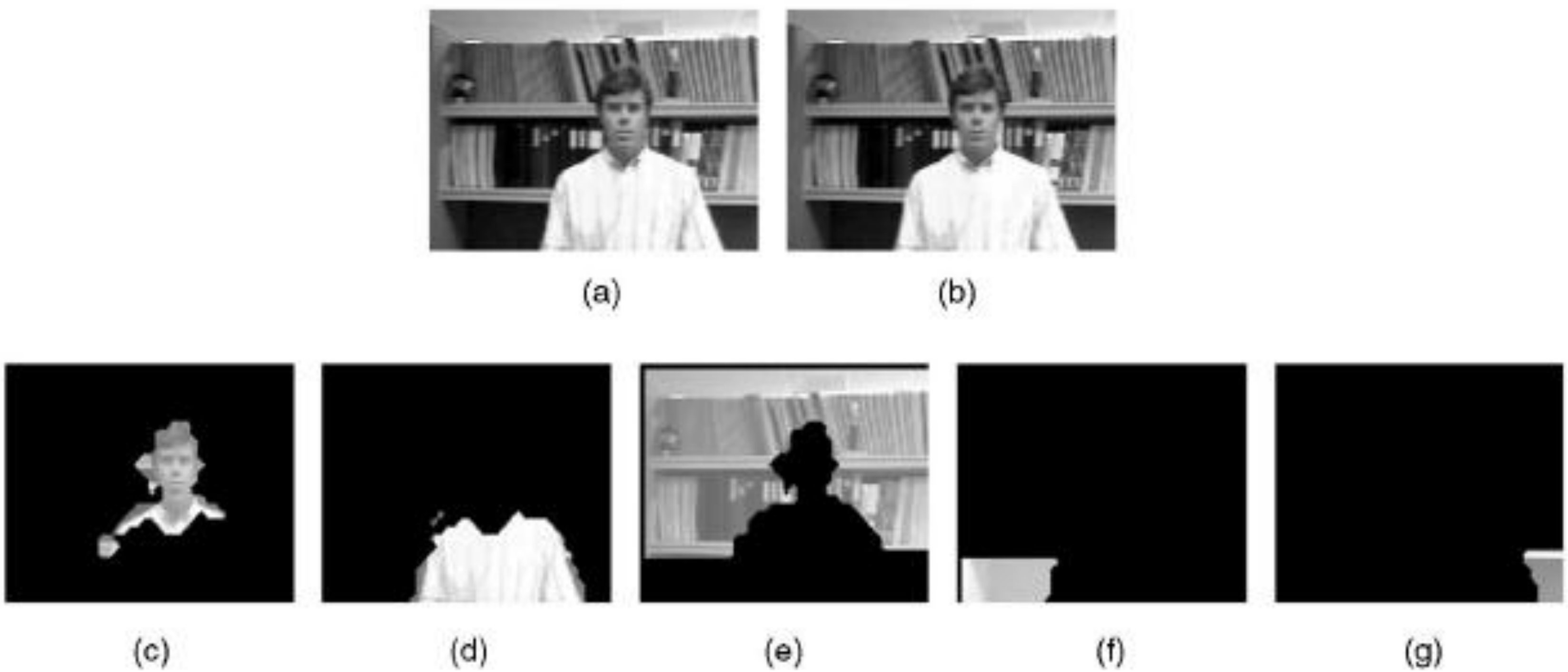

(a)
(b)
(c)


(a)
(b)
(c)
(d)



(a) (b) (c) (d)

(e) (f) (g) (h)



(a) (b)

(c) (d) (e) (f) (g)

Comparison of different graph cuts

- Ncut

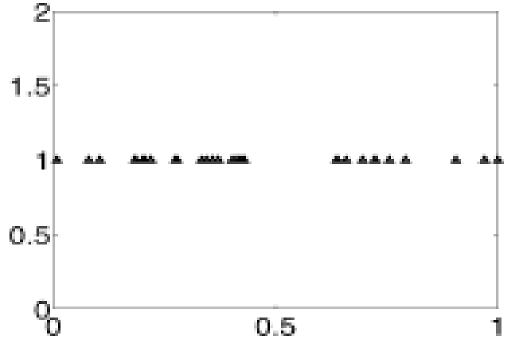
$$\min \frac{cut(A,\bar{A})}{vol(A)} + \frac{cut(A,\bar{A})}{vol(\bar{A})}$$

- Average cut

$$\min \frac{cut(A,\bar{A})}{|A|} + \frac{cut(A,\bar{A})}{|\bar{A}|}$$

- Average association

$$\max \frac{assoc(A,A)}{|A|} + \frac{assoc(\bar{A},\bar{A})}{|\bar{A}|}$$

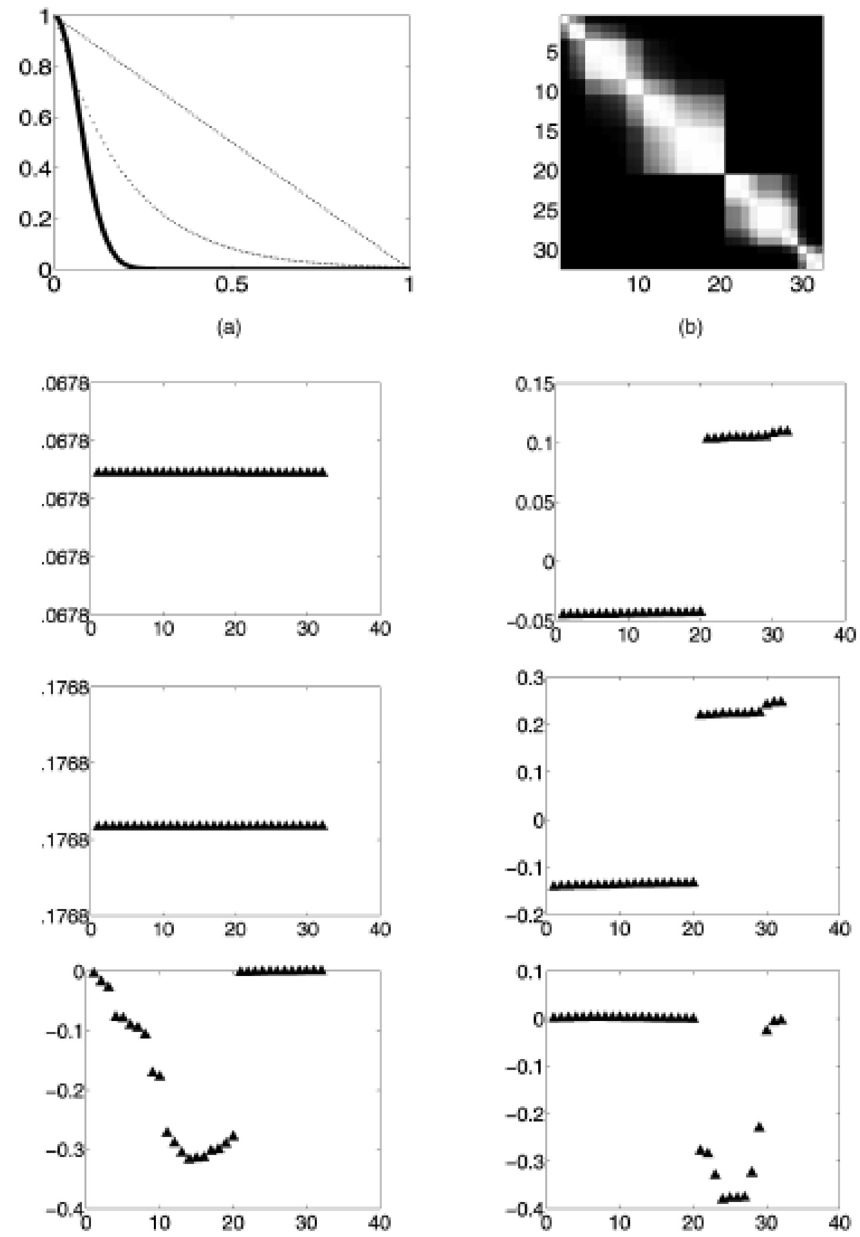


20 points~U(0,0.5)

12 points~U(0.65,1)

Weight function

Weight matrix



(a) (b)

Normalized Cut:

$$(D - W)x = \lambda D x$$

$$W x = (1 - \lambda) D x$$

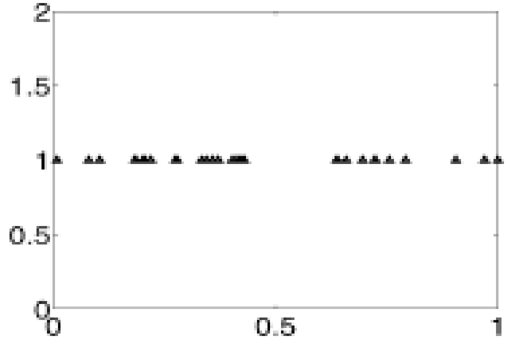
Average Cut:

$$(D - W)x = \lambda x$$

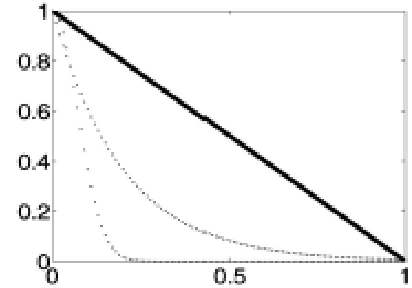
Average Association:

$$W x = \lambda x$$

(c) (d)

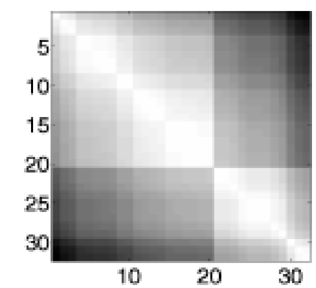


Weight function



(a)

Weight matrix



(b)

Normalized Cut:

$(D - W)x = \lambda D x$

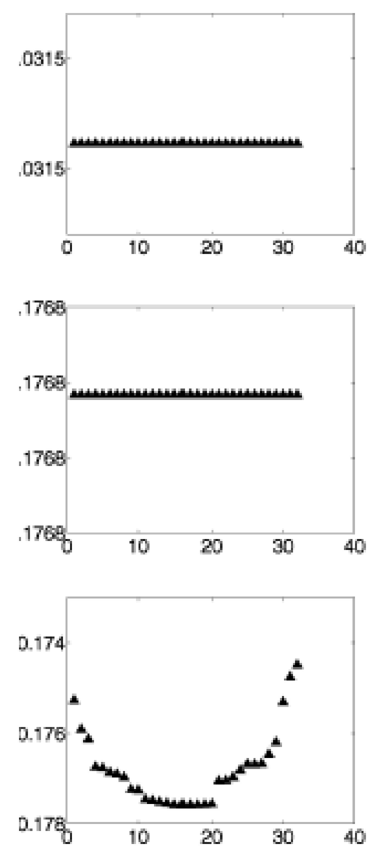
$W x = (1 - \lambda) D x$

Average Cut:

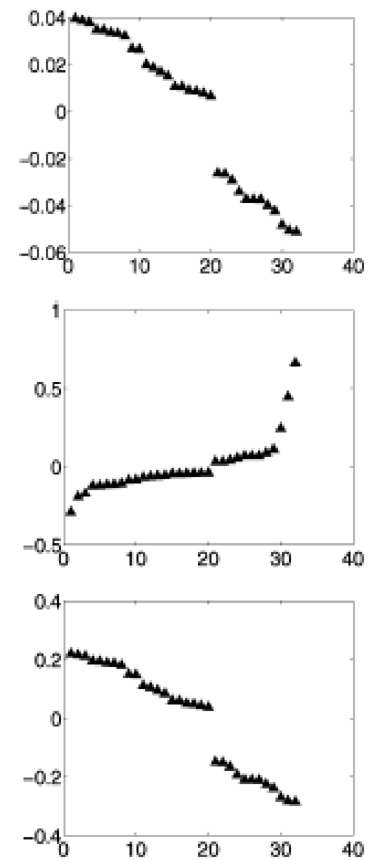
$(D - W)x = \lambda x$

Average Association:

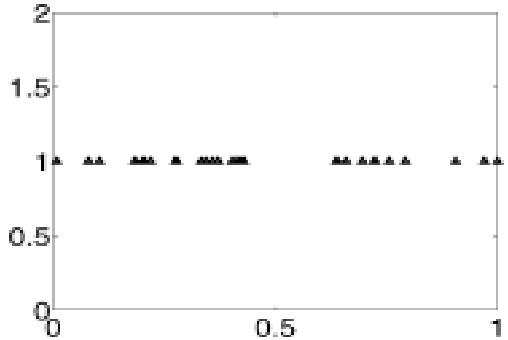
$W x = \lambda x$



(c)

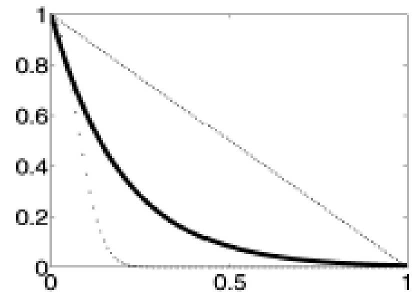


(d)

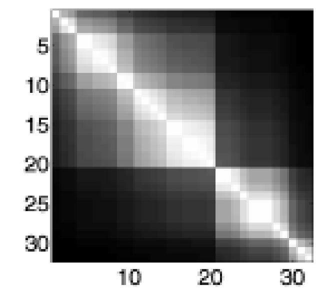


Weight function

Weight matrix



(a)



(b)

Normalized Cut:

$$(D - W)x = \lambda D x$$

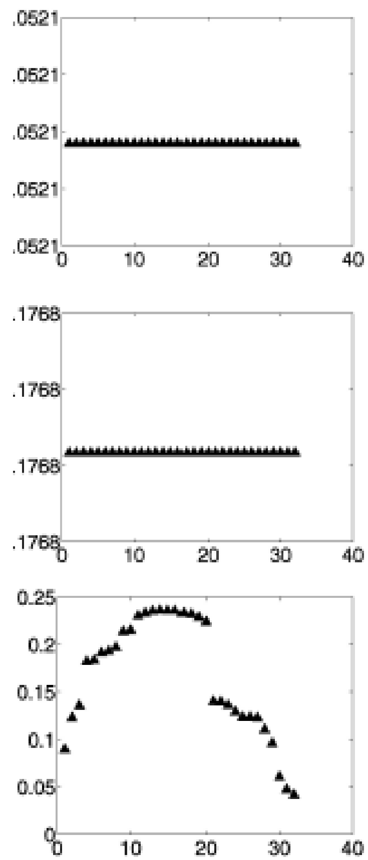
$$Wx = (1 - \lambda) D x$$

Average Cut:

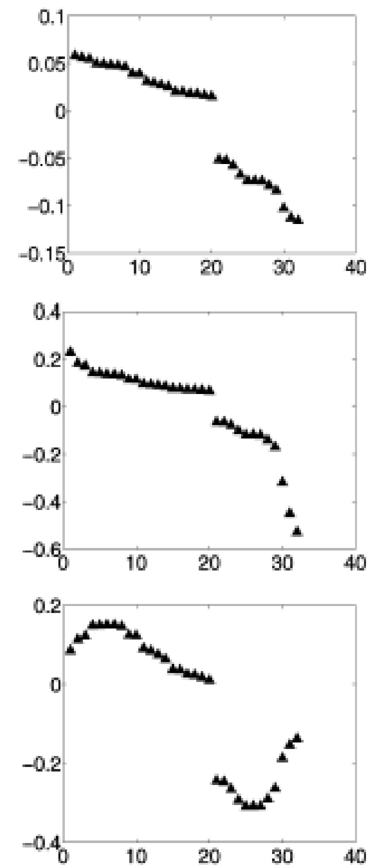
$$(D - W)x = \lambda x$$

Average Association:

$$Wx = \lambda x$$



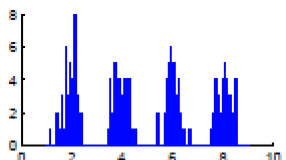
(c)



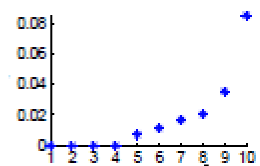
(d)

Practical issues

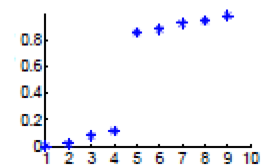
- Constructing similarity matrix
  - Gaussian distance $s(x_i, x_j) = \exp\left(-\|x_i - x_j\|^2 / (2\sigma^2)\right)$
  - Full connection vs. partial connection



Sample histogram

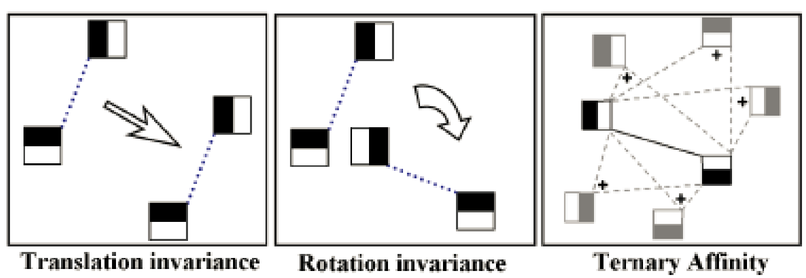


eigenvalue partial connection



eigenvalue full connection

  - Should be tuned for specific tasks(Ex. Cour, Gogin and Shi, AISTAT'05)



$$f(x_1, y_1, \theta_1; x_2, y_2, \theta_2) = \tilde{f}(x_2 - x_1;\ y_2 - y_1;\ \theta_2 - \theta_1)$$

Similarity matrix can be learned

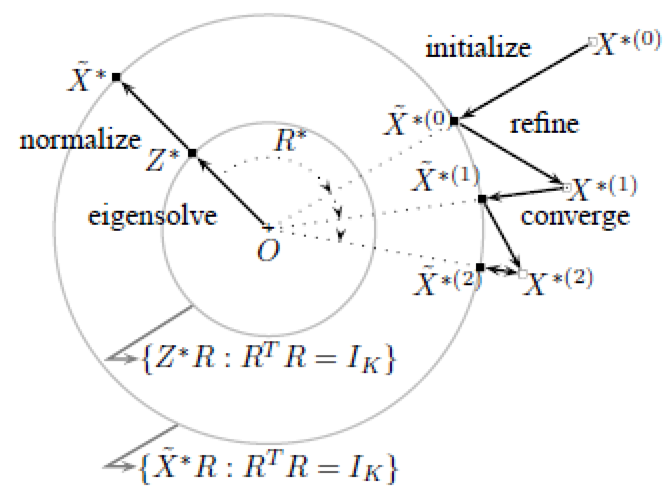
- Cour, Gogin and Shi, AISTAT'05
- Given: Labeled set I with known indicator vector $X^*(I)$, the cost function

$$\varepsilon(W, I) = \frac{1}{2} \| X_2[W(I)] - X^*(I) \|^2$$

- Find the optimum W using gradient method
- Bach and Jordan, NIPS'04

Relaxed vs. discrete

- How to obtain more accurate discrete clustering result from its relaxed solution?
- Orthogonal invariance: if Z is a solution to the relaxed k-way Ncut problem, so is ZR, R is the rotation matrix of $\mathbb{R}^k$ (Yu and Shi, ICCV'03; Bach and Jordan, NIPS'04)
- An iterative method to find a discrete solution X^* according to Z^*



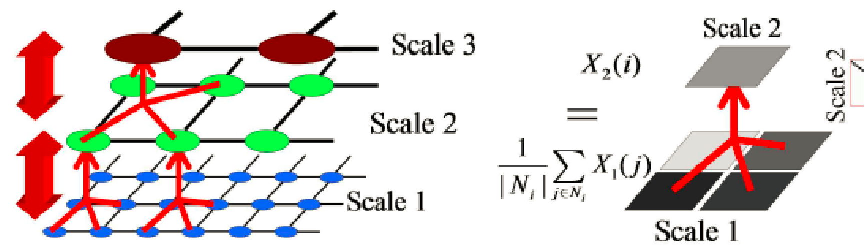
Multi-scale

- Cour, Benezit and Shi, CVPR'05
- Main concern: propagation of local grouping clues across multiple ranges
- Add another constrain across scales:

$X_s - partitioning\ vector\ of\ scale\ s$;

$\mathcal{N}_i - the\ neighbourhood\ of\ vertex\ i$;

$$X_{s+1}(i) = \frac{1}{|\mathcal{N}_i|} \sum_{j \in \mathcal{N}_i} X_s(j)$$



Other interpretations

- Random walks(Maila and Shi, NIPS'01)

$$Ncut(A,\overline{A}) = P(A \to \overline{A}) + P(\overline{A} \to A)$$

- Perturbation theory(Luxburg Tutorial'07)
  - The eigenvector deviation due to the matrix perturbation is bounded
  - View the actual W as a perturbated version of an ideal $\widetilde{W}$ with clusters disjoint, the eigenvectors should also approximate the ideal indicator vector

Pros and cons

- Pros
  - Ncuts does not make strong assumptions on the cluster forms(unlike k-mean, which assumes the clusters to be convex)
  - It's computational efficient

- Cons
  - Very sensitive to the selection of similarity matrix and parameters

Sources of materials

- Timothee Cour, Jianbo Shi, Nicolas Gogin, Learning Spectral Graph Segmentation, AISTAT 2005.
- Timothee Cour, Florence Benezit, Jianbo Shi, Spectral Segmentation with Multi-Scale Graph Decomposition , CVPR 2005.
- Jianbo Shi and Jitendra Malik, Normalized Cuts and Image Segmentation, TPAMI 2000.
- Stella X. Yu, Jianbo Shi, Multiclass Spectral Clustering, ICCV 2003.
- Ulrike von Luxburg, A Tutorial on Spectral Clustering
- Francis R. Bach, Michael I. Jordan, Learning Spectral Clustering