A Tutorial on Spectral Clustering

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Some historical notes

- Fiedler, 1973, 1975, graph Laplacian matrix
- Donath & Hoffman, 1973, bounds
- Pothen, Simon, Liou, 1990, Spectral graph partitioning (many related papers there after)
- Hagen & Kahng, 1992, Ratio-cut
- Chan, Schlag & Zien, multi-way Ratio-cut
- Chung, 1997, Spectral graph theory book
- Shi & Malik, 2000, Normalized Cut

Spectral Gold-Rush of 2001

9 papers on spectral clustering

- Meila & Shi, AI-Stat 2001. Random Walk interpreation of Normalized Cut
- Ding, He & Zha, KDD 2001. Perturbation analysis of Laplacian matrix on sparsely connected graphs
- Ng, Jordan & Weiss, NIPS 2001, K-means algorithm on the embeded eigen-space
- Belkin & Niyogi, NIPS 2001. Spectral Embedding
- Dhillon, KDD 2001, Bipartite graph clustering
- Zha et al, CIKM 2001, Bipartite graph clustering
- Zha et al, NIPS 2001. Spectral Relaxation of K-means
- Ding et al, ICDM 2001. MinMaxCut, Uniqueness of relaxation.
- Gu et al, K-way Relaxation of NormCut and MinMaxCut

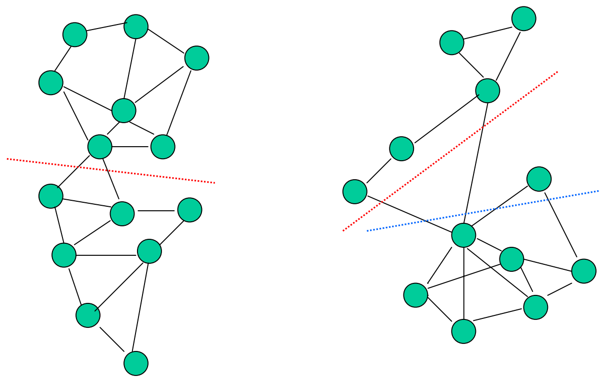
Part I: Basic Theory, 1973 – 2001

Spectral Graph Partitioning

MinCut: min cutsize

cutsize = # of cut edges

Constraint on sizes: |A| = |B|



2-way Spectral Graph Partitioning

Partition membership indicator: $q_i = \begin{cases} 1 & \textbf{if } i \in A \\ -1 & \textbf{if } i \in B \end{cases}$

$$J = CutSize = \frac{1}{4}\sum_{i,j} w_{ij}[q_i - q_j]^2$$

$$= \frac{1}{4}\sum_{i,j} w_{ij}[q_i^2 + q_j^2 - 2q_i q_j] = \frac{1}{2}\sum_{i,j} q_i[d_i\delta_{ij} - w_{ij}]q_j$$

$$= \frac{1}{2} q^T (D - W) q$$

Relax indicators q_i from discrete values to continuous values, the solution for min $J(q)$ is given by the eigenvectors of

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

(Fiedler, 1973, 1975)

(Pothen, Simon, Liou, 1990)

Properties of Graph Laplacian

Laplacian matrix of the Graph: $L = D - W$

- L is semi-positive definite $x^T L x \geq 0$ for any x.
- First eigenvector is $q_1=(1,\cdots,1)^T = e^T$ with $\lambda_1=0$.
- Second eigenvector q_2 is the desired solution.
  - The smaller λ_2, the better quality of the partitioning. Perturbation analysis gives

$$\lambda_2 = \frac{cutsize}{|A|} + \frac{cutsize}{|B|}$$

- Higher eigenvectors are also useful

Recovering Partitions

From the definition of cluster indicators:
Partitions A, B are determined by:

$$A = \{i \mid q_2(i) < 0\}, B = \{i \mid q_2(i) \geq 0\}$$

However, the objective function $J(q)$ is insensitive to additive constant c :

$$J = CutSize = \frac{1}{4}\sum_{i,j} w_{ij}[(q_i + c) - (q_j + c)]^2$$

Thus, we sort q_2 to increasing order, and cut in the middle point.

Multi-way Graph Partitioning

- Recursively applying the 2-way partitioning
  - Recursive 2-way partitioning
  - Using Kernigan-Lin to do local refinements
- Using higher eigenvectors
  - Using q_3 to further partitioning those obtained via q_2.
- Popular graph partitioning packages
  - Metis, Univ of Minnesota
  - Chaco, Sandia Nat'l Lab

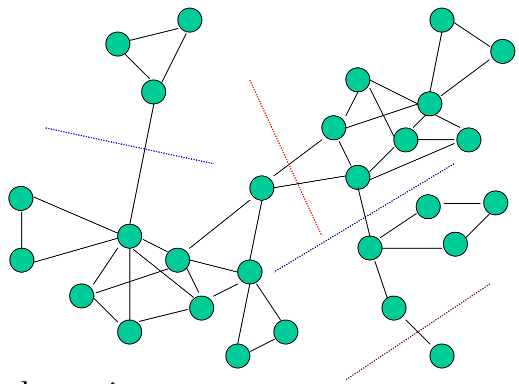
2-way Spectral Clustering

- Undirected graphs (pairwise similarities)
- Bipartite graphs (contingency tables)
- Directed graphs (web graphs)

Spectral Clustering

min cutsize , without explicit size constraints

But where to cut ?



Need to balance sizes

Clustering Objective Functions

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

- Ratio Cut

$$J_{Rcut}(A,B) = \frac{s(A,B)}{|A|} + \frac{s(A,B)}{|B|}$$

- Normalized Cut

$$d_A = \sum_{i \in A} d_i$$

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

$$= \frac{s(A,B)}{s(A,A)+s(A,B)} + \frac{s(A,B)}{s(B,B)+s(A,B)}$$

- Min-Max-Cut

$$J_{MMC}(A,B) = \frac{s(A,B)}{s(A,A)} + \frac{s(A,B)}{s(B,B)}$$

Ratio Cut (Hagen & Kahng, 1992)

Min similarity between A , B: $s(A,B) = \sum_{i\in A}\sum_{j\in B} w_{ij}$

Size Balance $J_{Rcut}(A,B) = \frac{s(A,B)}{|A|} + \frac{s(A,B)}{|B|}$ (Wei & Cheng, 1989)

Cluster membership indicator: $q(i) = \begin{cases} \sqrt{n_2/n_1 n} & \textbf{if } i \in A \\ -\sqrt{n_1/n_2 n} & \textbf{if } i \in B \end{cases}$

Normalization: $q^T q = 1, q^T e = 0$

Substitute q leads to $J_{Rcut}(q) = q^T(D-W)q$

Now relax q, the solution is 2nd eigenvector of L

Normalized Cut (Shi & Malik, 1997)

Min similarity between A & B: $s(A,B) = \sum_{i\in A}\sum_{j\in B} w_{ij}$

Balance weights $J_{Ncut}(A,B) = \frac{s(A,B)}{d_A} + \frac{s(A,B)}{d_B}$ $d_A = \sum_{i\in A} d_i$

Cluster indicator: $q(i) = \begin{cases} \sqrt{d_B/d_A d} & \textbf{if } i \in A \\ -\sqrt{d_A/d_B d} & \textbf{if } i \in B \end{cases}$ $d = \sum_{i\in G} d_i$

Normalization: $q^T D q = 1, q^T D e = 0$

Substitute q leads to $J_{Ncut}(q) = q^T(D-W)q$

$$\min_q q^T(D-W)q + \lambda(q^T D q - 1)$$

Solution is eigenvector of $(D-W)q = \lambda D q$

MinMaxCut (Ding et al 2001)

Min similarity between A & B: $s(A,B) = \sum_{i \in A} \sum_{j \in B} w_{ij}$

Max similarity within A & B: $s(A,A) = \sum_{i \in A} \sum_{j \in A} w_{ij}$

$$J_{MMC}(A,B) = \frac{s(A,B)}{s(A,A)} + \frac{s(A,B)}{s(B,B)}$$

Cluster indicator: $q(i) = \begin{cases} \sqrt{d_B / d_A d} & \textbf{if } i \in A \\ -\sqrt{d_A / d_B d} & \textbf{if } i \in B \end{cases}$

Substituting,

$$J_{MMC}(q) = \frac{1+\sqrt{d_B/d_A}}{J_m + \sqrt{d_B/d_A}} + \frac{1+\sqrt{d_A/d_B}}{J_m + \sqrt{d_A/d_B}} - 2 \qquad J_m = \frac{q^T W q}{q^T D q}$$

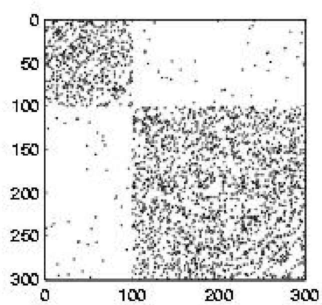
Because $\frac{dJ_{MMC}(J_m)}{dJ_m} < 0$ $\quad$ min $J_{\mathrm{mmc}} \Rightarrow$ max $J_{\mathrm{m}}(q)$

$$\Rightarrow \quad Wq = \xi Dq \quad \Rightarrow \quad (D-W)q = \lambda Dq$$

A simple example

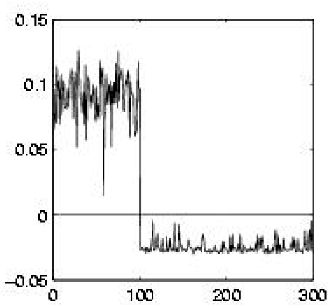
2 dense clusters, with sparse connections between them.

Adjacency matrix



(a)

Eigenvector q_2



(b)

Comparison of Clustering Objectives

- If clusters are well separated, all three give very similar and accurate results.
- When clusters are marginally separated, NormCut and MinMaxCut give better results
- When clusters overlap significantly, MinMaxCut tend to give more compact and balanced clusters.

$$J_{Ncut} = \frac{s(A,B)}{s(A,A)+\mathbf{s(A,B)}} + \frac{s(A,B)}{s(B,B)+\mathbf{s(A,B)}}$$

Cluster Compactness $\Rightarrow$ $\max s(A,A)$

2-way Clustering of Newsgroups

Newsgroups	RatioCut	NormCut	MinMaxCut
Atheism Comp.graphics	63.2 ± 16.2	97.2 ± 0.8	97.2 ± 1.1
Baseball Hockey	54.9 ± 2.5	74.4 ± 20.4	79.5 ± 11.0
Politics.mideast Politics.misc	53.6 ± 3.1	57.5 ± 0.9	83.6 ± 2.5

Cluster Balance Analysis I: Random Graph Model

- Random graph: edges are randomly assigned with probability p: $0 \le p \le 1$.
- RatioCut & NormCut show no size dependence

$$J_{\mathbf{Rcut}}(A,B) = \frac{p\,|A||B|}{|A|} + \frac{p\,|A||B|}{|B|} = np = \mathbf{constant}$$

$$J_{\mathbf{Ncut}}(A,B) = \frac{p\,|A||B|}{p\,|A|(n-1)} + \frac{p\,|A||B|}{p\,|B|(n-1)} = \frac{n}{n-1} = \mathbf{constant}$$

- MinMaxCut favors balanced clusters: $|A|=|B|$

$$J_{\mathbf{MMC}}(A,B) = \frac{p\,|A||B|}{p\,|A|(|A|-1)} + \frac{p\,|A||B|}{p\,|B|(|B|-1)} = \frac{|B|}{|A|-1} + \frac{|A|}{|B|-1}$$

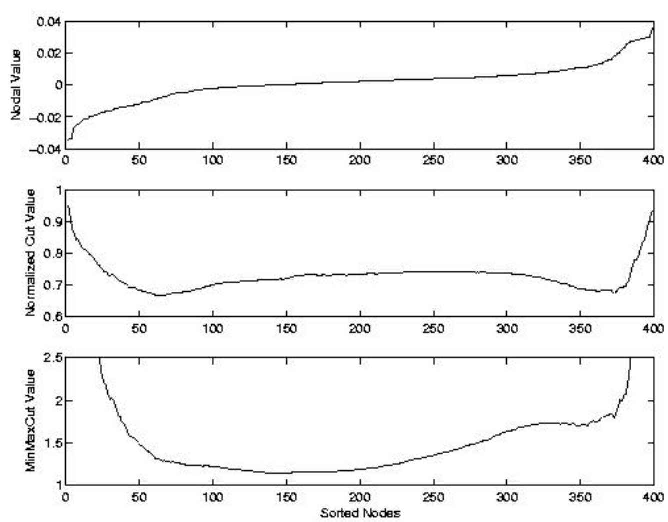
2-way Clustering of Newsgroups

Cluster Balance

Eigenvector

$J_{\text{Ncut}}(\text{i})$

$J_{\text{MMC}}(\text{i})$



Cluster Balance Analysis II:
Large Overlap Case

$$f = \frac{s(A,B)}{(1/2)[s(A,A)+s(B,B)]} > 0.5$$

Conditions for skewed cuts:

$$\textbf{NormCut}: s(A,A) \ \ge (\frac{1}{2f} - \frac{1}{2}) s(A,B) = s(A,B)/2$$

$$\textbf{MinMaxCut}: s(A,A) \ \ge \frac{1}{2f} s(A,B) = s(A,B)$$

Thus MinMaxCut is much less prone to skewed cuts

Spectral Clustering of Bipartite Graphs

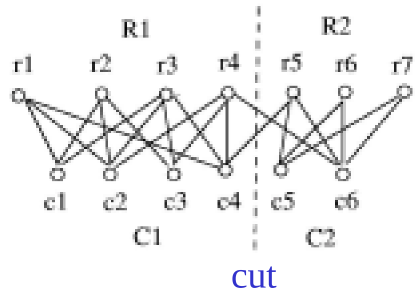
Simultaneous clustering of rows and columns of a contingency table (adjacency matrix B)

Examples of bipartite graphs

- Information Retrieval: word-by-document matrix
- Market basket data: transaction-by-item matrix
- DNA Gene expression profiles
- Protein vs protein-complex

Spectral Clustering of Bipartite Graphs

Simultaneous clustering of rows and columns
(adjacency matrix B)



$$s(B_{R_1,C_2}) = \sum_{r_i \in R_1} \sum_{c_j \in C_2} b_{ij}$$

min between-cluster sum of weights: $s(R_1,C_2)$, $s(R_2,C_1)$

max within-cluster sum of weights: $s(R_1,C_1)$, $s(R_2,C_2)$

$$J_{MMC}(C_1,C_2;R_1,R_2) = \frac{s(B_{R_1,C_2}) + s(B_{R_2,C_1})}{2s(B_{R_1,C_1})} + \frac{s(B_{R_1,C_2}) + s(B_{R_2,C_1})}{2s(B_{R_2,C_2})}$$

(Ding, AI-STAT 2003)

Bipartite Graph Clustering

Clustering indicators for rows and columns:

$$f(i) = \begin{cases} 1 & \text{if } r_i \in R_1 \\ -1 & \text{if } r_i \in R_2 \end{cases} \qquad g(i) = \begin{cases} 1 & \text{if } c_i \in C_1 \\ -1 & \text{if } c_i \in C_2 \end{cases}$$

$$B = \begin{pmatrix} B_{R_1,C_1} & B_{R_1,C_2} \\ B_{R_2,C_1} & B_{R_2,C_2} \end{pmatrix} \qquad W = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix} \qquad \mathbf{q} = \begin{pmatrix} \mathbf{f} \\ \mathbf{g} \end{pmatrix}$$

Substitute and obtain

$$J_{MMC}(C_1,C_2;R_1,R_2) = \frac{s(W_{12})}{s(W_{11})} + \frac{s(W_{12})}{s(W_{22})}$$

f,g are determined by

$$\left[\begin{pmatrix} D_r & \\ & D_c \end{pmatrix} - \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}\right]\begin{pmatrix} f \\ g \end{pmatrix} = \lambda \begin{pmatrix} D_r & \\ & D_c \end{pmatrix}\begin{pmatrix} f \\ g \end{pmatrix}$$

Clustering of Bipartite Graphs

Let

$$\tilde{B} = D_r^{-1/2} B D_c^{-1/2}, z = \begin{pmatrix} u \\ v \end{pmatrix} = Dq = \begin{pmatrix} D_r^{1/2} f \\ D_c^{1/2} g \end{pmatrix}$$

We obtain

$$\begin{pmatrix} 0 & \tilde{B} \\ \tilde{B}^T & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \lambda \begin{pmatrix} u \\ v \end{pmatrix}$$

Solution is SVD: $\tilde{B} = \sum_{k=1}^{m} u_k \lambda_k v_k^T$

(Zha et al, 2001, Dhillon, 2001)

Clustering of Bipartite Graphs

Recovering row clusters:

$$R_1 = \{r_i, | \; f_2(i) < z_r\}, R_2 = \{r_i, | \; f_2(i) \geq z_r\},$$

Recovering column clusters:

$$C_1 = \{c_i, | \; g_2(i) < z_c\}, C_2 = \{c_i, | \; g_2(i) \geq z_c\},$$

$z_r = z_c = 0$ are dividing points. Relaxation is invariant up to a constant shift.

Algorithm: search for optimal points i_{cut}, j_{cut}, let $z_r = f_2(i_{cut})$, $z_c = g_2(j_{cut})$, such that $J_{MMC}(C_1, C_2; R_1, R_2)$ is minimized.

(Zha et al, 2001)

Clustering of Directed Graphs

Min directed edge weights between A & B:

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

Max directed edges within A & B:

$$s(A,A) = \sum_{i \in A} \sum_{j \in A} (w_{ij} + w_{ji})$$

- Equivalent to deal with $\tilde{W} = W + W^T$
- All spectral methods apply to $\tilde{W}$
- For example, web graphs clustered in such way

(He, Ding, Zha, Simon, ICDM 2001)

K-way Spectral Clustering
$K \geq 2$

K-way Clustering Objectives

- Ratio Cut

$$J_{\text{Rcut}}(C_1,\cdots,C_K) = \sum_{<k,l>}\left(\frac{s(C_k,C_l)}{|C_k|}+\frac{s(C_k,C_l)}{|C_l|}\right)=\sum_k \frac{s(C_k,G-C_k)}{|C_k|}$$

- Normalized Cut

$$J_{\text{Ncut}}(C_1,\cdots,C_K) = \sum_{<k,l>}\left(\frac{s(C_k,C_l)}{d_k}+\frac{s(C_k,C_l)}{d_l}\right)=\sum_k \frac{s(C_k,G-C_k)}{d_k}$$

- Min-Max-Cut

$$J_{\text{MMC}}(C_1,\cdots,C_K) = \sum_{<k,l>}\left(\frac{s(C_k,C_l)}{s(C_k,C_k)}+\frac{s(C_k,C_l)}{s(C_l,C_l)}\right)=\sum_k \frac{s(C_k,G-C_k)}{s(C_k,C_k)}$$

K-way Spectral Relaxation

- Prove that the solution lie in the subspace spanned by the first k eigenvectors
- Ratio Cut
- Normalized Cut
- Min-Max-Cut

K-way Spectral Relaxation

Unsigned cluster indicators:

$$h_1 = (1\cdots1,0\cdots0,0\cdots0)^T$$
$$h_2 = (0\cdots0,1\cdots1,0\cdots0)^T$$
$$\cdots\cdots\cdots$$
$$h_k = (0\cdots0,0\cdots0,1\cdots1)^T$$

Re-write:

$$J_{\mathbf{Rcut}}(h_1,\cdots,h_k) = \frac{h_1^T(D-W)h_1}{h_1^T h_1} + \cdots + \frac{h_k^T(D-W)h_k}{h_k^T h_k}$$

$$J_{\mathbf{Ncut}}(h_1,\cdots,h_k) = \frac{h_1^T(D-W)h_1}{h_1^T Dh_1} + \cdots + \frac{h_k^T(D-W)h_k}{h_k^T Dh_k}$$

$$J_{\mathbf{MMC}}(h_1,\cdots,h_k) = \frac{h_1^T(D-W)h_1}{h_1^T Wh_1} + \cdots + \frac{h_k^T(D-W)h_k}{h_k^T Wh_k}$$

K-way Ratio Cut Spectral Relaxation

Unsigned cluster indicators: $x_k = (0\cdots0,\overbrace{1\cdots1}^{n_k},0\cdots0)^T / n_k^{1/2}$

Re-write: $J_{\mathbf{Rcut}}(x_1,\cdots,x_k) = x_1^T(D-W)x_1 + \cdots + x_k^T(D-W)x_k$

$$= \mathbf{Tr}(X^T(D-W)X) \qquad X = (x_1,\cdots,x_k)$$

$$\textbf{Optimize}: \min_X \mathbf{Tr}(X^T(D-W)X), \textbf{subject to} \quad X^T X = I$$

By K. Fan's theorem, optimal solution is eigenvectors: $X=(v_1,v_2,\ldots,v_k)$, $(D-W)v_k=\lambda_k v_k$

and lower-bound

$$\lambda_1 + \cdots + \lambda_k \le \min J_{\mathbf{Rcut}}(x_1,\cdots,x_k)$$

(Chan, Schlag, Zien, 1994)

K-way Normalized Cut Spectral Relaxation

Unsigned cluster indicators:

$$y_k = D^{1/2}(0\cdots 0,\overbrace{1\cdots 1}^{n_k},0\cdots 0)^T / \| D^{1/2} h_k \|$$

Re-write:

$$J_{\mathbf{Ncut}}(y_1,\cdots,y_k) = y_1^T(I-\tilde{W})y_1 + \cdots + y_k^T(I-\tilde{W})y_k$$
$$= \mathbf{Tr}(Y^T(I-\tilde{W})Y) \qquad \tilde{W} = D^{-1/2}WD^{-1/2}$$

$$\textbf{Optimize : } \min_Y \mathbf{Tr}(Y^T(I-\tilde{W})Y), \textbf{ subject to } \; Y^TY = I$$

By K. Fan's theorem, optimal solution is eigenvectors: $Y=(v_1,v_2, \ldots, v_k)$, $\quad (I-\tilde{W})v_k = \lambda_k v_k$

$$(D-W)u_k = \lambda_k D u_k, \quad u_k = D^{-1/2} v_k$$

$$\lambda_1 + \cdots + \lambda_k \le \min J_{\mathbf{Ncut}}(y_1,\cdots,y_k)$$

(Gu, et al, 2001)

K-way Min-Max Cut Spectral Relaxation

Unsigned cluster indicators:

$$y_k = D^{1/2}h_k / \| D^{1/2} h_k \| \qquad \tilde{W} = D^{-1/2}WD^{-1/2}$$

Re-write:

$$J_{\mathbf{MMC}}(y_1,\cdots,y_k) = \frac{1}{y_1^T\tilde{W}y_1} + \cdots + \frac{1}{y_k^T\tilde{W}y_k} - k$$

$$\textbf{Optimize : } \min_Y J_{MMC}(Y), \quad \textbf{subject to } \; Y^TY = I, \; y_k^T\tilde{W}y_k > 0.$$

Theorem. Optimal solution is by eigenvectors:
$Y=(v_1,v_2, \ldots, v_k)$, $\quad \tilde{W}v_k = \lambda_k v_k$

$$\frac{k^2}{\lambda_1 + \cdots + \lambda_k} - k \le \min J_{\mathbf{MMC}}(y_1,\cdots,y_k)$$

(Gu, et al, 2001)

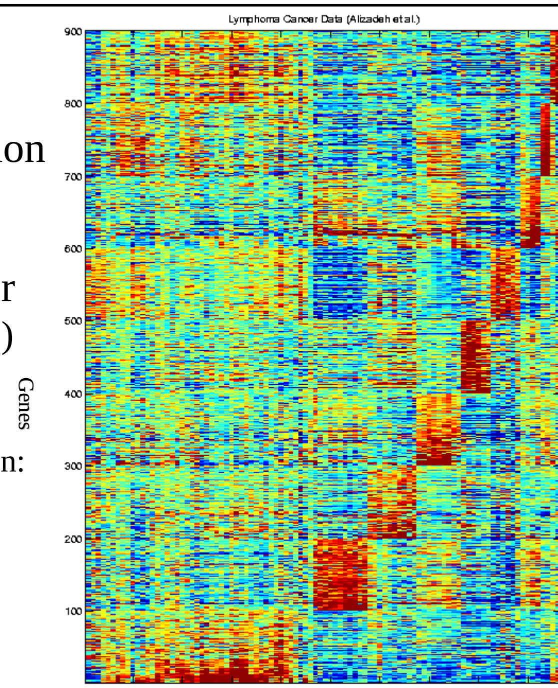
K-way Spectral Clustering

- Embedding (similar to PCA subspace approach)
  - Embed data points in the subspace of the *K* eigenvectors
  - Clustering embedded points using another algorithm, such as *K*-means (Shi & Malik, Ng et al, Zha, et al)
- Recursive 2-way clustering (standard graph partitioning)
  - If desired K is not power of 2, how optimcally to choose the next sub-cluster to split? (Ding, et al 2002)
- Both above approach do not use *K*-way clustering objective functions.
- Refine the obtained clusters using the *K*-way clustering objective function typically improve the results (Ding et al 2002).

DNA Gene expression

Lymphoma Cancer
(Alizadeh et al, 2000)

Effects of feature selection:
Select 900 genes out of
4025 genes



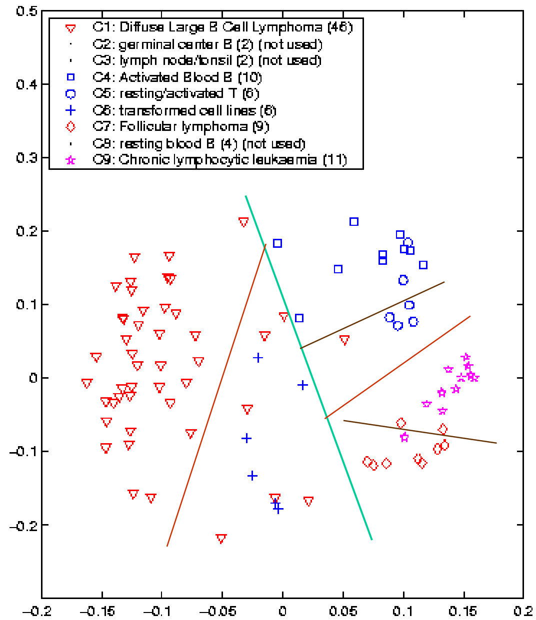
Lymphoma Cancer Tissue samples

B cell lymphoma go thru different stages

–3 cancer stages

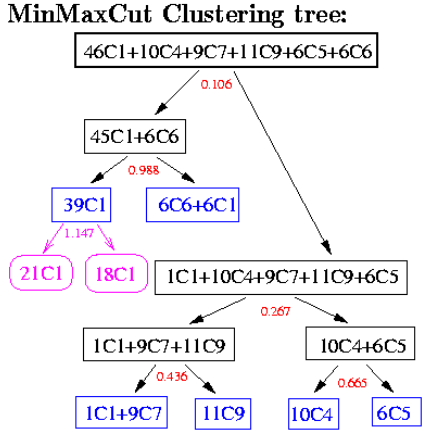
–3 normal stages

Key question: can we detect them automatically ?



PCA 2D Display

MinMaxCut Clustering tree:



Clustering results:

$$\begin{bmatrix} 39 & \cdot & 1 & \cdot & \cdot & 6 \\ \cdot & 10 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 9 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 11 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 6 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 6 \end{bmatrix}, \quad Q = 92.1\%$$

We believe OCI-Ly3, OCI-Ly10, DLCL-0042, and DLCL-0017 of C1 should belong to C6.

Brief summary of Part I

- Spectral graph partitioning as origin
- Clustering objective functions and solutions
- Extensions to bipartite and directed graphs
- Characteristics
  - Principled approach
  - Well-motivated objective functions
  - Clear, un-ambiguous
  - A framework of rich structures and contents
  - Everything is proved rigorously (within the relaxation framework, i.e., using continuous approximation of the discrete variables)
- Above results mostly done by 2001.
- More to come in Part II