A Tutorial on Spectral Clustering
Part 2: Advanced/related Topics

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Advanced/related Topics

- Spectral embedding: simplex cluster structure
- Perturbation analysis
- K-means clustering in embedded space
- Equivalence of K-means clustering and PCA
- Connectivity networks: scaled PCA & Green's function
- Extension to bipartite graphs: Correspondence analysis
- Random talks and spectral clustering
- Semi-definite programming and spectral clustering
- Spectral ordering (distance-sensitive ordering)
- Webpage spectral ranking: Page-Rank and HITS

Spectral Embedding: Simplex Cluster Structure

- Compute K eigenvectors of the Laplacian.
- Embed objects in the K-dim eigenspace

What is the structure of the clusters?

Simplex Embedding Theorem.

Assume objects are well characterized by spectral clustering objective functions. In the embedded space, objects aggregate to K distinct centroids:

- Centroids locate on K corners of a simplex
  - Simplex consists K basis vectors + coordinate origin
  - Simplex is rotated by an orthogonal transformation T
  - Columns of T are eigenvectors of a $K \times K$ embedding matrix Γ

(Ding, 2004)

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K-way Clustering Objectives

$$J = \sum_{1 \le p < q \le K} \frac{s(C_p, C_q)}{\rho(C_p)} + \frac{s(C_p, C_q)}{\rho(C_q)} = \sum_k \frac{s(C_p, G - C_q)}{\rho(C_p)}$$

$$\rho(C_k) = \begin{cases} n_k = |C_k| & \textbf{for Ratio Cut} \\ d(C_k) = \sum_{i \in C_k} d_i & \textbf{for Normalized Cut} \\ s(C_k, C_k) = \sum_{i \in C_k, j \in C_k} w_{ij} & \textbf{for MinMaxCut} \end{cases}$$

G - C_k is the graph complement of C_k

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Simplex Spectral Embedding Theorem

Simplex Orthogonal Transform Matrix $T = (\mathbf{t}_1, \cdots, \mathbf{t}_K)$

T are determined by: $\Gamma \mathbf{t}_k = \lambda_k \mathbf{t}_k$

Spectral Perturbation Matrix $\Gamma = \Omega^{-\frac{1}{2}} \overline{\Gamma} \Omega^{-\frac{1}{2}}$

$$\overline{\Gamma} = \begin{bmatrix} h_{11} & -s_{12} & \cdots & -s_{1K} \\ -s_{21} & h_{22} & \cdots & -s_{2K} \\ \vdots & \vdots & \cdots & \vdots \\ -s_{K1} & -s_{K2} & \cdots & h_{KK} \end{bmatrix}$$

$$s_{pq} = s(C_p, C_q)$$

$$h_{kk} = \sum_{p|p \neq k} s_{kp}$$

$$\Omega = \mathbf{diag}[\rho(C_1), \cdots, \rho(C_k)]$$

Properties of Spectral Embedding

- Original basis vectors:

$$h_k = (0 \cdots 0, \overbrace{1 \cdots 1}^{n_k}, 0 \cdots 0) / n_k$$

- Dimension of embedding is K-1: (q_2, ... q_K)
  - $q_1 = (1, \ldots, 1)^T$ is constant & trivial
  - Eigenvalues of Γ (=eigenvalues of D-W)
  - Eigenvalues determine how well clustering objective function characterize the data
- Exact solution for K=2

2-way Spectral Embedding (Exact Solution)

Eigenvalues

$$\lambda_{\mathrm{Rcut}} = \frac{s(C_1,C_2)}{n(C_1)} + \frac{s(C_1,C_2)}{n(C_2)},\ \lambda_{\mathrm{Ncut}} = \frac{s(C_1,C_2)}{d(C_1)} + \frac{s(C_1,C_2)}{d(C_2)},\ \lambda_{\mathrm{MMC}} = \frac{s(C_1,C_2)}{s(C_1,C_1)} + \frac{s(C_1,C_2)}{s(C_2,C_2)}$$

Recover the original 2-way clustering objectives

For Normalized Cut, orthogonal transform T rotates

$$h_1 = (1\cdots 1,0\cdots 0)^T\ ,\quad h_2 = (0\cdots 0,1\cdots 1)^T$$

into

$$q_1 = (1\cdots 1)^T,\quad q_2 = (a,\cdots,a,-b,\cdots,-b)^T$$

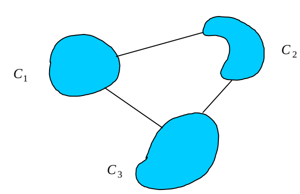
Spectral clustering inherently consistent! (Ding et al, KDD'01)

Perturbation Analysis

$$Wq = \lambda Dq \qquad \hat{W}z = (D^{-1/2}WD^{-1/2})z = \lambda z \quad q = D^{-1/2}z$$

Assume data has 3 dense clusters sparsely connected.

$$W = \begin{bmatrix} W_{11} & W_{12} & W_{13} \\ W_{21} & W_{22} & W_{23} \\ W_{31} & W_{32} & W_{33} \end{bmatrix}$$



Off-diagonal blocks are between-cluster connections, assumed small and are treated as a perturbation

(Ding et al, KDD'01)

Perturbation Analysis

0th order:

$$W^{(0)} = \begin{bmatrix} W_{11} & & \\ & W_{22} & \\ & & W_{33} \end{bmatrix} \qquad \hat{W}^{(0)} = \begin{bmatrix} \hat{W}_{11}^{(0)} & & \\ & \hat{W}_{22}^{(0)} & \\ & & \hat{W}_{33}^{(0)} \end{bmatrix}$$

1st order:

$$W^{(1)} = \begin{bmatrix} & W_{12} & W_{13} \\ W_{21} & & W_{23} \\ W_{31} & W_{32} & \end{bmatrix} \qquad \hat{W}^{(1)} = \begin{bmatrix} \hat{W}_{11} - \hat{W}_{11}^{(0)} & \hat{W}_{12} & \hat{W}_{13} \\ \hat{W}_{21} & \hat{W}_{22} - \hat{W}_{22}^{(0)} & \hat{W}_{23} \\ \hat{W}_{31} & \hat{W}_{32} & \hat{W}_{33} - \hat{W}_{33}^{(0)} \end{bmatrix}$$

$$\hat{W}_{pq}^{(0)} = D_{pp}^{-1/2} W_{pq} D_{qq}^{-1/2}$$

$$\hat{W}_{pq} = (D_{p1} + D_{p2} + D_{p3})^{-1/2} W_{pq} (D_{q1} + D_{q2} + D_{q3})^{-1/2}$$

K-means clustering

- Developed in 1960's (Lloyd, MacQueen, etc)
- Computationally Efficient (order-*mN*)
- Widely used in practice
  – Benchmark to evaluate other algorithms

Given *n* points in *m*-dim: $X = (x_1, x_2, \cdots, x_n)$

K-means $\min J_K = \sum_{k=1}^{K} \sum_{i \in C_k} || x_i - c_k ||^2$

K-means Clustering in Spectral Embedded Space

Simplex spectral embedding theorem provides theoretical basis for K-means clustering in the embedded eigenspace

- Cluster centroids are well separated (corners of the simplex)
- *K*-means clustering is invariant under (i) coordinate rotation $x \rightarrow Tx$, and (ii) shift $x \rightarrow x + a$
- Thus orthogonal transform T in simplex embedding unnecessary

• Many variants of K-means (Ng et al, Bach & Jordan, Zha et al, Shi & Xu, etc)

We have proved

Spectral embedding + *K*-means clustering is the appropriate method

We now show :

K-means itself is solved by PCA

Equivalence of *K*-means Clustering and Principal Component Analysis

- Cluster indicators specify the solution of *K*-means clustering
- Principal components are eigenvectors of the Gram (Kernel) matrix = data projections in the principal directions of the covariance matrix
- Optimal solution of K-means clustering: continuous solution of the discrete cluster indicators of *K*-means are given by Principal components

(Zha et al, NIPS'01; Ding & He, 2003)

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Principal Component Analysis (PCA)

- Widely used in large number of different fields
  - Best low-rank approximation (SVD Theorem, Eckart-Young, 1930) : Noise reduction
  - Unsupervised dimension reduction
  - Many generalizations
- Conventional perspective is inadequate to explain the effectiveness of PCA
- New results: Principal components are cluster indicators for well-motivated clustering objective

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Principal Component Analysis

n points in m-dim: $X = (x_1, x_2, \cdots, x_n)$

Principal directions: u_k

Covariance $S = XX^T$ $\quad XX^T u_k = \lambda_k u_k$

Principal components: v_k

Gram (Kernel) matrix $X^T X$ $\quad X^T X v_k = \lambda_k v_k$

Singular Value Decomposition: $X = \sum_{k=1}^{m} \lambda_k u_k v_k^T$

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2-way K-means Clustering

Cluster membership indicator:

$$q(i) = \begin{cases} +\sqrt{n_2 / n_1 n} & \text{if } i \in C_1 \\ -\sqrt{n_1 / n_2 n} & \text{if } i \in C_2 \end{cases}$$

$$J_K = n\langle x^2 \rangle - J_D, \quad J_D = \frac{n_1 n_2}{n}\left[2\frac{d(C_1,C_2)}{n_1 n_2} - \frac{d(C_1,C_1)}{n_1^2} - \frac{d(C_2,C_2)}{n_2^2} \right]$$

Define distance matrix: $D = (d_{ij}),\ d_{ij} = |x_i - x_j|^2$

$$J_D = -q^T D q = -q^T \tilde{D} q = 2 q^T X^T X q$$

$\tilde{D}$ is the centered distance matrix

$$\min J_K \Rightarrow \max J_D$$

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2-way K-means Clustering

Cluster indicator satisfy: $\sum_i q(i) = 0, \sum_i q^2(i) = 1$

Relax the restriction q (i) take discrete values. Let it take continuous values in [-1,1]. Solution for q is the eigenvector of the Gram matrix.

Theorem: The (continuous) optimal solution of q is given by the principal component v_1 .

Clusters C_1, C_2 are determined by:

$$C_1 = \{i \mid v_1(i) < 0\}, C_2 = \{i \mid v_1(i) \geq 0\}$$

Once C_1, C_2 are computed, iterate ***K***-mean to convergence

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Multi-way K-means Clustering

Unsigned Cluster membership indicators $h_1, \cdots, h_K$:

$$\begin{array}{ccc} C_1 & C_2 & C_3 \end{array}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = (h_1, h_2, h_3)$$

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Multi-way K-means Clustering

For $K \geq 2$, $J_K = \sum_i x_i^2 - \sum_{k=1}^{K} \frac{1}{n_k} \sum_{i,j \in C_k} x_i^T x_j$

(Unsigned) Cluster membership indicators $h_1, \cdots, h_K$:

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

$$J_K = \sum_i x_i^2 - \sum_{k=1}^{K} h_k^T X^T X h_k$$

Let $H = (h_1, \cdots, h_K)$

$$J_K = \sum_i x_i^2 - \mathrm{Tr}(H_k^T X^T X H_k)$$

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Multi-way K-means Clustering

Regularized Relaxation of *K*-means Clustering

Redundancy in $h_1, \cdots, h_K$: $\sum_{k=1}^{K} n_k^{1/2} h_k = e = (11 \cdots 1)^T$

Transform to signed indicator vectors q_1 - q_k via the k x k orthogonal matrix T:

$$(q_1, ..., q_k) = (h_1, \cdots, h_k) T \qquad Q_k = H_k T$$

Require 1st column of T = $(n_1^{1/2}, \cdots, n_k^{1/2})^T / n^{1/2}$

Thus $q_1 = e / n^{1/2} = \text{const}$

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Regularized Relaxation of *K*-means Clustering

$$J_K = Tr(Y^T Y) - Tr(Q_{k-1}^T Y^T Y Q_{k-1})$$

(Regularized relaxation) $$Q_{k-1} = (q_2, \ldots, q_k)$$

Theorem: The optimal solutions of $q_2 \cdots q_k$ are given by the principal components $v_2 \cdots v_k$. J_K is bounded below by total variance minus sum of K eigenvalues of covariance:

$$n\overline{y^2} - \sum_{k=1}^{K-1} \lambda_k < \min J_K < n\overline{y^2}$$

Scaled PCA

similarity matrix $S=(s_{ij})$ (generated from XX^T)

$$D = \mathrm{diag}(d_1, \cdots, d_n) \qquad d_i = s_{i.}$$

Nonlinear re-scaling: $\tilde{S} = D^{-\frac{1}{2}} S D^{-\frac{1}{2}}, \tilde{s}_{ij} = s_{ij} / (s_{i.} s_{j.})^{1/2}$

Apply SVD on $\tilde{S} \Rightarrow$

$$S = D^{\frac{1}{2}} \tilde{S} D^{\frac{1}{2}} = D^{\frac{1}{2}} \sum_k z_k \lambda_k z_k^T D^{\frac{1}{2}} = D \left[\sum_k q_k \lambda_k q_k^T \right] D$$

$q_k = D^{-1/2} z_k$ is the scaled principal component

Subtract trivial component $\lambda_0 = 1,\ z_0 = d^{1/2}/s..,\ q_0 = 1$

$$\Rightarrow \quad S - dd^T/s.. = D \sum_{k=1} q_k \lambda_k q_k^T D$$

(Ding, et al, 2002)

Optimality Properties of Scaled PCA

Scaled principal components have optimality properties:

Ordering

– Adjacent objects along the order are similar
– Far-away objects along the order are dissimilar
– Optimal solution for the permutation index are given by scaled PCA.

Clustering

– Maximize within-cluster similarity
– Minimize between-cluster similarity
– Optimal solution for cluster membership indicators given by scaled PCA.

Difficulty of *K*-way clustering

- 2-way clustering uses a single eigenvector
- *K*-way clustering uses several eigenvectors
- How to recover 0-1 cluster indicators *H*?

eigenvectors : $Q = (q_1, ..., q_k)$

has both positive and negative entries

indicators : $H = (h_1, \cdots, h_k)$ $\quad Q = HT$

Avoid computing the transformation *T*:

- Do *K*-means, which is invariant under *T*
- Compute connectivity network QQ^T, which cancels *T*

Connectivity Network

$$C_{ij} = \begin{cases} 1 & \text{if } i, j \text{ belong to same cluster} \\ 0 & \text{otherwise} \end{cases}$$

SPCA provides $C \cong D \sum_{k=1}^{K} q_k \lambda_k q_k^T D$

Green's function : $C \approx G = \sum_{k=2}^{K} q_k \frac{1}{1-\lambda_k} q_k^T$

Projection matrix: $C \approx P \equiv \sum_{k=1}^{K} q_k q_k^T$

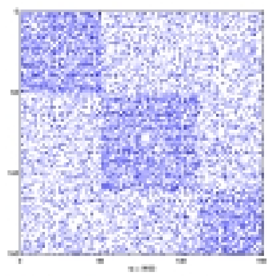
(Ding et al, 2002)

Connectivity network

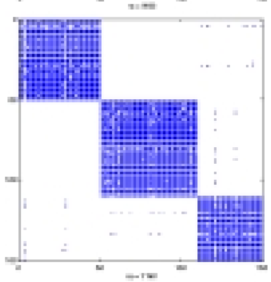
- Similar to Hopfield network
- Mathematical basis: projection matrix
- Show self-aggregation clearly
- Drawback: how to recover clusters
  - Apply *K*-means directly on *C*
  - Use linearized assignment with cluster crossing and spectral ordering (ICML'04)

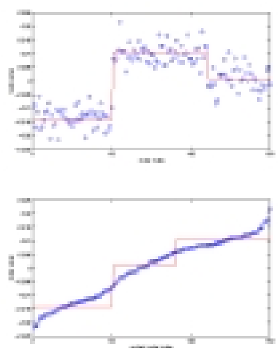
Connectivity network: Example 1

Similarity matrix W



Connectivity matrix





$\lambda_2 = 0.300, \bar{\lambda}_2 = 0.268$

Between-cluster connections suppressed

Within-cluster connections enhanced

Effects of self-aggregation

Connectivity of Internet Newsgroups

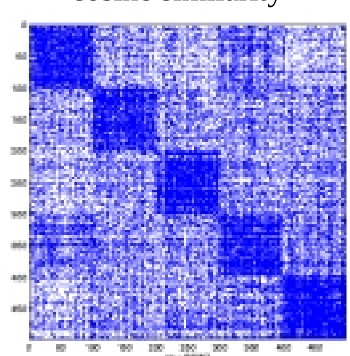
NG2: comp.graphics
NG9: rec.motorcycles
NG10: rec.sport.baseball
NG15:sci.space
NG18:talk.politics.mideast

100 articles from each group.
1000 words
Tf.idf weight. Cosine similarity

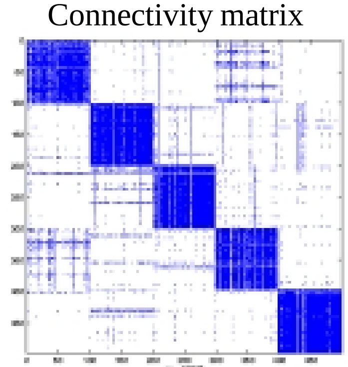
Spectral Clustering 89%

Direct *K*-means 66%

cosine similarity

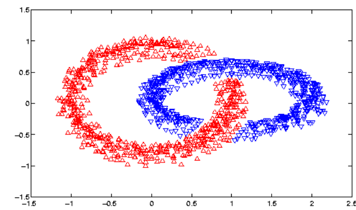


Connectivity matrix

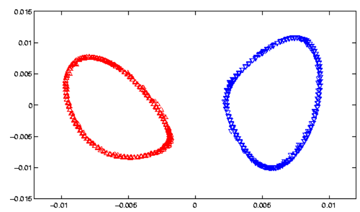


Spectral embedding is not topology preserving

700 3-D data points form 2 interlock rings



In eigenspace, they shrink and separate



Correspondence Analysis (CA)

- Mainly used in graphical display of data
- Popular in France (Benzécri, 1969)
- Long history
  - Simultaneous row and column regression (Hirschfeld, 1935)
  - Reciprocal averaging (Richardson & Kuder, 1933; Horst, 1935; Fisher, 1940; Hill, 1974)
  - Canonical correlations, dual scaling, etc.
- Formulation is a bit complicated ("convoluted" Jolliffe, 2002, p.342)
- "A neglected method", (Hill, 1974)

Scaled PCA on a Contingency Table ⇒ Correspondence Analysis

Nonlinear re-scaling: $\tilde{P} = D_r^{-\frac{1}{2}} P D_c^{-\frac{1}{2}}, \ \tilde{p}_{ij} = p_{ij} / (p_{i.} p_{j.})^{1/2}$

Apply SVD on $\tilde{P}$ Subtract trivial component

$$P - rc^T / p_{..} = D_r \sum_{k=1} f_k \lambda_k g_k^T D_c$$

$$r = (p_{1.}, \cdots, p_{n.})^T$$

$$c = (p_{.1}, \cdots, p_{.n})^T$$

$$f_k = D_r^{-\frac{1}{2}} u_k, \ g_k = D_c^{-\frac{1}{2}} v_k$$

are the scaled row and column principal component (standard coordinates in CA)

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Information Retrieval

Bell Lab tech memos

5 comp-sci and 4 applied-math memo titles:

C1: Human machine interface for lab ABC computer applications

C2: A survey of user opinion of computer system response time

C3: The EPS user interface management system

C4: System and human system engineering testing of EPS

C5: Relation of user-perceived response time to error management

M1: The generation of random, binary, unordered trees

M2: The intersection graph of paths in trees

M3: Graph minors IV: widths of trees and well-quasi-ordering

M4: Graph minors: A survey

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Word-document matrix: row/col clustering

words \ docs	c4	c1	c3	c5	c2	m4	m3	m2	m1
human	1	1							
EPS	1		1						
interface		1	1						
system	2		1		1				
computer					1				
user				1	1				
response				1	1				
time				1	1				
survey					1	1			
minors						1	1		
graph						1	1	1	
tree							1	1	1

Bipartite Graph: 3 types of Connectivity networks

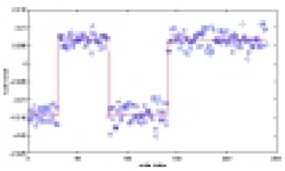
$$Q_K Q_K^T = \begin{bmatrix} F_K F_K^T & F_K G_K^T \\ G_K F_K^T & G_K G_K^T \end{bmatrix} \qquad Q_K = (\mathbf{q}_1, \cdots, \mathbf{q}_K) = \begin{bmatrix} F_K \\ G_K \end{bmatrix}$$

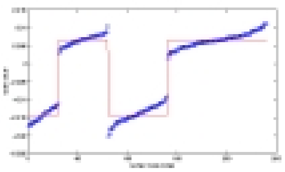
$$F_K F_K^T = \begin{bmatrix} \mathbf{e}_{r_1}\mathbf{e}_{r_1}^T / 2s_{11} & 0 \\ 0 & \mathbf{e}_{r_2}\mathbf{e}_{r_2}^T / 2s_{22} \end{bmatrix}$$ row-row clustering

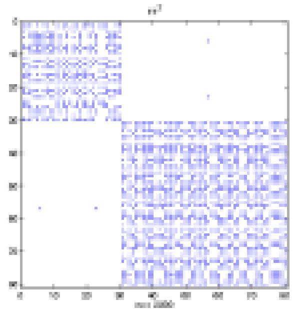
$$G_K G_K^T = \begin{bmatrix} \mathbf{e}_{c_1}\mathbf{e}_{c_1}^T / 2s_{11} & 0 \\ 0 & \mathbf{e}_{c_2}\mathbf{e}_{c_2}^T / 2s_{22} \end{bmatrix}$$ Column-column clustering

$$F_K G_K^T = \begin{bmatrix} \mathbf{e}_{r_1}\mathbf{e}_{c_1}^T / 2s_{11} & 0 \\ 0 & \mathbf{e}_{r_2}\mathbf{e}_{c_2}^T / 2s_{22} \end{bmatrix}$$ Row-column association

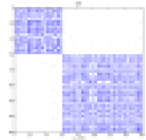
Example



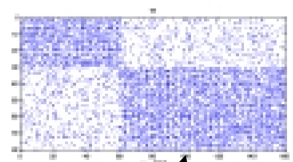




column-column: GG^T

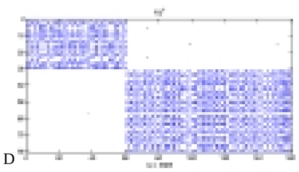


row-row: FF^T



Original data matrix

$\lambda_2 = 0.456, \bar{\lambda}_2 = 0.477$



row-column: FG^T

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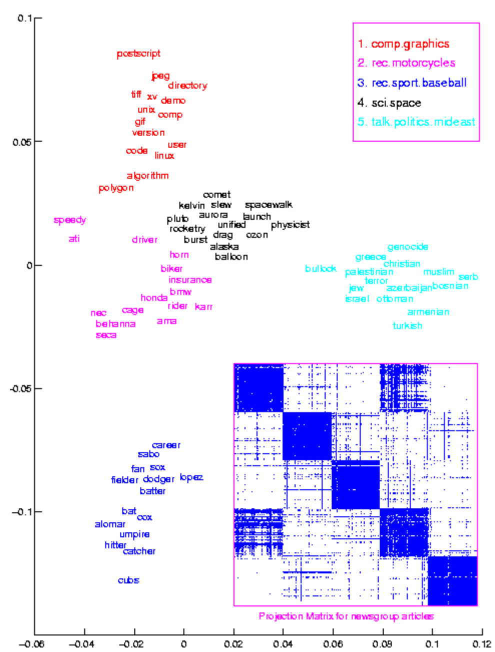
Internet Newsgroups

Simultaneous clustering of documents and words



Random Walks and Normalized Cut

Similarity matrix W, $\quad P = D^{-1}W$ Stochastic matrix

$\pi^T P = \pi^T \quad \Rightarrow$ equilibrium distribution: $\quad \pi = d$

$$Px = \lambda x \;\Rightarrow\; Wx = \lambda Dx \;\Rightarrow\; (D-W)x = (1-\lambda)Dx$$

Random walks between *A,B:*

$$J_{NormCut} = \frac{P(A \to B)}{\pi(A)} + \frac{P(B \to A)}{\pi(B)}$$

(Meila & Shi, 2001)

PageRank: $\quad P = \alpha L D_{out}^{-1} + (1-\alpha)ee^T$

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Semi-definite Programming for Normalized Cut

Normalized Cut :

$$y_k = D^{1/2}(0\cdots0,\overbrace{1\cdots1}^{n_k},0\cdots0)^T / \| D^{1/2}h_k \|$$

$$\tilde{W} = D^{-1/2}WD^{-1/2}$$

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

$\Rightarrow \mathrm{Tr}[(I-\tilde{W})YY^T] \qquad \Rightarrow \min\limits_{Z} \mathrm{Tr}[(I-\tilde{W})Z] \qquad \boxed{Z = YY^T}$

$$\boxed{s.t.\, Z \ge 0,\;\; Z \succ 0, Zd = d, \mathrm{Tr}\, Z = K,\;\; Z = Z^T}$$

Compute Z via SDP. $Z=Y'Y'^T$.
$Y''=D^{-1/2}Y'$. K-means on Y''.

(Xing & Jordan, 2003)

Z = connectivity network

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Spectral Ordering

Hill, 1970, spectral embedding

Find coordinate x to minimize

$$J = \sum_{ij} (x_i - x_j)^2 w_{ij} = x^T (D - W) x$$

Solution are eigenvectors of Laplacian

Barnard, Pothen, Simon, 1993, envelop reduction of sparse matrix: find ordering such that the envelop is minimized

$$\min \sum_{ij} (i-j)^2 w_{ij} \quad \Rightarrow \quad \min \sum_{ij} (\pi_i - \pi_j)^2 w_{ij}$$

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Distance-sensitive ordering

Ordering is determined by permutation indexes

4-variable. For a given ordering, there are 3 *distance*=1 pairs, two *d*=2 pairs, one *d*=3 pair.

$$\begin{bmatrix} 0 & 1 & 2 & 3 \\ & 0 & 1 & 2 \\ & & 0 & 1 \\ & & & 0 \end{bmatrix}$$

$$\pi(1,\cdots,n) = (\pi_1,\cdots,\pi_n)$$

$$J_d(\pi) = \sum_{i=1}^{n-d} s_{\pi_i,\pi_{i+d}}$$

$$\min_{\pi} J, \; J(\pi) = \sum_{d=1}^{n-1} d^2 J_d(\pi)$$

The larger distance, the larger weights. Large distance similarities reduced more than small distance similarities

(Ding & He, ICML'04) 40

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Distance-sensitive ordering

Theorem. The continuous optimal solution for the discrete inverse permutation indexes are given by the scaled principal component q_1.

The shifted and scaled inverse permutation indexes

$$q_i = \frac{\pi_i^{-1} - (n+1)/2}{n/2} = \{\frac{1-n}{n}, \frac{3-n}{n}, \cdots, \frac{n-1}{n}\}$$

Relax the restriction on q. Allow it be continuous.

Solution for q becomes the eigenvector of

$$(D-S)q = \lambda Dq$$

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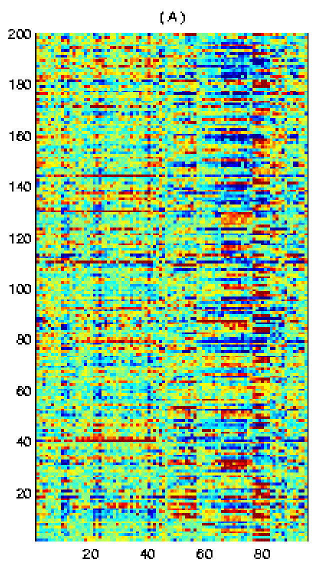
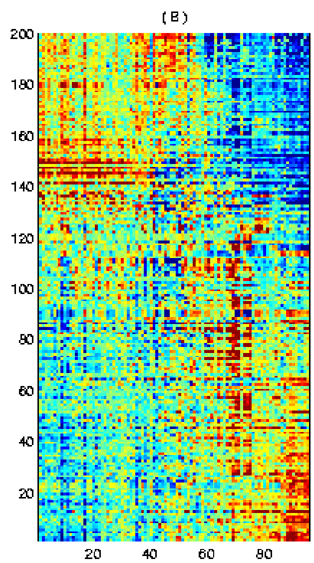
Re-ordering of Genes and Tissues





$$r = \frac{J(\pi)}{J(\text{random})}$$

$$r = 0.18$$

$$r_{d=1} = \frac{J_{d=1}(\pi)}{J_{d=1}(\text{random})}$$

$$r_{d=1} = 3.39$$

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C. Ding, RECOMB 2002

Webpage Spectral Ranking

Rank webpages from the hyperlink topology.

L : adjacency matrix of the web subgraph

PageRank (Page & Brin): rank according to principal eigenvector π (equilibrium distribution)

$$\pi T = \pi, \; T = 0.8 D_{out}^{-1} L + 0.2 e e^T$$

HITS (Kleinberg): rank according to principal eigenvector of authority matrix

$$(L^T L) q = \lambda q$$

Eigenvectors can be obtained in closed-form

Webpage Spectral Ranking

HITS (Kleinberg) ranking algorithm

Assume web graph is fixed degree sequence random graph (Aiello, Chung, Lu, 2000)

Theorem. Eigenvalues of $L^T L$

$$\lambda_1 > h_1 > \lambda_2 > h_2 > \cdots\cdots, \; h_i = d_i - \frac{d_i^2}{n-1}$$

Eigenvectors: $$u_k = \left(\frac{d_1}{\lambda_k - h_1}, \frac{d_2}{\lambda_k - h_2}, \cdots, \frac{d_n}{\lambda_k - h_n}\right)^T$$

Principal eigenvector u_1 is monotonic decreasing if $d_1 > d_2 > d_3 > \cdots\cdots$

$\Rightarrow$ HITS ranking is identical to indegree ranking

(Ding, et al, SIAM Review '04)

Webpage Spectral Ranking

PageRank: weight normalization

HITS : mutual reinforcement

Combine PageRank and HITS. Generalize. ⇒

Ranking based on a similarity graph $S = L^T D_{out}^{-1} L$

Random walks on this similarity graph has the equilibrium distribution: $(d_1, d_2, \cdots, d_n)^T / 2E$

PageRank ranking is identical to indegree ranking

(1st order approximation, due to combination of PageRank & HITS)

(Ding, et al, SIGIR'02)

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PCA: a Unified Framework for clustering and ordering

- PCA is equivalent to *K*-means Clustering
- Scaled PCA has two optimality properties
  - Distance sensitive ordering
  - Min-max principle Clustering
- SPCA on contingency table ⇒ Correspondence Analysis
  - Simultaneous ordering of rows and columns
  - Simultaneous clustering of rows and columns
- Resolve open problems
  - Relationship between Correspondence Analysis and PCA (open problem since 1940s)
  - Relationship between PCA and *K*-means clustering (open problem since 1960s)

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Spectral Clustering:

a rich spectrum of topics

a comprehensive framework for learning

A tutorial & review of spectral clustering

Tutorial website will post all related papers (send your papers)

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