



Spectral clustering

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主要参考文献: A Tutorial on Spectral Clustering





Agenda

- Brief Clustering Review
- Similarity Graph
- Graph Laplacian
- Spectral Clustering Algorithm
- Graph Cut Point of View
- Practical Details





Brief Clustering Review

- Similarity Graph
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子科技士等 Brief Clustering Review



Clustering

Groups together "similar" instances in the data sample

Basic clustering problem:

- distribute data into k different groups such that data points similar to each other are in the same group
- Similarity between data points is defined in terms of some distance metric (can be chosen)

Clustering is useful for:

- Similarity/Dissimilarity analysis
 Analyze what data points in the sample are close to each other
- Dimensionality reduction
 High dimensional data replaced with a group (cluster) label

子科技士学 Brief Clustering Review



K-MEANS CLUSTERING

• Description

Given a set of observations $(\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_n)$, where each observation is a *d*-dimensional real vector, *k*-means clustering aims to partition the *n* observations into *k* sets $(k \le n)$ $\mathbf{S} = \{S_1, S_2, ..., S_k\}$ so as to minimize the within-cluster sum of squares (WCSS):

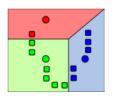
$$\underset{S}{\operatorname{arg\,min}} \sum_{i=1}^{k} \sum_{x_{i} \in S_{i}} ||x_{j} - u_{i}||^{2}$$

where μ_i is the mean of points in S_i .

• Standard Algorithm



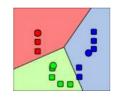
1) k initial "means" (in this case k=3) are randomly selected from the data set.



2) k clusters are created by associating every observation with the nearest mean.



3) The centroid of each of the k clusters becomes the new means.



4) Steps 2 and 3 are repeated until convergence has been reached.





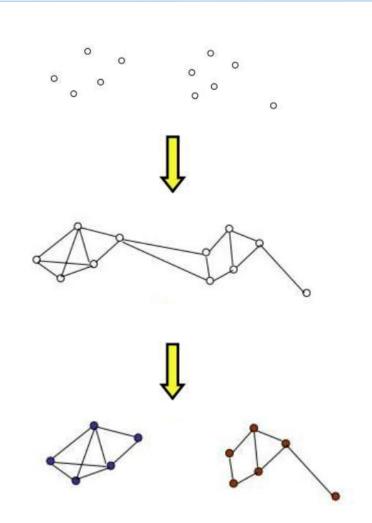
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First - graph representation of data (largely, application dependent)

Then - graph partitioning



Disconnected graph components



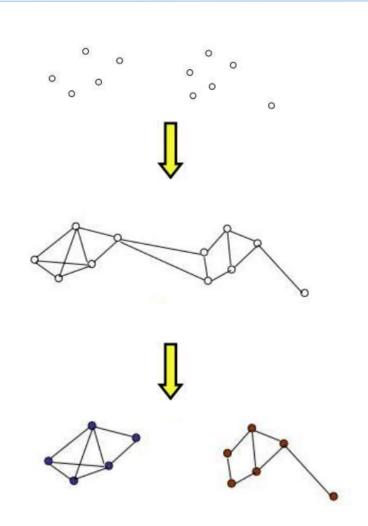
Groups of points (Weakly connections in between components Strongly connections within components)





First - graph representation of data (largely, application dependent)

Then - graph partitioning



Disconnected graph components



Groups of points (Weakly connections in between components Strongly connections within components)



・ 科域大学 Similarity Graph

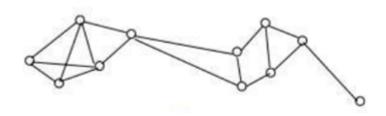


set of n data points x_1, \ldots, x_n with similarites $s_{i,j} \ge 0$ between all pairs of data points x_i, \ldots, x_j

 $\mathbf{\uparrow}$ represent in a similarity graph G = (V, E)

each vertex v_i represents a data point x_i two vertices are connected, if $s_{i,j}$ is larger than a certain threshold, and the edge ist weighted by $s_{i,j}$



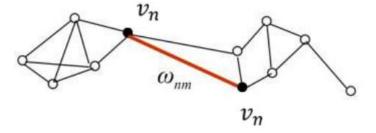


we want to find a partition of the graph such that the edges between different groups have very low weights (which means that points in different clusters are dissimilar from each other) and the edges within a group have high weights (which means that points within the same cluster are similar to each other).

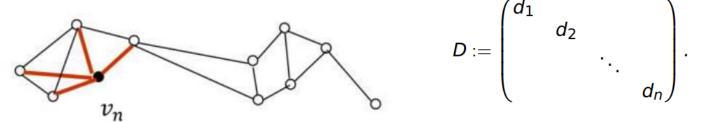


$$G=(V,E)$$
:

- Vertex set $V = \{v_1, \dots, v_n\}$
- Weighted adjacency matrix $W = (w_{ij}) i, j = 1, ..., n \quad w_{ij} \ge 0$



• Degree $d_i = \sum_{j=1}^n w_{ij}$



• Degree matrix Diagonal matrix with the degrees $d_1, ..., d_n$ on the diagonal.

子科技大学 Graph notation

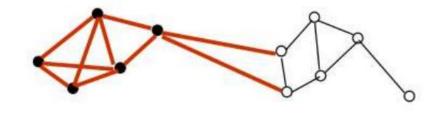


$$G=(V,E)$$
:

- Indicator Vector $\mathbb{1}_A = (f_1, ..., f_n)' \in \mathbb{R}^n$ $f_i \in \{0,1\}$
- "Size" of a subset $A \subset V$

$$|A| := \text{the number of vertices in } A$$

 $vol(A) := \sum_{i=1}^{n} d_i$



- A subset A of a graph is connected if any two vertices in A can be joined by a path such that all intermediate points also lie in A.
- Connected Component it is connected and if there are no connections between vertices in A and \bar{A} . The nonempty sets A_1, \dots, A_k form a partition of the graph if $A_i \cap A_i = \emptyset$ and $A_1 \cup \cdots \cup A_k = V$.



SIMILARITY GRAPH



ε-neighborhood graph

Connect all points whose pairwise distances are smaller than ε

$$W_{ij} = \left\{egin{array}{ll} 0 & s_{ij} > \epsilon \ \epsilon & s_{ij} \leq \epsilon \end{array}
ight.$$

• *k*-nearest neighbor graph

Connect vertex v_i with vertex v_j if v_j is among the k-nearest neighbors of v_i .

$$W_{ij} = W_{ji} = egin{cases} 0 & x_i
otin KNN(x_j) \ and \ x_j
otin KNN(x_i) \ exp(-rac{||x_i - x_j||_2^2}{2\sigma^2}) & x_i
otin KNN(x_j) \ or \ x_j
otin KNN(x_i) \end{cases}$$

fully connected graph

Connect all points with positive similarity with each other

$$W_{ij} = S_{ij} = exp(-rac{\left|\left|x_i - x_j
ight|
ight|_2^2}{2\sigma^2})$$

All the above graphs are regularly used in spectral clustering!





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Unnormalized Graph Laplacian

$$d_i = \sum_{j=1}^n w_{ij}$$

$$L = D - W$$

For every vector $f \in \mathbb{R}^n$ we have

$$f'Lf = \frac{1}{2} \sum_{i,j=1}^{n} w_{ij} (f_i - f_j)^2.$$

By the definition of d_i ,

$$f'Lf = f'Df - f'Wf = \sum_{i=1}^{n} d_i f_i^2 - \sum_{i,j=1}^{n} f_i f_j w_{ij}$$
$$= \frac{1}{2} \left(\sum_{i=1}^{n} d_i f_i^2 - 2 \sum_{i,j=1}^{n} f_i f_j w_{ij} + \sum_{i=1}^{n} d_j f_j^2 \right) = \frac{1}{2} \sum_{i,j=1}^{n} w_{ij} (f_i - f_j)^2.$$



• Unnormalized Graph Laplacian

$$d_i = \sum_{j=1}^n w_{ij}$$

$$L = D - W$$

Proposition 1 (Properties of L) The matrix L satisfies the following properties:

1. For every vector $f \in \mathbb{R}^n$ we have

$$f'Lf = \frac{1}{2} \sum_{i,j=1}^{n} w_{ij} (f_i - f_j)^2.$$

- 2. L is symmetric and positive semi-definite.
- 3. The smallest eigenvalue of L is 0, the corresponding eigenvector is the constant one vector $\mathbb{1}$.
- 4. L has n non-negative, real-valued eigenvalues $0 = \lambda_1 \le \lambda_2 \le \ldots \le \lambda_n$.



• Unnormalized Graph Laplacian

$$d_i = \sum_{j=1}^n w_{ij}$$

$$L = D - W$$

Proposition 2 (Number of connected components and the spectrum of L) Let G be an undirected graph with non-negative weights. Then the multiplicity k of the eigenvalue 0 of L equals the number of connected components A_1, \ldots, A_k in the graph. The eigenspace of eigenvalue 0 is spanned by the indicator vectors $1_{A_1}, \ldots, 1_{A_k}$ of those components.

Proof:

When k = 1, a graph consisting of only one connected component we thus only have the constant one vector \mathbb{I} as eigenvector with eigenvalue 0, which obviously is the indicator vector of the connected component.

When k > 1, L can be written in a block form. the spectrum of L is given by the union of the spectra of L_i , and the corresponding eigenvectors of L are the eigenvectors of L_i , filled with 0 at the positions of the other blocks.

$$L = egin{pmatrix} L_1 & & & & \ & L_2 & & & \ & & \ddots & & \ & & & L_k \end{pmatrix}$$





Normalized Graph Laplacian

$$L_{sym} := D^{-\frac{1}{2}}LD^{-\frac{1}{2}} = I - D^{-\frac{1}{2}}WD^{-\frac{1}{2}}$$
$$L_{rw} := D^{-1}L = I - D^{-1}W$$

We denote the first matrix by L_{sym} as it is a symmetric matrix, and the second one by L_{rw} as it is closely related to a random walk.





Normalized Graph Laplacian

Proposition 3 (Properties of L_{sym} and L_{rw}) The normalized Laplacians statisfy the following properties:

1. For every
$$f \in \mathbb{R}^n$$
 we have $f'L_{sym}f = \frac{1}{2}\sum_{i,j=1}^n w_{ij}^2 \left(\frac{f_i}{\sqrt{d_i}} - \frac{f_j}{\sqrt{d_j}}\right)^2$

- 2. λ is an eigenvalue of L_{rw} with eigenvector u if and only if λ is an eigenvalue of L_{sym} with eigenvector $w = D^{1/2}u$.
- 3. λ is an eigenvalue of L_{rw} with eigenvector u if and only if λ and u solve the generalized eigen problem $Lu = \lambda Du$.
- 4. 0 is an eigenvalue of L_{rw} with the constant one vector 1 as eigenvector. 0 is an eigenvalue of L_{sym} with eigenvector $D^{1/2}\mathbb{1}$.
- 5. L_{sym} and L_{rw} are positive semi-definite and have n non-negative real-valued eigenvalues $0 = \lambda_i \le \lambda_2 \le \cdots \le \lambda_n$.

$$L_{sym} := D^{-\frac{1}{2}}LD^{-\frac{1}{2}} = I - D^{-\frac{1}{2}}WD^{-\frac{1}{2}}$$
$$L_{rw} := D^{-1}L = I - D^{-1}W$$





• Normalized Graph Laplacian

$$L_{sym} := D^{-\frac{1}{2}}LD^{-\frac{1}{2}} = I - D^{-\frac{1}{2}}WD^{-\frac{1}{2}}$$

$$L_{rw} := D^{-1}L = I - D^{-1}W$$

Proposition 4 (Number of connected components and spectra of L_{sym} and L_{rw})

Let G be an undirected graph with non-negative weights. Then the multiplicity k of the eigenvalue 0 of both L_{sym} and L_{rw} equals the number of connected components A_1, \ldots, A_k in the graph. For L_{rw} the eigenspace of 0 is spanned by the indicator vectors $\mathbb{1}_{A_i}$ of those components. For L_{sym} , the eigenspace of 0 is spanned by the vectors $D^{1/2}\mathbb{1}_{A_i}$.





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Unnormalized Graph Laplacian

$$L = D - W$$

Unnormalized spectral clustering

Input: Similarity matrix $S \in \mathbb{R}^{n \times n}$, number k of clusters to construct.

- ullet Construct a similarity graph by one of the ways described in Section 2. Let W be its weighted adjacency matrix.
- ullet Compute the unnormalized Laplacian L.
- Compute the first k eigenvectors u_1, \ldots, u_k of L.
- ullet Let $U \in \mathbb{R}^{n \times k}$ be the matrix containing the vectors u_1, \dots, u_k as columns.
- ullet For $i=1,\ldots,n$, let $y_i\in\mathbb{R}^k$ be the vector corresponding to the i-th row of U.
- Cluster the points $(y_i)_{i=1,...,n}$ in \mathbb{R}^k with the k-means algorithm into clusters C_1,\ldots,C_k .

Output: Clusters A_1, \ldots, A_k with $A_i = \{j | y_j \in C_i\}$.





Normalized Graph Laplacian

$$L_{rw} := D^{-1}L = I - D^{-1}W$$

Normalized spectral clustering according to Shi and Malik (2000)

Input: Similarity matrix $S \in \mathbb{R}^{n \times n}$, number k of clusters to construct.

- ullet Construct a similarity graph by one of the ways described in Section 2. Let W be its weighted adjacency matrix.
- Compute the unnormalized Laplacian L.
- Compute the first k generalized eigenvectors u_1, \ldots, u_k of the generalized eigenproblem $Lu = \lambda Du$.
- ullet Let $U \in \mathbb{R}^{n \times k}$ be the matrix containing the vectors u_1, \dots, u_k as columns.
- ullet For $i=1,\ldots,n$, let $y_i\in\mathbb{R}^k$ be the vector corresponding to the i-th row of U.
- ullet Cluster the points $(y_i)_{i=1,\dots,n}$ in \mathbb{R}^k with the k-means algorithm into clusters C_1,\dots,C_k .

Output: Clusters A_1, \ldots, A_k with $A_i = \{j | y_j \in C_i\}$.





• Normalized Graph Laplacian

$$L_{sym} := D^{-\frac{1}{2}}LD^{-\frac{1}{2}} = I - D^{-\frac{1}{2}}WD^{-\frac{1}{2}}$$

Normalized spectral clustering according to Ng, Jordan, and Weiss (2002)

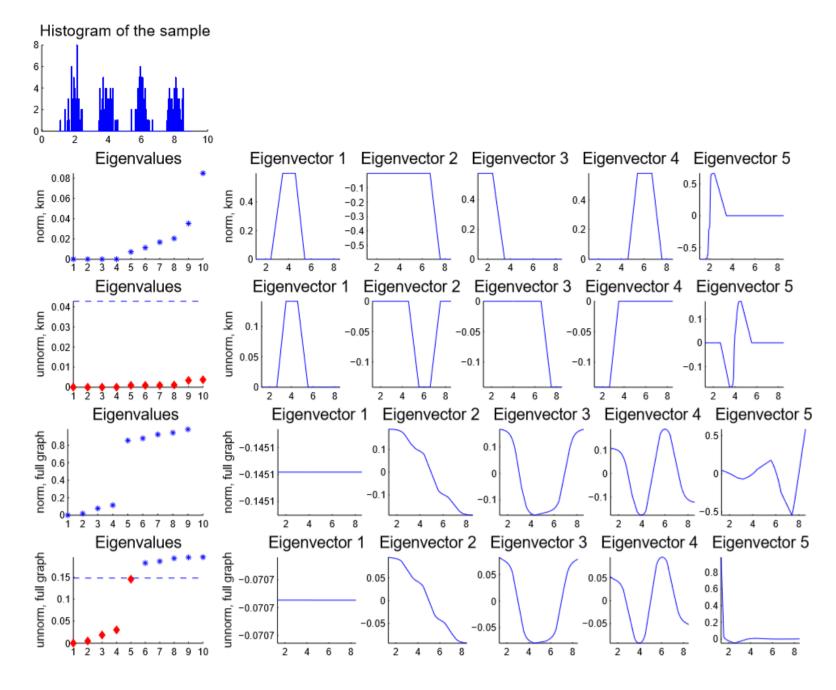
Input: Similarity matrix $S \in \mathbb{R}^{n \times n}$, number k of clusters to construct.

- ullet Construct a similarity graph by one of the ways described in Section 2. Let W be its weighted adjacency matrix.
- ullet Compute the normalized Laplacian $L_{ exttt{sym}}$.
- Compute the first k eigenvectors u_1, \ldots, u_k of L_{sym} .
- ullet Let $U \in \mathbb{R}^{n \times k}$ be the matrix containing the vectors u_1, \dots, u_k as columns.
- Form the matrix $T \in \mathbb{R}^{n \times k}$ from U by normalizing the rows to norm 1, that is set $t_{ij} = u_{ij}/(\sum_k u_{ik}^2)^{1/2}$.
- ullet For $i=1,\ldots,n$, let $y_i\in\mathbb{R}^k$ be the vector corresponding to the i-th row of T.
- ullet Cluster the points $(y_i)_{i=1,\ldots,n}$ with the k-means algorithm into clusters C_1,\ldots,C_k .

Output: Clusters A_1, \ldots, A_k with $A_i = \{j | y_j \in C_i\}$.



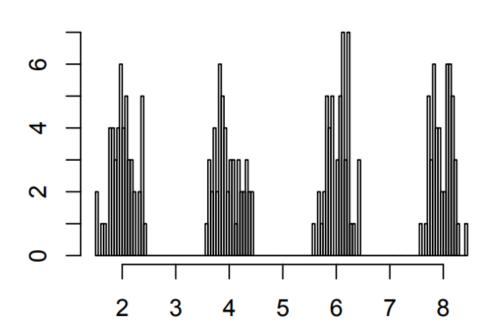


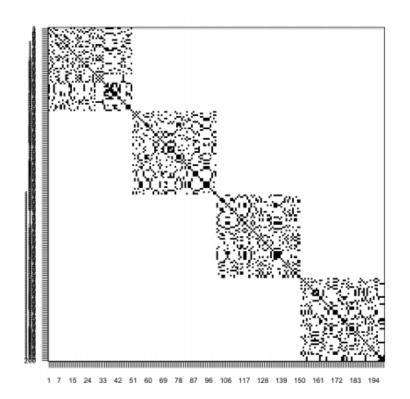


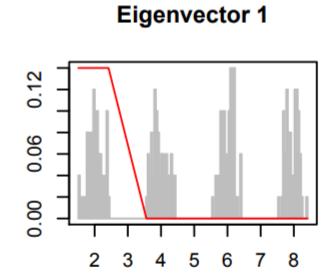


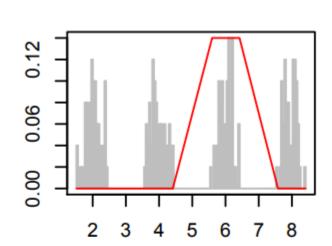


Histogram of the sample

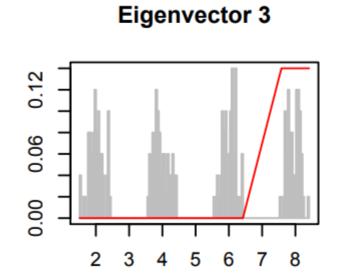


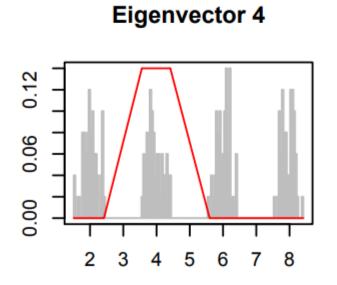


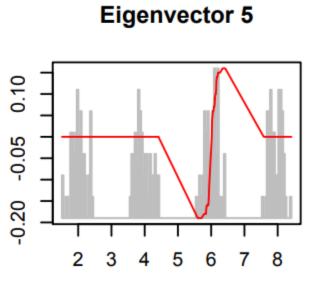




Eigenvector 2











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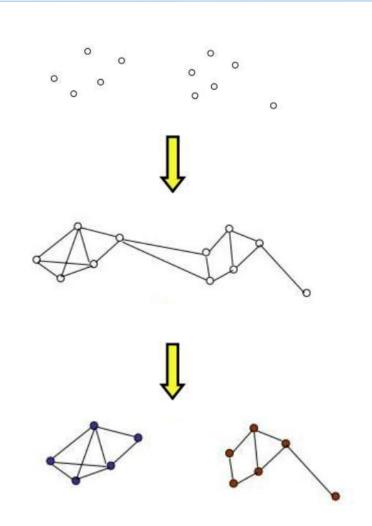


Graph Cut Point of View



First - graph representation of data (largely, application dependent)

Then - graph partitioning



Disconnected graph components



Groups of points(Weakly connections in between components Strongly connections within components)





$$G=(V,E)$$
:

• For two not necessarily disjoint set $A, B \subset V$, we define

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

• Minicut: choosing a partition $A_1, A_2, ..., A_K$ which minimizes

$$cut(A_1, ..., A_k) := \frac{1}{2} \sum_{i=1}^k W(A_i, \overline{A_i})$$

Cut between 2 sets $cut(A_1, A_2) = \sum_{n \in A_1} \sum_{m \in A_2} w_{nm}$

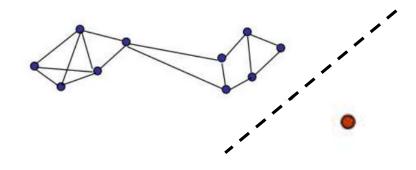


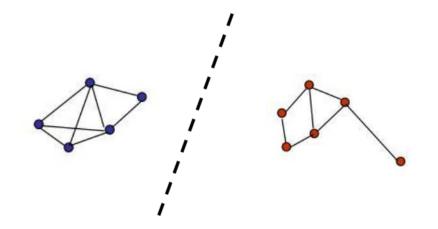




Problems!!!

Sensitive to outliers





What we get

What we want





Solutions

|A| := the number of vertices in A

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

RatioCut(Hagen and Kahng, 1992)

$$RatioCut(A_1, ..., A_k) := \frac{1}{2} \sum_{i=1}^k \frac{W(A_i, \overline{A_i})}{|A_i|} = \sum_{i=1}^k \frac{cut(A_i, \overline{A_i})}{|A_i|}$$

Ncut(Shi and Malik, 2000)

$$Ncut(A_1,...,A_k) := \frac{1}{2} \sum_{i=1}^k \frac{W(A_i,\overline{A_i})}{vol(A_i)} = \sum_{i=1}^k \frac{cut(A_i,\overline{A_i})}{vol(A_i)}$$





Problem!!!

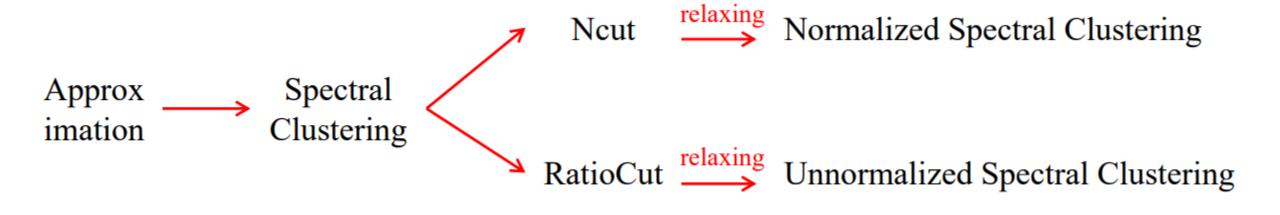
NP hard

Solution!!!

Approximation

$$RatioCut(A_1, \dots, A_k) := \frac{1}{2} \sum_{i=1}^k \frac{W(A_i, \overline{A_i})}{|A_i|} = \sum_{i=1}^k \frac{cut(A_i, \overline{A_i})}{|A_i|}$$

$$Ncut(A_1, ..., A_k) := \frac{1}{2} \sum_{i=1}^k \frac{W(A_i, \overline{A_i})}{vol(A_i)} = \sum_{i=1}^k \frac{cut(A_i, \overline{A_i})}{vol(A_i)}$$







Our goal is to solve the optimization problem:

$$\min_{A\subset V}RatioCut(A,\bar{A})$$

We first rewrite the problem in a more convenient form. Given a subset $A \subset V$ we define the vector $f = (f_1, \ldots, f_n)' \in \mathbb{R}^n$ with entries

$$f_i = egin{cases} \sqrt{|\overline{A}|/|A|} & ext{if } v_i \in A \ -\sqrt{|A|/|\overline{A}|} & ext{if } v_i \in \overline{A}. \end{cases}$$





$$f_i = \begin{cases} \sqrt{|\bar{A}|/|A|}, & \text{if } v_i \in A \\ -\sqrt{|\bar{A}|/|A|}, & \text{if } v_i \in \bar{A} \end{cases}$$

$$f'Lf = \frac{1}{2} \sum_{i,j=1}^{n} w_{ij} (f_i - f_j)^2$$

$$RatioCut(A_1, ..., A_k) := \frac{1}{2} \sum_{i=1}^k \frac{W(A_i, \overline{A_i})}{|A_i|} = \sum_{i=1}^k \frac{cut(A_i, \overline{A_i})}{|A_i|}$$

$$cut(A_1, ..., A_k) := \frac{1}{2} \sum_{i=1}^k W(A_i, \overline{A_i}) \qquad W(A, B) := \sum_{i \in A, j \in B} w_{ij}$$

$$= \frac{1}{2} \sum_{i \in A, j \in \overline{A}} w_{ij} \left(\sqrt{\frac{|\overline{A}|}{|A|}} + \sqrt{\frac{|A|}{|\overline{A}|}} \right)^{2} + \frac{1}{2} \sum_{i \in \overline{A}, j \in A} w_{ij} \left(-\sqrt{\frac{|\overline{A}|}{|A|}} - \sqrt{\frac{|A|}{|\overline{A}|}} \right)^{2}$$

$$= \operatorname{cut}(A, \overline{A}) \left(\frac{|\overline{A}|}{|A|} + \frac{|A|}{|\overline{A}|} + 2 \right)$$

$$= \operatorname{cut}(A, \overline{A}) \left(\frac{|A| + |\overline{A}|}{|A|} + \frac{|A| + |\overline{A}|}{|\overline{A}|} \right)$$

$$= |V| \cdot \operatorname{RatioCut}(A, \overline{A}).$$





Additionally, we have

$$\sum_{i=1}^{n} f_i = \sum_{i \in A} \sqrt{\frac{|\overline{A}|}{|A|}} - \sum_{i \in \overline{A}} \sqrt{\frac{|A|}{|\overline{A}|}} = |A| \sqrt{\frac{|\overline{A}|}{|A|}} - |\overline{A}| \sqrt{\frac{|A|}{|\overline{A}|}} = 0$$

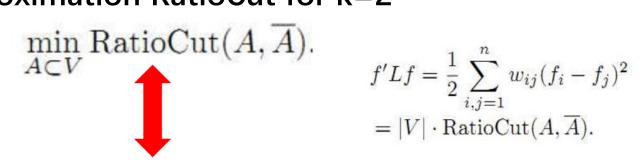
The vector f as defined before is orthogonal to the constant one vector \mathbb{I} .

f satisfies

$$||f||^2 = \sum_{i=1}^n f_i^2 = |A| \frac{|\overline{A}|}{|A|} + |\overline{A}| \frac{|A|}{|\overline{A}|} = |\overline{A}| + |A| = n.$$







$$f'Lf = \frac{1}{2} \sum_{i,j=1}^{n} w_{ij} (f_i - f_j)^2$$
$$= |V| \cdot \text{RatioCut}(A, \overline{A}).$$

 $\min_{A\subset V} f'Lf \text{ subject to } f\perp \mathbb{1} \quad ||f|| = \sqrt{n}.$



Relaxation !!!

 $\min_{f \in \mathbb{R}^n} f' L f \text{ subject to } f \perp \mathbb{1}, \ \|f\| = \sqrt{n}.$



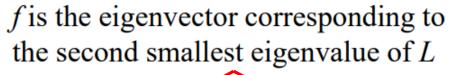
Rayleigh-Ritz Theorem

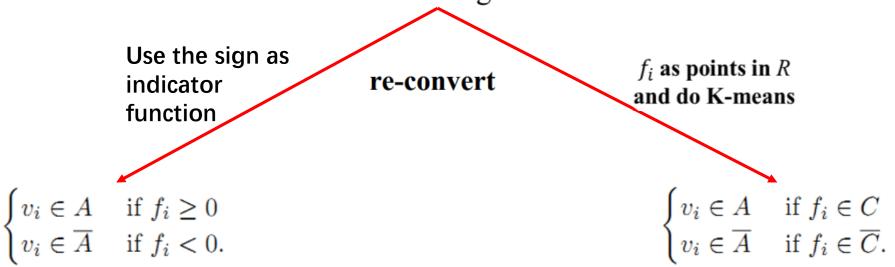
f is the eigenvector corresponding to the second smallest eigenvalue of L (the smallest eigenvalue of L is 0 with eigenvector \mathbb{I})

$$f_i = \begin{cases} \sqrt{|\overline{A}|/|A|} & \text{if } v_i \in A \\ -\sqrt{|A|/|\overline{A}|} & \text{if } v_i \in \overline{A}. \end{cases}$$









Only works for k = 2

More General, works for any k



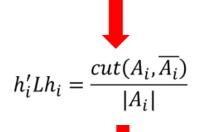


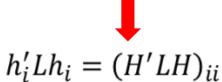
Approximation RatioCut for arbitrary k

Given a partition of V into k sets $A_1, A_2, ..., A_k$, we define k indicator vectors

$$h_j = (h_{1,j}, ..., h_{n,j})'$$
 by

$$h_{i,j} = \begin{cases} \frac{1}{\sqrt{|A_j|}}, & \text{if } v_i \in A_j \\ 0, & \text{otherwise} \end{cases}$$
 $(i=1,...,n; j=1,...,k)$





 $H \in \mathbb{R}^{n \times k}$, containing those k Indicator vectors as columns. Columns in H are orthonormal to each other, that is H'H = I

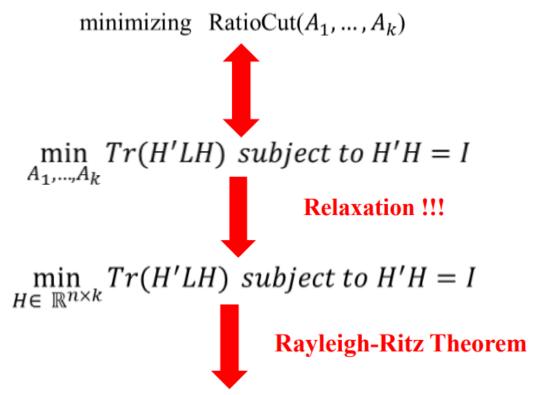
RatioCut
$$(A_1, \dots, A_k) = \sum_{i=1}^k h'_i L h_i = \sum_{i=1}^k (H'LH)_{ii} = \text{Tr}(H'LH),$$





Approximation RatioCut for arbitrary k

Problem reformulation:



Optimal H is the first k eigenvectors of L as columns.

$$h_{i,j} = \begin{cases} \frac{1}{\sqrt{|A_j|}}, & \text{if } v_i \in A_j \\ 0, & \text{otherwise} \end{cases}$$





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PRACTICAL DETAILS



Constructing the similarity graph

- Similarity Function Itself Make sure that points which are considered to be "very similar" by the similarity function are also closely related in the application the data comes from.
- Type of Similarity Graph Which one to choose from those three types.
 General recommendation: k-nearest neighbor graph.
- 3. Parameters of Similarity Graph(k or ε)
 - KNN: k in order of log(n);
 - mutual KNN: k significantly larger than standard KNN;
 - 3. ε -neighborhood graph: longest edge of MST;
 - 4. fully connected graph: σ in order of the mean distance of a point to its k-th nearest neighbor. Or choose $k = \varepsilon$.



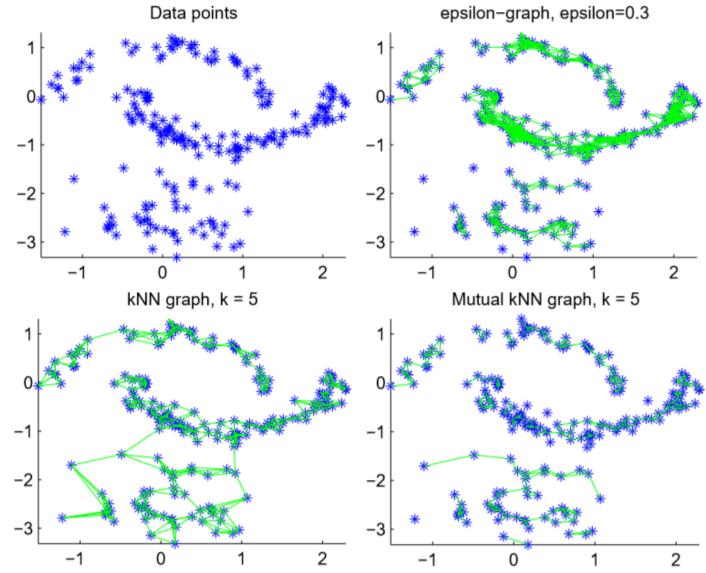


Figure 3: Different similarity graphs, see text for details.



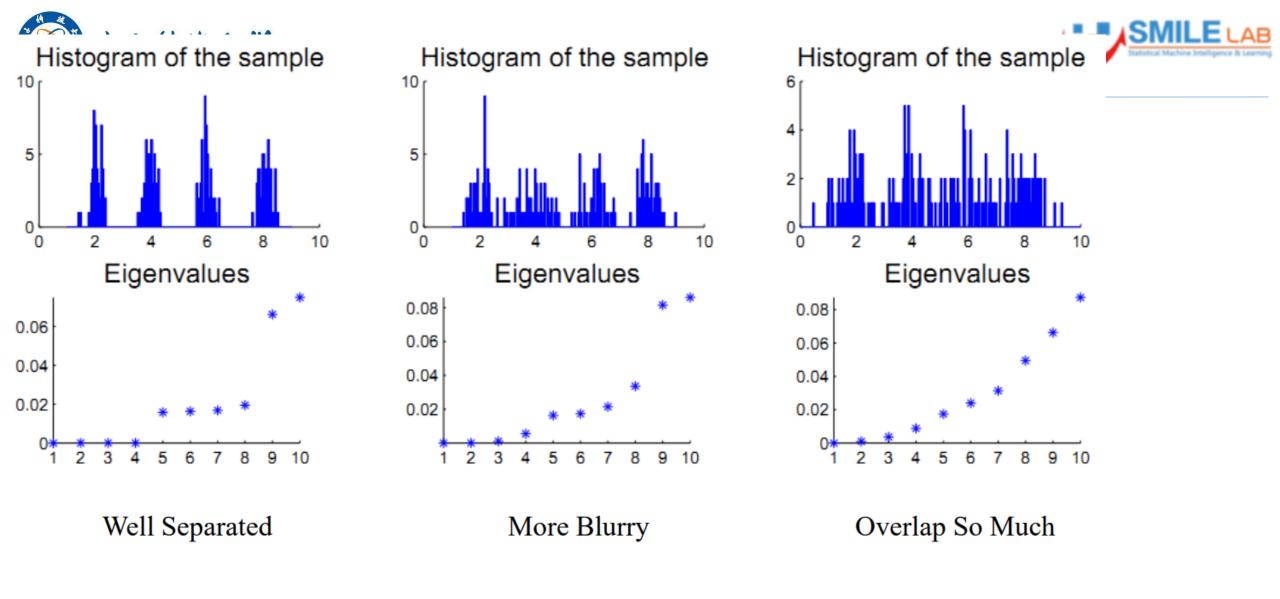


Computing Eigenvectors

- 1. How to compute the first eigenvectors efficiently for large L
- Numerical eigensolvers converge to some orthonormal basis of the eigenspace.

Number of Clusters

- General Strategies
- 2. Eigengap heuristic(Choose the number k such that all eigenvalues $\lambda_1, ... \lambda_k$ are very small, but λ_{k+1} is relatively large)



Eigengap Heuristic usually works well if the data contains very well pronounced clusters, but in ambiguous cases it also returns ambiguous results.





Spectral clustering

- 1. Does not make strong assumptions on the form of the clusters ⇒ can solve very general problems like intertwined spirals
- 2.can be implemented efficiently even for large data sets (as the adjacency matrix is sparse)
- adjacency matrix is sparse)
 3.no issues of getting stuck in local minima or restarting the algorithm for several times with different initializations

but

- 1.choosing a good similarity graph is not trivial
- 2.spectral clustering can be quite unstable under different choices of the parameters for the similarity graph

Spectral clustering cannot serve as a "black box algorithm" which automatically detects the correct clusters in any given data set. But itcan be considered as a powerful tool which can produce good results if applied with care.





Thanks!