CS247: ADVANCED DATA MINING

Graph and Network: Spectral Clustering and Label Propagation

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Methods to Learn

	Vector Data	Text Data	Graph & Network	Recommender Systems
Classification	**Naïve Bayes; Logistic Regression; NN**		**Label Propagation**	
Clustering	**K-means; kernel k-means; Mixture Models**	**PLSA; LDA**	**Spectral Clustering**	Matrix Factorization
Prediction	**NN**			Collaborative Filtering; Factorization machine; Hybrid CF; Recommendation with graph regularization
Ranking			**PageRank**	
Similarity Search			**P-PageRank**	
Representation Learning		**Word embedding**	Network embedding	Deep collaborative learning

Graph: Clustering and Classification

- Graph Laplacians 
- Spectral Clustering
- Label Propagation
- Summary

What are Graph Laplacian Matrices?

- They are matrices defined as functions of graph adjacency or weight matrix
- A tool to study graphs
- There is a field called spectral graph theory studying those matrices

Examples of Graph Laplacians

- Given an undirected and weighted graph $G = (V, E)$, with weight matrix W
  - $W_{ij} = W_{ji} \geq 0$
  - n: total number of nodes
  - Degree for node $v_i \in V$: $d_i = \sum_j w_{ij}$
  - Degree matrix D: a diagonal matrix with degrees on the diagonal, i.e., $D_{ii} = d_i$ and $D_{ij} = 0 \; if \; i \neq j$
- Three examples of graph Laplacians
  - The unnormalized graph Laplacian
    - $L = D - W$
  - The normalized graph Laplacians
    - Symmetric: $L_{sym} = D^{-1/2} L D^{-1/2}$
    - Random walk related: $L_{rw} = D^{-1} L$

The Unnormalized Graph Laplacian

- Definition: $L = D - W$
- Properties of L
  - For any vector $f \in R^n$

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

  - L is symmetric and positive semi-definite
  - The smallest eigenvalue of L is 0, and the corresponding eigenvector is the constant one vector $\mathbf{1}$
    - $\mathbf{1}$ is an all-one vector with n dimensions
    - An eigenvector can be scaled by multiplying a nonzero scalar α
  - L has n non-negative, real-valued eigenvalues:

$$0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$$

Question

- Will self loops in graph change L?

Number of Connected Components

- The multiplicity k of the eigenvalue 0 of L equals the number of connected components
  - Consider $k = 1$, i.e., a connected graph, and f, the corresponding eigenvector for 0

$$0 = f' L f = \sum_{i,j=1}^{n} w_{ij}(f_i - f_j)^2$$

  - Every element of f has to be equal to each other

K connected components

- The graph can be represented as a block diagonal matrix, and so do matrix L

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

  - For each block L_i, it has eigenvalue 0 with corresponding constant one eigenvector
  - For L, it has k eigenvalues with 0, with corresponding eigenvectors as indicator vectors
    - $\mathbf{1}_{A_i}$ is an indicator vector, with ones for nodes in A_i, i.e., the nodes in component i, and zeros elsewhere

The normalized graph Laplacians

- Symmetric:
  - $L_{sym} = D^{-1/2} L D^{-1/2} = I - D^{-1/2} W D^{-1/2}$
- Random walk related:
  - $L_{rw} = D^{-1} L = I - D^{-1} W$

Properties of L_{sym} and L_{rw}

- For any vector $f \in R^n$

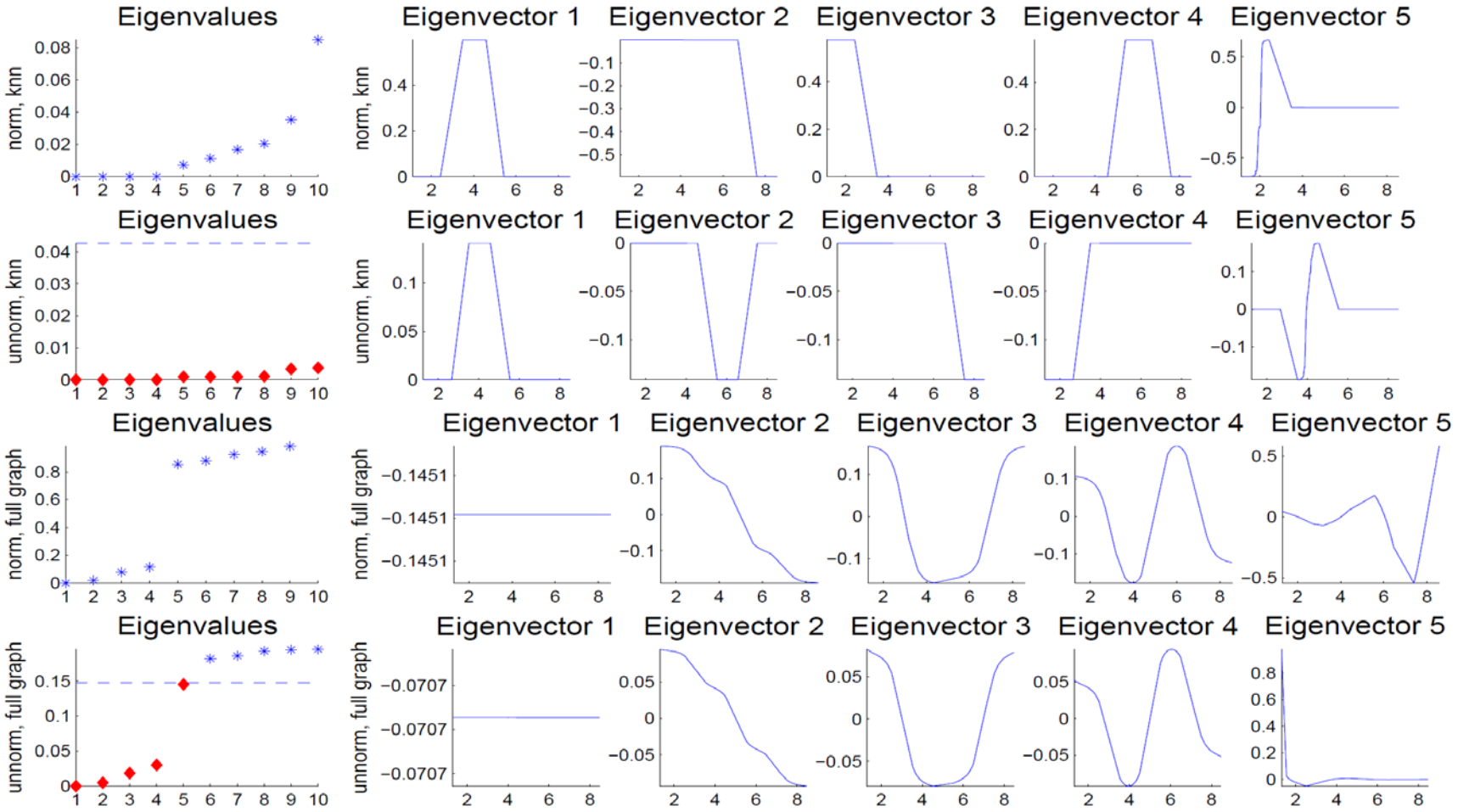
$$f' L_{sym} f = \frac{1}{2} \sum_{i,j=1}^{n} w_{ij} \left(\frac{f_i}{\sqrt{d_i}} - \frac{f_j}{\sqrt{d_j}} \right)^2$$

- λ is an eigenvalue of $\boldsymbol{L_{rw}}$ with eigenvector $v \Leftrightarrow \lambda$ is an eigenvalue of $\boldsymbol{L_{sym}}$ with eigenvector $w = D^{1/2} v$
- λ is an eigenvalue of $\boldsymbol{L_{rw}}$ with eigenvector $v \Leftrightarrow \lambda$ and v solves the generalized eigen problem $Lv = \lambda D v$
- 0 is an eigenvalue of $\boldsymbol{L_{rw}}$ with eigenvector $\mathbf{1}$. 0 is an eigenvalue of $\boldsymbol{L_{sym}}$ with eigenvector $D^{1/2}\mathbf{1}$
- $\boldsymbol{L_{sym}}$ and $\boldsymbol{L_{rw}}$ are positive semi-definite, and have n non-negative real-valued eigenvalues

$$0 = \lambda_1 \leq \ldots \leq \lambda_n$$

Example

- Graph built upon Gaussian mixture model with four components



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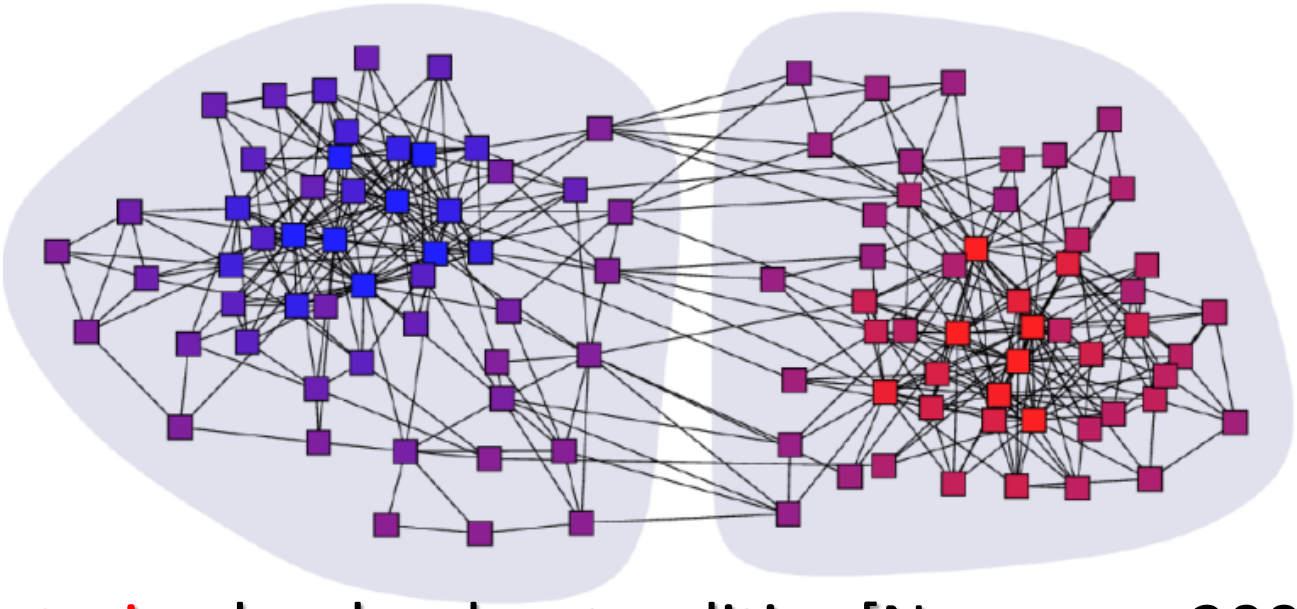
Clustering Graphs and Network Data

- Applications
  - Bi-partite graphs, e.g., customers and products, authors and conferences
  - Web search engines, e.g., click through graphs and Web graphs
  - Social networks, friendship/coauthor graphs



Clustering books about politics [Newman, 2006]

Example of Graph Clustering

- Reference: ICDM'09 Tutorial by Chris Ding
- Example:
  - Clustering supreme court justices according to

W =

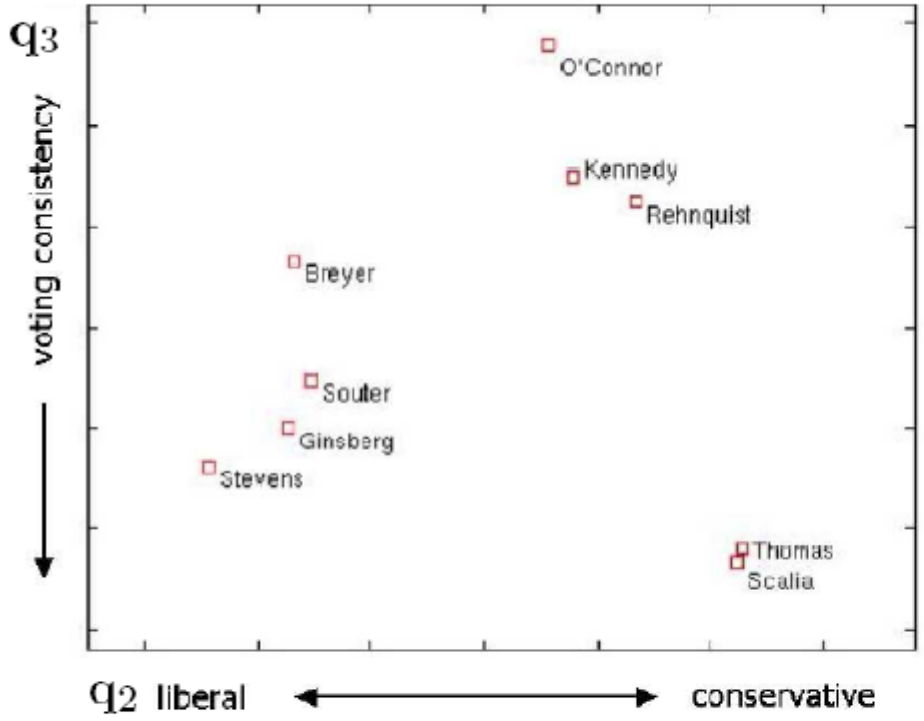
Number of times (%) two Justices voted in agreement

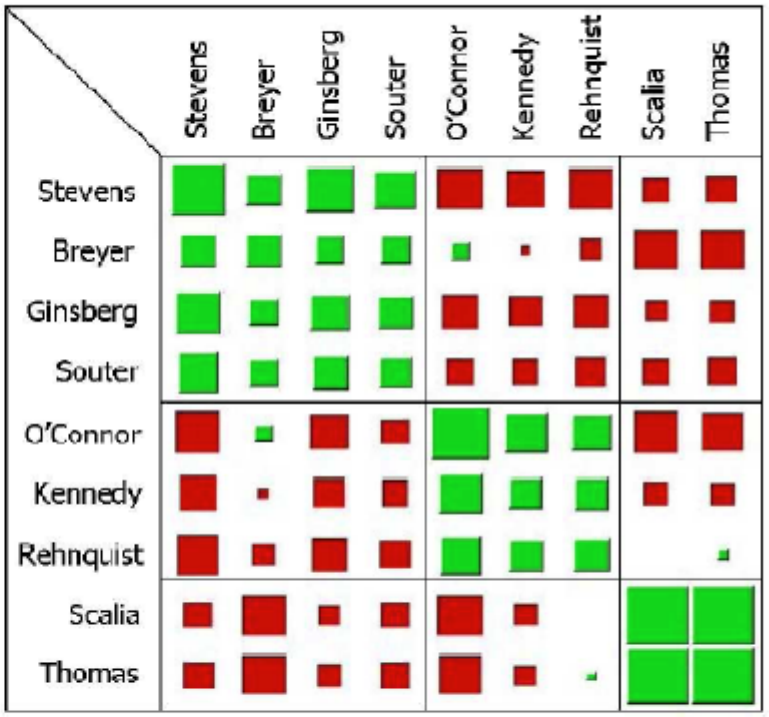
	Ste	Bre	Gin	Sou	O'Co	Ken	Reh	Sca	Tho
Stevens	–	62	66	63	33	36	25	14	15
Breyer	62	–	72	71	55	47	43	25	24
Ginsberg	66	72	–	78	47	49	43	28	26
Souter	63	71	78	–	55	50	44	31	29
O'Connor	33	55	47	55	–	67	71	54	54
Kennedy	36	47	49	50	67	–	77	58	59
Rehnquist	25	43	43	44	71	77	–	66	68
Scalia	14	25	28	31	54	58	66	–	79
Thomas	15	24	26	29	54	59	68	79	–

Table 1: From the voting record of Justices 1995 Term – 2004 Term, the number of times two justices voted in agreement (in percentage). (Data source: from July 2, 2005 *New York Times*. Originally from *Legal Affairs*; *Harvard Law Review*)

Example: Continue

$$C = \mathbf{q}_2\mathbf{q}_2^T + \mathbf{q}_3\mathbf{q}_3^T$$





- Three groups in the Supreme Court:
  - Left leaning group, center-right group, right leaning group.

Spectral Clustering Algorithms

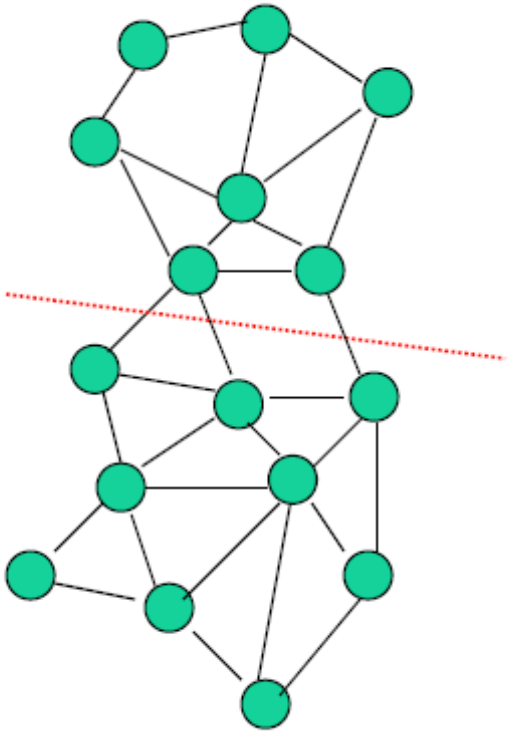
- Goal: cluster nodes in the graph into k clusters
- Idea: Leverage the first k eigenvectors of L
- Major steps:
  - Compute the first k eigenvectors, $v_1, v_2, \ldots, v_k$, of L
  - Each node i is then represented by k values $y_i = (v_{1i}, v_{2i}, \ldots, v_{ki})$
  - Cluster y_i's using k-means

Variants of Spectral Clustering Algorithms

- Normalized spectral clustering according to Shi and Malik (2000)
  - Compute the first k eigenvectors, $v_1, v_2, \ldots, v_k$, of L_{rw}
- Normalized spectral clustering according to Ng, Jordan, and Weiss (2002)
  - Compute the first k eigenvectors, $v_1, v_2, \ldots, v_k$, of L_{sym}
  - Normalizing y_i to have norm 1

Connections to Graph Cuts

- Min-Cut
  - Minimize the # of cut of edges to partition a graph into 2 disconnected components



Objective Function of Min-Cut

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)

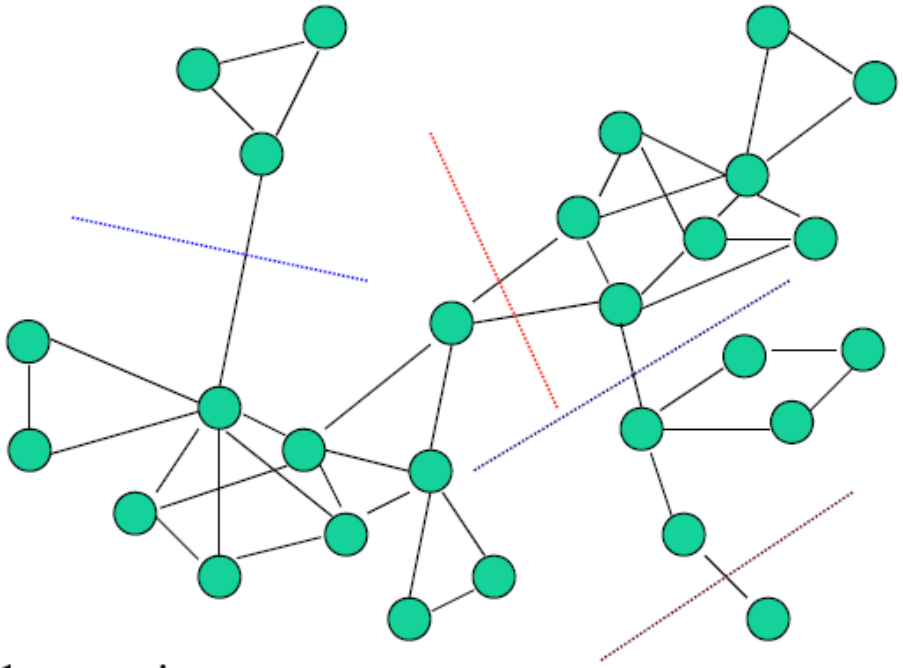
Algorithm

- Step 1:
  - Calculate Graph Laplacian matrix: $L = D - W$
- Step 2:
  - Calculate the second eigenvector q
    - Q: Why second?
- Step 3:
  - Bisect q (e.g., 0) to get two clusters

Minimum Cut with Constraints

minimize cutsize without explicit size constraints

But where to cut ?



Need to balance sizes

Other Objective Functions

- Ratio Cut (Hangen & Kahng, 1992)

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

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

- Normalized Cut (Shi & Malik, 2000)

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

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

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

- Min-Max-Cut (Ding et al, 2001)

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

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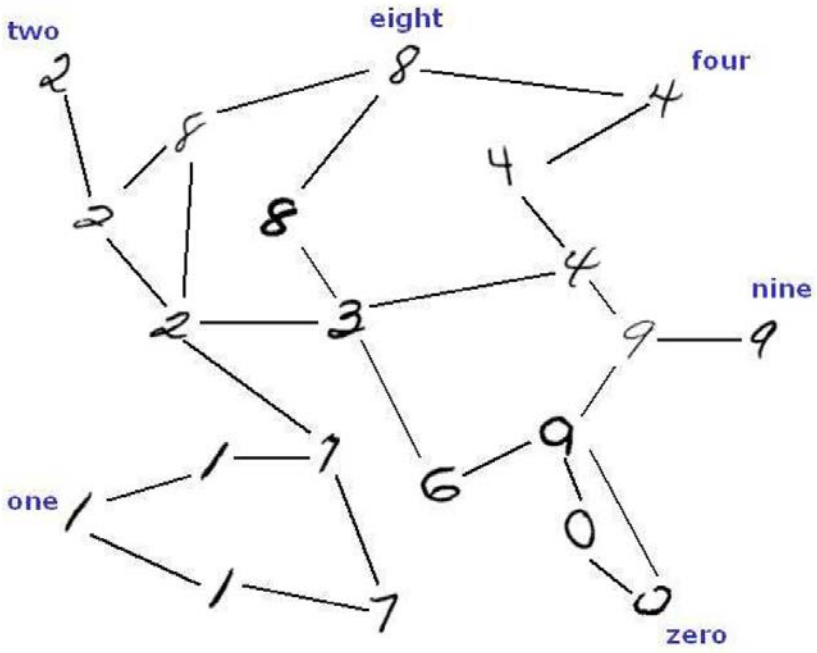
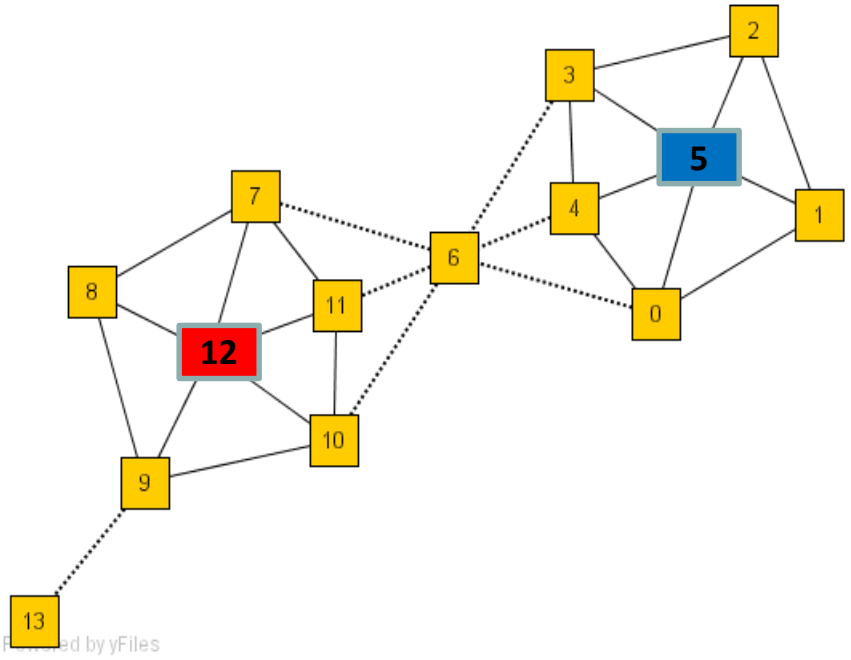
Label Propagation in the Network

- Given a network, some nodes are given labels, can we classify the unlabeled nodes by using link information?
  - E.g., Node 12 belongs to **Class 1**, Node 5 Belongs to **Class 2**





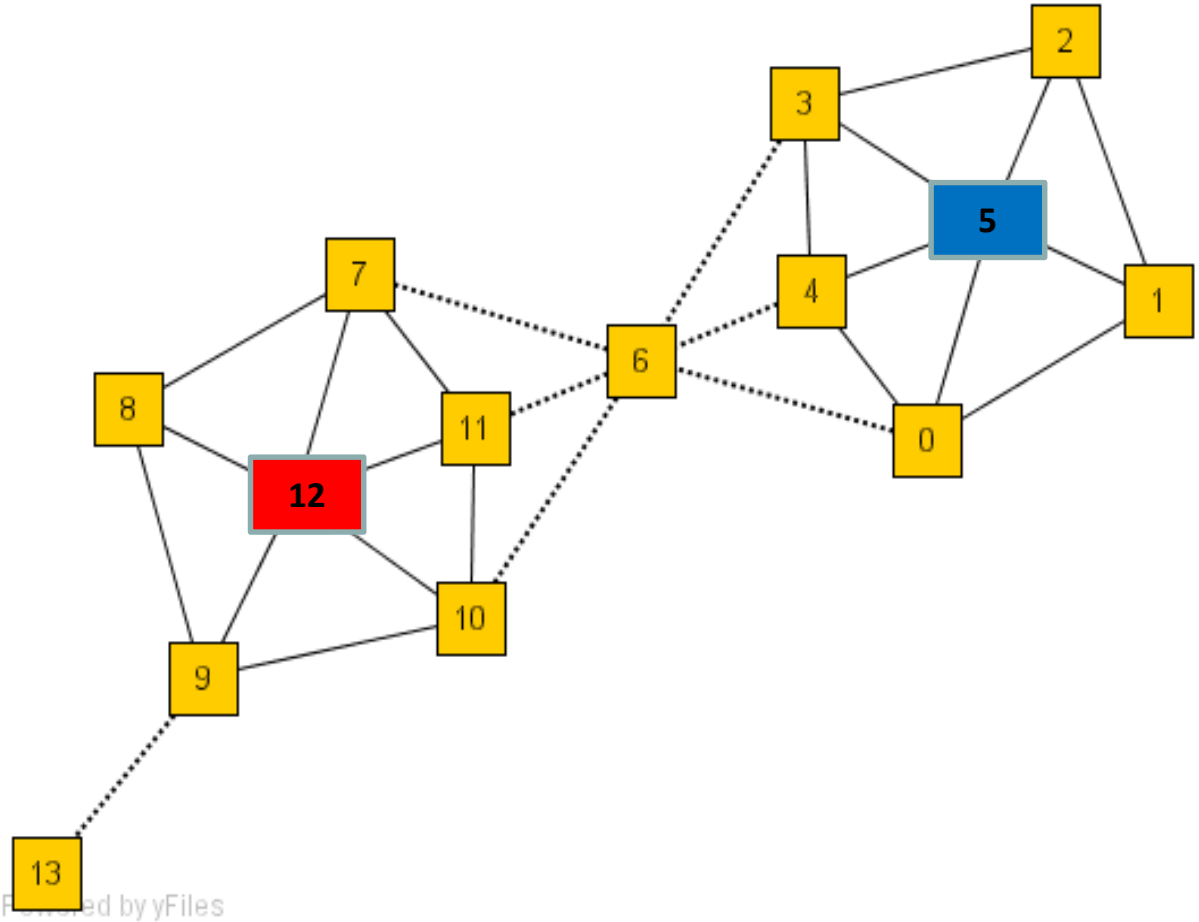
Problem Formalization for Label Propagation

- Given n nodes
  - l with labels (e.g., $Y_1, Y_2, \ldots, Y_l$ *are known*)
  - u without labels (e.g., $Y_{l+1}, Y_{l+2}, \ldots, Y_n$ are unknown)
  - Y *is the* $n \times K$ *label matrix*
    - K is the number of labels (classes)
    - Y_{ik} denotes the probability node i belonging to class k
- The weighted adjacency matrix is W
- The probabilistic transition matrix T
  - $T_{ij} = P(j \to i) = \frac{w_{ij}}{\sum_{i'} w_{i'j}}$

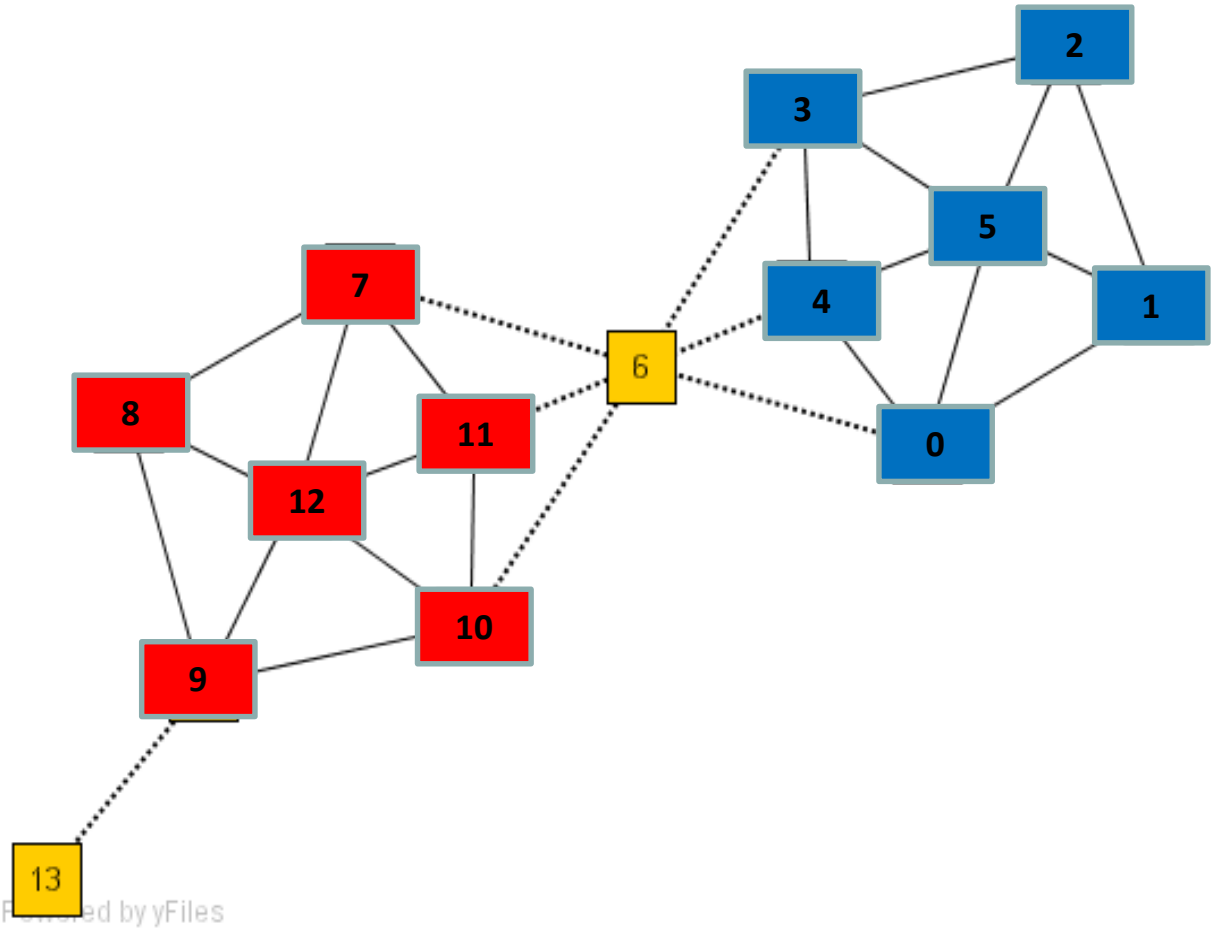
The Label Propagation Algorithm

- Step 1: Propagate $Y \leftarrow TY$
  - $Y_i = \sum_j T_{ij} Y_j = \sum_j P(j \rightarrow i) Y_j$
  - Initialization of Y for unlabeled ones is not important
- Step 2: Row-normalize Y
  - The summation of the probability of each object belonging to each class is 1
- Step 3: Reset the labels for the labeled nodes. Repeat 1-3 until Y converges

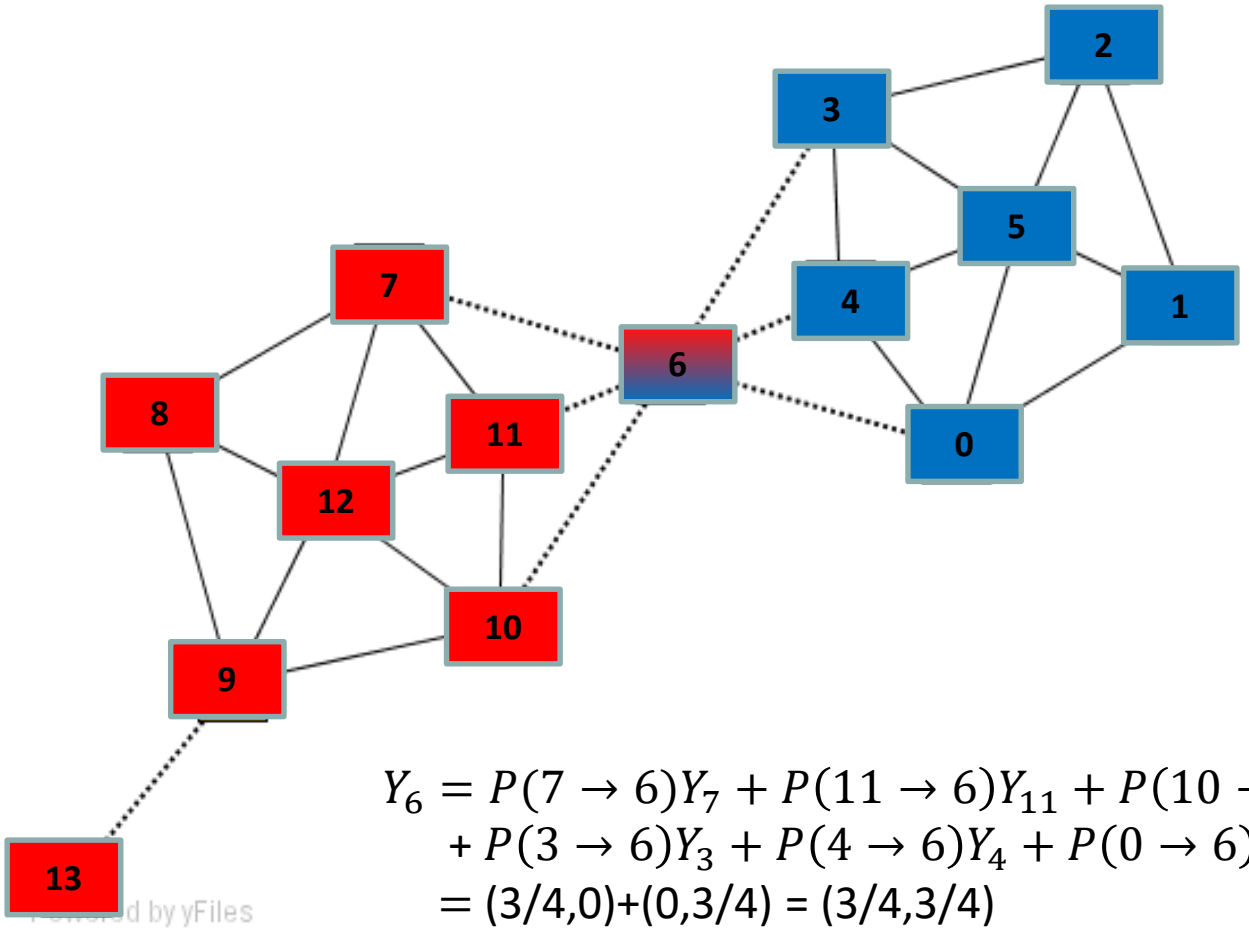
Example: Iter = 0



Example: Iter = 1



Example: Iter = 2



$$Y_6 = P(7 \to 6)Y_7 + P(11 \to 6)Y_{11} + P(10 \to 6)Y_{10} + P(3 \to 6)Y_3 + P(4 \to 6)Y_4 + P(0 \to 6)Y_0$$

$$= (3/4,0)+(0,3/4) = (3/4,3/4)$$

After normalization, $Y_6 = (\frac{1}{2}, \frac{1}{2})$

Other Label Propagation Algorithms

- Energy minimizing and harmonic function
  - Semi-Supervised Learning Using Gaussian Fields and Harmonic Functions
    - By Xiaojin Zhu et al., ICML'03
    - https://www.aaai.org/Papers/ICML/2003/ICML03-118.pdf
- Graph regularization
  - Learning with Local and Global Consistency
    - By Denny Zhou et al., NIPS'03
    - http://papers.nips.cc/paper/2506-learning-with-local-and-global-consistency.pdf

From Energy Minimizing Perspective

- Consider a binary classification problem
  - $y \in \{0,1\}$
- Let $f: V \rightarrow R$, which maps a node to a real number
  - $f(i) = y_i$, if i is labeled
  - $f = \begin{pmatrix} f_l \\ f_u \end{pmatrix}$
- The energy function
  - $$E(f) = \frac{1}{2} \sum_{i,j} w_{ij} \left(f(i) - f(j)\right)^2$$
  - Intuition: if two nodes are connected, they should share similar labels

Minimizing Energy Function Results in Harmonic Function

- Note $E(f) = f'(D - W)f = f'Lf$!
- *Goal: find f such that $E(f)$ is minimized, and f_l is fixed*
- *Solution:*
  - $(D - W)f = 0$

Solve f_u

- *Consider W as a block matrix*

$$W = \begin{bmatrix} W_{ll} & W_{lu} \\ W_{ul} & W_{uu} \end{bmatrix}$$

- *Closed form solution of f_u:*

$$f_u = (D_{uu} - W_{uu})^{-1} W_{ul} f_l = (I - P_{uu})^{-1} P_{ul} f_l$$

  - $Where\ P = D^{-1}W$

- *Iterative solution of f_u:*

  - $f_u = (\sum_{t=0} P_{uu}^t) P_{ul} f_l \Rightarrow f_u^t = P_{uu} f_u^{t-1} + P_{ul} f_l$
  - $As\ (I - P_{uu})^{-1} = I + P_{uu} + P_{uu}^2 + \cdots$

From Graph Regularization Perspective

- Let F be n*K matrix with nonnegative entries
  - For node i, pick the label k such that F_{ik} is the maximum on among all the k
- Let Y be n*K matrix with $y_{ik} = 1$, if node i is labeled as class k, and 0 otherwise.
- Cost function:
- **Smoothness constraint + fitting constraint**

$$\mathcal{Q}(F) = \frac{1}{2}\left(\sum_{i,j=1}^{n} W_{ij} \left\| \frac{1}{\sqrt{D_{ii}}} F_i - \frac{1}{\sqrt{D_{jj}}} F_j \right\|^2 + \mu \sum_{i=1}^{n} \left\| F_i - Y_i \right\|^2 \right)$$

Solve F

- Note the first component is related to $\text{trace}\left(F' L_{sym} F\right)$
- Closed form solution:
  - $\left.\frac{\partial \mathcal{Q}}{\partial F}\right|_{F=F^*} = F^* - SF^* + \mu(F^* - Y) = 0$
    - $\Rightarrow F^* = (1-\alpha)(I - \alpha S)^{-1} Y$
  - Where $S = D^{-1/2} W D^{-1/2}$, $\alpha = \frac{1}{1+\mu}$ is a value between 0 and 1
- Iterative solution:
  - $$F(t+1) = \alpha S F(t) + (1-\alpha) Y$$

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Summary

- Graph Laplacians are keys to understand graphs
  - Unnormalized graph Laplacians
  - Normalized graph Laplacians
- Spectral clustering
  - Leverage eigenvectors of graph Laplacians to conduct clustering on graphs
  - Has close relationship with graph cuts
- Label propagation
  - Semi-supervised node classification on graphs
  - Also related to graph Laplacians

References

- A Tutorial on Spectral Clustering by U. Luxburg http://www.kyb.mpg.de/fileadmin/user_upload/files/publications/attachments/Luxburg07_tutorial_4488%5B0%5D.pdf
- Learning from Labeled and Unlabeled Data with Label Propagation
  - By Xiaojin Zhu and Zoubin Ghahramani
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