CS6220: DATA MINING TECHNIQUES

Mining Graph/Network Data

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Methods to Learn

	Matrix Data	Set Data	Sequence Data	Time Series	Graph & Network
Classification	Decision Tree; Naïve Bayes; Logistic Regression SVM; kNN		HMM		Label Propagation
Clustering	K-means; hierarchical clustering; DBSCAN; Mixture Models; kernel k-means				SCAN; Spectral Clustering
Frequent Pattern Mining		Apriori; FP-growth	GSP; PrefixSpan		
Prediction	Linear Regression			Autoregression	
Similarity Search				DTW	P-PageRank
Ranking					PageRank

Mining Graph/Network Data

• Graph / Network Data



- Ranking on Graph / Network
- Graph/Network Clustering
- Graph/Network Classification
- Summary

Graph, Graph, Everywhere



Aspirin





Yeast protein interaction network



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Why Graph Mining?

- Graphs are ubiquitous
 - Chemical compounds (Cheminformatics)
 - Protein structures, biological pathways/networks (Bioinformactics)
 - Program control flow, traffic flow, and workflow analysis
 - XML databases, Web, and social network analysis
- Graph is a general model
 - Trees, lattices, sequences, and items are degenerated graphs
- Diversity of graphs
 - Directed vs. undirected, labeled vs. unlabeled (edges & vertices), weighted, with angles & geometry (topological vs. 2-D/3-D)
- Complexity of algorithms: many problems are of high complexity

Representation of a Graph

- G = < V, E >
 - $V = \{u_1, ..., u_n\}$: node set
 - $E \subseteq V \times V$: edge set
- Adjacency matrix
 - $A = \{a_{ij}\}, i, j = 1, ..., n$
 - $a_{ij} = 1, if < u_i, u_j > \in E$
 - $a_{ij} = 0$, if $\langle u_i, u_j \rangle \notin E$
 - Undirected graph vs. Directed graph
 - $A = A^{\mathrm{T}} vs. A \neq A^{\mathrm{T}}$
 - Weighted graph
 - Use W instead of A, where w_{ij} represents the weight of edge $< u_i, u_j >$

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Ranking on Graph / Network

PageRank

Personalized PageRank

The History of PageRank

- PageRank was developed by Larry Page (hence the name Page-Rank) and Sergey Brin.
- It is first as part of a research project about a new kind of search engine. That project started in 1995 and led to a functional prototype in 1998.
- Shortly after, Page and Brin founded Google.

Ranking web pages

- Web pages are not equally "important"
 - <u>www.cnn.com</u> vs. a personal webpage
- Inlinks as votes
 - The more inlinks, the more important
- Are all inlinks equal?
 - Recursive question!

Simple recursive formulation

- Each link's vote is proportional to the importance of its source page
- If page P with importance x has n outlinks, each link gets x/n votes
- Page P's own importance is the sum of the votes on its inlinks

Matrix formulation

- Matrix M has one row and one column for each web page
- Suppose page j has n outlinks
 - If j -> i, then $M_{ij}=1/n$
 - Else M_{ij}=0
- M is a column stochastic matrix
 - Columns sum to 1
- Suppose r is a vector with one entry per web page
 - r_i is the importance score of page i
 - Call it the rank vector
 - |**r**| = 1

Eigenvector formulation

The flow equations can be written

r = Mr

- So the rank vector is an eigenvector of the stochastic web matrix
 - In fact, its first or principal eigenvector, with corresponding eigenvalue 1

Example



$$\begin{array}{ccccccc} y & a & m \\ y & 1/2 & 1/2 & 0 \\ a & 1/2 & 0 & 1 \\ m & 0 & 1/2 & 0 \end{array}$$

r = Mr



Power Iteration method

- Simple iterative scheme (aka relaxation)
- Suppose there are N web pages
- Initialize: $\mathbf{r}^{0} = [1/N,...,1/N]^{T}$
- Iterate: $\mathbf{r}^{k+1} = \mathbf{M}\mathbf{r}^k$
- Stop when $|\mathbf{r}^{k+1} \mathbf{r}^k|_1 < \varepsilon$
 - $|\mathbf{x}|_1 = \sum_{1 \le i \le N} |x_i|$ is the L₁ norm
 - Can use any other vector norm e.g., Euclidean

Power Iteration Example



 \boldsymbol{r}_1 \boldsymbol{r}_2 **r**₃ r_0

Random Walk Interpretation

- Imagine a random web surfer
 - At any time t, surfer is on some page P
 - At time t+1, the surfer follows an outlink from P uniformly at random
 - Ends up on some page Q linked from P
 - Process repeats indefinitely
- Let p(t) be a vector whose ith component is the probability that the surfer is at page i at time t
 - **p**(t) is a probability distribution on pages

*The stationary distribution

- Where is the surfer at time t+1?
 - Follows a link uniformly at random
 - p(t+1) = Mp(t)
- Suppose the random walk reaches a state such that p(t+1) = Mp(t) = p(t)
 - Then **p**(t) is called a stationary distribution for the random walk
- Our rank vector r satisfies r = Mr
 - So it is a stationary distribution for the random surfer

*Existence and Uniqueness

A central result from the theory of random walks (aka Markov processes):

For graphs that satisfy certain conditions, the stationary distribution is unique and eventually will be reached no matter what the initial probability distribution at time t = 0.

Spider traps

- A group of pages is a spider trap if there are no links from within the group to outside the group
 - Random surfer gets trapped
- Spider traps violate the conditions needed for the random walk theorem

Microsoft becomes a spider trap



Random teleports

- The Google solution for spider traps
- At each time step, the random surfer has two options:
 - With probability β , follow a link at random
 - With probability 1-β, jump to some page uniformly at random
 - Common values for β are in the range 0.8 to 0.9
- Surfer will teleport out of spider trap within a few time steps

Random teleports ($\beta = 0.8$)



Random teleports ($\beta = 0.8$)



PageRank

- Construct the N-by-N matrix A as follows
 - $\mathbf{M}^*_{ij} = \beta \mathbf{M}_{ij} + (1-\beta)/\mathbf{N}$
- Verify that M^{*} is a stochastic matrix
- The page rank vector r is the principal eigenvector of this matrix

• satisfying $\mathbf{r} = \mathbf{M}^* \mathbf{r}$

 Equivalently, r is the stationary distribution of the random walk with teleports

Dead ends

- Pages with no outlinks are "dead ends" for the random surfer
 - Nowhere to go on next step

Microsoft becomes a dead end



Dealing with dead-ends

Teleport

- Follow random teleport links with probability 1.0 from dead-ends
- Adjust matrix accordingly
- Prune and propagate
 - Preprocess the graph to eliminate dead-ends
 - Might require multiple passes
 - Compute page rank on reduced graph
 - Approximate values for deadends by propagating values from reduced graph

Computing PageRank

- Key step is matrix-vector multiplication
 - $\mathbf{r}^{new} = \mathbf{M}^* \mathbf{r}^{old}$
- Easy if we have enough main memory to hold M^{*}, r^{old}, r^{new}
- Say N = 1 billion pages
 - We need 4 bytes for each entry (say)
 - 2 billion entries for vectors, approx 8GB
 - Matrix **M**^{*} has N² entries
 - 10¹⁸ is a large number!

Rearranging the equation

$$\begin{aligned} \mathbf{r} &= \mathbf{M}^* \mathbf{r}, \text{ where} \\ \mathbf{M}^*_{ij} &= \beta \mathbf{M}_{ij} + (1 - \beta) / \mathbf{N} \\ \mathbf{r}_i &= \sum_{1 \leq j \leq \mathbf{N}} \mathbf{M}^*_{ij} \mathbf{r}_j \\ \mathbf{r}_i &= \sum_{1 \leq j \leq \mathbf{N}} [\beta \mathbf{M}_{ij} + (1 - \beta) / \mathbf{N}] \mathbf{r}_j \\ &= \beta \sum_{1 \leq j \leq \mathbf{N}} \mathbf{M}_{ij} \mathbf{r}_j + (1 - \beta) / \mathbf{N} \sum_{1 \leq j \leq \mathbf{N}} \mathbf{r}_j \\ &= \beta \sum_{1 \leq j \leq \mathbf{N}} \mathbf{M}_{ij} \mathbf{r}_j + (1 - \beta) / \mathbf{N}, \text{ since } |\mathbf{r}| = 1 \\ \mathbf{r} &= \beta \mathbf{M} \mathbf{r} + [(1 - \beta) / \mathbf{N}]_{\mathbf{N}} \end{aligned}$$

where $[x]_N$ is an N-vector with all entries x

Sparse matrix formulation

- We can rearrange the page rank equation:
 - $\mathbf{r} = \beta \mathbf{M} \mathbf{r} + [(1-\beta)/N]_N$
 - $[(1-\beta)/N]_N$ is an N-vector with all entries $(1-\beta)/N$
- M is a sparse matrix!
 - 10 links per node, approx 10N entries
- So in each iteration, we need to:
 - Compute $\mathbf{r}^{\text{new}} = \beta \mathbf{M} \mathbf{r}^{\text{old}}$
 - Add a constant value $(1-\beta)/N$ to each entry in \mathbf{r}^{new}

Sparse matrix encoding

- Encode sparse matrix using only nonzero entries
 - Space proportional roughly to number of links
 - say 10N, or 4*10*1 billion = 40GB
 - still won't fit in memory, but will fit on disk

source node	degree	destination nodes	
0	3	1, 5, 7	
1	5	17, 64, 113, 117, 245	
2	2	13, 23	

Personalized PageRank

- Query-dependent Ranking
 - For a query webpage q, which webpages are most important to q?
 - The relative important webpages to different queries would be different

Calculation of P-PageRank

- Recall PageRank calculation:
 - $r = \beta M r + [(1-\beta)/N]_{N}$ or

•
$$\mathbf{r} = \beta \mathbf{Mr} + (1-\beta) q_0$$
, where $q_0 = \begin{pmatrix} 1/N \\ 1/N \\ ... \\ 1/N \end{pmatrix}$

• Replace q_0 with $q_0 =$

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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]

- Graph clustering methods
 - Density-based clustering: SCAN (Xu et al., KDD'2007)
 - Spectral clustering
 - Modularity-based approach
 - Probabilistic approach
 - Nonnegative matrix factorization



SCAN: Density-Based Clustering of Networks

- How many clusters?
- What size should they be?
- What is the best partitioning?
- Should some points be segregated?



Application: Given simply information of who associates with whom, could one identify clusters of individuals with common interests or special relationships (families, cliques, terrorist cells)?

A Social Network Model

- Cliques, hubs and outliers
 - Individuals in a tight social group, or clique, know many of the same people, regardless of the size of the group
 - Individuals who are <u>hubs</u> know many people in different groups but belong to no single group. Politicians, for example bridge multiple groups
 - Individuals who are <u>outliers</u> reside at the margins of society. Hermits, for example, know few people and belong to no group
- The Neighborhood of a Vertex
 - Define Γ(v) as the immediate neighborhood of a vertex (i.e. the set of people that an individual knows)



Structure Similarity

The desired features tend to be captured by a measure we call Structural Similarity

$$\sigma(v,w) = \frac{|\Gamma(v) \cap \Gamma(w)|}{\sqrt{|\Gamma(v)||\Gamma(w)|}}$$



 Structural similarity is large for members of a clique and small for hubs and outliers

Structural Connectivity [1]

- \mathcal{E} -Neighborhood: $N_{\mathcal{E}}(v) = \{ w \in \Gamma(v) \mid \sigma(v, w) \ge \mathcal{E} \}$
- Core: $CORE_{\varepsilon,\mu}(v) \Leftrightarrow |N_{\varepsilon}(v)| \ge \mu$
- Direct structure reachable:

 $DirRECH_{\varepsilon,\mu}(v,w) \Leftrightarrow CORE_{\varepsilon,\mu}(v) \land w \in N_{\varepsilon}(v)$

- Structure reachable: transitive closure of direct structure reachability
- Structure connected:

 $CONNECT_{\varepsilon,\mu}(v,w) \Leftrightarrow \exists u \in V : RECH_{\varepsilon,\mu}(u,v) \land RECH_{\varepsilon,\mu}(u,w)$

[1] M. Ester, H. P. Kriegel, J. Sander, & X. Xu (KDD'96) "A Density-Based Algorithm for Discovering Clusters in Large Spatial Databases

Structure-Connected Clusters

- Structure-connected cluster C
 - Connectivity: $\forall v, w \in C: CONNECT_{\varepsilon,\mu}(v, w)$
 - Maximality: $\forall v, w \in V : v \in C \land REACH_{\varepsilon, u}(v, w) \Longrightarrow w \in C$
- Hubs:
 - Not belong to any cluster
 - Bridge to many clusters
- Outliers:
 - Not belong to any cluster
 - Connect to less clusters







































Running Time

- Running time = O(|E|)
- For sparse networks = O(|V|)



Spectral Clustering

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

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



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

Spectral Graph Partition

Min-Cut

• Minimize the # of cut of edges



Objective Function

2-way Spectral Graph Partitioning

Partition membership indicator:
$$q_{i} = \begin{cases} 1 & \text{if } i \in A \\ -1 & \text{if } i \in B \end{cases}$$
$$J = CutSize = \frac{1}{4} \sum_{i,j} w_{ij} [q_{i} - q_{j}]^{2}$$
$$= \frac{1}{4} \sum_{i,j} w_{ij} [q_{i}^{2} + q_{j}^{2} - 2q_{i}q_{j}] = \frac{1}{2} \sum_{i,j} q_{i} [d_{i}\delta_{ij} - w_{ij}]q_{j}$$
$$= \frac{1}{2} q^{T} (D - W)q$$

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)

Minimum Cut with Constraints

minimize cutsize without explicit size constraints

But where to cut ?



Need to balance sizes

New Objective Functions

• Ratio Cut (Hangen & Kahng, 1992) $J_{Rcut}(A,B) = \frac{s(A,B)}{|A|} + \frac{s(A,B)}{|B|}$

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

• 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)

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

Other References

- A Tutorial on Spectral Clustering by U. Luxburg http://www.kyb.mpg.de/fileadmin/user_u
 - pload/files/publications/attachments/Lux
 - burg07 tutorial 4488%5B0%5D.pdf

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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 and Node 5 Belongs to Class 2



Reference

- Learning from Labeled and Unlabeled
 Data with Label Propagation
 - By Xiaojin Zhu and Zoubin Ghahramani
 - http://www.cs.cmu.edu/~zhuxj/pub/CMU-CALD-02-107.pdf

Problem Formalization

Given n nodes

- l with labels $(Y_1, Y_2, \dots, Y_l \text{ are known})$
- u without labels $(Y_{l+1}, Y_{l+2}, \dots, Y_n$ are unknown)
- *Y* is the *n* × *C* label matrix
 - C is the number of labels (classes)
- The adjacency matrix is W
- The probabilistic transition matrix T

•
$$T_{ij} = P(j \rightarrow i) = \frac{w_{ij}}{\sum_k w_{kj}}$$

The Label Propagation Algorithm

- Step 1: Propagate $Y \leftarrow TY$
- 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

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Summary

- Graph / Network Data
 - Adjacency matrix
- Ranking on Graph / Network
 - PageRank
 - Personalized PageRank
- Network Clustering
 - SCAN
 - Spectral clustering
- Network classification
 - Label propagation