## CS6220: DATA MINING TECHNIQUES

## Mining Graph/Network Data

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## Methods to Learn

|  | Matrix Data | Set Data | Sequence <br> 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 <br> Pattern <br> Mining |  | Apriori; FP-growth | GSP; <br> PrefixSpan |  |  |
| Prediction | Linear Regression |  |  | Autoregression |  |
| Similarity Search |  |  |  | DTW | P-PageRank |
| Ranking |  |  |  |  | PageRank |
|  |  |  |  |  | 2 |

## 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


## 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

- $G=<V, E>$
- $V=\left\{u_{1}, \ldots, u_{n}\right\}$ : node set
- $E \subseteq V \times V$ : edge set
- Adjacency matrix
- $A=\left\{a_{i j}\right\}, i, j=1, \ldots, n$
- $a_{i j}=1, i f<u_{i}, u_{j}>\in E$
- $a_{i j}=0, i f<u_{i}, u_{j}>\notin E$
- Undirected graph vs. Directed graph
- $A=A^{\mathrm{T}}$ vs. $A \neq A^{\mathrm{T}}$
- Weighted graph
- Use $W$ instead of $A$, where $w_{i j}$ 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"

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


## Eigenvector formulation

-The flow equations can be written

$$
\mathrm{r}=\mathrm{Mr}
$$

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


## Example



$\mathbf{r}=\mathbf{M r}$

## Power Iteration method

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


## Power Iteration Example



| y |  |  |  |  |  |  |
| :--- | :---: | :---: | :---: | :--- | :--- | :--- | ---: |
| $\mathrm{a}=$ | $1 / 3$ | $1 / 3$ | $5 / 12$ | $3 / 8$ |  | $2 / 5$ |
| m | $1 / 3$ | $1 / 2$ | $1 / 3$ | $11 / 24$ | $\ldots$ | $2 / 5$ |
| $1 / 3$ | $1 / 6$ | $1 / 4$ | $1 / 6$ |  | $1 / 5$ |  |
| $r_{0}$ | $r_{1}$ | $r_{2}$ | $r_{3}$ | $\ldots$ | $r^{*}$ |  |

## Random Walk Interpretation

- Imagine a random web surfer
- At any time t , surfer is on some page P
- At time $\mathrm{t}+1$, the surfer follows an outlink from P uniformly at random
- Ends up on some page Q linked from $P$
- Process repeats indefinitely
- Let $\mathbf{p}(\mathrm{t})$ be a vector whose $\mathrm{i}^{\text {th }}$ component is the probability that the surfer is at page $i$ at time $t$
$\cdot \mathrm{p}(\mathrm{t})$ is a probability distribution on pages


## *The stationary distribution

-Where is the surfer at time $t+1$ ?

- Follows a link uniformly at random
- $\mathbf{p}(\mathrm{t}+1)=\mathbf{M p}(\mathrm{t})$
- Suppose the random walk reaches a state such that $\mathbf{p}(\mathrm{t}+1)=\mathbf{M p}(\mathrm{t})=\mathbf{p}(\mathrm{t})$
- Then $\mathbf{p}(t)$ is called a stationary distribution for the random walk
- Our rank vector $\mathbf{r}$ satisfies $\mathbf{r}=\mathbf{M r}$
- 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 $\beta$, follow a link at random
- With probability $1-\beta$, jump to some page uniformly at random
- Common values for $\beta$ are in the range 0.8 to 0.9
- Surfer will teleport out of spider trap within a few time steps


## Random teleports ( $\beta=0.8$ )




0.8 \begin{tabular}{|ccc|}
\hline $1 / 2$ \& $1 / 2$ \& 0 <br>
$1 / 2$ \& 0 \& 0 <br>
0 \& $1 / 2$ \& 1

 \left\lvert\,$\quad+0.2$

\hline $1 / 3$ \& $1 / 3$ \& $1 / 3$ <br>
$1 / 3$ \& $1 / 3$ \& $1 / 3$ <br>
$1 / 3$ \& $1 / 3$ \& $1 / 3$ <br>
\hline
\end{tabular}\right.

|  | $7 / 15$ | $7 / 15$ | $1 / 15$ |
| :--- | :--- | :--- | :--- |
| a | $7 / 15$ | $1 / 15$ | $1 / 15$ |
| m | $1 / 15$ | $7 / 15$ | $13 / 15$ |
|  |  |  |  |

## Random teleports ( $\beta=0.8$ )



## PageRank

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



$$
0.8 \begin{array}{|ccc|}
\hline 1 / 2 & 1 / 2 & 0 \\
1 / 2 & 0 & 0 \\
0 & 1 / 2 & 0
\end{array} \quad+0.2 \begin{array}{lll}
1 / 3 & 1 / 3 & 1 / 3 \\
1 / 3 & 1 / 3 & 1 / 3 \\
1 / 3 & 1 / 3 & 1 / 3
\end{array}
$$



## 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
- $\mathbf{r}^{\text {new }}=\mathbf{M}^{*} \mathbf{r}^{\text {old }}$
- Easy if we have enough main memory to hold $\mathbf{M}^{*}, \mathbf{r}^{\text {old }}, \mathbf{r}^{\text {new }}$
- Say N = 1 billion pages
- We need 4 bytes for each entry (say)
- 2 billion entries for vectors, approx 8GB
- Matrix $\mathbf{M}^{*}$ has $\mathbf{N}^{2}$ entries
- $10^{18}$ is a large number!


## Rearranging the equation

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

where $[\mathrm{x}]_{\mathrm{N}}$ is an N -vector with all entries x

## Sparse matrix formulation

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


## Sparse matrix encoding

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

| source <br> 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:
$\cdot \mathbf{r}=\beta \mathbf{M r}+[(1-\beta) / \mathrm{N}]_{\mathrm{N}}$ or
$\cdot \mathrm{r}=\beta \mathbf{M r}+(1-\beta) q_{0}$, where $q_{0}=\left(\begin{array}{c}1 / N \\ 1 / N \\ \ldots \\ 1 / N\end{array}\right)$
- For P-PageRank
- Replace $q_{0}$ with $q_{0}=\left(\begin{array}{c}0 \\ 0 \\ \ldots \\ 1 \\ \ldots \\ 0\end{array}\right) \quad$ qth webpage


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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]

## Algorithms

- 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 hubs know many people in different groups but belong to no single group. Politicians, for example bridge multiple groups
- Individuals who are outliers reside at the margins of society. Hermits, for example, know few people and belong to no group
- The Neighborhood of a Vertex
- Define $\Gamma(v)$ 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

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



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



## Structural Connectivity [1]

- $\varepsilon$-Neighborhood: $\quad N_{\varepsilon}(v)=\{w \in \Gamma(v) \mid \sigma(v, w) \geq \varepsilon\}$
- Core:

$$
\operatorname{CORE}_{\varepsilon, \mu}(v) \Leftrightarrow\left|N_{\varepsilon}(v)\right| \geq \mu
$$

- Direct structure reachable:

$$
\operatorname{DirRECH}_{\varepsilon, \mu}(v, w) \Leftrightarrow \operatorname{CORE}_{\varepsilon, \mu}(v) \wedge w \in N_{\varepsilon}(v)
$$

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

$$
\operatorname{CONNECT}_{\varepsilon, \mu}(v, w) \Leftrightarrow \exists u \in V: R E C H_{\varepsilon, \mu}(u, v) \wedge R E C H_{\varepsilon, \mu}(u, w)
$$

[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 $\mathbf{C}$
- Connectivity:

$$
\forall v, w \in C: \operatorname{CONNECT}_{\varepsilon, \mu}(v, w)
$$

- Maximality:

$$
\forall v, w \in V: v \in C \wedge R E A C H_{\varepsilon, \mu}(v, w) \Rightarrow w \in C
$$

- Hubs:
- Not belong to any cluster
- Bridge to many clusters
- Outliers:
- Not belong to any cluster
- Connect to less clusters



## Algorithm



## Algorithm



## Algorithm



## Algorithm



## Algorithm



## Algorithm



## Algorithm



## Algorithm



## Algorithm



## Algorithm



## Algorithm



## Algorithm



## Algorithm



## Running Time

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


Num. of Vertices
[2] A. Clauset, M. E. J. Newman, \& C. Moore, Phys. Rev. E 70, 066111 (2004).

## Spectral Clustering

## - Reference: ICDM’09 Tutorial by Chris Ding <br> - Example:

- Clustering supreme court justices according to

Number of times (\%) two Justices voted in agreement

|  | Ste | Bre | Gin | Sou | O' $^{\prime}$ o | 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: $\quad q_{i}=\left\{\begin{array}{cc}1 & \text { if } i \in A \\ -1 & \text { if } i \in B\end{array}\right.$

$$
\begin{aligned}
J & =\text { CutSize }=\frac{1}{4} \sum_{i, j} w_{i j}\left[q_{i}-q_{j}\right]^{2} \\
& =\frac{1}{4} \sum_{i, j} w_{i j}\left[q_{i}^{2}+q_{j}^{2}-2 q_{i} q_{j}\right]=\frac{1}{2} \sum_{i, j} q_{i}\left[d_{i} \delta_{i j}-w_{i j}\right] q_{j} \\
& =\frac{1}{2} q^{T}(D-W) q
\end{aligned}
$$

Relax indicators $q_{\mathrm{i}}$ from discrete values to continuous values, the solution for $\min J(q)$ is given by the eigenvectors of

$$
\begin{equation*}
(D-W) q=\lambda q \tag{Fiedler,1973,1975}
\end{equation*}
$$

## 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)

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

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

- Normalized Cut (Shi \& Malik, 2000)

$$
\begin{aligned}
J_{\text {Nout }}(A, B) & =\frac{s(A, B)}{d_{A}}+\frac{s(A, B)}{d_{B}} \\
& =\frac{s(A, B)}{s(A, A)+s(A, B)}+\frac{s(A, B)}{s(B, B)+s(A, B)}
\end{aligned}
$$

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

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

## 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/ ${ }^{\sim}$ zhuxj/pub/CMU-CALD-02-107.pdf


## Problem Formalization

- Given n nodes
-1 with labels ( $Y_{1}, Y_{2}, \ldots, Y_{l}$ are known)
- u without labels $\left(Y_{l+1}, Y_{l+2}, \ldots, Y_{n}\right.$ are unknown)
- $Y$ is the $n \times C$ label matrix
- $C$ is the number of labels (classes)
- The adjacency matrix is W
- The probabilistic transition matrix T
- $T_{i j}=P(j \rightarrow i)=\frac{w_{i j}}{\Sigma_{k} w_{k j}}$


## The Label Propagation Algorithm

- Step 1: Propagate $Y \leftarrow T Y$
- 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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- Graph / Network Data
- Adjacency matrix
- Ranking on Graph / Network
- PageRank
- Personalized PageRank
- Network Clustering
- SCAN
- Spectral clustering
- Network classification
- Label propagation

