

### Tools for large graph mining WWW 2008 tutorial Part 3: Matrix tools for graph mining

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### **Tutorial outline**

- Part 1: Structure and models for networks
  - What are properties of large graphs?
  - How do we model them?
- Part 2: Dynamics of networks
  - Diffusion and cascading behavior
  - How do viruses and information propagate?
- Part 3: Matrix tools for mining graphs
  - Singular value decomposition (SVD)
  - Random walks
- Part 4: Case studies
  - 240 million MSN instant messenger network
  - Graph projections: how does the web look like



### About part 3

 Introduce matrix and tensor tools through real mining applications

- Goal: find patterns, rules, clusters, outliers, ...
  - in matrices and
  - in tensors



### What is this part about?

- Connection of matrix tools and networks
- Matrix tools
  - Singular Value Decomposition (SVD)
  - Principal Component Analysis (PCA)
  - Webpage ranking algorithms: HITS, PageRank
  - CUR decomposition
  - Co-clustering (in part 4 of the tutorial)
- Tensor tools
  - Tucker decomposition
- Applications



### Why matrices? Examples

- Social networks
- Documents and terms
- Authors and terms

	John		Peter	Mary	Nick	•••
John Peter Mary Nick		0	11	22	55	
		5	0	6	7	
•••						



### Why tensors? Example

- Tensor:
  - n-dimensional generalization of matrix

#### SIGMOD'07

	data	mining	classif.	tree	•••
John Peter Mary Nick	13	11	22	55	
Peter	5	4	6	7	
Mary					
N1CK					
•••					



### Why tensors? Example

- Tensor:
  - n-dimensional generalization of matrix





### Tensors are useful for 3 or more modes

Terminology: 'mode' (or 'aspect'):



Leskovec&Faloutsos, WWW 2008



## **Motivating applications**

- Why matrices are important?
- Why tensors are useful?
  - P1: social networks
  - P2: web & text mining
  - P3: network forensics
  - P4: sensor networks









#### Network forensics







#### Tensor

**CMU SCS** 

- Formally,  $\mathcal{X} \in \mathbf{R}^{N_1 imes \dots imes N_M}$
- Generalization of matrices
- Represented as multi-array, (~ data cube).





### Dynamic Data model

#### Tensor Streams

A sequence of Mth order tensors

$$\mathcal{X}_1 \dots \mathcal{X}_t$$
 where  $\mathcal{X}_i \in \mathbf{R}^{N_1 imes \dots imes N_M}$ 

*t* is increasing over time





### SVD: Examples of Matrices

- Example/Intuition: Documents and terms
- Find patterns, groups, concepts





### Singular Value Decomposition (SVD) $\mathbf{X} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^{\mathsf{T}}$





### SVD as spectral decomposition



- Best rank-k approximation in L2 and Frobenius
- SVD only works for static matrices (a single 2<sup>nd</sup> order tensor)





#### • $\mathbf{A} = \mathbf{U} \Sigma \mathbf{V}^{\mathsf{T}}$ - example:















#### • $\mathbf{A} = \mathbf{U} \Sigma \mathbf{V}^{\mathsf{T}}$ - example:













### SVD - Interpretation

- 'documents', 'terms' and 'concepts':
- Q: if A is the document-to-term matrix, what is A<sup>T</sup> A?
- A: term-to-term ([m x m]) similarity matrix Q: A A<sup>T</sup> ?
- A: document-to-document ([n x n]) similarity matrix



#### SVD properties

 V are the eigenvectors of the covariance matrix A<sup>T</sup>A

#### U are the eigenvectors of the Gram (innerproduct) matrix AA<sup>T</sup>

Further reading:

1. Ian T. Jolliffe, *Principal Component Analysis* (2<sup>nd</sup> ed), Springer, 2002.

2. Gilbert Strang, Linear Algebra and Its Applications (4th ed), Brooks Cole, 2005 rt 3-23



## Principal Component Analysis (PCA) SVD $\mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T$



- PCA is an important application of SVD
- Note that U and V are dense and may have negative entries



### **PCA** interpretation

#### best axis to project on: ('best' = min sum of squares of projection errors)

Term2 ('lung')







- Problem definition:
  - given the web and a query
  - find the most 'authoritative' web pages for this query

Step 0: find all pages containing the query terms Step 1: expand by one move forward and backward

Further reading:

1. J. Kleinberg. Authoritative sources in a hyperlinked environment. SODA 1998



Step 1: expand by one move forward and backward





- on the resulting graph, give high score (= 'authorities') to nodes that many important nodes point to
- give high importance score ('hubs') to nodes that point to good 'authorities'





observations

- recursive definition!
- each node (say, 'i'-th node) has both an authoritativeness score a<sub>i</sub> and a hubness score h<sub>i</sub>



Let **A** be the adjacency matrix:

the (*i,j*) entry is 1 if the edge from *i* to *j* exists Let **h** and **a** be [n x 1] vectors with the 'hubness' and 'authoritativiness' scores.

Then:



Then:

$$a_i = h_k + h_l + h_m$$





1

### Kleinberg's algorithm: HITS

symmetrically, for the 'hubness':



$$h_{i} = a_{n} + a_{p} + a_{q}$$
  
that is  
$$h_{i} = \text{Sum}(q_{j}) \quad \text{over all } j \text{ that } (i,j)$$
  
edge exists  
or  
$$h = A a$$



# In conclusion, we want vectors **h** and **a** such that:

h = A a a = A<sup>⊤</sup> h

That is:

 $\mathbf{a} = \mathbf{A}^{\mathsf{T}}\mathbf{A} \mathbf{a}$ 



a is a <u>right singular vector</u> of the adjacency matrix A (by dfn!), a.k.a the <u>eigenvector</u> of A<sup>T</sup>A

Starting from random **a'** and iterating, we'll eventually converge

Q: to which of all the eigenvectors? why?

A: to the one of the strongest eigenvalue,  $(\mathbf{A}^{\mathsf{T}}\mathbf{A})^{\mathsf{k}}\mathbf{a} = \lambda_1^{\mathsf{k}}\mathbf{a}$ 



### Kleinberg's algorithm - discussion

- 'authority' score can be used to find 'similar pages' (how?)
- closely related to 'citation analysis', social networks / 'small world' phenomena


# Motivating problem: PageRank

# Given a directed graph, find its most interesting/central node



A node is important, if it is connected with important nodes (recursive, but OK!)



#### Motivating problem – PageRank solution

# Given a directed graph, find its most interesting/central node

Proposed solution: Random walk; spot most 'popular' node (-> steady state prob. (ssp))



A node has high ssp, if it is connected with high ssp nodes (recursive, but OK!)



#### Let A be the transition matrix (= adjacency matrix); let B be the transpose, column-normalized - then





• B p = p











- thus, p is the eigenvector that corresponds to the highest eigenvalue (=1, since the matrix is columnnormalized)
- Why does such a p exist?
  - p exists if B is nxn, nonnegative, irreducible [Perron–Frobenius theorem]



- In short: imagine a particle randomly moving along the edges
- compute its steady-state probabilities (ssp)

Full version of algo: with occasional random jumps

Why? To make the matrix irreducible



# Full Algorithm

- With probability 1-c, fly-out to a random node
- Then, we have **p** = c **B p** + (1-c)/n **1** => **p** = (1-c)/n [**I** c **B**]<sup>-1</sup> **1**







#### Motivation of CUR or CMD

- SVD, PCA all transform data into some abstract space (specified by a set basis)
  - Interpretability problem
  - Loss of sparsity



# **PCA** - interpretation





#### CUR

- Example-based projection: use actual rows and columns to specify the subspace
- Given a matrix A∈R<sup>m×n</sup>, find three matrices C∈ R<sup>m×c</sup>, U∈ R<sup>c×r</sup>, R∈ R<sup>r×n</sup>, such that ||A-CUR|| is small





#### CUR

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- Given a matrix A∈R<sup>m×n</sup>, find three matrices C∈ R<sup>m×c</sup>, U∈ R<sup>c×r</sup>, R∈ R<sup>r×n</sup>, such that ||A-CUR|| is small



U is the pseudo-inverse of X:  $U = X^{\dagger} = (U^T U)^{-1} U^T$ 



#### CUR (cont.)

- Key question:
  - How to select/sample the columns and rows?
- Uniform sampling
- Biased sampling
  - CUR w/ absolute error bound
  - CUR w/ relative error bound

Reference:

- 1. Tutorial: Randomized Algorithms for Matrices and Massive Datasets, SDM'06
- 2. Drineas et al. Subspace Sampling and Relative-error Matrix Approximation: Column-Row-Based Methods, ESA2006
- 3. Drineas et al., Fast Monte Carlo Algorithms for Matrices III: Computing a Compressed Approximate Matrix Decomposition, SIAM Journal on Computing, 2006.



#### The sparsity property – pictorially:

 $\sim$ 





=

SVD/PCA: Destroys sparsity









#### The sparsity property





#### Matrix tools - summary

- SVD:
  - optimal for L2 VERY popular (HITS, PageRank, Karhunen-Loeve, Latent Semantic Indexing, PCA, etc etc)
- C-U-R (CMD etc)
  - near-optimal; sparsity; interpretability



#### **TENSORS**



#### Reminder: SVD



Best rank-k approximation in L2



**Reminder: SVD** 



Best rank-k approximation in L2



### Goal: extension to >=3 modes





# Tensors: Main points

- 2 major types of tensor decompositions: Kruskal and Tucker
- both can be solved with ``alternating least squares'' (ALS)
- Details follow we start with terminology:



# Kruskal's Decomposion - intuition







# **Tucker Decomposition - intuition**



- author x keyword x conference
- A: author x author-group
- B: keyword x keyword-group
- C: conf. x conf-group
- G: how groups relate to each other Leskovec&Faloutsos, WWW 2008



**CMU SCS** 

#### 2-d analog of Tucker decomposition



**CMU SCS** med. doc cs doc med. terms .05 .05 .05 0 0 0 .05 .05 .05 0 0 0 0 0 .05 .05 .05 0 cs terms 0 .05 .05 .05 term group x 0 0 doc. group .04 .04 0 .04 .04 .04 common terms .04 .04 .04 0 .04 .04 .3 0 .36 .36 .28 0 .5 0 0 .054 .054 .042 0 0 0 0 0 .3 0 .28 .36 .36 0 0 0 .5 .054 .054 .042 0 0 0 0 .2 .2 .5 0 0 0 0 .042 .054 .054 0 .5 0 .042 .054 .054 0 0 0 0 doc x 0 .036 .036 028 .028 .036 .5 .036 0 doc group .036 .028 .028 0 .5 .036 .036 .036 0

term x term-group



#### **Tensor tools - summary**

- Two main tools
  - PARAFAC
  - Tucker
- Both find row-, column-, tube-groups
  - but in PARAFAC the three groups are identical
- To solve: Alternating Least Squares
- Toolbox: from Tamara Kolda: http://csmr.ca.sandia.gov/~tgkolda/TensorToolbox/



#### P1: Environmental sensor monitoring





## P1: sensor monitoring









voltage

hum.

temp.



- <sup>1</sup><sup>st</sup> factor consists of the main trends:
  - Daily periodicity on time
  - Uniform on all locations
  - Temp, Light and Volt are positively correlated while negatively correlated with Humid



## P1: sensor monitoring







light

- 2<sup>nd</sup> factor captures an atypical trend:
  - Uniformly across all time
  - Concentrating on 3 locations
  - Mainly due to voltage
- Interpretation: two sensors have low battery, and the other one has high battery.

hum.

voltage

temp.



# P3: Social network analysis

- Multiway latent semantic indexing (LSI)
  - Monitor the change of the community structure over time





# P3: Social network analysis (cont.)



- Two groups are correctly identified: Databases and Data mining
- People and concepts are drifting over time



## P4: Network anomaly detection



- Reconstruction error gives indication of anomalies.
- Prominent difference between normal and abnormal ones is mainly due to the unusual scanning activity (confirmed by the campus admin).



# P5: Web graph mining

- How to order the importance of web pages?
  - Kleinberg's algorithm HITS
  - PageRank
  - Tensor extension on HITS (TOPHITS)





# Kleinberg's Hubs and Authorities (the HITS method)



#### Sparse adjacency matrix and its SVD:

 $x_{ij} = \begin{cases} 1 & \text{if page } i \text{ links to page } j \\ 0 & \text{otherwise} \end{cases}$ 

$$\mathbf{X} \approx \sum_{r} \sigma_r \, \mathbf{h}_r \circ \mathbf{a}_r$$





#### **CMU SCS**

# **HITS Authorities on Sample Data**

1st Principal Factor													
	.97	www.ibm.com											
.24 www.alphaw 2nd Princi				cipal Fa	actor								
.08 .05 .02 .01 .01		www-128.ibm www.develop www.researc www.redbook news.com.co	.99 www.lenign .11 www2.lehig .06 www.lehigh .06 www.lehigh	gh du ha .75 java.sun.c hs .38 www.sun. eh .36 developer cc24 see.sun.c	3rd Princ java.sun.co www.sun.c developers. see.sun.co www.sama	com s.sun. 4th Pri com .60 www.pue		4th Prin www.puel	We started our crawl from http://www-neos.mcs.anl.gov/neos, and crawled 4700 pages, resulting in 560 cross-linked hosts.				
				www.leo.le www.distar fp1.cc.lehio	nc .13 nc .12 gh .08 .08 .08	docs.sun.c blogs.sun.c sunsolve.su www.sun-c news.com.	com com un.co atalo	.45 .35 .31 .22 .20 .16	www.whit www.irs.g travel.stat www.gsa. www.ssa. www.cens	gov te .g .97 .g .18	e.gov 6th Princip mathpost.as math.la.asu. www.asu.edu	u.edu edu	
a fe	uth or 1	ority scores <sup>st</sup> topic	<sup>3</sup> fo	ithority sc r 2 <sup>nd</sup> topic ✓	;			.14 .13 .13	www.govt www.kids www.usde		www.act.org www.eas.asu archives.mat	h.utk.edu	
from		=	h	+						.02 .02 .02 .02	www.geom.u www.fulton.a www.amstat www.maa.org	su.edu .org	
for 1 <sup>st</sup> topic for 2 <sup>nd</sup> topic Leskovec&Faloutsos, WWW 2008										4-71			

#### Three-Dimensional View of the Web



Kolda, Baderve Kernvut S. MOSV 2008



# **Topical HITS (TOPHITS)**

<u>Main Idea</u>: Extend the idea behind the HITS model to incorporate term (i.e., topical) information.

$$\mathbf{\mathfrak{X}} \approx \sum_{r=1}^{R} \lambda_r \, \mathbf{h}_r \circ \mathbf{a}_r$$





# **Topical HITS (TOPHITS)**

<u>Main Idea</u>: Extend the idea behind the HITS model to incorporate term (i.e., topical) information.

$$\mathbf{\mathfrak{X}} \approx \sum_{r=1}^{R} \lambda_r \, \mathbf{h}_r \circ \mathbf{a}_r \circ \mathbf{t}_r$$





# TOPHITS Terms & Authorities on Sample Data





## Conclusions

- Real data are often in high dimensions with multiple aspects (modes)
- Matrices and tensors provide elegant theory and algorithms
- Several research problems are still open
  - skewed distribution, anomaly detection, streaming algorithms, distributed/parallel algorithms, efficient out-of-core processing



#### References

 Slides borrowed from SIGMOD '07 tutorial by Falutsos, Kolda and Sun.