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15-826: Multimedia Databases and Data Mining

Lecture #20: Tensor decompositions

C. Faloutsos

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Must-read Material

- Tamara G. Kolda and Brett W. Bader. Tensor decompositions and applications. Technical Report SAND2007-6702, Sandia National Laboratories, Albuquerque, NM and Livermore, CA, November 2007

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Outline

Goal: 'Find similar / interesting things'

- Intro to DB
- Indexing - similarity search
- Data Mining

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Indexing - Detailed outline

- primary key indexing
- secondary key / multi-key indexing
- spatial access methods
- fractals
- text
- Singular Value Decomposition (SVD)
  - …
  - Tensors
- multimedia
- ...

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Most of foils by

- Dr. Tamara Kolda (Sandia N.L.)
- csmr.ca.sandia.gov/~tgkolda

- Dr. Jimeng Sun (CMU -> IBM)
- www.cs.cmu.edu/~jimeng

3h tutorial: www.cs.cmu.edu/~christos/TALKS/SDM-tut-07/

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Outline

- Motivation - Definitions
- Tensor tools
- Case studies

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Motivation 0: Why "matrix"?

- Why matrices are important?

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Examples of Matrices:
Graph - social network

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

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Examples of Matrices:
cloud of n-d points

	chol#	blood#	age	..	...
John	13	11	22	55	...
Peter	5	4	6	7	...
Mary	...	...	...	...	...
Nick	...	...	...	...	...
...	...	...	...	...	...

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Examples of Matrices:
Market basket

- **market basket** as in Association Rules

	milk	bread	choc.	wine	...
John	13	11	22	55	...
Peter	5	4	6	7	...
Mary	...	...	...	...	...
Nick	...	...	...	...	...
...	...	...	...	...	...

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Examples of Matrices:
Documents and terms

	data	mining	classif.	tree	...
Paper#1	13	11	22	55	...
Paper#2	5	4	6	7	...
Paper#3	...	...	...	...	...
Paper#4	...	...	...	...	...
...	...	...	...	...	...

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Examples of Matrices:
Authors and terms

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

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Examples of Matrices:
sensor-ids and time-ticks

	temp1	temp2	humid.	pressure	...
t1	13	11	22	55	…
t2	5	4	6	7	…
t3	…	…	…	…	…
t4	…	…	…	…	…
…	…	…	…	…	…

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Motivation: Why tensors?

- Q: what is a tensor?

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Motivation 2: Why tensor?

- A: N-D generalization of matrix:

KDD'07	data	mining	classif.	tree	...
John	13	11	22	55	…
Peter	5	4	6	7	…
Mary	…	…	…	…	…
Nick	…	…	…	…	…
…	…	…	…	…	…

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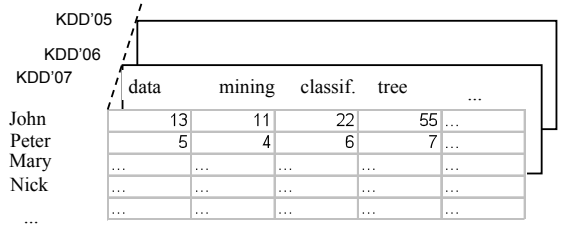
Motivation 2: Why tensor?

- A: N-D generalization of matrix:



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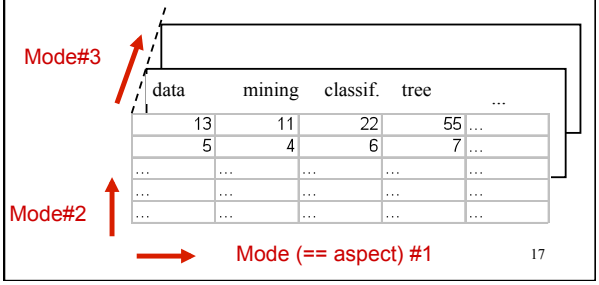
Tensors are useful for 3 or more modes

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



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Motivating Applications

- Why matrices are important?
- Why tensors are useful?
  - P1: social networks
  - P2: web mining

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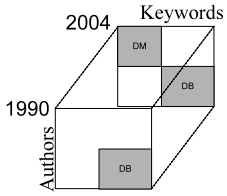
P1: Social network analysis

- Traditionally, people focus on static networks and find community structures
- We plan to monitor the change of the community structure over time



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P2: Web graph mining

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

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Outline

- Motivation – Definitions
- Tensor tools
- Case studies

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- Tensor Basics
- Tucker
- PARAFAC

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Tensor Basics

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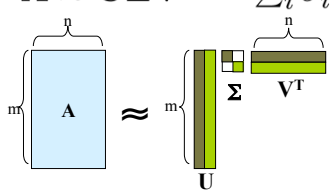
Reminder: SVD

$$\mathbf{A} \approx \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T = \sum_i \sigma_i \mathbf{u}_i \circ \mathbf{v}_i$$



– Best rank-k approximation in L2

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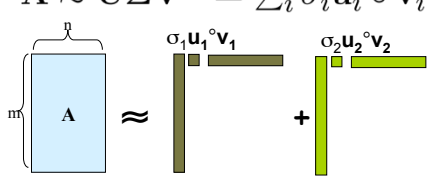
Reminder: SVD

$$\mathbf{A} \approx \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T = \sum_i \sigma_i \mathbf{u}_i \circ \mathbf{v}_i$$



– Best rank-k approximation in L2

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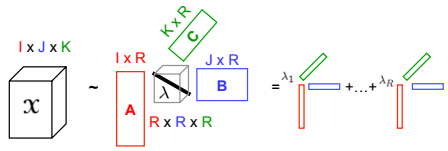
Goal: extension to >=3 modes



$$\mathcal{X} \approx [\![\lambda\,;\mathbf{A},\mathbf{B},\mathbf{C}]\!] = \sum_r \lambda_r\, \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r$$

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Main points:

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

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Specially Structured Tensors

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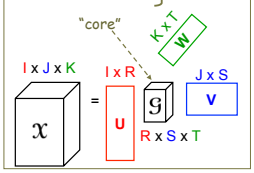
Specially Structured Tensors

- Tucker Tensor

$$\mathcal{X} = \mathcal{G} \times_1 \mathbf{U} \times_2 \mathbf{V} \times_3 \mathbf{W}$$
$$= \sum_r \sum_s \sum_t g_{rst}\, \mathbf{u}_r \circ \mathbf{v}_s \circ \mathbf{w}_t$$
$$\equiv [\![\mathcal{G}\,; \mathbf{U}, \mathbf{V}, \mathbf{W}]\!]$$

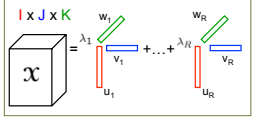
Our Notation



- Kruskal Tensor

$$\mathcal{X} = \sum_r \lambda_r\, \mathbf{u}_r \circ \mathbf{v}_r \circ \mathbf{w}_r$$
$$\equiv [\![\lambda\,; \mathbf{U}, \mathbf{V}, \mathbf{W}]\!]$$

Our Notation



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details

Specially Structured Tensors

- Tucker Tensor

$$\mathcal{X} = \mathcal{G} \times_1 \mathbf{U} \times_2 \mathbf{V} \times_3 \mathbf{W}$$
$$= \sum_r \sum_s \sum_t g_{rst}\, \mathbf{u}_r \circ \mathbf{v}_s \circ \mathbf{w}_t$$
$$\equiv [\![\mathcal{G}\,; \mathbf{U}, \mathbf{V}, \mathbf{W}]\!]$$

In matrix form:

$$\mathbf{X}_{(1)} = \mathbf{U}\mathbf{G}_{(1)}(\mathbf{W} \otimes \mathbf{V})^{\mathsf{T}}$$
$$\mathbf{X}_{(2)} = \mathbf{V}\mathbf{G}_{(2)}(\mathbf{W} \otimes \mathbf{U})^{\mathsf{T}}$$
$$\mathbf{X}_{(3)} = \mathbf{W}\mathbf{G}_{(3)}(\mathbf{V} \otimes \mathbf{U})^{\mathsf{T}}$$

$$\mathrm{vec}(\mathcal{X}) = (\mathbf{W} \otimes \mathbf{V} \otimes \mathbf{U})\mathrm{vec}(\mathcal{G})$$

- Kruskal Tensor

$$\mathcal{X} = \sum_r \lambda_r\, \mathbf{u}_r \circ \mathbf{v}_r \circ \mathbf{w}_r$$
$$\equiv [\![\lambda\,; \mathbf{U}, \mathbf{V}, \mathbf{W}]\!]$$

In matrix form:

Let $\mathbf{\Lambda} = \mathrm{diag}(\lambda)$

$$\mathbf{X}_{(1)} = \mathbf{U}\,\mathbf{\Lambda}\,(\mathbf{W} \odot \mathbf{V})^{\mathsf{T}}$$
$$\mathbf{X}_{(2)} = \mathbf{V}\,\mathbf{\Lambda}\,(\mathbf{W} \odot \mathbf{U})^{\mathsf{T}}$$
$$\mathbf{X}_{(3)} = \mathbf{W}\,\mathbf{\Lambda}\,(\mathbf{V} \odot \mathbf{U})^{\mathsf{T}}$$

$$\mathrm{vec}(\mathcal{X}) = (\mathbf{W} \odot \mathbf{V} \odot \mathbf{U})\,\lambda$$

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Tensor Decompositions

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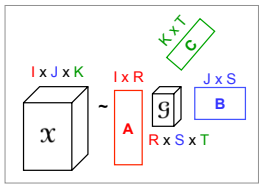
Tucker Decomposition - intuition



- author x keyword x conference
- A: author x author-group
- B: keyword x keyword-group
- C: conf. x conf-group
- $\mathcal{G}$: how groups relate to each other

Needs elaboration!

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Intuition behind core tensor

- 2-d case: co-clustering
- [Dhillon et al. Information-Theoretic Co-clustering, KDD'03]

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$$\begin{array}{c|c} & n \\ \hline m & \begin{bmatrix} .05 & .05 & .05 & 0 & 0 & 0 \\ .05 & .05 & .05 & 0 & 0 & 0 \\ 0 & 0 & 0 & .05 & .05 & .05 \\ 0 & 0 & 0 & .05 & .05 & .05 \\ .04 & .04 & 0 & .04 & .04 & .04 \\ .04 & .04 & .04 & 0 & .04 & .04 \end{bmatrix} \end{array}$$

eg, terms x documents

$$\begin{array}{c|c} & k \\ \hline m & \begin{bmatrix} .5 & 0 & 0 \\ .5 & 0 & 0 \\ 0 & .5 & 0 \\ 0 & .5 & 0 \\ 0 & 0 & .5 \\ 0 & 0 & .5 \end{bmatrix} \end{array} \begin{array}{c|c} & l \\ \hline k & \begin{bmatrix} .3 & 0 \\ 0 & .3 \\ .2 & .2 \end{bmatrix} \end{array} \begin{array}{c|c} & n \\ \hline l & \begin{bmatrix} .36 & .36 & .28 & 0 & 0 & 0 \\ 0 & 0 & 0 & .28 & .36 & .36 \end{bmatrix} \end{array} = \begin{bmatrix} .054 & .054 & .042 & 0 & 0 & 0 \\ .054 & .054 & .042 & 0 & 0 & 0 \\ 0 & 0 & 0 & .042 & .054 & .054 \\ 0 & 0 & 0 & .042 & .054 & .054 \\ .036 & .036 & 028 & .028 & .036 & .036 \\ .036 & .036 & .028 & .028 & .036 & .036 \end{bmatrix}$$

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med. doc

cs doc

$$\begin{bmatrix} .05 & .05 & .05 & 0 & 0 & 0 \\ .05 & .05 & .05 & 0 & 0 & 0 \\ 0 & 0 & 0 & .05 & .05 & .05 \\ 0 & 0 & 0 & .05 & .05 & .05 \\ .04 & .04 & 0 & .04 & .04 & .04 \\ .04 & .04 & .04 & 0 & .04 & .04 \end{bmatrix}$$

med. terms

cs terms

common terms

term group x doc. group

$$\begin{bmatrix} .5 & 0 & 0 \\ .5 & 0 & 0 \\ 0 & .5 & 0 \\ 0 & .5 & 0 \\ 0 & 0 & .5 \\ 0 & 0 & .5 \end{bmatrix} \begin{bmatrix} .3 & 0 \\ 0 & .3 \\ .2 & .2 \end{bmatrix} \begin{bmatrix} .36 & .36 & .28 & 0 & 0 & 0 \\ 0 & 0 & 0 & .28 & .36 & .36 \end{bmatrix} = \begin{bmatrix} .054 & .054 & .042 & 0 & 0 & 0 \\ .054 & .054 & .042 & 0 & 0 & 0 \\ 0 & 0 & 0 & .042 & .054 & .054 \\ 0 & 0 & 0 & .042 & .054 & .054 \\ .036 & .036 & 028 & .028 & .036 & .036 \\ .036 & .036 & .028 & .028 & .036 & .036 \end{bmatrix}$$

doc x doc group

term x term-group

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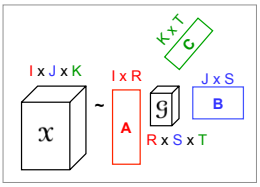
Tucker Decomposition



$$\mathcal{X} \approx [\![\mathcal{G} \; ; \mathbf{A}, \mathbf{B}, \mathbf{C}]\!]$$

Given A, B, C, the optimal core is:

$$\mathcal{G} = [\![\mathcal{X} \; ; \mathbf{A}^{\dagger}, \mathbf{B}^{\dagger}, \mathbf{C}^{\dagger}]\!]$$

- Proposed by Tucker (1966)
- AKA: Three-mode factor analysis, three-mode PCA, orthogonal array decomposition
- **A**, **B**, and **C** generally assumed to be orthonormal (generally assume they have full column rank)
- $\mathcal{G}$ is <u>not</u> diagonal
- Not unique

Recall the equations for converting a tensor to a matrix

$$\mathbf{X}_{(1)} = \mathbf{A}\mathbf{G}_{(1)}(\mathbf{C} \otimes \mathbf{B})^{\mathsf{T}}$$
$$\mathbf{X}_{(2)} = \mathbf{B}\mathbf{G}_{(2)}(\mathbf{C} \otimes \mathbf{A})^{\mathsf{T}}$$
$$\mathbf{X}_{(3)} = \mathbf{C}\mathbf{G}_{(3)}(\mathbf{B} \otimes \mathbf{A})^{\mathsf{T}}$$
$$\text{vec}(\mathcal{X}) = (\mathbf{C} \otimes \mathbf{B} \otimes \mathbf{A})\text{vec}(\mathcal{G})$$

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Outline

- Motivation – Definitions
- Tensor tools
- Case studies

- Tensor Basics
- Tucker
- PARAFAC

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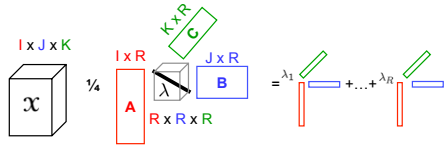
CANDECOMP/PARAFAC Decomposition



$$\mathcal{X} \approx [\![\lambda\,;\mathbf{A},\mathbf{B},\mathbf{C}]\!] = \sum_r \lambda_r\, \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r$$

- CANDECOMP = Canonical Decomposition (Carroll & Chang, 1970)
- PARAFAC = Parallel Factors (Harshman, 1970)
- Core is diagonal (specified by the vector λ)
- Columns of **A**, **B**, and **C** are not orthonormal
- If R is *minimal*, then R is called the **rank** of the tensor (Kruskal 1977)
- Can have rank($\mathcal{X}$) > min{I,J,K}

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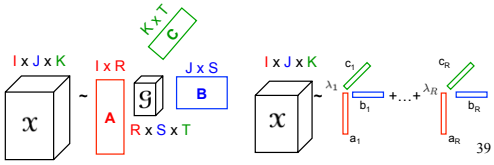
IMPORTANT

Tucker vs. PARAFAC Decompositions

- Tucker
  - Variable transformation in each mode
  - Core G may be dense
  - A, B, C generally orthonormal
  - Not unique
- PARAFAC
  - Sum of rank-1 components
  - No core, i.e., superdiagonal core
  - A, B, C may have linearly dependent columns
  - Generally unique



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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/

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Outline

- Motivation - Definitions
- Tensor tools
- Case studies

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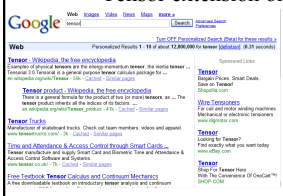
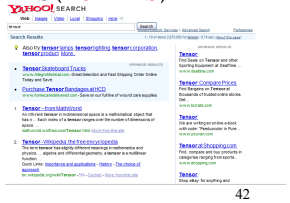
P1: Web graph mining

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





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P1: Web graph mining

- T. G. Kolda, B. W. Bader and J. P. Kenny, ***Higher-Order Web Link Analysis Using Multilinear Algebra***, ICDM 2005: ICDM, pp. 242-249, November 2005, doi:10.1109/ICDM.2005.77. [PDF]

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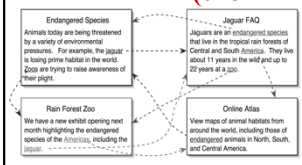
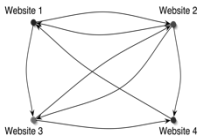
Kleinberg's Hubs and Authorities (the HITS method)

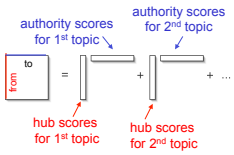


Sparse adjacency matrix and its SVD:

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

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





Kleinberg, JACM, 1999

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HITS Authorities on Sample Data

1st Principal Factor

.97	www.ibm.com
.24	www.alphaw
.08	www-128.ibm
.05	www.develop
.02	www.researc
.01	www.redbook
.01	news.com.co

2nd Principal Factor

.99	www.lehigh.edu
.11	www2.lehigh
.06	www.lehigha
.06	www.lehighs
.02	www.bethleh
.02	www.adobe.c
.02	lewisweb.cc.
.02	www.leo.lehi
.02	www.distanc
.02	fp1.cc.lehigh

3rd Principal Factor

.75	java.sun.com
.38	www.sun.com
.36	developers.sun.
.24	see.sun.com
.16	www.samag.co
.13	docs.sun.com
.12	blogs.sun.com
.08	sunsolve.sun.co
.08	www.sun-catalo
.08	news.com.com

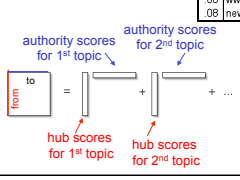
4th Principal Factor

.60	www.pueblo.gsa.gov
.45	www.whitehouse.gov
.35	www.irs.gov
.31	travel.state
.22	www.gsa.g
.20	www.ssa.g
.16	www.censu
.14	www.govbe
.13	www.kids.g
.13	www.usdoj

6th Principal Factor

.97	mathpost.asu.edu
.18	math.la.asu.edu
.17	www.asu.edu
.04	www.act.org
.03	www.eas.asu.edu
.02	archives.math.utk.edu
.02	www.geom.uiuc.edu
.02	www.fulton.asu.edu
.02	www.amstat.org
.02	www.maa.org

We started our crawl from http://www-neos.mcs.anl.gov/neos, and crawled 4700 pages, resulting in 560 cross-linked hosts.



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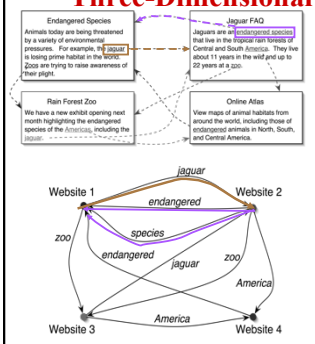
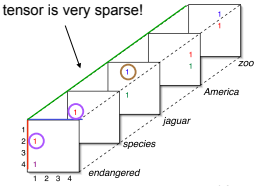
Three-Dimensional View of the Web



$$x_{ijk} = \begin{cases} 1 & \text{if page } i \rightarrow \text{page } j \\ & \text{with term } k \\ 0 & \text{otherwise} \end{cases}$$

Observe that this tensor is very sparse!



Kolda, Bader, Kenny, ICDM05

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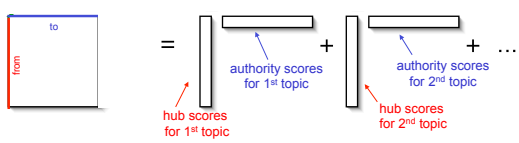
Topical HITS (TOPHITS)

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

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



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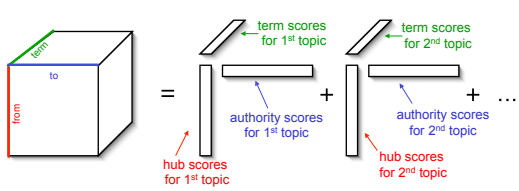
Topical HITS (TOPHITS)

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

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



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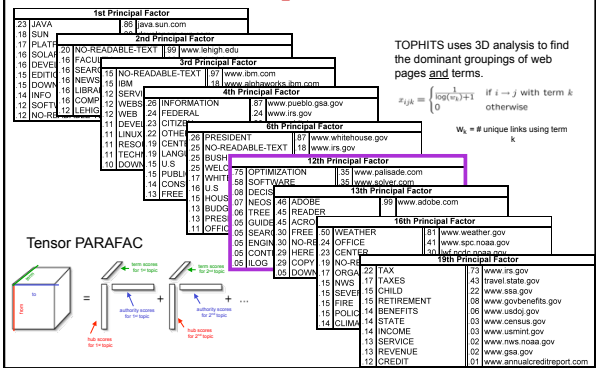
TOPHITS Terms & Authorities on Sample Data



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GigaTensor: Scaling Tensor Analysis Up By 100 Times – Algorithms and Discoveries

U Kang
Evangelos Papalexakis
Abhay Harpale
Christos Faloutsos

KDD 2012

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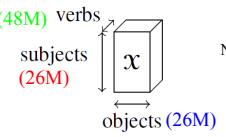
P2: N.E.L.L. analysis

- NELL: Never Ending Language Learner
  - Q1: dominant concepts / topics?
  - Q2: synonyms for a given new phrase?

"Eric Clapton plays guitar"
"Barrack Obama is the president of U.S."



NELL (Never Ending Language Learner)
Nonzeros =144M

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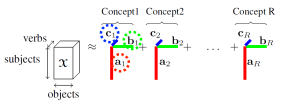
A1: Concept Discovery

- Concept Discovery in Knowledge Base



Noun Phrase 1	Noun Phrase 2	Context
Concept 1: "Web Protocol"		
internet	protocol	'np1' 'stream' 'np2'
file	software	'np1' 'marketing' 'np2'
data	suite	'np1' 'dating' 'np2'
Concept 2: "Credit Cards"		
credit	information	'np1' 'card' 'np2'
Credit	debt	'np1' 'report' 'np2'
library	number	'np1' 'cards' 'np2'
Concept 3: "Health System"		
health	provider	'np1' 'care' 'np2'
child	providers	'np' 'insurance' 'np2'
home	system	'np1' 'service' 'np2'
Concept 4: "Family Life"		
life	rest	'np2' 'of' 'my' 'np1'
family	part	'np2' 'of' 'his' 'np1"
body	years	'np2' 'of' 'her' 'np1'

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A1: Concept Discovery

Noun Phrase 1	Noun Phrase 2	Context
Concept 1: "Web Protocol"		
internet	protocol	'np1' 'stream' 'np2'
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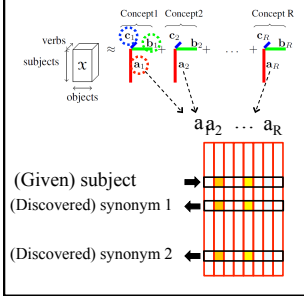
A2: Synonym Discovery

- Synonym Discovery in Knowledge Base



(Given) Noun Phrase	(Discovered) Potential Synonyms
pollutants	dioxin, sulfur dioxide, greenhouse gases, particulates, nitrogen oxide, air pollutants, cholesterol
disabilities	infections, dizziness, injuries, diseases, drowsiness, stiffness, injuries
vodafone	verizon, comcast
Christian history	European history, American history, Islamic history, history
disbelief	dismay, disgust, astonishment
cyberpunk	online-gaming
soul	body

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A2: Synonym Discovery

(Given) Noun Phrase	(Discovered) Potential Synonyms
pollutants	dioxin, sulfur dioxide, greenhouse gases, particulates, nitrogen oxide, air pollutants, cholesterol
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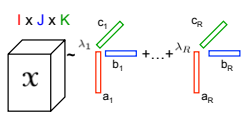
Conclusions

- Real data are often in high dimensions with multiple aspects (modes)
- Matrices and tensors provide elegant theory and algorithms



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