# Tensor Decompositions for Analyzing Multi-link Graphs

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## Linear Algebra, Graph Analysis, Informatics

- Network analysis and bibiliometrics
- PageRank [Brin & Page, 1998]
  - Transition matrix of a Markov chain:  $\mathbf{M}$
  - Ranks: Mr = r
- HITS [Kleinberg, 1998]
  - Adjacency matrix of the Web graph:  ${\bf L}$
  - Hubs:  $\mathbf{L}\mathbf{L}^T\mathbf{y} = \mathbf{y}$
  - Authorities:  $\mathbf{L}^T \mathbf{L} \mathbf{x} = \mathbf{x}$
- Latent Semantic Analysis (LSA) [Dumais, et al., 1988]
  - Vector space model of documents (term-document matrix): A
  - Truncated SVD:  $\mathbf{A} \approx \mathbf{T} \mathbf{\Sigma} \mathbf{D}^{\mathsf{T}} = \sum_{r=1}^{k} \sigma_r \mathbf{t}_r \mathbf{d}_r^T$
  - Maps terms and documents to the "same" k-dimensional space





## **Multi-Link Graphs**



- Nodes (one type) connected by multiple types of links
  - Node x Node x Connection
- Two types of nodes connected by multiple types of links
  - Node A x Node B x Connection
- Multiple types of nodes connected by multiple types of links
  - Node A x Node B x Node C x Connection
  - Directed and undirected links



#### Tensors



#### Other names for tensors

- Multidimensional array
- N-way array
- Tensor order
  - Number of dimensions
- Other names for dimension
  - Mode
  - Way

#### Example

- The matrix A (at left) has order 2.
- The tensor  $\mathfrak{X}$  (at left) has order 3 and its 3<sup>rd</sup> mode is of size *K*.



#### Tensors



## Tensor Unfolding: Converting a Tensor to a Matrix



#### **Tensor n-Mode Multiplication**

$$\mathbf{X} \in \mathbb{R}^{I \times J \times K}, \ \mathbf{B} \in \mathbb{R}^{M \times J}, \ \mathbf{a} \in \mathbb{R}^{I}$$

#### **Tensor Times Matrix**

$$\mathbf{\mathcal{Y}} = \mathbf{\mathcal{X}} \times_{\mathbf{2}} \mathbf{B} \in \mathbb{R}^{I \times M \times K}$$

$$y_{imk} = \sum_{j} x_{ijk} \ b_{mj}$$
$$\mathbf{Y}_{(2)} = \mathbf{B}\mathbf{X}_{(2)}$$

Multiply each row (mode-2) fiber by **B** 



**Tensor Times Vector** 

$$\mathbf{Y} = \mathbf{X} \,\bar{\mathbf{x}}_{1} \,\mathbf{a} \in \mathbb{R}^{J \times K}$$
$$y_{jk} = \sum_{i} x_{ijk} \,a_{i}$$

Compute the dot product of **a** and each column (mode-1) fiber





## **Outer, Kronecker, & Khatri-Rao Products**





#### **Specially Structured Tensors**

#### **Tucker Tensor**

#### Kruskal Tensor

$$\mathbf{\mathfrak{X}} = \sum_{r} \lambda_r \ \mathbf{u}_r \circ \mathbf{v}_r \circ \mathbf{w}_r$$
  
 $\equiv \llbracket \mathbf{\lambda} ; \mathbf{U}, \mathbf{V}, \mathbf{W} 
rbracket 
ightarrow rac{\mathbf{O}ur}{\mathbf{Notation}}$ 





## **Specially Structured Tensors**

#### **Tucker Tensor**

$$\begin{split} \mathbf{\mathfrak{X}} &= \mathbf{\mathfrak{G}} \times_{1} \mathbf{U} \times_{2} \mathbf{V} \times_{3} \mathbf{W} \\ &= \sum_{r} \sum_{s} \sum_{t} g_{rst} \, \mathbf{u}_{r} \circ \mathbf{v}_{s} \circ \mathbf{w}_{t} \\ &\equiv \llbracket \mathbf{\mathfrak{G}} ; \mathbf{U}, \mathbf{V}, \mathbf{W} \rrbracket \end{split}$$

In matrix form:

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

$$\mathsf{vec}(\mathfrak{X}) = (\mathbf{W} \otimes \mathbf{V} \otimes \mathbf{U})\mathsf{vec}(\mathfrak{G})$$

#### **Kruskal Tensor**

$$egin{aligned} &\mathfrak{X} = \sum_r \lambda_r \; \mathbf{u}_r \circ \mathbf{v}_r \circ \mathbf{w}_r \ &\equiv \llbracket oldsymbol{\lambda} \; ; \mathbf{U}, \mathbf{V}, \mathbf{W} 
brace \end{aligned}$$

In matrix form: Let  $\Lambda = \text{diag}(\lambda)$   $\mathbf{X}_{(1)} = \mathbf{U} \Lambda (\mathbf{W} \odot \mathbf{V})^{\mathsf{T}}$   $\mathbf{X}_{(2)} = \mathbf{V} \Lambda (\mathbf{W} \odot \mathbf{U})^{\mathsf{T}}$  $\mathbf{X}_{(3)} = \mathbf{W} \Lambda (\mathbf{V} \odot \mathbf{U})^{\mathsf{T}}$ 

 $\operatorname{vec}(\mathfrak{X}) = (\mathbf{W} \odot \mathbf{V} \odot \mathbf{U}) \lambda$ 



#### **Tucker Decomposition**

Three-mode factor analysis Three-mode PCA *N*-mode PCA Higher-order SVD (HO-SVD)



[Tucker, 1966] [Kroonenberg, et al. 1980] [Kapteyn et al., 1986] [De Lathauwer et al., 2000]

## $\boldsymbol{\mathfrak{X}} \approx [\![\boldsymbol{\mathfrak{G}} \text{ ; } \mathbf{A}, \mathbf{B}, \mathbf{C}]\!]$

Given **A**, **B**, **C**, the optimal core is:  $\mathbf{\mathcal{G}} = [\![\mathbf{\mathcal{X}}; \mathbf{A}^{\dagger}, \mathbf{B}^{\dagger}, \mathbf{C}^{\dagger}]\!]$ 

- A, B, and C may be orthonormal (generally, full column rank)
- G is <u>not</u> diagonal
- Decomposition is **not** unique



## **CANDECOMP/PARAFAC (CP) Decomposition**



- **CANDECOMP** = Canonical Decomposition
- **PARAFAC** = Parallel Factors
- Core is *diagonal* (specified by the vector  $\lambda$ )
- Columns of A, B, and C are not orthonormal

[Carroll & Chang, 1970] [Harshman, 1970]



## **CP Alternating Least Squares (CP-ALS)**



#### Khatri-Rao Pseudoinverse

$$\begin{aligned} (\mathbf{B} \odot \mathbf{A})^{\dagger} &= \\ \left( \left( \mathbf{B}^{\mathsf{T}} \mathbf{B} \right) * \left( \mathbf{A}^{\mathsf{T}} \mathbf{A} \right) \right)^{\dagger} \left( \mathbf{B} \odot \mathbf{A} \right)^{\mathsf{T}} \end{aligned}$$

- Fix **A**, **B**, and **A**, solve for **C**:  $\min_{C} \| \mathcal{X} - [\lambda; \mathbf{A}, \mathbf{B}, \mathbf{C}] \| \equiv \min_{C} \| \mathbf{X}_{(3)} - \mathbf{C} \mathbf{A} (\mathbf{B} \odot \mathbf{A})^{\mathsf{T}} \|$ [Smilde et al., 2004]
- Optimal **C** is the least squares solution:

$$\mathbf{C} = \mathbf{X}_{(3)} \left( \mathbf{B} \odot \mathbf{A} \right) \left( \left( \mathbf{B}^{\mathsf{T}} \mathbf{B} \right) * \left( \mathbf{A}^{\mathsf{T}} \mathbf{A} \right) \right)^{\dagger} \mathbf{\Lambda}^{-1}$$

• Successively solve for each component (**C**,**B**,**A**)



## **CP Alternating Least Squares (CP-ALS)**

 $\mathsf{CP-ALS}(\mathfrak{X}, R, M, \epsilon)$ 

- 1  $m \leftarrow 0$
- 2  $\mathbf{A} \leftarrow R$  principal eigenvectors of  $\mathbf{X}_{(1)}\mathbf{X}_{(1)}^{\mathsf{T}}$
- 3  $\mathbf{B} \leftarrow R$  principal eigenvectors of  $\mathbf{X}_{(2)}\mathbf{X}_{(2)}^{\mathsf{T}}$
- 4 repeat

5

 $m \leftarrow m + 1$ 

 $\mathbf{C} \leftarrow \mathbf{X}_{(3)}(\mathbf{B} \odot \mathbf{A}) \left( \left( \mathbf{B}^{\mathsf{T}} \mathbf{B} \right) * \left( \mathbf{A}^{\mathsf{T}} \mathbf{A} \right) \right)^{\dagger}$ 6 Normalize columns of C to length 1 7  $\mathbf{B} \leftarrow \mathbf{X}_{(2)}(\mathbf{C} \odot \mathbf{A}) \left( \left( \mathbf{C}^{\mathsf{T}} \mathbf{C} \right) * \left( \mathbf{A}^{\mathsf{T}} \mathbf{A} \right) \right)^{\dagger}$ 8 Normalize columns of B to length 1 9  $\mathbf{A} \leftarrow \mathbf{X}_{(1)}(\mathbf{C} \odot \mathbf{B}) \left( \left( \mathbf{C}^{\mathsf{T}} \mathbf{C} \right) * \left( \mathbf{B}^{\mathsf{T}} \mathbf{B} \right) \right)^{\dagger}$ 10 Store column norms of A in  $\lambda$  and 11 normalize columns of A to length 1until m > M or  $\| \mathbf{X} - [ \mathbf{\lambda} ; \mathbf{A}, \mathbf{B}, \mathbf{C} ] \| \| < \epsilon$ 12 return  $\lambda \in \mathbb{R}^R$  ;  $\mathbf{A} \in \mathbb{R}^{I \times R}$  ;  $\mathbf{B} \in \mathbb{R}^{J \times R}$  ;  $\mathbf{C} \in \mathbb{R}^{K \times R}$ 13 such that  $\mathfrak{X} \approx \llbracket \lambda$  ;  $\mathbf{A}, \mathbf{B}, \mathbf{C} \rrbracket$ 



## **Analyzing SIAM Publication Data**

#### 1999-2004 SIAM Journal Data 5022 Documents

Tensor Toolbox (MATLAB) [T. Kolda, B. Bader, 2007]

Google" [tensor toolbox

Journal Name Articles SIAM J APPL DYN SYST 32 SIAM J APPL MATH 548 SIAM J COMPUT 540 SIAM J CONTROL OPTIM 577 SIAM J DISCRETE MATH 260 SIAM J MATH ANAL 420 I MATRIX ANAL A SIAM 423 SIAM J NUMER ANAL 611 344 SIAM J OPTIMIZ SIAM J SCI COMPUT 656 SIAM PROC S 469 SIAM REV 142

	Total in	Per Document		nt	
	Collection	Average	Maximum	Minimum	
Unique terms	16617	148.32	831	17	
abstracts	15752	128.06	802	11	
titles	5164	10.16	33	1	
keywords	5248	10.10	40	2	
Authors	6891	2.19	13	1	
Citations (within collection)	2659	0.53	12	0	



#### **SIAM Data: Why Tensors?**





## **SIAM Data: Tensor Construction**



Slice (k)	Description	Nonzeros	$\sum_{i}\sum_{j}x_{ijk}$
1	Abstract Similarity	28476	7695.28
2	Title Similarity	120236	33285.79
3	Keyword Similarity	115412	16201.85
4	Author Similarity	16460	8027.46
5	Citation	2659	5318.00

Frontal Slices  $\mathbf{X}_k$ 

- $\mathbf{X}_1 = \mathbf{T}^{\mathsf{T}}\mathbf{T}$  where  $t_{ij} = f_{ij} \log_2(N/N_i)$  for terms in the abstracts
  - $f_{ij}$  is the frequency of term *i* in document *j*
  - $N_i$  is the number of documents that term *i* appears in
- $\mathbf{X}_2 = \mathbf{T}^T \mathbf{T}$  for terms in the **titles**
- $X_3 = T^T T$  for terms in the author-supplied keywords

•  $\mathbf{X}_4 = \mathbf{W}^\mathsf{T} \mathbf{W}$  where  $w_{ij} = \begin{cases} 1/\sqrt{M_j} & \text{if author } i \text{ wrote document } j \\ 0 & \text{otherwise,} \end{cases}$ 

•  $x_{ij5} = \begin{cases} 2 & \text{if document } i \text{ cites document } j \\ 0 & \text{otherwise.} \end{cases}$ 

not symmetric



## **SIAM Data: CP Applications**

$$\mathfrak{X} \approx \llbracket \boldsymbol{\lambda} ; \mathbf{A}, \mathbf{B}, \mathbf{C} 
rbracket = \sum_r \lambda_r \ \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r$$

- **Community Identification** •  $(\mathbf{a}_r, \mathbf{b}_r, \mathbf{c}_r)$  Communities of papers connected by different link types Latent Document Similarity •  $\alpha \mathbf{A} \mathbf{A} \mathbf{A}^{\mathsf{T}} + \beta \mathbf{B} \mathbf{A} \mathbf{B}^{\mathsf{T}}$  Using tensor decompositions for LSA-like analysis Analysis of a Body of Work via Centroids ۲  $\alpha \mathbf{A} \Lambda \mathbf{g}_A + \beta \mathbf{B} \Lambda \mathbf{g}_B$  Body of work defined by query terms Body of work defined by authorship **Author Disambiguation** •  $\alpha \mathbf{a}_{i}^{\mathsf{T}} \mathbf{g}_{A} + \beta \mathbf{b}_{i}^{\mathsf{T}} \mathbf{g}_{B}$  List of most prolific authors in collection changes Multiple author disambiguation Journal Prediction
  - Co-reference information to define journal characteristics



### **SIAM Data: Document Similarity**

Link Analysis: Hubs and Authorities on the World Wide Web, C.H.Q. Ding, H. Zha, X. He, P. Husbands, and H.D. Simon, SIREV, 2004.

- **CP decomposition,**  $R = 10: \mathfrak{X} \approx [\lambda; \mathbf{A}, \mathbf{B}, \mathbf{C}] = \sum_{r=1}^{\infty} \lambda_r \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r$ lacksquare
- Similarity scores:  $S = \frac{1}{2}AA^{T} + \frac{1}{2}BB^{T}$

Score	Title
0.000079	Ordering anisotropy and factored sparse approximate inverses
0.000079	Robust approximate inverse preconditioning for the conjugate gradient method
0.000077	An interior point algorithm for large-scale nonlinear programming
0.000073	Primal-dual interior-point methods for semidefinite programming in finite precision
0.000068	Some new search directions for primal-dual interior point methods in semidefinite programming
0.000068	A fast and high-quality multilevel scheme for partitioning irregular graphs
0.000067	Reoptimization with the primal-dual interior point method
0.000065	Superlinear convergence of primal-dual interior point algorithms for nonlinear programming
0.000064	A robust primal-dual interior-point algorithm for nonlinear programs
0.000063	Orderings for factorized sparse approximate inverse preconditioners

Interior Point Methods Sparse approximate inverses (Arguably distantly related) **Graph Partitioning** 

(Not related) (Related)



## **SIAM Data: Document Similarity**

Link Analysis: Hubs and Authorities on the World Wide Web, C.H.Q. Ding, H. Zha, X. He, P. Husbands, and H.D. Simon, *SIREV*, 2004.

- **CP decomposition,**  $R = 30: \mathfrak{X} \approx [\lambda; \mathbf{A}, \mathbf{B}, \mathbf{C}] = \sum_{r=1}^{30} \lambda_r \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r$
- Similarity scores:  $S = \frac{1}{2}AA^{T} + \frac{1}{2}BB^{T}$

Score	Title
0.000563	Skip graphs
0.000356	Random lifts of graphs
0.000354	A fast and high-quality multilevel scheme for partitioning irregular graphs
0.000322	The minimum all-ones problem for trees
0.000306	Rankings of directed graphs
0.000295	Squarish k-d trees
0.000284	Finding the k-shortest paths
0.000276	On floor-plan of plane graphs
0.000275	1-Hyperbolic graphs
0.000269	Median graphs and triangle-free graphs

#### **Graphs (Related)**



- **CP decomposition,** R = 20:  $\mathfrak{X} \approx [\lambda; \mathbf{A}, \mathbf{B}, \mathbf{C}] = \sum_{r=1}^{20} \lambda_r \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r$
- Computed centroids of top 20 authors' papers ( $g_A, g_B$ )
- **Disambiguation scores:**  $s = \frac{1}{2}Ag_A + \frac{1}{2}Bg_B$
- Scored all authors with same last name, first initial



**Disambiguation Scores for Various CP Tensor Decompositions (+ = correct; o = incorrect)** 



**Disambiguation Scores for Various CP Tensor Decompositions (+ = correct; o = incorrect)** 



**Disambiguation Scores for Various CP Tensor Decompositions (+ = correct; o = incorrect)** 



#### **SIAM Data: Journal Prediction**

- CP decomposition, R = 30, vectors from B
- Bagged ensemble of decision trees (n = 100)
- 10-fold cross validation
- 43% overall accuracy

ID	Journal Name	Size	Correct	Mislabeled as
1	SIAM J APPL DYN SYST	1%	0%	2 (44%)
2	SIAM J APPL MATH	11%	58%	6 (10%)
3	SIAM J COMPUT	11%	56%	11 (20%)
4	SIAM J CONTROL OPTIM	11%	60%	2 (10%)
5	SIAM J DISCRETE MATH	5%	15%	3 (47%)
6	SIAM J MATH ANAL	8%	26%	2 (29%)
7	SIAM J MATRIX ANAL A	8%	56%	10 (19%)
8	SIAM J NUMER ANAL	12%	50%	10 (16%)
9	SIAM J OPTIMIZ	7%	66%	4 (16%)
10	SIAM J SCI COMPUT	13%	36%	8 (21%)
11	SIAM PROC S	9%	32%	3 (38%)
12	SIAM REV	3%	5%	2 (34%)



#### **SIAM Data: Journal Prediction**



## **Tensors and HPC**

#### Sparse tensors

- Data partitioning and load balancing issues
- Partially sorted coordinate format
  - Optimize unfolding for single mode
- Scalable decomposition algorithms
  - CP, Tucker, PARAFAC2, DEDICOM, INDSCAL, ...
    - Different operations, data partitioning issues

#### Applications

- Network analysis, web analysis, multi-way clustering, data fusion, cross-language IR, feature vector generation
  - Different operations, data partitioning issues
- Leverage Sandia's Trilinos packages
  - Data structures, load balancing, SVD, Eigen.



### Papers Most Similar to Authors' Centroids

#### John R. Gilbert (3 articles in data)

~	-		
20	30	Title	
10			

R

2	1	MSP A class of parallel multistep successive sparse approximate inverse preconditioning strategies
4	2	A factored approximate inverse preconditioner with pivoting
5	3	Algebraic multilevel methods and sparse approximate inverses
1	4	The recursive inverse eigenvalue problem
3	5	Efficient and stable solution of M-matrix linear systems of (block) Hessenberg form
19	6	A robust and efficient ILU that incorporates the growth of the inverse triangular factors
7	7	Orderings for factorized sparse approximate inverse preconditioners
8	8	Solving complex-valued linear systems via equivalent real formulations
18	9	On the relations between ILUs and factored approximate inverses
10	10	Scalable parallel preconditioning with the sparse approximate inverse of triangular matrices

#### **Bruce A. Hendrickson (5 articles in data)**

R				
20	30	Title		
1	1	Norms of large Toeplitz band matrices		
2	2	Special ultrametric matrices and graphs		
4	3	A chart of backward errors for singly and doubly structured eigenvalue problems		
3	4	Fast and stable algorithms for banded plus semiseparable systems of linear equations		
6	5	Convex noncommutative polynomials have degree two or less		
7	6	A bound for the inverse of a lower triangular Toeplitz matrix		
9	7	Computing the minimum eigenvalue of symmetric positive definite Toeplitz matrix by Newton		
10	8	Spectral characterizations for Hermitian centrosymmetric K-matrices and Hermitian skew-centro		
12	9	A Korovkin-based approximation of multilevel Toeplitz matrices (with rectangular unstructured		
5	10	Recognizing perfect 2-split graphs		



## Tensor Decompositions for Analyzing Multi-link Graphs

#### **Danny Dunlavy**

Email: dmdunla@sandia.gov

Web Page: http://www.cs.sandia.gov/~dmdunla







## High-Order Analogue of the Matrix SVD

• Matrix SVD:

$$\mathbf{X} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^{\mathsf{T}} = \begin{bmatrix} \mathbf{\sigma}_{1} & \mathbf{\sigma}_{2} & \mathbf{\sigma}_{R} \\ \mathbf{\sigma}_{1} & \mathbf{\sigma}_{2} & \mathbf{\sigma}_{R} \\ \mathbf{\sigma}_{1} & \mathbf{\sigma}_{2} & \mathbf{\sigma}_{R} \\ \mathbf{\sigma}_{1} & \mathbf{\sigma}_{2} & \mathbf{\sigma}_{1} \\ \mathbf{\sigma}_{2} & \mathbf{\sigma}_{1} & \mathbf{\sigma}_{2} \\ \mathbf{\sigma}_{1} & \mathbf{\sigma}_{2} & \mathbf{\sigma}_{1} \\ \mathbf{\sigma}_{2} & \mathbf{\sigma}_{2} & \mathbf{\sigma}_{1} \\ \mathbf{\sigma}_{2} & \mathbf{\sigma}_{2} & \mathbf{\sigma}_{2} \\ \mathbf{\sigma}_{3} & \mathbf{\sigma}_{4} & \mathbf{\sigma}_{4} \\ \mathbf{\sigma}_{4} & \mathbf{\sigma}_{4} & \mathbf{\sigma}_{4} \\ \mathbf{\sigma}_{4} & \mathbf{\sigma}_{4} & \mathbf{\sigma}_{4} \\ \mathbf{\sigma}_{4} & \mathbf{\sigma}_{4} & \mathbf{\sigma}_{4} & \mathbf{\sigma}_{4} & \mathbf{\sigma}_{4} \\ \mathbf{\sigma}_{4} & \mathbf{\sigma}_{4}$$

• Tucker Tensor (finding bases for each subspace):

$$\mathbf{X} = \boldsymbol{\Sigma} \times_1 \mathbf{U} \times_2 \mathbf{V} = \llbracket \boldsymbol{\Sigma} ; \mathbf{U}, \mathbf{V} \rrbracket$$

• Kruskal Tensor (sum of rank-1 components):

$$\mathbf{X} = \sum_{r=1}^{R} \sigma_r \, \mathbf{u}_r \circ \mathbf{v}_r = \llbracket \boldsymbol{\sigma} ; \mathbf{U}, \mathbf{V} \rrbracket$$



## **Other Tensor Applications at Sandia**

• Tensor Toolbox (MATLAB) [Kolda/Bader, 2007]

http://csmr.ca.sandia.gov/~tgkolda/TensorToolbox/

#### • TOPHITS (Topical HITS) [Kolda, 2006]

- HITS plus **terms** in dimension 3
- Decomposition: CP

#### Cross Language Information Retrieval [Chew et al., 2007]

- Different languages in dimension 3
- Decomposition: PARAFAC2

#### • Temporal Analysis of E-mail Traffic [Bader et al., 2007]

- Directed e-mail graph with time in dimension 3
- Decomposition: DEDICOM

