



Multilinear Algebra for Analyzing Data with Multiple Linkages

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In collaboration with:

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Sandia National Labs

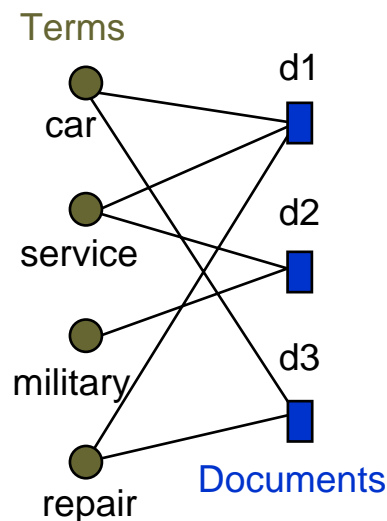
MMDS, Stanford, CA, June 21-24, 2006



Linear Algebra plays an important role in Graph Analysis

- PageRank
 - Brin & Page (1998)
 - Page, Brin, Motwani, Winograd (1999)
- HITS (hubs and authorities)
 - Kleinberg (1998/99)
- Latent Semantic Indexing (LSI)
 - Dumais, Furnas, Landauer, Deerwester, and Harshman (1988)
 - Deerwester, Dumais, Landauer, Furnas, and Harshman (1990)

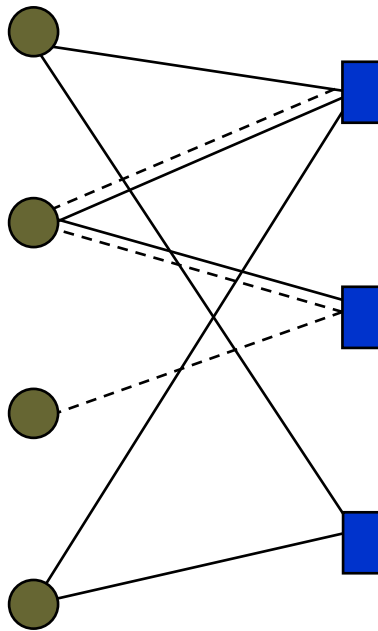
$$A \approx T \Sigma D^T = \sum_r \sigma_r t_{\bullet r} \circ d_{\bullet r}$$



One Use of LSI: Maps terms and documents to the “same” k-dimensional space.



Multi-Linear Algebra can be used in more complex graph analyses

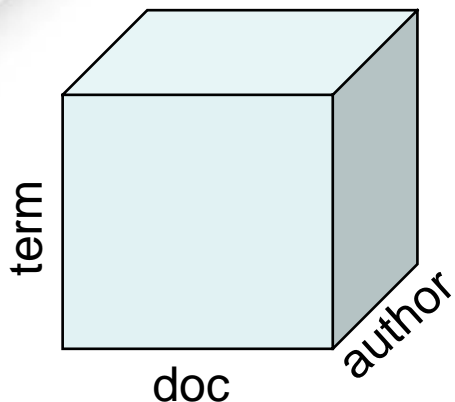


- Nodes (one type) connected by multiple types of links
 - Node x Node x Connection
- Two types of nodes connected by multiple types of links
 - Node A x Node B x Connection
- Multiple types of nodes connected by a single link
 - Node A x Node B x Node C
- Multiple types of nodes connected by multiple types of links
 - Node A x Node B x Node C x Connection
- Etc...



Analyzing Publication Data: Term x Doc x Author

1999-2004
SIAM Journal Data
(except SIREV)



6928 terms
4411 documents
6099 authors
464645 nonzeros

$A =$ term-document matrix

$$a_{ij} = \frac{(1 + \log_2 f_{ij}) \log_2(N/n_i)}{d_j}$$

$B =$ author-document matrix

$$b_{kj} = \begin{cases} 1/\sqrt{m_j} & \text{if author } k \text{ wrote document } j \\ 0 & \text{otherwise} \end{cases}$$

Terms must appear in at least 3 documents and no more than 10% of all documents. Moreover, it must have at least 2 characters and no more than 30.

Form tensor \mathcal{X} as: $x_{ijk} = a_{ij}b_{jk}$

Element (i,j,k) is nonzero only if author k wrote document j using term i .

$$\mathcal{X} \approx \sum_r \lambda_r \mathbf{t}_{\bullet r} \circ \mathbf{d}_{\bullet r} \circ \mathbf{a}_{\bullet r}$$



A tensor is a multidimensional array

NOTATION

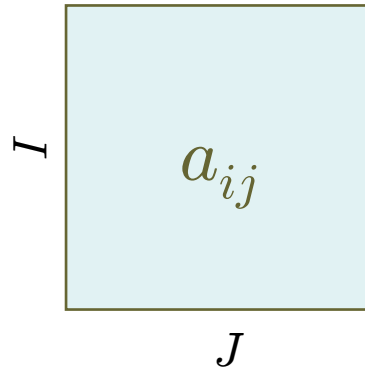
s scalar

\mathbf{a} vector

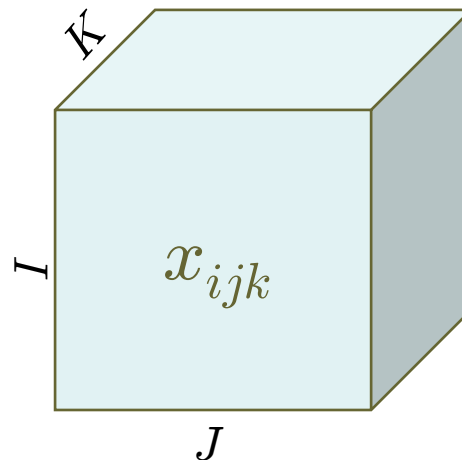
\mathbf{B} matrix

\mathcal{X} tensor

An $I \times J$ matrix



An $I \times J \times K$ tensor

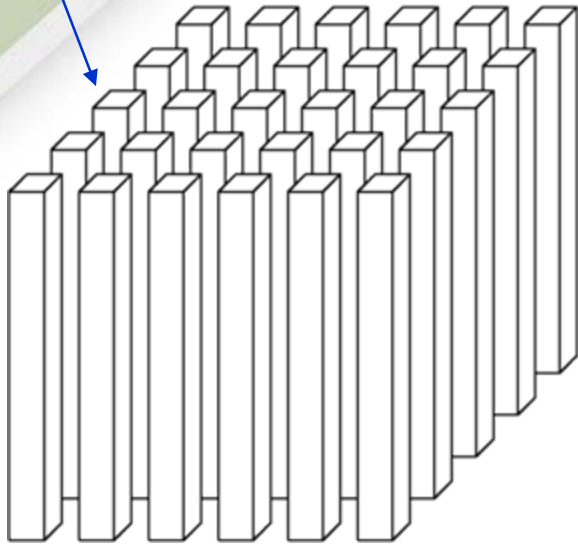


- Other names for tensors...
 - Multi-way array
 - N-way array
- The “order” of a tensor is the number of dimensions
- Other names for dimension...
 - Mode
 - Way
- Example
 - The matrix \mathbf{A} (at left) has order 2.
 - The tensor \mathcal{X} (at left) has order 3 and its 3rd mode is of size K .



Tensor “fibers” generalize the concept of rows and columns

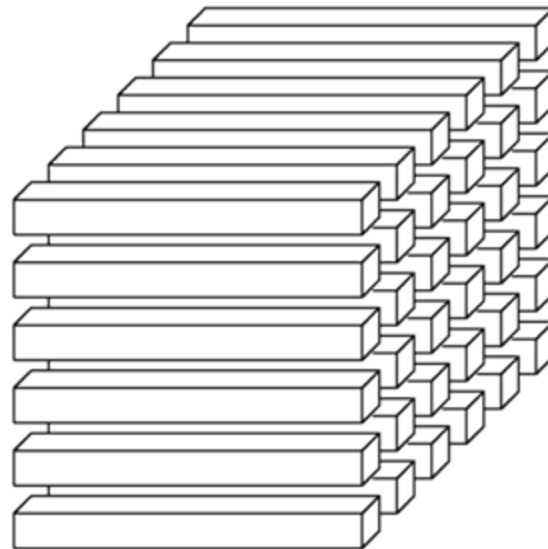
$x_{\bullet 13}$



Column Fibers

$$x_{\bullet jk}$$

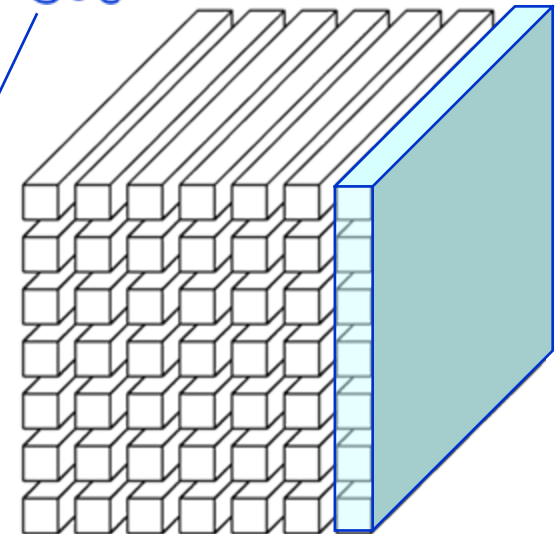
$x_{3\bullet 6}$



Row Fibers

$$x_{i\bullet k}$$

“Slice” $x_{\bullet 6\bullet}$



Tube Fibers

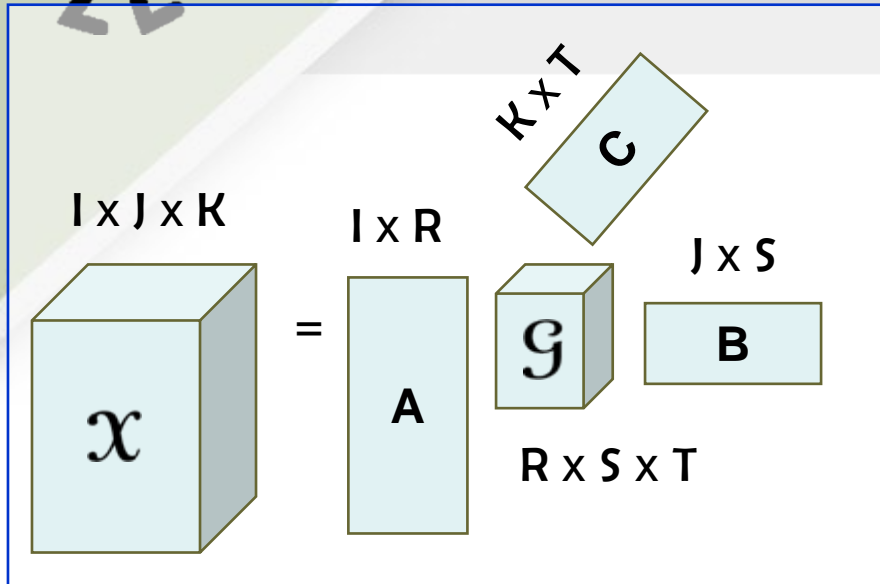
$$x_{ij\bullet}$$

NOTE

There’s no naming scheme past 3 dimensions; instead, we just say, e.g., the 4th-mode fibers.



Tucker Decomposition



$$\mathcal{X} = \sum_{r=1}^R \sum_{s=1}^S \sum_{t=1}^T g_{rst} \mathbf{a}_{\bullet r} \circ \mathbf{b}_{\bullet s} \circ \mathbf{c}_{\bullet t}$$

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

- Proposed by Tucker (1966)
- Also known as: Three-mode factor analysis, three-mode PCA, orthogonal array decomposition
- \mathbf{A} , \mathbf{B} , and \mathbf{C} may be orthonormal (generally assume they have full column rank)
- \mathcal{G} is not diagonal
- Not unique

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

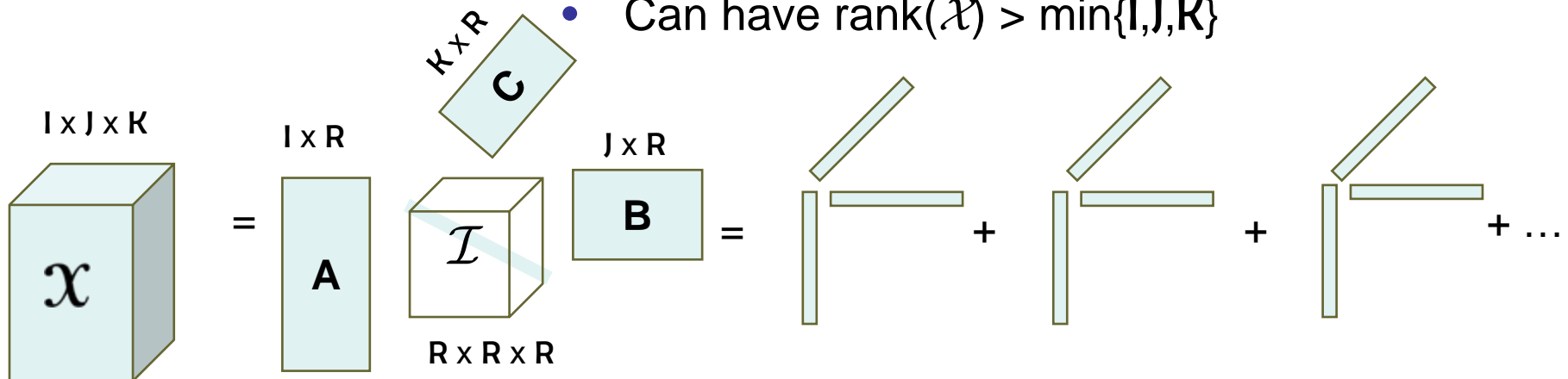


CANDECOMP/PARAFAC

$$\mathcal{X} = \sum_{r=1}^R \mathbf{a}_{\bullet r} \circ \mathbf{b}_{\bullet r} \circ \mathbf{c}_{\bullet r}$$

$$\mathcal{X} = [\mathbf{A}, \mathbf{B}, \mathbf{C}]$$

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





Combining Tucker and PARAFAC

Have: Tensor \mathcal{X} of size $M \times N \times P$

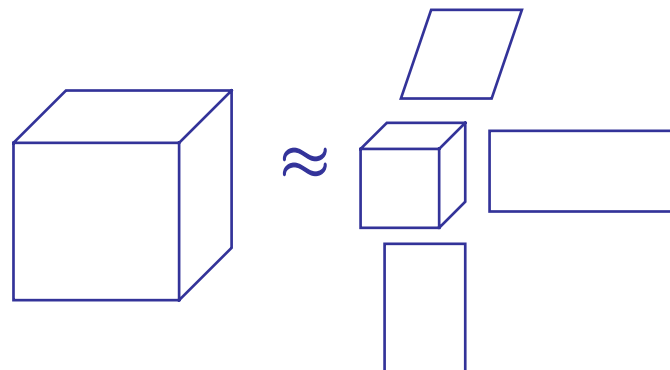
Want: $\mathcal{X} \approx \lambda[\mathbf{T}, \mathbf{D}, \mathbf{A}]$

Step 1: Choose orthonormal compression matrices for each dimension:

\mathbf{U} of size $M \times I$

\mathbf{V} of size $N \times J$

\mathbf{W} of size $P \times K$

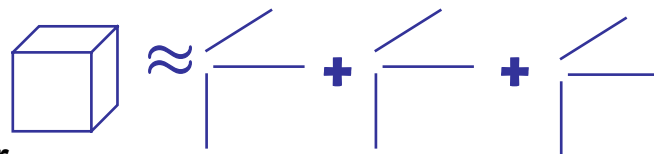


Step 2: Form reduced tensor (implicitly)

$$\hat{\mathcal{X}} = [\mathcal{X}; \mathbf{U}^T, \mathbf{V}^T, \mathbf{W}^T] \Rightarrow \mathcal{X} \approx [\hat{\mathcal{X}}; \mathbf{U}, \mathbf{V}, \mathbf{W}]$$

Step 3: Compute PARAFAC on reduced tensor

$$\hat{\mathcal{X}} \approx \hat{\lambda}[\hat{\mathbf{T}}, \hat{\mathbf{D}}, \hat{\mathbf{A}}]$$



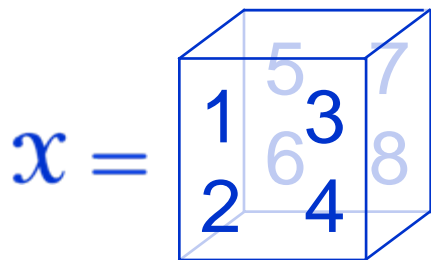
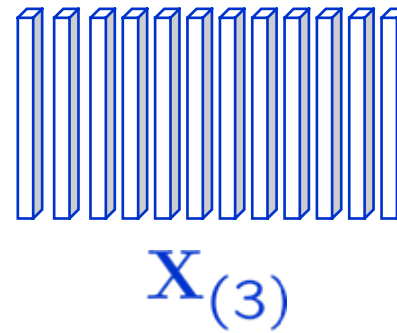
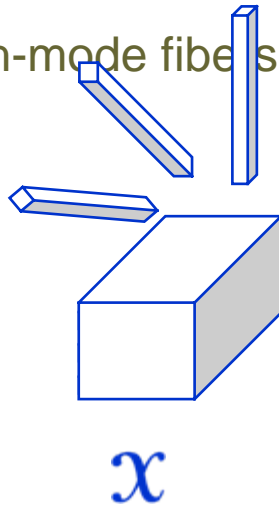
Step 4: Convert to PARAFAC of full tensor

$$\mathcal{X} \approx \hat{\lambda} [\mathbf{U}\hat{\mathbf{T}}, \mathbf{V}\hat{\mathbf{D}}, \mathbf{W}\hat{\mathbf{A}}] \equiv \lambda [\mathbf{T}, \mathbf{D}, \mathbf{A}]$$



Matricize: $X_{(n)}$

The n th-mode fibers are rearranged to be the columns of a matrix



$$X_{(1)} = \begin{bmatrix} 1 & 3 & 5 & 7 \\ 2 & 4 & 6 & 8 \end{bmatrix}$$

$$X_{(2)} = \begin{bmatrix} 1 & 2 & 5 & 6 \\ 3 & 4 & 7 & 8 \end{bmatrix}$$

$$X_{(3)} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \end{bmatrix}$$



Tucker and PARAFAC Matrix Representations

Fact 1:

$$([\mathcal{G} ; \mathbf{A}, \mathbf{B}, \mathbf{C}])_{(1)} = \mathbf{A} \mathbf{G}_{(1)} (\mathbf{C} \otimes \mathbf{B})^T$$

Fact 2:

$$([\mathbf{A}, \mathbf{B}, \mathbf{C}])_{(1)} = \mathbf{A} (\mathbf{C} \odot \mathbf{B})^T$$

Khatri-Rao Matrix Product (Columnwise Kronecker Product):

$$\mathbf{C} \odot \mathbf{B} = \begin{bmatrix} \mathbf{c}_{\bullet 1} \otimes \mathbf{b}_{\bullet 1} & \mathbf{c}_{\bullet 2} \otimes \mathbf{b}_{\bullet 2} & \cdots & \mathbf{c}_{\bullet R} \otimes \mathbf{b}_{\bullet R} \end{bmatrix}$$

Special pseudo-inverse structure:

$$((\mathbf{C} \odot \mathbf{B})^T)^\dagger = (\mathbf{C} \odot \mathbf{B}) (\mathbf{C}^T \mathbf{C} * \mathbf{B}^T \mathbf{B})^{-1}$$



Implicit Compressed PARAFAC ALS

Have: $\hat{\mathbf{X}} = [\mathbf{X} ; \mathbf{U}^T, \mathbf{V}^T, \mathbf{W}^T]$

Want: $\hat{\mathbf{X}} \approx [\hat{\mathbf{T}}, \hat{\mathbf{D}}, \hat{\mathbf{A}}]$

Consider the problem of fixing the 2nd and 3rd factors and solving just for the 1st.

$$\min_{\hat{\mathbf{T}}} \|\hat{\mathbf{X}} - [\hat{\mathbf{T}}, \hat{\mathbf{D}}, \hat{\mathbf{A}}]\| \quad \min_{\hat{\mathbf{T}}} \|\hat{\mathbf{X}}_{(1)} - \hat{\mathbf{T}}(\hat{\mathbf{A}} \odot \hat{\mathbf{D}})^T\|$$

$$\hat{\mathbf{T}} = \hat{\mathbf{X}}_{(1)}((\hat{\mathbf{A}} \odot \hat{\mathbf{D}})^T)^\dagger$$

$$\hat{\mathbf{T}} = \hat{\mathbf{X}}_{(1)}(\hat{\mathbf{A}} \odot \hat{\mathbf{D}})\mathbf{Z}^{-1} \quad \text{with} \quad \mathbf{Z} = \hat{\mathbf{A}}^T \hat{\mathbf{A}} * \hat{\mathbf{D}}^T \hat{\mathbf{D}}$$

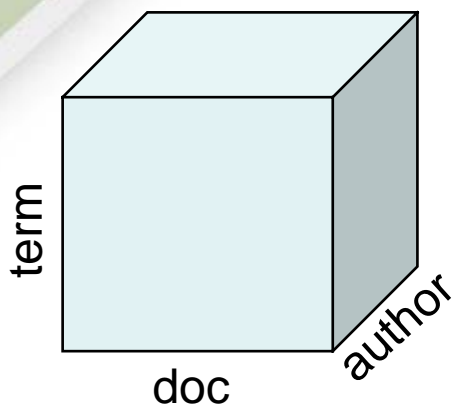
$$\hat{\mathbf{T}} = \mathbf{U}^T \mathbf{X}_{(1)} (\mathbf{W} \otimes \mathbf{V}) (\hat{\mathbf{A}} \odot \hat{\mathbf{D}}) \mathbf{Z}^{-1}$$

$$\hat{\mathbf{T}} = \mathbf{U}^T \mathbf{X}_{(1)} (\mathbf{W} \hat{\mathbf{A}} \odot \mathbf{V} \hat{\mathbf{D}}) \mathbf{Z}^{-1}$$

$$(\hat{\mathbf{T}}\mathbf{Z})_{\bullet r} = \mathbf{U}^T \mathbf{X}_{(1)} [(\mathbf{W} \hat{\mathbf{A}})_{\bullet r} \otimes (\mathbf{V} \hat{\mathbf{D}})_{\bullet r}] \quad \text{Update columnwise}$$



Back to the Problem: Term x Doc x Author



6928 documents
4411 terms
6099 authors
464645 nonzeros

$$A = \text{term-document matrix}$$
$$a_{ij} = \frac{(1 + \log_2 f_{ij}) \log_2(N/n_i)}{d_j}$$

$B =$ author-document matrix

$$b_{kj} = \begin{cases} 1/\sqrt{m_j} & \text{if author } k \text{ wrote document } j \\ 0 & \text{otherwise} \end{cases}$$

Terms must appear in at least 3 documents and no more than 10% of all documents. Moreover, it must have at least 2 characters and no more than 30.

Form tensor \mathcal{X} as: $x_{ijk} = a_{ij}b_{jk}$

Element (i,j,k) is nonzero only if author k wrote document j using term i .

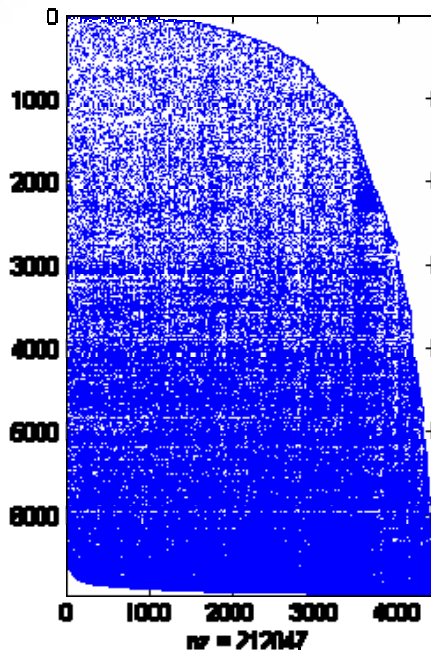
$$\mathcal{X} \approx \sum_r \lambda_r \mathbf{t}_{\bullet r} \circ \mathbf{d}_{\bullet r} \circ \mathbf{a}_{\bullet r}$$



Original problem is “overly” sparse

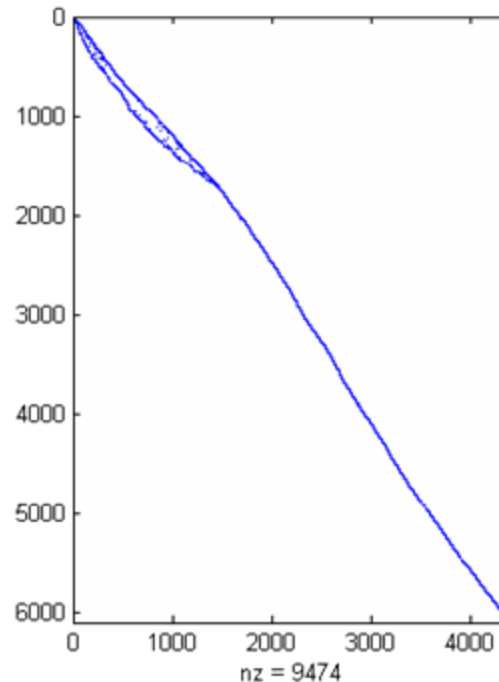
A = term-document matrix

$$a_{ij} = \frac{(1 + \log_2 f_{ij}) \log_2(N/n_i)}{d_j}$$

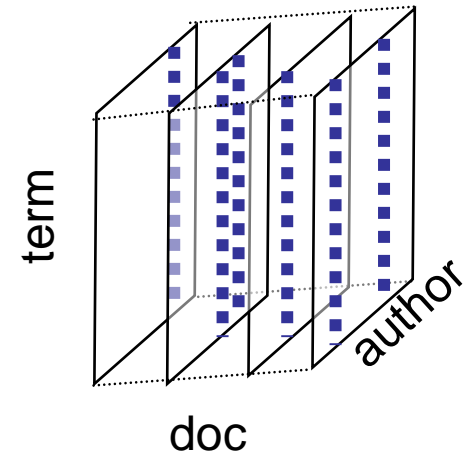


B = author-document matrix

$$b_{ij} = \begin{cases} 1/\sqrt{m_j} & \text{if author } i \text{ wrote document } j \\ 0 & \text{otherwise} \end{cases}$$



Result: Resulting tensor has just a few nonzero columns in each lateral slice.



Experimentally, PARAFAC seems to overfit such data and not do a good job of “mixing” different authors.



Compression Matrices & PARAFAC

$$\mathcal{X} \approx [\hat{\mathcal{X}} ; \mathbf{U}, \mathbf{V}, \mathbf{W}]$$

\mathbf{A} = term-document matrix

$$\mathbf{A} \approx \mathbf{U}_A \mathbf{\Sigma}_A \mathbf{V}_A^T \quad (\text{rank } 100)$$

$$\mathbf{U} = \mathbf{U}_A^T, \mathbf{V} = \mathbf{V}_A^T,$$

\mathbf{C} = term-author matrix

$$c_{ik} = \sum_j x_{ijk}$$

$$\mathbf{C} \approx \mathbf{U}_C \mathbf{\Sigma}_C \mathbf{V}_C^T \quad (\text{rank } 100)$$

$$\mathbf{W} = \mathbf{V}_C^T,$$

Run rank-100 PARAFAC on compressed tensor.
Reassemble results.



Three-Way Fingerprints

- Each of the Terms, Docs, and Authors has a rank-k ($k=100$) fingerprint from the PARAFAC approximation
- All items can be directly compared in “concept space”
- Thus, we can compare any of the following
 - Term-Term
 - Doc-Doc
 - Term-Doc
 - Author-Author
 - Author-Term
 - Author-Doc
- The fingerprints can be used as inputs for clustering, classification, etc.

$$\mathcal{X} \approx \lambda [[\mathbf{T}, \mathbf{D}, \mathbf{A}]]$$

$$\text{score} = \mathbf{u}^T \Lambda \mathbf{v}$$



MATLAB Results

- Go to MATLAB

```
~~~~~ Group 1 ~~~~~
```

```
Weight = 0.649794
```

```
0.2291772 3474 Vortex motion law for the Schrodinger-Ginzburg-Landua equations
0.2280338 1633 Vortex state of d-wave superconductors in the Ginzburg-Landau energy
0.2233726 320 Studies of a Ginzburg-Landau model for d-wave superconductors
0.2183914 3340 Vortices in p-wave superconductivity
0.2056138 485 Numerical solution of the three-dimensional Ginzburg-Landau models using artificial boundary
-0.0130460 463 Layer stripping for a transversely isotropic elastic medium
-0.0132632 1151 Scattering of time-harmonic electromagnetic waves by anisotropic inhomogeneous scatterers or impenetrable
-0.0133375 1206 Phase equations for relaxation oscillators
-0.0135059 2592 On the two-dimensional gas expansion for compressible Euler equations
-0.0141843 3091 A thermomechanical model for energetic materials with phase transformations
0.4828654 3387 landau
0.4489465 2614 ginzburg
0.2688777 6130 superconductivity
0.2611251 6771 vortex
0.2227376 6772 vortices
-0.0120339 1964 elastic
-0.0120368 1620 design
-0.0120543 3767 mesh
-0.0144529 2554 gas
-0.0153897 5462 scattering
0.7300468 1322 du q
0.3112497 3142 lin tc
0.2275581 814 chapman sj
0.1382164 4991 spirn d
0.1048653 3133 lin fg
-0.0182970 5898 yao pf
-0.0188236 2045 han wm
-0.0244190 2947 laurencot p
-0.0281511 2393 izhikevich em
-0.0318239 3369 manservisi s
```

```
Return to continue, jump to rank, or '0' (zero) to quit: |
```

Find terms similar to 'tensor'

Match 1: tensor (6261)

No. docs in which the term appears: 61

No. authors that use the term: 118

Norm of matching item: 1.934519e-001

-- Top 10 matches for PARAFAC --

Score 2.73e-001: tensor (6261)

Score 2.35e-001: multilinear (3955)

Score 2.15e-001: tensors (6262)

Score 2.06e-001: svds (6182)

Score 2.04e-001: deficient (1520)

Score 2.00e-001: valuable (6660)

Score 1.97e-001: confirms (1160)

Score 1.94e-001: hyper (2860)

Score 1.93e-001: displacement (1787)

Score 1.92e-001: div (1814)

-- Top 10 matches for SVD --

Score 1.17e-001: decomposition (1498)

Score 1.13e-001: squares (5891)

Score 1.07e-001: rank (4980)

Score 9.75e-002: least (3437)

Score 9.20e-002: singular (5724)

Score 7.89e-002: tensor (6261)

Score 7.21e-002: elasticity (1965)

Score 6.22e-002: orthogonal (4327)

Score 6.19e-002: mixed (3837)

Score 5.71e-002: elastic (1964)

Find documents similar to 'tensor'

Match 1: tensor (6261)

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-- Top 10 matches for PARAFAC --

Score 2.21e-001: On the best rank-1 and rank-(R1R2...R-N) approximation of higher-order tensors (1224)

Score 2.01e-001: Efficient solution of the rank-deficient linear least squares problem (148)

Score 1.87e-001: On the best rank-1 approximation of higher-order supersymmetric tensors (2570)

Score 1.86e-001: Orthogonal tensor decompositions (2180)

Score 1.82e-001: A counterexample to the possibility of an extension of the Eckart-Young low-rank approximation theorem

Score 1.78e-001: Least squares solution of matrix equation $AXB(*)+CYD*=E-*$ (3192)

Score 1.74e-001: Least-squares methods for incompressible Newtonian fluid flow Linear stationary problems (4244)

Score 1.74e-001: Least-squares methods for linear elasticity (4243)

Score 1.73e-001: Tensor methods for large sparse nonlinear least squares problems (1119)

Score 1.69e-001: Multilevel boundary functionals for least-squares mixed finite element methods (396)

-- Top 10 matches for SVD --

Score 5.78e-002: A counterexample to the possibility of an extension of the Eckart-Young low-rank approximation theorem

Score 5.77e-002: On the best rank-1 and rank-(R1R2...R-N) approximation of higher-order tensors (1224)

Score 5.59e-002: Least-squares methods for linear elasticity (4243)

Score 5.35e-002: First-order system least squares for the stress-displacement formulation Linear elasticity (3431)

Score 4.98e-002: Rank-one approximation to high order tensors (2369)

Score 4.72e-002: Least-squares methods for incompressible Newtonian fluid flow Linear stationary problems (4244)

Score 4.51e-002: First-order system least squares for linear elasticity Numerical results (1178)

Score 4.43e-002: Orthogonal tensor decompositions (2180)

Score 4.39e-002: Layer stripping for a transversely isotropic elastic medium (463)

Score 3.91e-002: First-order system least squares for the Stokes and linear elasticity equations Further results (1178)

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Find authors similar to 'tensor'
```

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Match 1: tensor (6261)
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No. authors that use the term: 118
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```
Norm of matching item: 1.934519e-001
```

```
-- Top 10 matches for PARAFAC --
```

```
Score 1.91e-001: vandewalle j (5451)
```

```
Score 1.84e-001: delathauwer l (1181)
```

```
Score 1.83e-001: quintanaorti g (4293)
```

```
Score 1.83e-001: quintanaorti es (4292)
```

```
Score 1.83e-001: petitet a (4109)
```

```
Score 1.76e-001: chen y (873)
```

```
Score 1.76e-001: shim sy (4846)
```

```
Score 1.73e-001: demoor b (1199)
```

```
Score 1.68e-001: barlow jl (288)
```

```
Score 1.66e-001: cai zq (693)
```

Find terms similar to Dhillon

Match 1: dhillon is (1239)

No. terms used by author: 68

No. documents written by author: 1

Norm of matching item: 5.289941e-002

-- Top 10 matches for PARAFAC --

Score 2.27e-001: bidiagonal (575)

Score 2.26e-001: qr (4907)

Score 2.11e-001: ldlt (3424)

Score 2.08e-001: lapack (3391)

Score 2.07e-001: columns (1000)

Score 2.04e-001: column (999)

Score 2.03e-001: revealing (5308)

Score 2.03e-001: pivoting (4579)

Score 2.02e-001: rank (4980)

Score 1.98e-001: bjoerck (610)

Find authors similar to Dhillon

Match 1: dhillon is (1239)

No. terms used by author: 68

No. documents written by author: 1

Norm of matching item: 5.289941e-002

-- Top 10 matches for PARAFAC --

Score 3.11e-001: dhillon is (1239)

Score 3.11e-001: parlett bn (4024)

Score 2.28e-001: drmac z (1315)

Score 2.19e-001: molera jm (3625)

Score 2.16e-001: jessup er (2437)

Score 2.04e-001: dopico fm (1292)

Score 2.04e-001: moro j (3661)

Score 2.02e-001: jubete f (2495)

Score 2.02e-001: pruneda re (4253)

Score 2.02e-001: castillo e (761)

Find terms similar to OLeary DP

Match 1: oleary dp (3913)

No. terms used by author: 114

No. documents written by author: 2

Norm of matching item: 2.567276e-001

-- Top 10 matches for PARAFAC --

Score 2.35e-001: ill (2906)

Score 2.15e-001: tikhonov (6334)

Score 2.12e-001: posed (4667)

Score 2.07e-001: regularization (5142)

Score 2.05e-001: conditioned (1138)

Score 2.02e-001: clustered (940)

Score 2.01e-001: unmixed (6601)

Score 2.01e-001: regularizing (5145)

Score 1.95e-001: regularisation (5140)

Score 1.95e-001: regularized (5144)

Find authors similar to OLeary DP

Match 1: oleary dp (3913)

No. terms used by author: 114

No. documents written by author: 2

Norm of matching item: 2.567276e-001

-- Top 10 matches for PARAFAC --

Score 2.55e-001: oleary dp (3913)

Score 2.37e-001: kilmer me (2645)

Score 2.30e-001: hansen pc (2056)

Score 2.18e-001: o'leary dp (3889)

Score 2.10e-001: gulliksson m (1956)

Score 2.10e-001: wedin pa (5695)

Score 2.09e-001: maass p (3306)

Score 2.08e-001: mante c (3372)

Score 2.07e-001: jin qn (2458)

Score 2.05e-001: johnston pr (2470)

Find authors like H.Y. Zha

Match 1: zha hy (5990)

No. terms used by author: 164

No. documents written by author: 5

Norm of matching item: 3.795614e-001

-- Top 10 matches for PARAFAC --

Score 3.55e-001: zha hy (5990)

Score 3.46e-001: simon hd (4890)

Score 3.36e-001: zhang zy (6025)

Score 3.28e-001: simon h (4889)

Score 3.19e-001: fundelic re (1645)

Score 3.09e-001: zha h (5989)

Score 2.94e-001: zhang t (6013)

Score 2.81e-001: vandooren p (5453)

Score 2.77e-001: golub g (1820)

Score 2.75e-001: dopico fm (1292)


```
Find authors similar to 'svd'
```

```
Match 1: svd (6181)
```

```
No. docs in which the term appears: 24
```

```
No. authors that use the term: 36
```

```
Norm of matching item: 1.789480e-001
```

```
-- Top 10 matches for PARAFAC --
```

```
Score 3.28e-001: delathauwer l (1181)
```

```
Score 3.23e-001: golub g (1820)
```

```
Score 3.23e-001: vandooren p (5453)
```

```
Score 3.21e-001: dopico fm (1292)
```

```
Score 3.21e-001: moro j (3661)
```

```
Score 3.20e-001: fundelic re (1645)
```

```
Score 3.13e-001: jessup er (2437)
```

```
Score 3.12e-001: zha h (5989)
```

```
Score 3.12e-001: demmel j (1197)
```

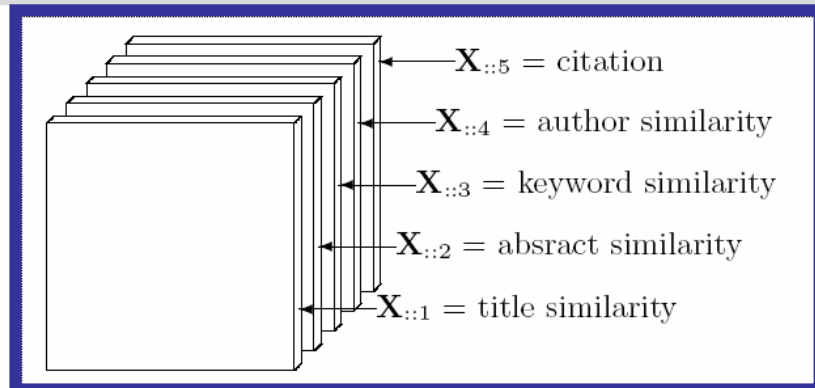
```
Score 3.12e-001: vandewalle j (5451)
```

```
>> |
```

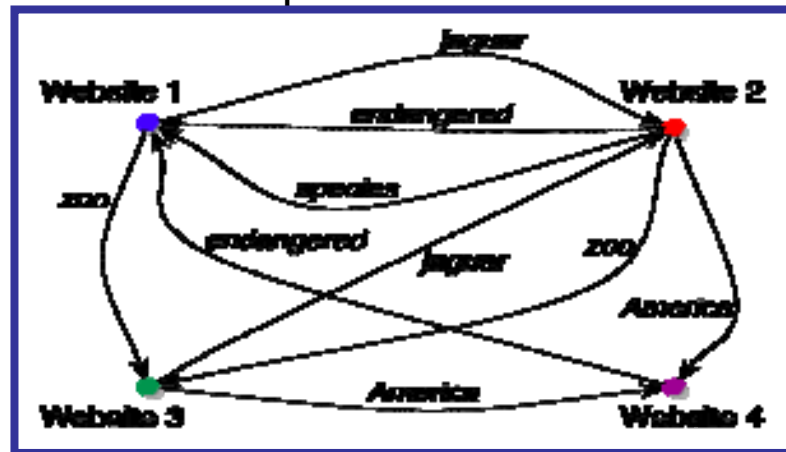


Wrap-Up

- Higher-order LSI for term-doc-author tensor
- Tucker-PARAFAC combination for sparse tensors
 - Spasre Tensor Toolbox (release summer 2006)
- Mathematical manipulations
 - Kolda, Tech. Rep. SAND2006-2081
- Thanks to Kevin Boyack for journal data
- For more info: Tammy Kolda, tgkolda@sandia.gov



Dunlavy, Kolda, Kegelmeyer,
Tech. Rep. SAND2006-2079



Kolda, Bader, Kenny, ICDM05