

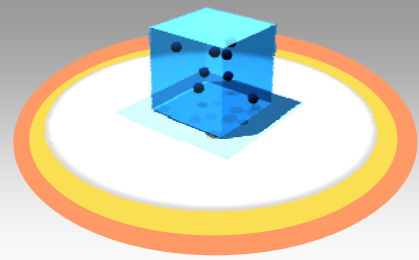
# Tensor Decompositions and Data Mining

Tammy Kolda

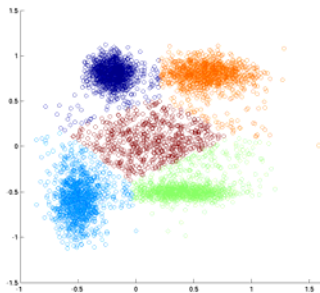
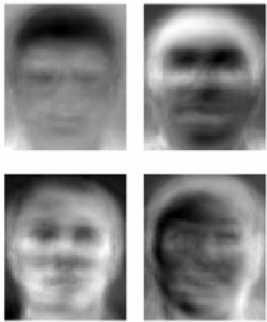
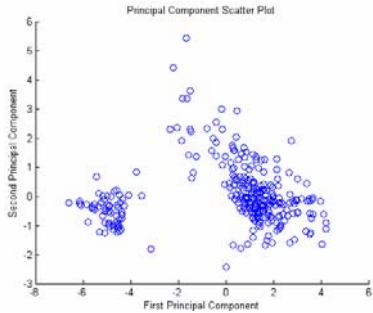
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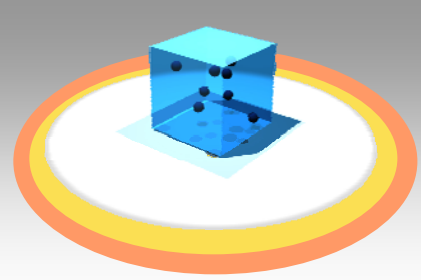
<http://csmr.ca.sandia.gov/~tgkolda/>



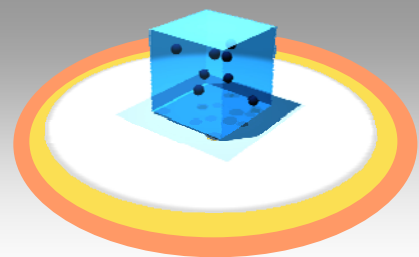
# Matrix decompositions are important to data mining



- **Principal Component Analysis (PCA)** – singular value decomposition (SVD) of object-feature matrix to define primary features
- **Latent semantic indexing (LSI)** – SVD of term-document matrix to project terms and documents into conceptual space (Dumais et al., CHI88)
- **Eigenfaces** – EVD of covariance matrix derived from facial images (Turk & Pentland, CVPR91)
- **PageRank** – EVD of specialized Markov matrix representing the web (Page et al., WWW7, 1998)
- **HITS** – SVD of adjacency matrix of the web graph to compute hubs and authorities (Kleinberg, JACM, 1999)
- **K-means and SVD equivalency** – Under certain conditions, the SVD is shown to be the relaxed solution of K-means clustering problem (Ding and He, ICML04)

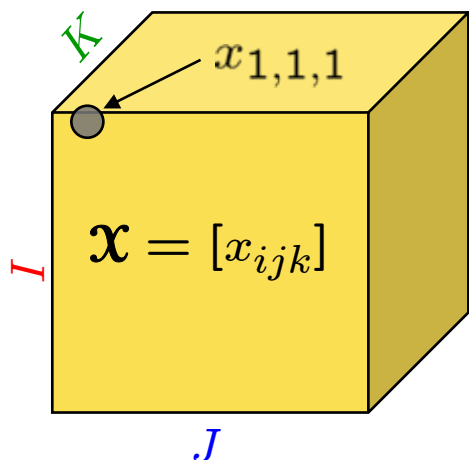


# Tensor Basics



# A tensor is a multidimensional array

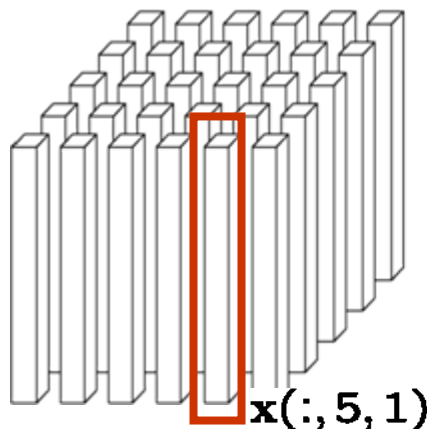
An  $I \times J \times K$  tensor



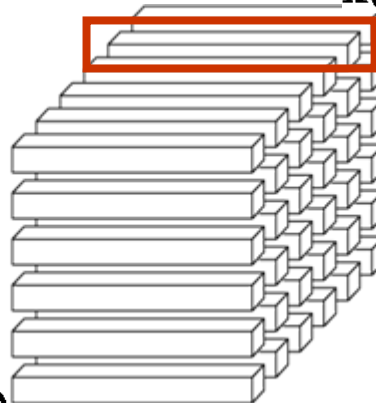
3<sup>rd</sup> order or 3-way tensor

Mode 1 has dimension  $I$   
 Mode 2 has dimension  $J$   
 Mode 3 has dimension  $K$

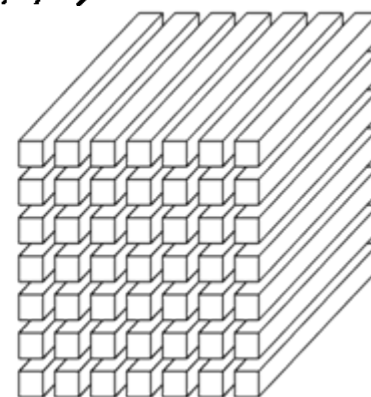
Column (Mode-1)  
Fibers



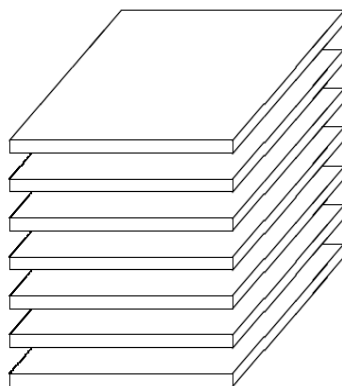
Row (Mode-2)  
Fibers



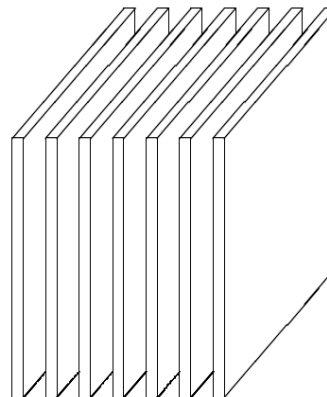
Tube (Mode-3)  
Fibers



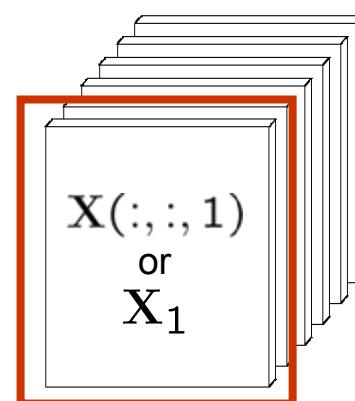
Horizontal Slices

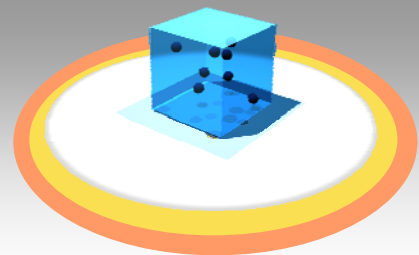


Lateral Slices

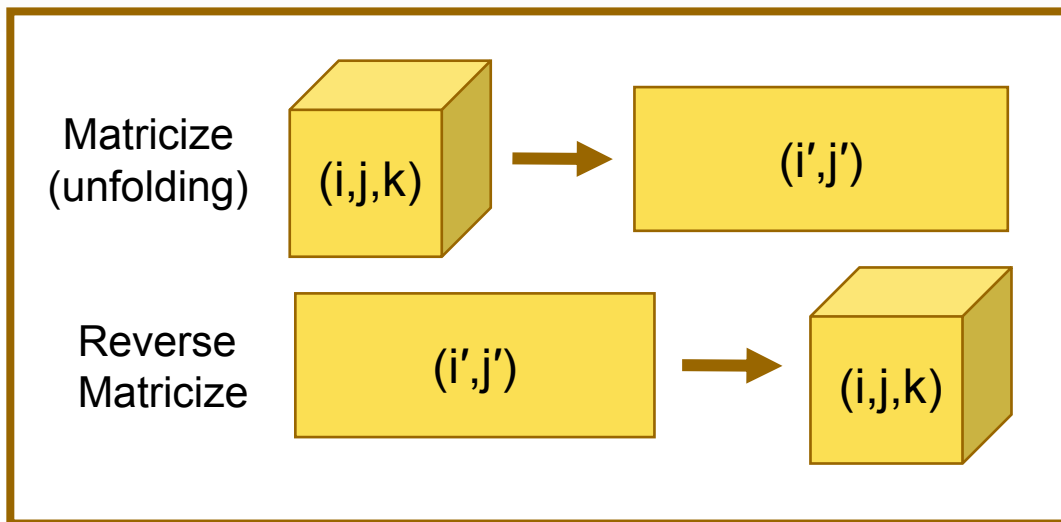


Frontal Slices

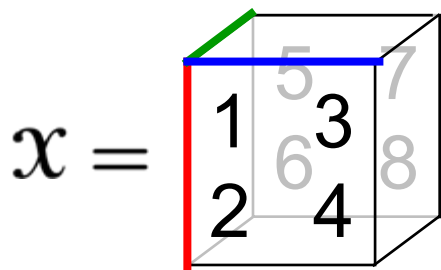
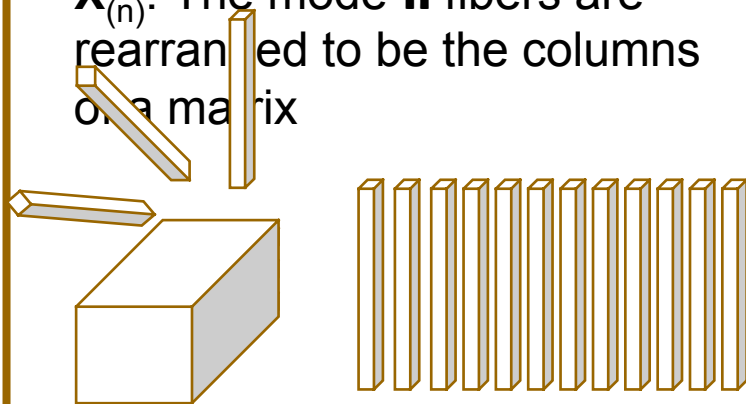




# Unfolding: Converting a Tensor to a Matrix



$\mathbf{X}_{(n)}$ : The mode- $n$  fibers are rearranged to be the columns of a matrix



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

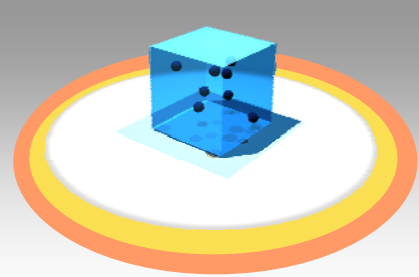
$$\mathbf{X}_{(2)} = \begin{bmatrix} 1 & 2 & 5 & 6 \\ 3 & 4 & 7 & 8 \end{bmatrix}$$

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

$\mathcal{X}$

$\mathbf{X}_{(3)}$

$$\text{vec}(\mathcal{X}) = \text{vec}(\mathbf{X}_{(1)}) = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \end{bmatrix}$$



# Tensor Mode-n Multiplication

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

- Tensor Times Matrix

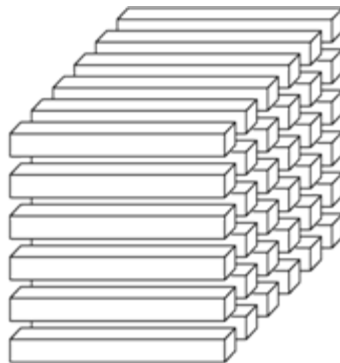
$$\mathcal{Y} = \mathcal{X} \times_2 \mathbf{B} \in \mathbb{R}^{I \times M \times K}$$

$$y_{imk} = \sum_j x_{ijk} b_{mj}$$

$$\mathbf{Y}_{(2)} = \mathbf{B} \mathbf{X}_{(2)}$$

Multiply each  
mode-2 fiber  
by  $\mathbf{B}$ :

$$\mathbf{y}_{i:k} = \mathbf{B} \mathbf{x}_{i:k}$$



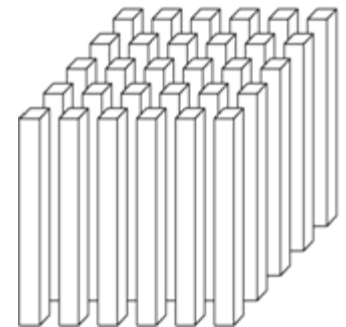
- Tensor Times Vector

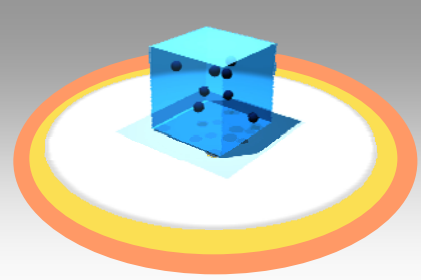
$$\mathcal{Y} = \mathcal{X} \bullet_1 \mathbf{a} \in \mathbb{R}^{J \times K}$$

$$y_{jk} = \sum_i x_{ijk} a_i$$

Compute the  
dot product of  
 $\mathbf{a}$  and each  
mode-1 fiber:

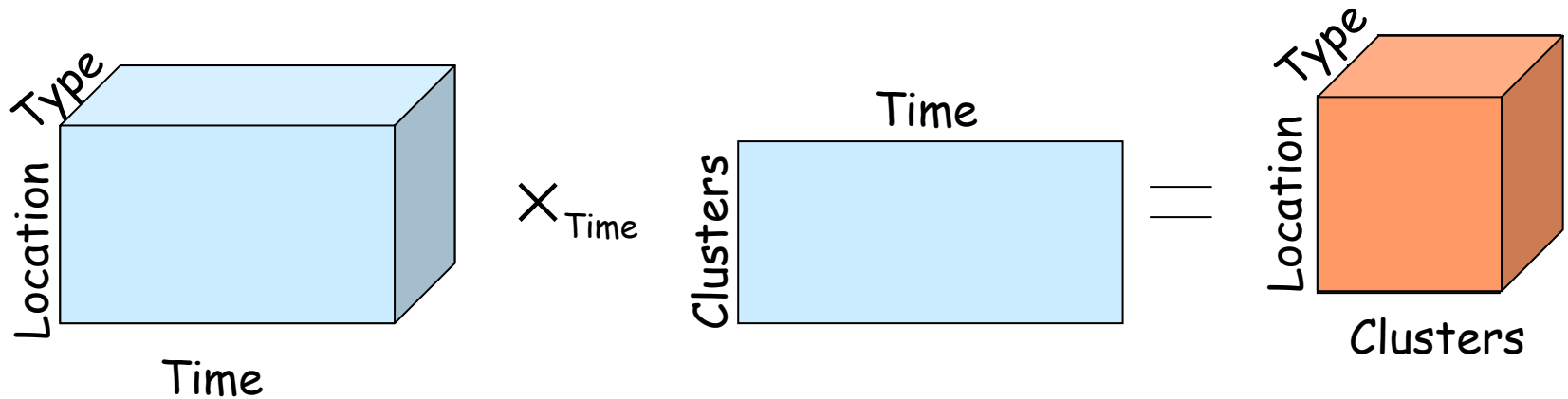
$$y_{jk} = (\mathbf{x}_{:jk})^\top \mathbf{a}$$



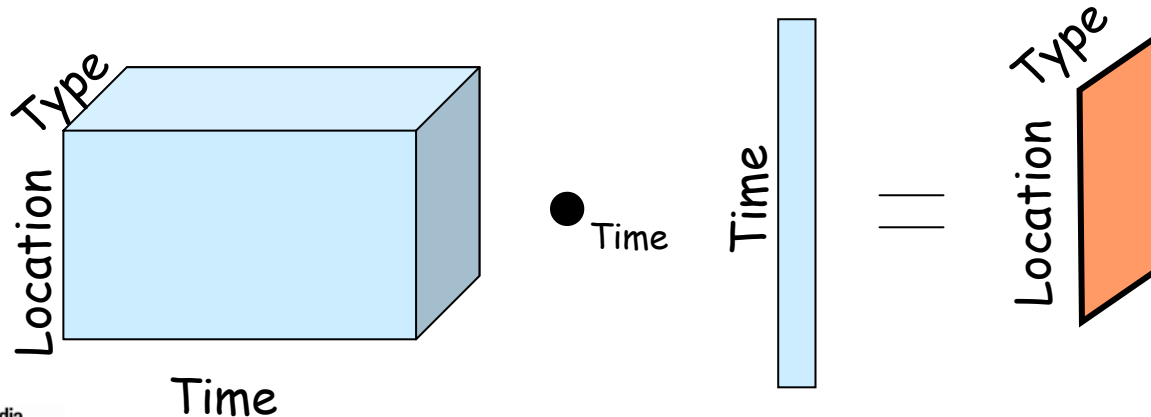


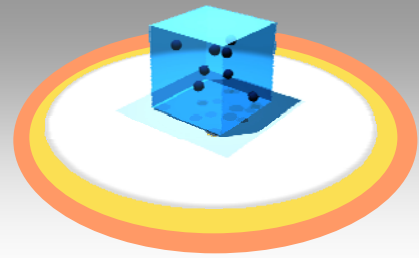
# Mode-n Multiplication Example

Tensor times a matrix:



Tensor times a vector:





# What is the higher-order analogue of the Matrix SVD?

Two views of the matrix SVD:

$$X = U \Sigma V^T = \text{[Red Box]} \begin{bmatrix} \diagup \\ \diagdown \end{bmatrix} \text{[Blue Box]} = \sigma_1 \begin{bmatrix} \text{[Red Box]} \\ \text{[Red Box]} \end{bmatrix} \begin{bmatrix} \text{[Blue Box]} \end{bmatrix} + \sigma_2 \begin{bmatrix} \text{[Red Box]} \\ \text{[Red Box]} \end{bmatrix} \begin{bmatrix} \text{[Blue Box]} \end{bmatrix} + \dots + \sigma_R \begin{bmatrix} \text{[Red Box]} \\ \text{[Red Box]} \end{bmatrix} \begin{bmatrix} \text{[Blue Box]} \end{bmatrix}$$

Finding bases for row and column subspaces:

$$X = \Sigma \times_1 U \times_2 V$$



Tucker  
Decomposition

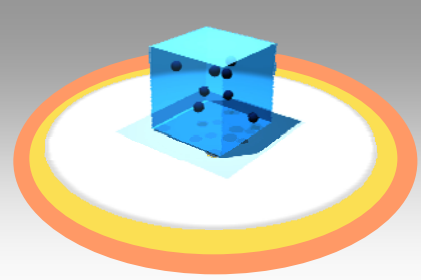
Sum of  $R$  rank-1 matrix factors (where  $R$  is the rank):

$$X = \sum_{r=1}^R \sigma_r \mathbf{u}_r \circ \mathbf{v}_r$$



CANDECOMP/  
PARAFAC





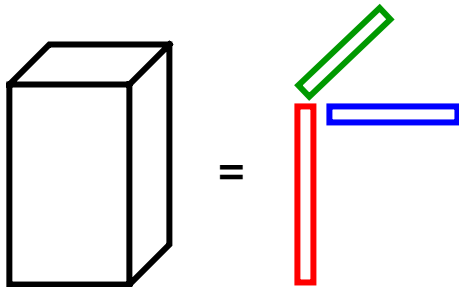
# Tucker Decomposition

# Outer Products & Kronecker Products

3-Way Outer Product

$$\mathcal{X} = \mathbf{a} \circ \mathbf{b} \circ \mathbf{c}$$

$$x_{ijk} = a_i b_j c_k$$



Rank-1 Tensor

Vector Kronecker Product

$$(\mathbf{a} \otimes \mathbf{b})^T = [a_1 \mathbf{b}^T \quad a_2 \mathbf{b}^T \quad \cdots \quad a_N \mathbf{b}^T]$$

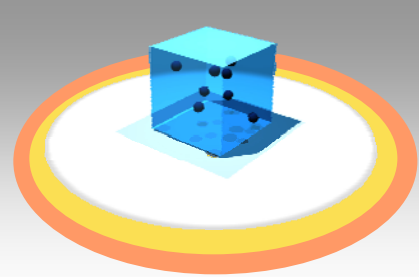
Matrix Kronecker Product

$$\begin{aligned} \underset{M \times N}{\mathbf{A}} \otimes \underset{P \times Q}{\mathbf{B}} &= \begin{bmatrix} a_{11}\mathbf{B} & a_{12}\mathbf{B} & \cdots & a_{1N}\mathbf{B} \\ a_{21}\mathbf{B} & a_{22}\mathbf{B} & \cdots & a_{2N}\mathbf{B} \\ \vdots & \vdots & \ddots & \vdots \\ a_{M1}\mathbf{B} & a_{M2}\mathbf{B} & \cdots & a_{MN}\mathbf{B} \end{bmatrix} \\ &\underset{MP \times NQ}{=} [\mathbf{a}_1 \otimes \mathbf{b}_1 \quad \mathbf{a}_1 \otimes \mathbf{b}_2 \quad \cdots \quad \mathbf{a}_N \otimes \mathbf{b}_Q] \end{aligned}$$

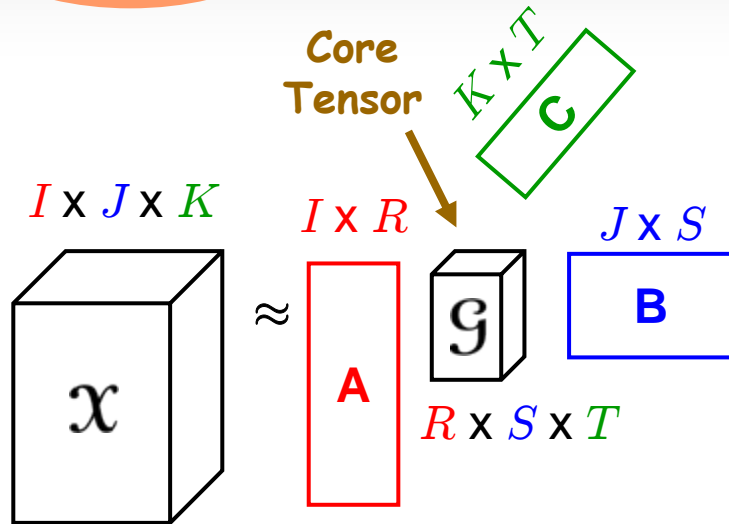
Observe

The Kronecker product and outer product yield the same results, just shaped differently:

$$\mathcal{X} = \mathbf{a} \circ \mathbf{b} \circ \mathbf{c} \Rightarrow \text{vec}(\mathcal{X}) = \mathbf{c} \otimes \mathbf{b} \otimes \mathbf{a}$$



# Tucker Decomposition

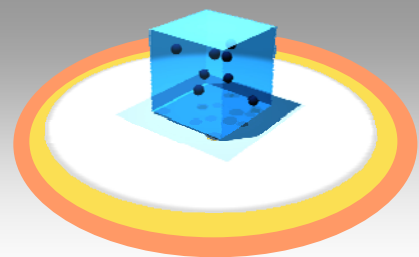


$$\mathcal{X} \approx \mathcal{G} \times_1 \mathbf{A} \times_2 \mathbf{B} \times_3 \mathbf{C}$$

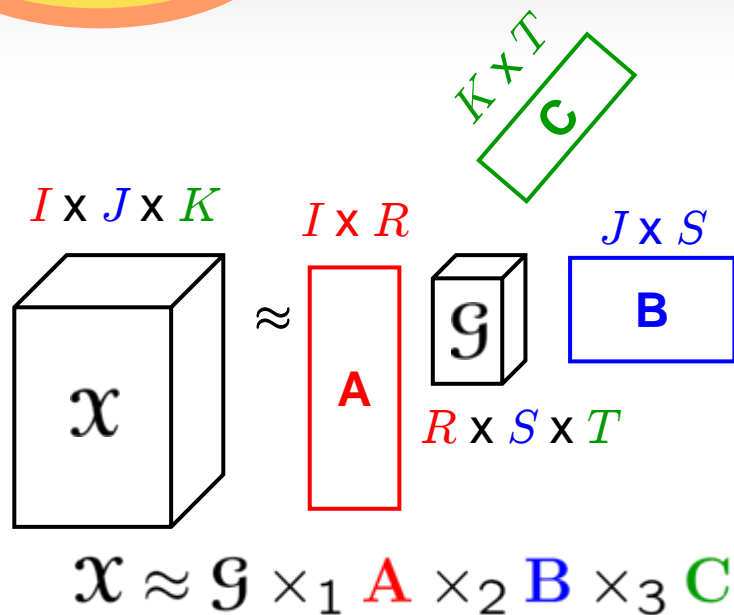
$$\mathcal{X} = \underbrace{\sum_{r=1}^R \sum_{s=1}^S \sum_{t=1}^T g_{rst} \mathbf{a}_r \circ \mathbf{b}_s \circ \mathbf{c}_t}_{\text{RST rank-1 factors}}$$

- Also known as: three-mode factor analysis, three-mode PCA, orthogonal array decomposition
- Dimensions  $R$ ,  $S$ ,  $T$  chosen by the user.
- $\mathbf{A}$ ,  $\mathbf{B}$ , and  $\mathbf{C}$  may be orthonormal (generally assume full column rank)
- $\mathcal{G}$  is not diagonal
- Not unique

See Tucker, *Psychometrika*, 1966; see also Hitchcock, 1927.



# Matrix & Vector Forms of Tucker Decomposition



## "Matricized" Tucker

$$\mathbf{X}_{(1)} \approx \mathbf{A} \mathbf{G}_{(1)} (\mathbf{C} \otimes \mathbf{B})^T$$

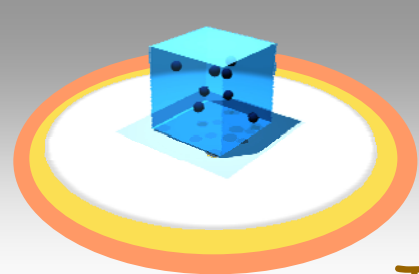
$$\mathbf{X}_{(2)} \approx \mathbf{B} \mathbf{G}_{(2)} (\mathbf{C} \otimes \mathbf{A})^T$$

$$\mathbf{X}_{(3)} \approx \mathbf{C} \mathbf{G}_{(3)} (\mathbf{B} \otimes \mathbf{A})^T$$

## "Vectorized" Tucker

$$\text{vec}(\mathcal{X}) \approx (\mathbf{C} \otimes \mathbf{B} \otimes \mathbf{A}) \text{vec}(\mathcal{G}) \Rightarrow \text{Given } \mathbf{A}, \mathbf{B}, \mathbf{C}, \text{ with orthonormal columns, the optimal core is:}$$

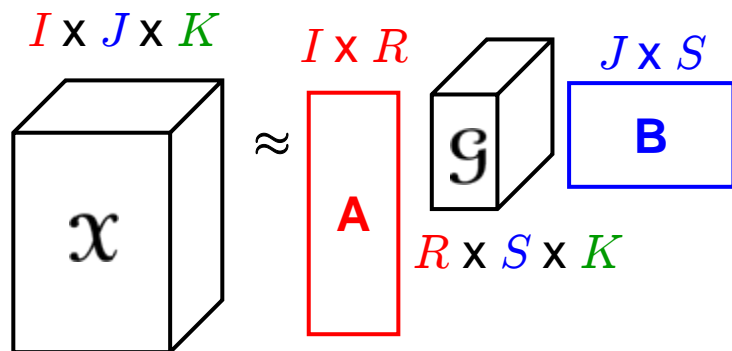
$$\mathcal{G} = \mathcal{X} \times_1 \mathbf{A}^\dagger \times_2 \mathbf{B}^\dagger \times_3 \mathbf{C}^\dagger$$



# Tucker Variations

Details

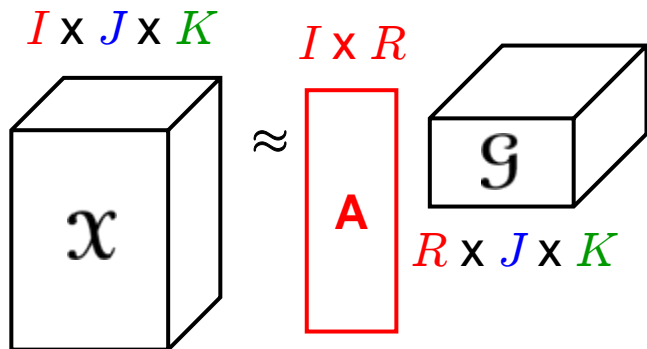
## Tucker 2



$$\mathcal{X} = \mathcal{G} \times_1 \mathbf{A} \times_2 \mathbf{B} \times_3 \mathbf{I}$$

$$\mathbf{X}_{(3)} \approx \mathbf{G}_{(3)} (\mathbf{B} \otimes \mathbf{A})^\top$$

## Tucker 1



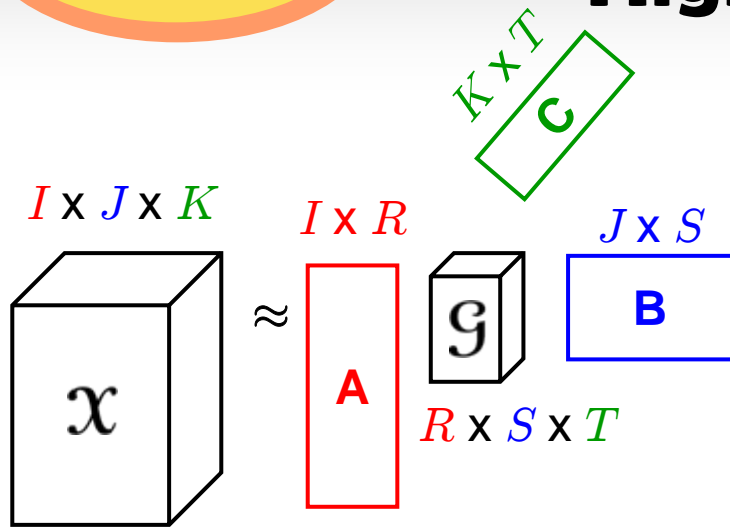
$$\mathcal{X} = \mathcal{G} \times_1 \mathbf{A} \times_2 \mathbf{I} \times_3 \mathbf{I}$$

$$\mathbf{X}_{(1)} \approx \mathbf{A} \mathbf{G}_{(1)}$$

Can be solved via SVD.

See Kroonenberg & De Leeuw, *Psychometrika*, 1980 for discussion.

# Fitting Tucker via the Higher Order SVD (HO-SVD)



$$\mathcal{X} \approx \mathcal{G} \times_1 \mathbf{A} \times_2 \mathbf{B} \times_3 \mathbf{C}$$

Not optimal, but often used to initialize other algorithms.

$\mathbf{A}$  = leading  $\mathbf{R}$  left singular vectors of  $\mathbf{X}_{(1)}$

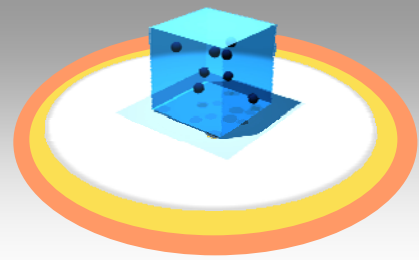
$\mathbf{B}$  = leading  $\mathbf{S}$  left singular vectors of  $\mathbf{X}_{(2)}$

$\mathbf{C}$  = leading  $\mathbf{T}$  left singular vectors of  $\mathbf{X}_{(3)}$

(Observe connection to Tucker 1)

$$\mathcal{G} = \mathcal{X} \times_1 \mathbf{A}^\dagger \times_2 \mathbf{B}^\dagger \times_3 \mathbf{C}^\dagger$$

De Lathauwer, De Moor, & Vandewalle, SIMAX, 2000.  
Also known as “Method 1” in Tucker, 1966.



# Fitting Tucker via Alternating Least Squares (ALS)

1. Initialize  $A$ ,  $B$ ,  $C$ .

2. Repeat the following steps until “convergence”:

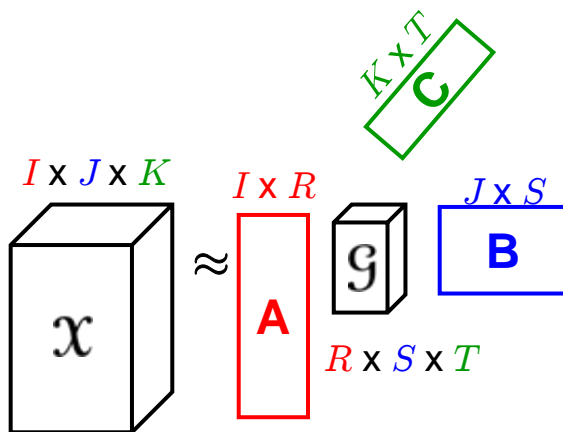
$A$  = leading  $R$  left singular vectors of  $X_{(1)}(C \otimes B)$

$B$  = leading  $S$  left singular vectors of  $X_{(2)}(C \otimes A)$

$C$  = leading  $T$  left singular vectors of  $X_{(3)}(B \otimes A)$

3. Finally, set:

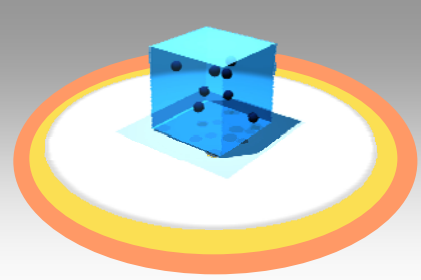
$$\mathcal{G} = \mathcal{X} \times_1 A^\dagger \times_2 B^\dagger \times_3 C^\dagger$$



See Kroonenberg & De Leeuw, *Psychometrika*, 1980, and De Lathauwer, De Boor, and Vandewalle, *SIMAX*, 2000.

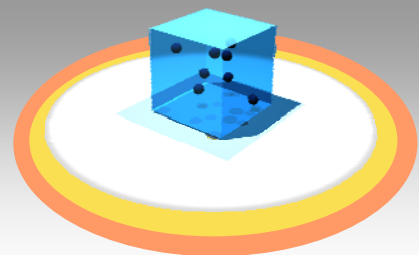


Newton-Grassmann method proposed by Eldén and Savas, 2007.



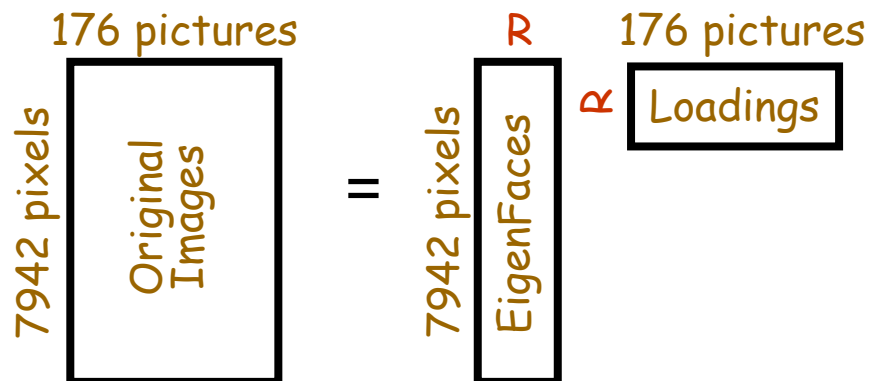
# Application: TensorFaces



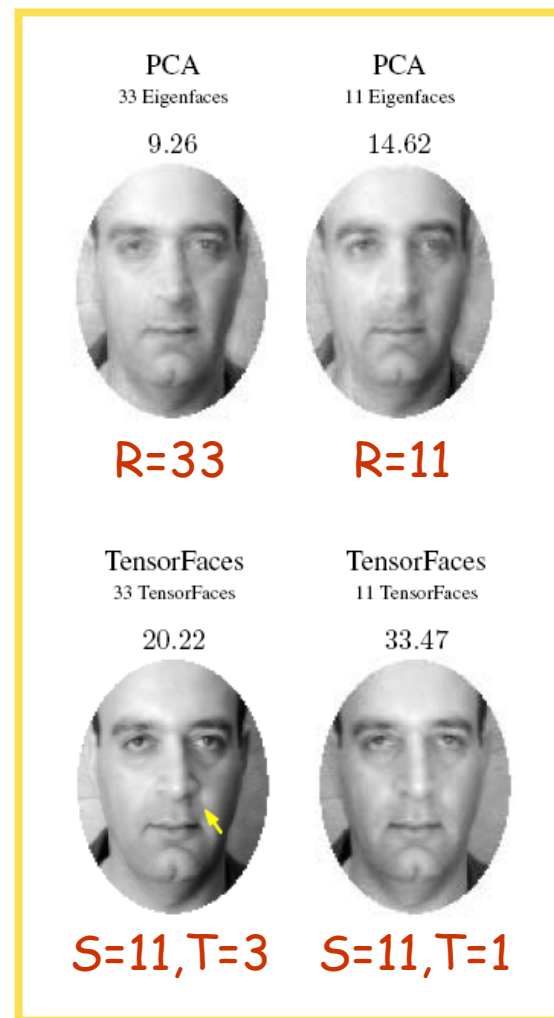
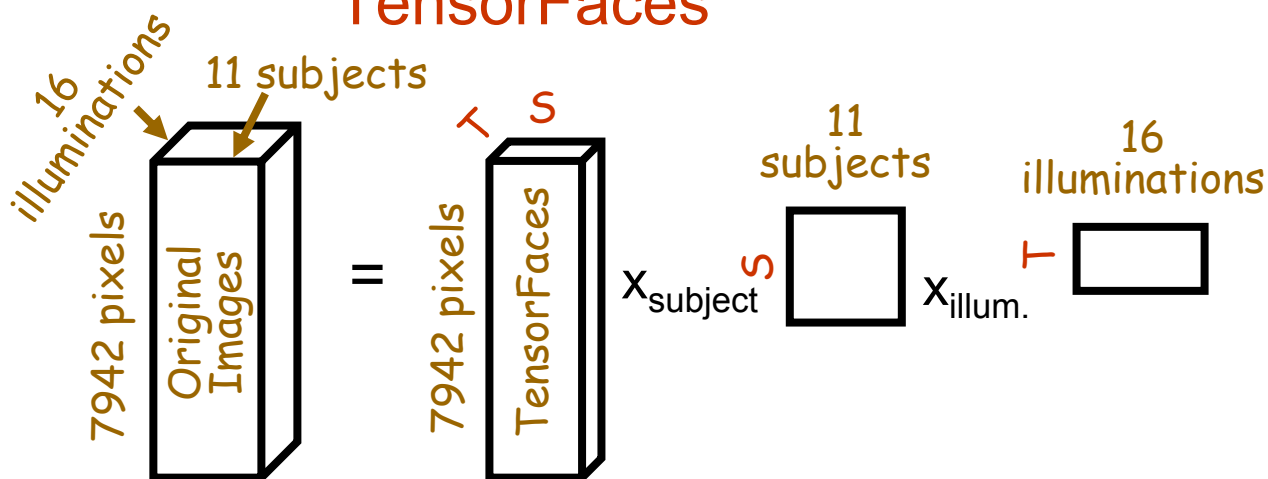


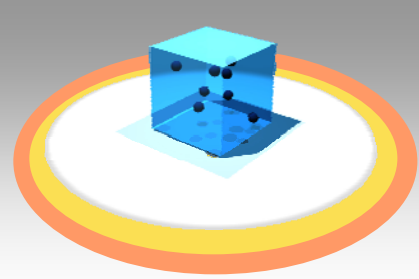
# TensorFaces: An Application of the Tucker2 Decomposition

## EigenFaces



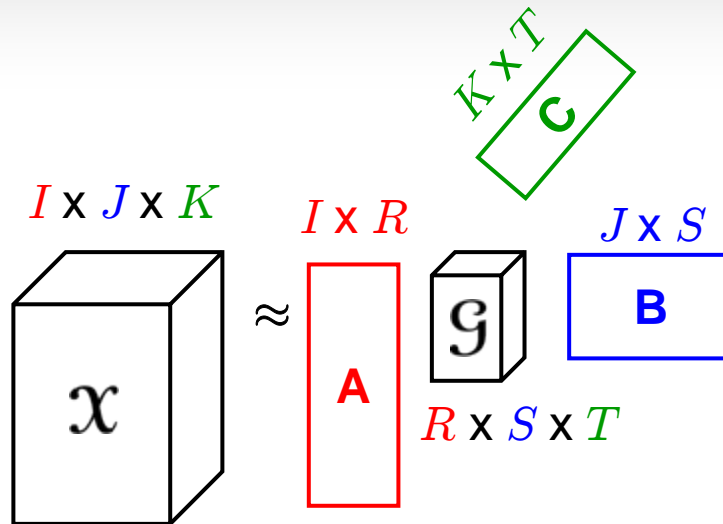
## TensorFaces





# Issue: Tucker is Not Unique

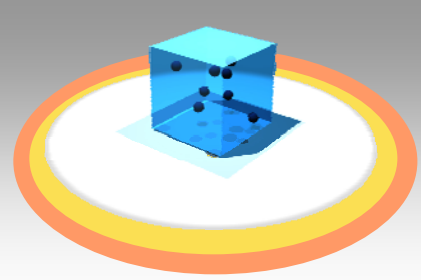
Details



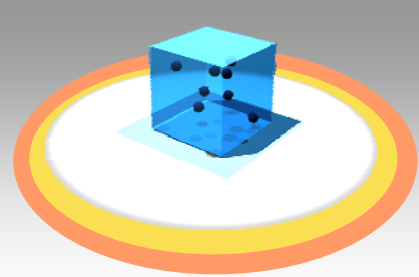
Tucker decomposition is not unique. Let  $Y$  be an  $R \times R$  orthogonal matrix. Then...

$$\mathcal{X} \approx \mathcal{G} \times_1 \mathbf{A} \times_2 \mathbf{B} \times_3 \mathbf{C} = (\mathcal{G} \times_1 \mathbf{Y}^T) \times_1 (\mathbf{A} \mathbf{Y}) \times_2 \mathbf{B} \times_3 \mathbf{C}$$

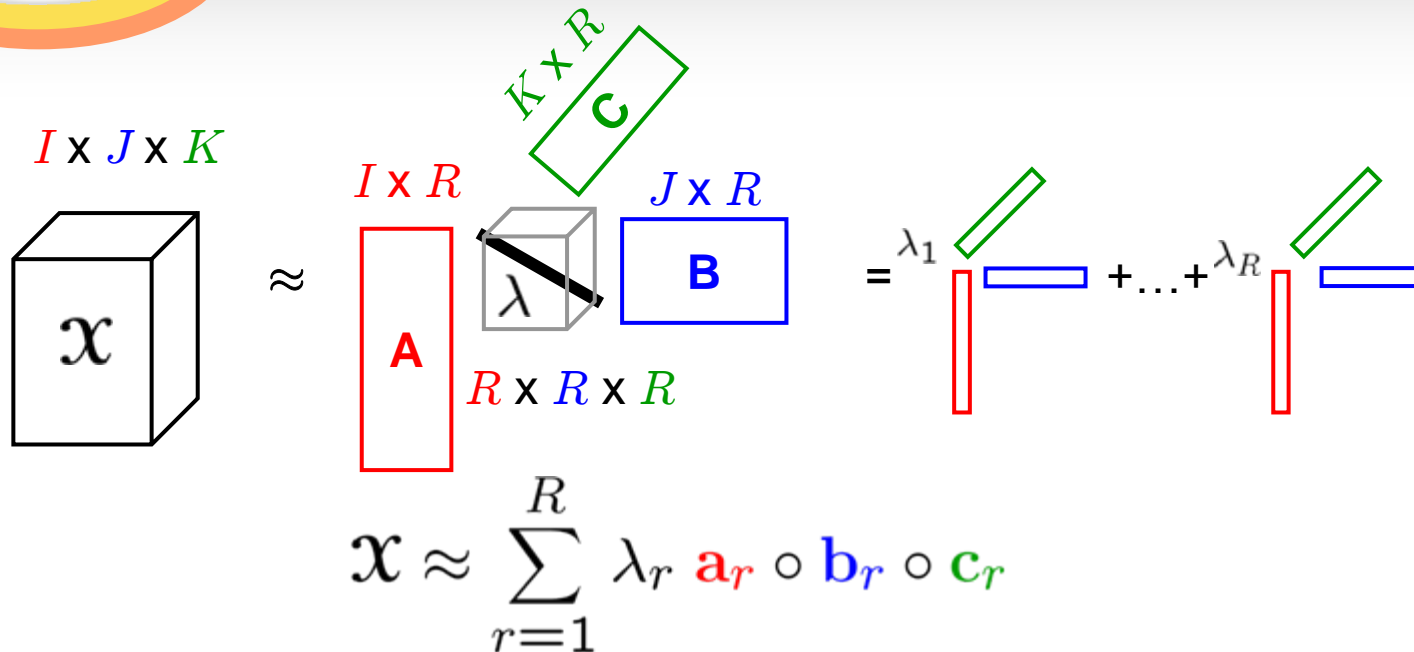
$$\mathbf{X}_{(1)} \approx \mathbf{A} \mathbf{G}_{(1)} (\mathbf{C} \otimes \mathbf{B})^T = \mathbf{A} \mathbf{Y} \mathbf{Y}^T \mathbf{G}_{(1)} (\mathbf{C} \otimes \mathbf{B})^T$$



# **CANDECOMP/PARAFAC Decomposition**

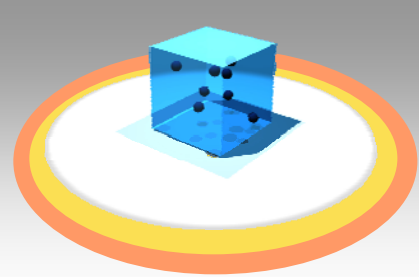


# CANDECOMP/PARAFAC (CP)



- CANDECOMP = Canonical Decomposition,
- PARAFAC = Parallel Factors
- Optional core is diagonal (specified by the vector  $\lambda$ )
- Columns of  $\mathbf{A}$ ,  $\mathbf{B}$ , and  $\mathbf{C}$  are not orthonormal
- Exact decomposition is often unique

Carroll & Chang, *Psychometrika*, 1970, Harshman, 1970 – plus Hitchcock, 1927.



# CP & Tensor Rank

$I \times J \times K$

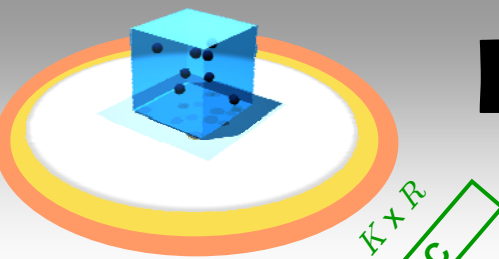
$$\mathcal{X} = \sum_{r=1}^R \lambda_r \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r$$

Tensor Rank: The rank of a tensor  $\mathcal{X}$ , denoted  $\text{rank}(\mathcal{X})$ , is the smallest number of rank-1 factors that generate  $\mathcal{X}$  as their sum.

- No straightforward method to determine the rank of a specific tensor
- Maximum rank = maximum achievable rank
  - $2 \times 2 \times 2$  tensor = 3,  $3 \times 3 \times 2$  tensor = 4
- Typical rank = occurs with probability greater than zero
  - $2 \times 2 \times 2$  tensor =  $\{2,3\}$ ,  $3 \times 3 \times 2 = \{3,4\}$
- Border Rank = Minimum number of rank-1 tensors sufficient to approximate given tensor with arbitrarily small nonzero error
  - “Best” low-rank approximation may not exist

See also Kruskal, *LAA*, 1977; Kruskal, 1989; J. M. F. Ten Berge, *Psychometrika*, 1991; Bini et al., *Inform. Process. Lett.*, 1979

# Matrix & Vector Forms of CP Decomposition



$$\begin{aligned}
 \mathcal{X} &\approx \begin{matrix} I \times J \times K \\ \text{red box} \end{matrix} \begin{matrix} I \times R \\ \text{red box} \end{matrix} \begin{matrix} K \times R \\ \text{green box } C \end{matrix} \begin{matrix} J \times R \\ \text{blue box } B \end{matrix} \\
 &= \lambda_1 \begin{matrix} \text{red box} \end{matrix} \begin{matrix} \text{blue box} \end{matrix} + \dots + \lambda_R \begin{matrix} \text{red box} \end{matrix} \begin{matrix} \text{blue box} \end{matrix} \\
 \mathcal{X} &\approx \sum_{r=1}^R \lambda_r \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r
 \end{aligned}$$

Matrix Khatri-Rao Product

$$\underset{M \times R}{A} \odot \underset{N \times R}{B} = \begin{bmatrix} \mathbf{a}_1 \otimes \mathbf{b}_1 & \mathbf{a}_2 \otimes \mathbf{b}_2 & \cdots & \mathbf{a}_R \otimes \mathbf{b}_R \end{bmatrix} \underset{MN \times R}{}$$

"Matricized" CP

$$X_{(1)} \approx \mathbf{A} \Lambda (\mathbf{C} \odot \mathbf{B})^T$$

$$X_{(2)} \approx \mathbf{B} \Lambda (\mathbf{C} \odot \mathbf{A})^T$$

$$X_{(3)} \approx \mathbf{C} \Lambda (\mathbf{B} \odot \mathbf{A})^T$$

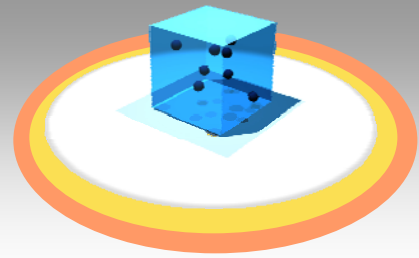
$$\Lambda = \text{diag}(\lambda)$$

"Vectorized" CP

$$\text{vec}(\mathcal{X}) \approx (\mathbf{C} \odot \mathbf{B} \odot \mathbf{A}) \lambda$$

Useful Fact

$$(\mathbf{A} \odot \mathbf{B})^\dagger = ((\mathbf{A}^T \mathbf{A}) * (\mathbf{B}^T \mathbf{B}))^\dagger (\mathbf{A} \odot \mathbf{B})^T$$



# Fitting CP via Alternating Least Squares (ALS)

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

$$\overset{I \times J \times K}{\mathcal{X}} = \lambda_1 \begin{array}{c} \text{green diagonal} \\ \text{red vertical} \end{array} \text{blue horizontal} + \dots + \lambda_R \begin{array}{c} \text{green diagonal} \\ \text{red vertical} \end{array} \text{blue horizontal}$$

1. Initialize A, B, C.
2. Repeat the following steps until “convergence”:

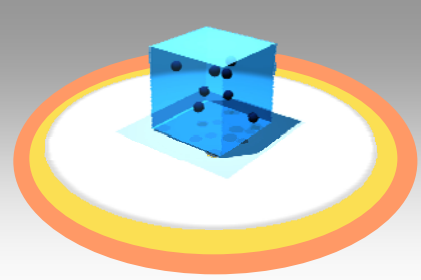
$$\mathbf{A} = \mathbf{X}_{(1)} (\mathbf{C} \odot \mathbf{B}) (\mathbf{C}^T \mathbf{C} * \mathbf{B}^T \mathbf{B})^\dagger$$

$$\mathbf{B} = \mathbf{X}_{(2)} (\mathbf{C} \odot \mathbf{A}) (\mathbf{C}^T \mathbf{C} * \mathbf{A}^T \mathbf{A})^\dagger$$

$$\mathbf{C} = \mathbf{X}_{(3)} (\mathbf{B} \odot \mathbf{A}) (\mathbf{B}^T \mathbf{B} * \mathbf{A}^T \mathbf{A})^\dagger$$

(normalize each matrix in turn to get  $\Lambda$ )

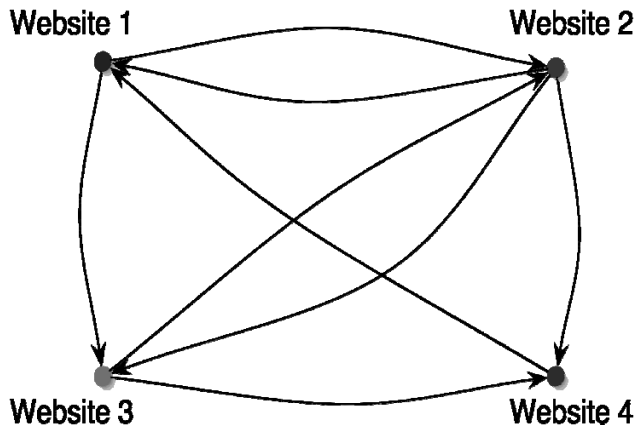
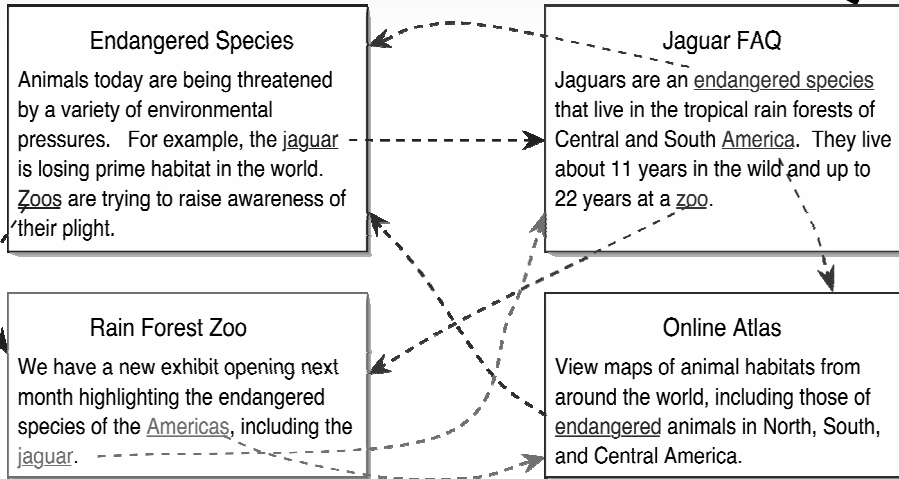
Survey: Tomasi & Bro, Computational Statistics & Data Analysis, 2006.



# Application: TOPHITS



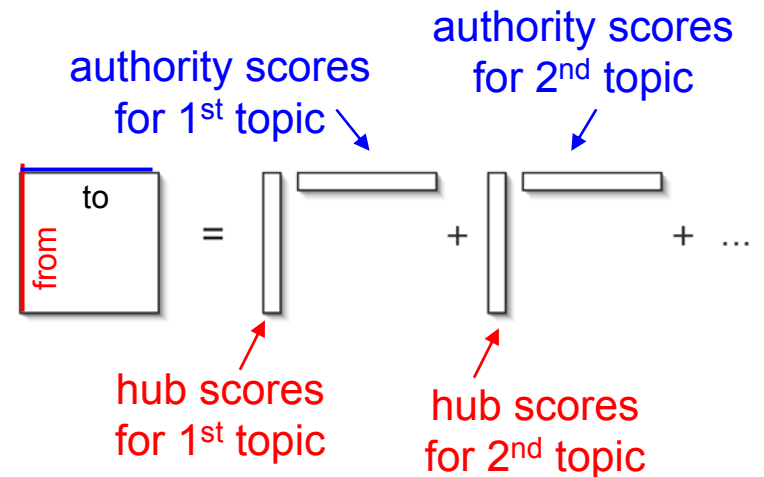
# Hubs and Authorities (the HITS method)

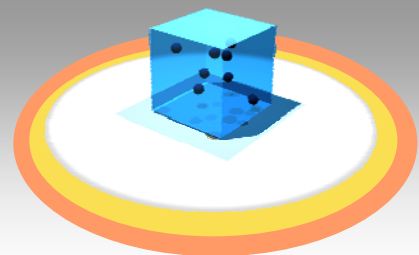


Sparse adjacency matrix and its SVD:

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

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





# HITS Authorities on Sample Data

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

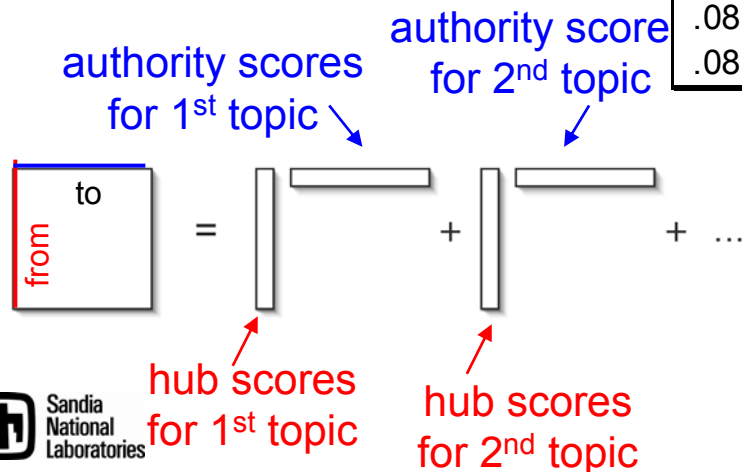
1st Principal Factor	
.97	www.ibm.com
.24	www.alphaw
.08	www-128.ibm
.05	www.develop
.02	www.research
.01	www.redbook
.01	news.com.cc

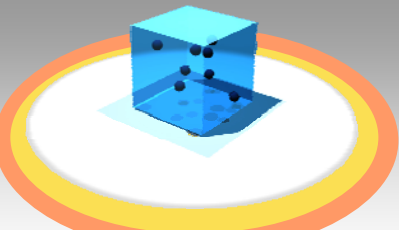
2nd Principal Factor	
.99	www.lehigh.edu
.11	www2.lehigh.edu
.06	www.lehigha
.06	www.lehighs
.02	www.bethleh
.02	www.adobe.c
.02	lewisweb.cc.
.02	www.leo.lehi
.02	www.distanc
.02	fp1.cc.lehigh

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.cc
.08	www.sun-catalo
.08	news.com.com

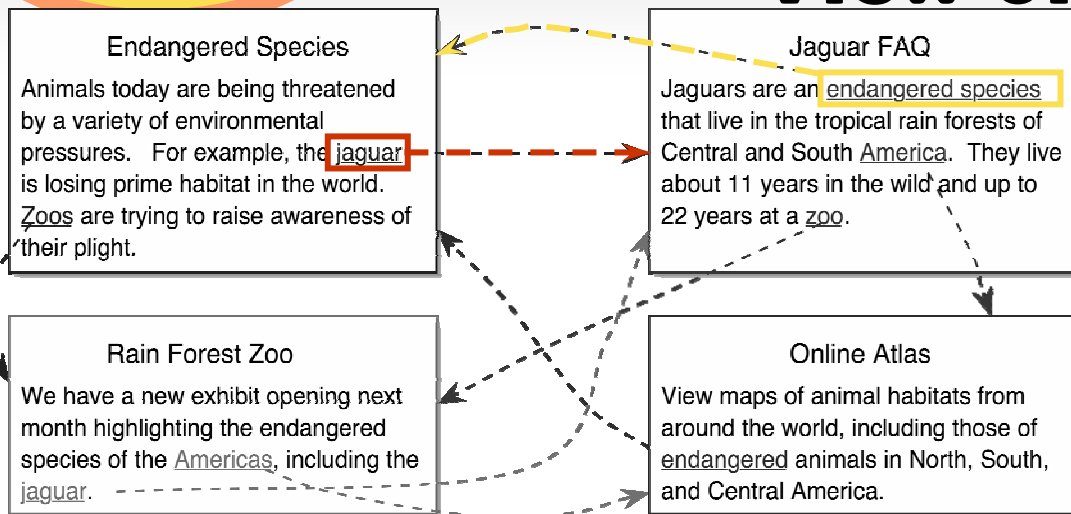
4th Principal Factor	
.60	www.pueblo.gsa.gov
.45	www.whitehouse.gov
.35	www.irs.gov
.31	travel.state
.22	www.gsa.g
.20	www.ssa.g
.16	www.censu
.14	www.govbe
.13	www.kids.g
.13	www.usdoj

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





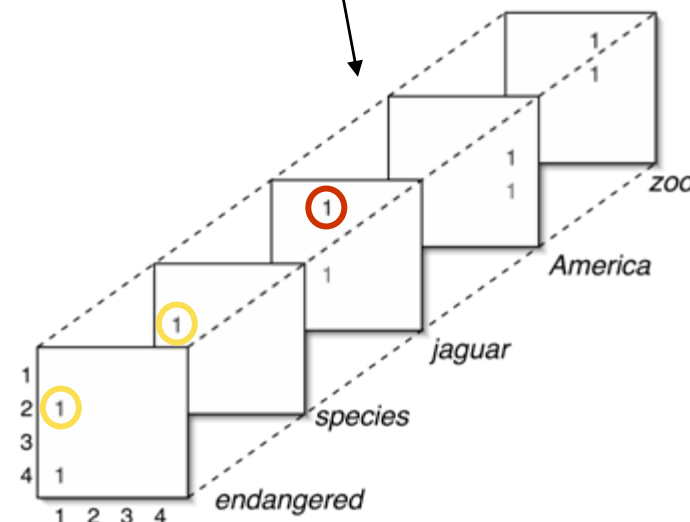
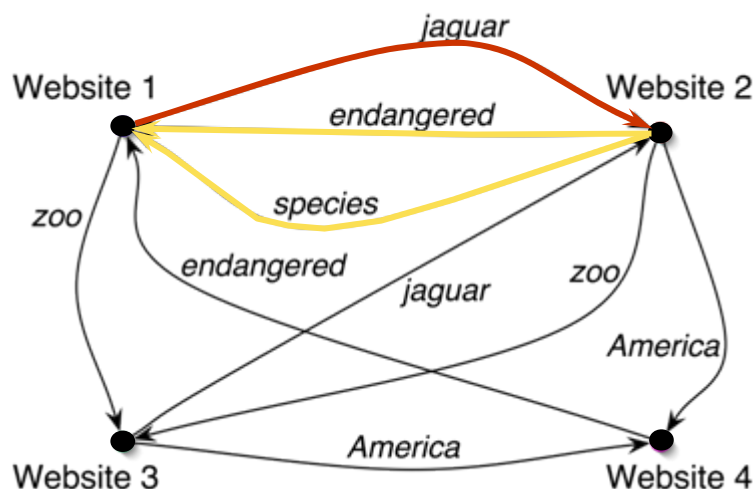
# TOPHITS – A Three-Dimensional View of the Web

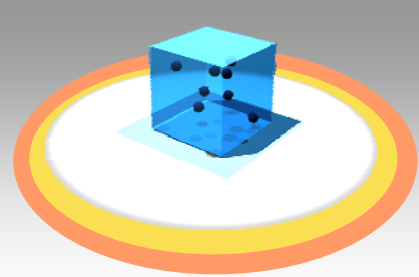


**Tensor Definition**

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

Observe that this tensor is very sparse!

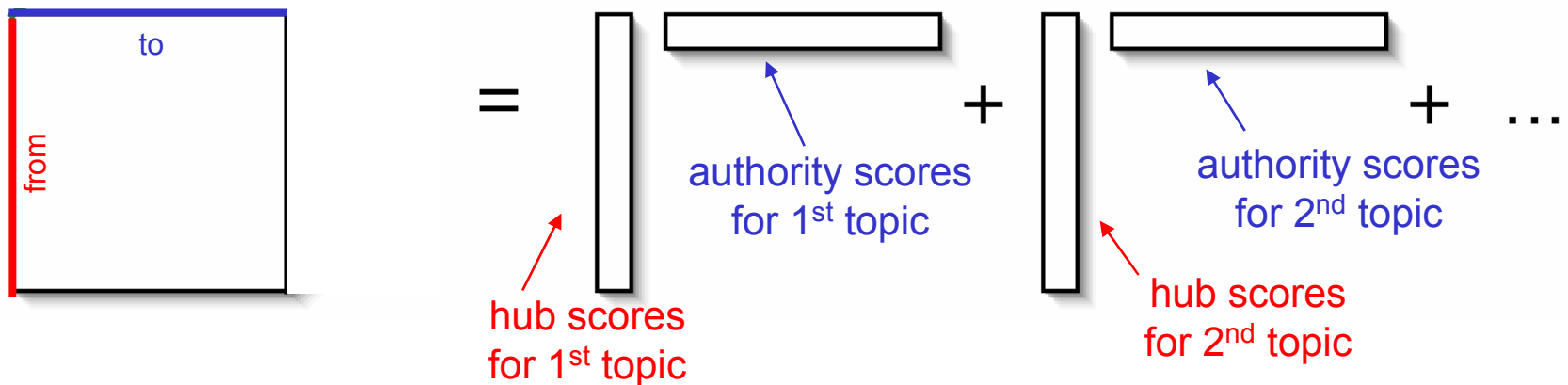


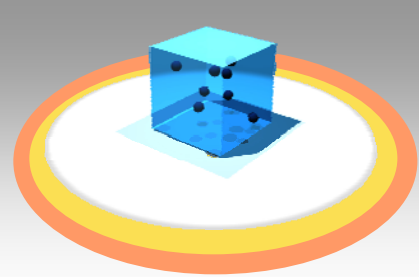


# Topical HITS (TOPHITS)

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

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

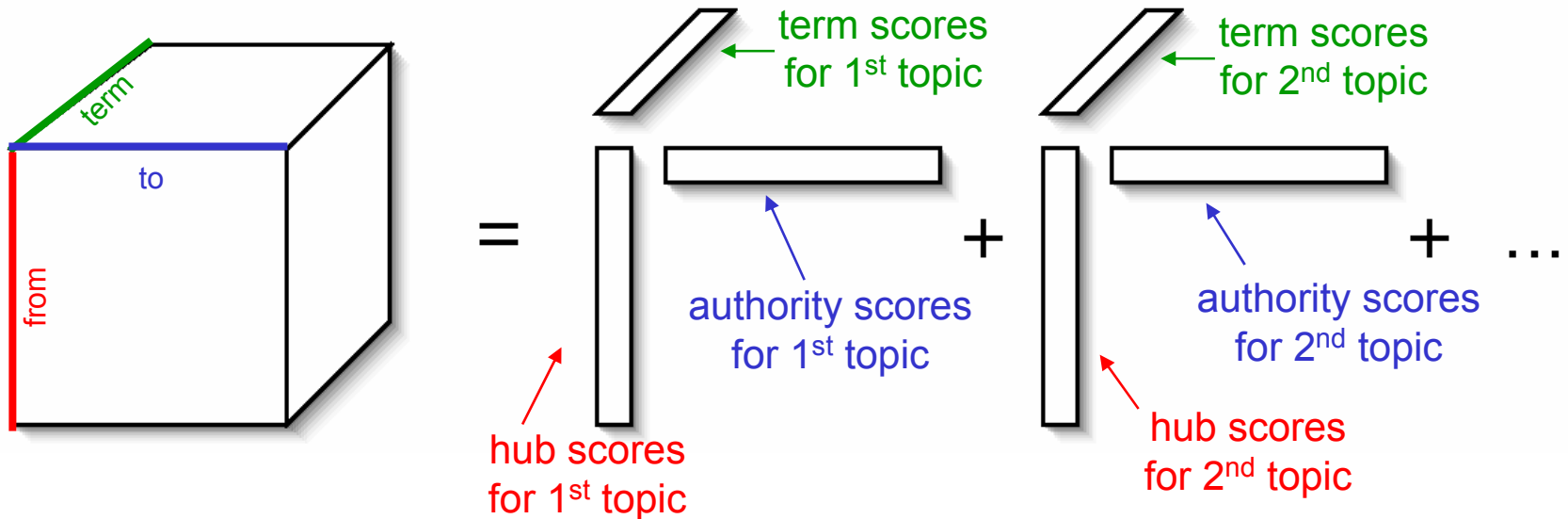




# Topical HITS (TOPHITS)

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

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



# TOPHITS Terms & Authorities

## on Sample Data

TOPHITS uses 3D analysis to find the dominant groupings of web pages and terms.

$$x_{ijk} = \begin{cases} \frac{1}{\log(w_k)+1} & \text{if } i \rightarrow j \text{ with term } k \\ 0 & \text{otherwise} \end{cases}$$

$w_k$  = # unique links using term k

**1st Principal Factor**

.23	JAVA	.86	java.sun.com
.18	SUN	.38	developers.sun.com

**2nd Principal Factor**

.20	NO-READABLE-TEXT	.99	www.lehigh.edu
-----	------------------	-----	----------------

**3rd Principal Factor**

.15	NO-READABLE-TEXT	.97	www.ibm.com
.15	IBM	.18	www.alphaworks.ibm.com

**4th Principal Factor**

.26	INFORMATION	.87	www.pueblo.gsa.gov
.24	FEDERAL	.24	www.irs.gov

**6th Principal Factor**

.26	PRESIDENT	.87	www.whitehouse.gov
.25	NO-READABLE-TEXT	.18	www.irs.gov

**12th Principal Factor**

.75	OPTIMIZATION	.35	www.palisade.com
.58	SOFTWARE	.35	www.solver.com

**13th Principal Factor**

.46	ADOBE	.99	www.adobe.com
-----	-------	-----	---------------

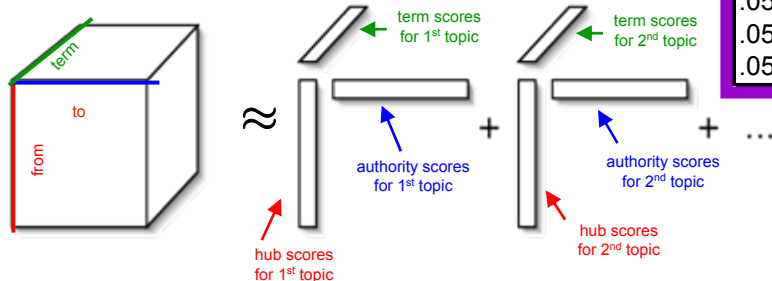
**16th Principal Factor**

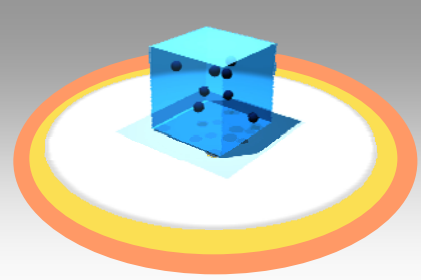
.50	WEATHER	.81	www.weather.gov
.24	OFFICE	.41	www.spc.noaa.gov
.23	CENTER	.30	lwf.ncdc.noaa.gov

**19th Principal Factor**

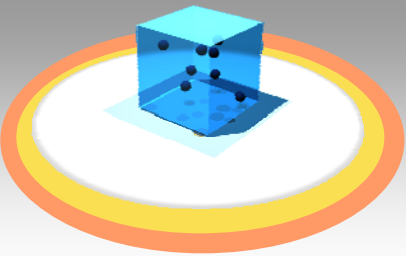
.22	TAX	.73	www.irs.gov
.17	TAXES	.43	travel.state.gov
.15	CHILD	.22	www.ssa.gov
.15	RETIREMENT	.08	www.govbenefits.gov
.15	BENEFITS	.06	www.usdoj.gov
.14	STATE	.03	www.census.gov
.14	INCOME	.03	www.usmint.gov
.13	SERVICE	.02	www.nws.noaa.gov
.13	REVENUE	.02	www.gsa.gov
.12	CREDIT	.01	www.annualcreditreport.com

Tensor PARAFAC



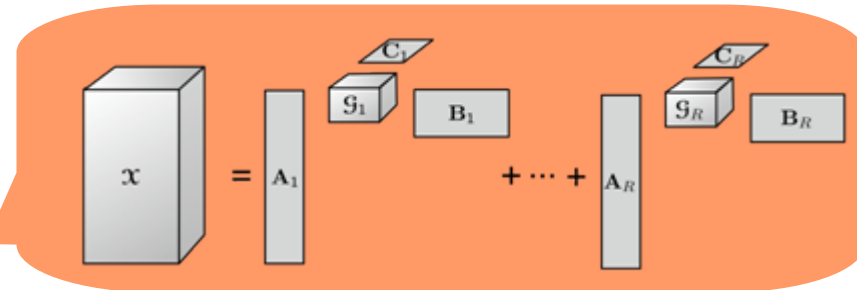
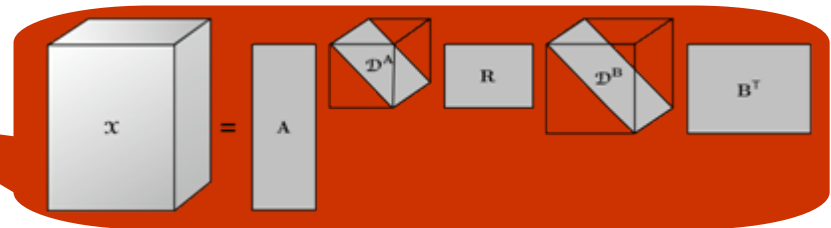
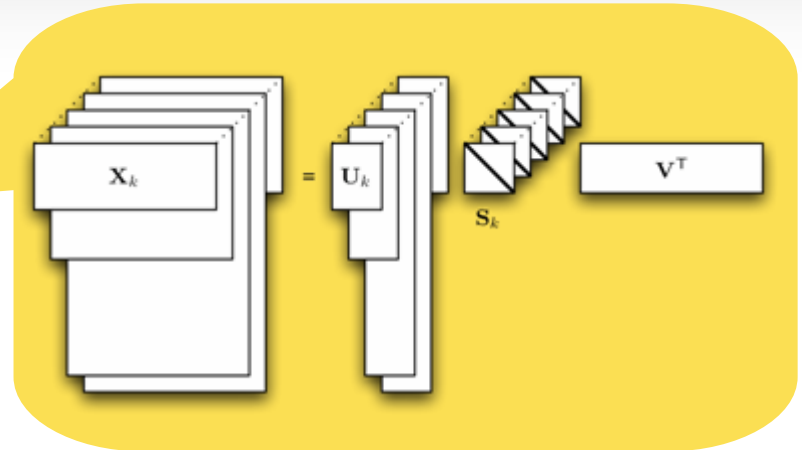


# Other Decompositions

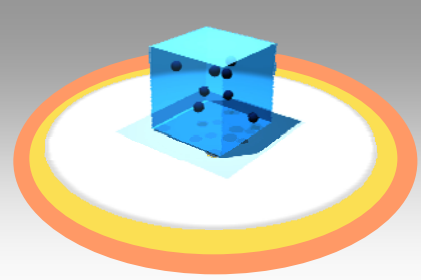


# Other Decompositions

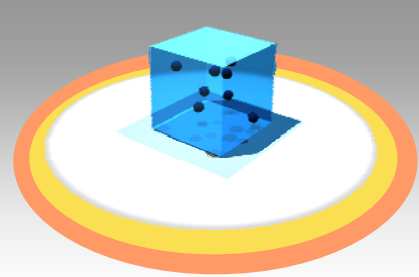
- **INDSCAL**: Individual Differences in Scaling (Carroll & Chang, 1972)
- **PARAFAC2** (Harshman, 1978)
- **CANDELINC**: Linearly constrained CP (Carroll, Pruzansky, Kruskal, 1980)
- **DEDICOM**: Decomposition into directional components (Harshman, 1972)
- **PARATUCK2**: Generalization of DEDICOM (Harshman & Lundy, 1996)
- **Nonnegative tensor factorizations** (Bro and De Jung, 1997; Paatero, 1997; Welling and Weber, 2001; etc.)
- **Block factorizations** (De Lathauwer, 2007; etc.)







# PARAFAC2



# Yet another view of PARAFAC

$I \times J \times K$

$$\mathcal{X} = \text{rank-1 tensor} + \dots + \text{rank-1 tensor}$$

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

$$\mathbf{X}_{(1)} \approx \mathbf{A}(\mathbf{C} \odot \mathbf{B})^T$$

$$\mathbf{X}_{(2)} \approx \mathbf{B}(\mathbf{C} \odot \mathbf{A})^T$$

$$\mathbf{X}_{(3)} \approx \mathbf{C}(\mathbf{B} \odot \mathbf{A})^T$$

$$\text{vec}(\mathcal{X}) \approx (\mathbf{C} \odot \mathbf{B} \odot \mathbf{A})\mathbf{1}$$

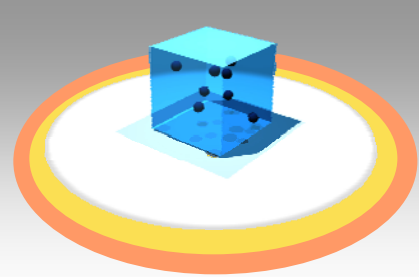
$$\mathbf{X}_k = \mathbf{A} \mathbf{S}_k \mathbf{B}^T$$

$\mathbf{S}_k = \text{diag}(k^{\text{th}} \text{ row of } \mathbf{C})$

$$\mathbf{X}_k = \mathbf{A} \mathbf{S}_k \mathbf{B}^T$$

This representation only works for 3<sup>rd</sup>-order tensors.

Looks like SVD.

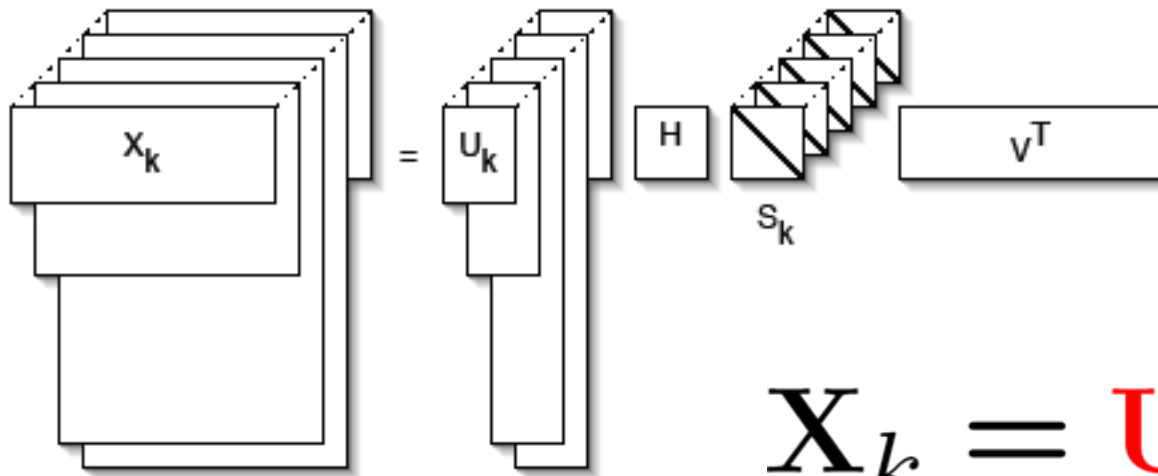


# PARAFAC2

(not, strictly speaking, a tensor decomposition)

PARAFAC

$$X_k = \mathbf{A} \mathbf{S}_k \mathbf{B}^T$$



Not a tensor,  
but similar

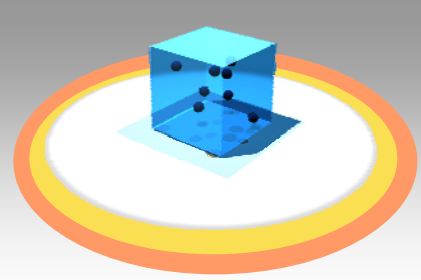
$$X_k = \mathbf{U}_k \mathbf{H} \mathbf{S}_k \mathbf{v}^T$$

orthonormal  
columns

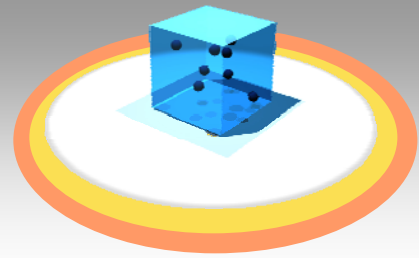
diagonal

used to enforce  
uniqueness

R. A. Harshman, *UCLA Working Papers in Phonetics*, 1972.

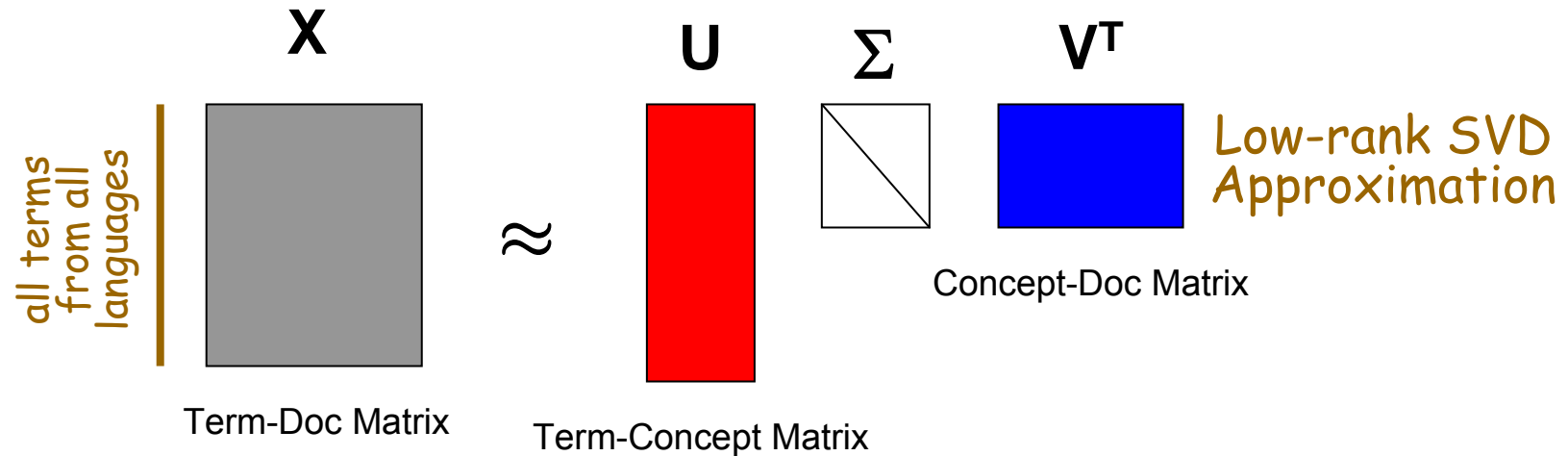


# **Application: Cross-Language Information Retrieval**



# Latent Semantic Indexing (LSI) in Multilingual Environment

Step 1: Compute SVD on Parallel Corpus for training. Each “document” consists of all its translations.



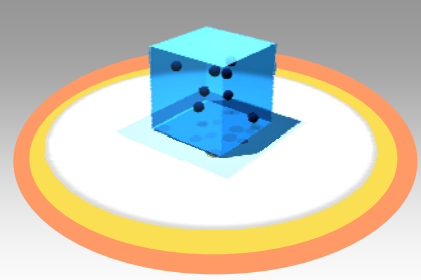
Step 2: Map test documents to concept space. Each document is only a single translation.

$$\hat{Y} = UY$$

Same U for all languages.

Goal

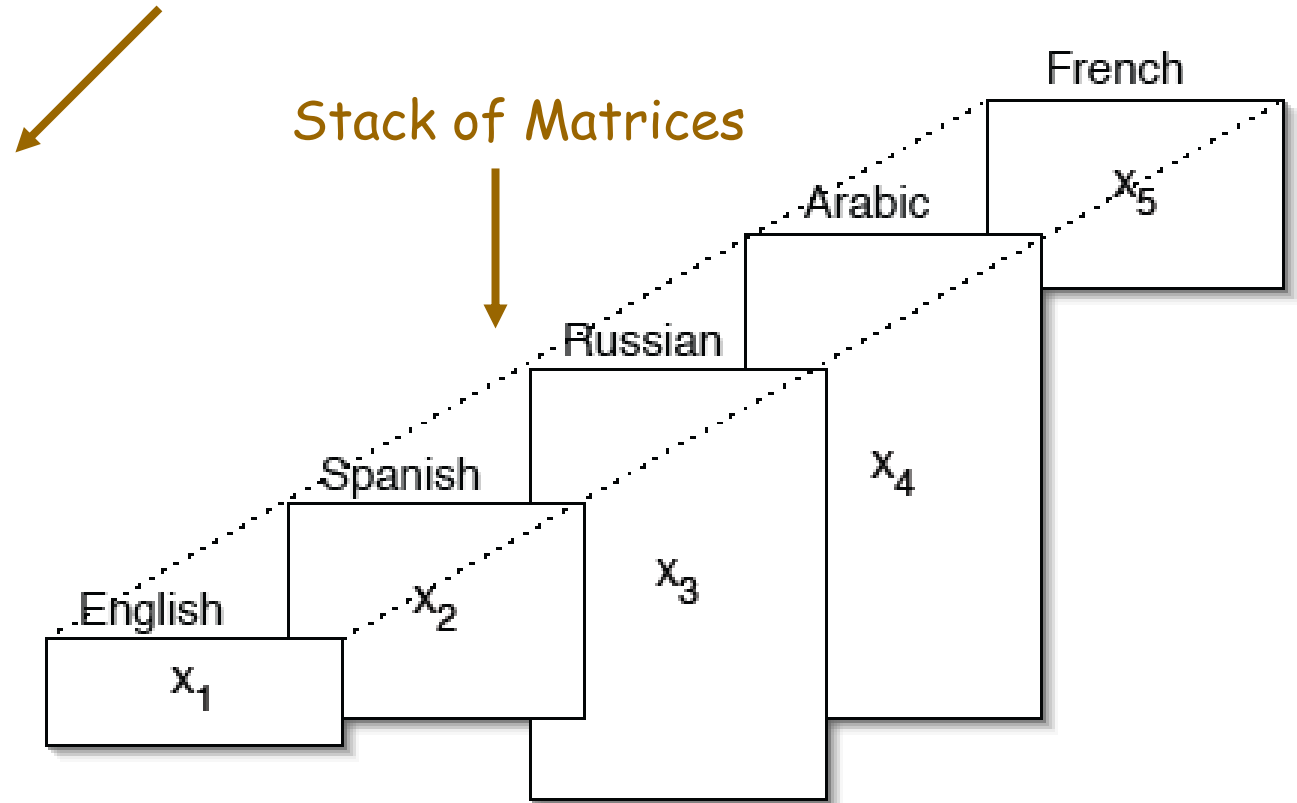
Different translations of the same document should be nearby in concept space.

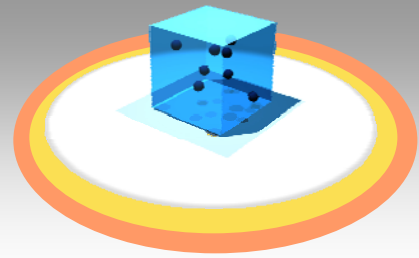


# A Different View

$x_1$
$x_2$
$x_3$
$x_4$
$x_5$

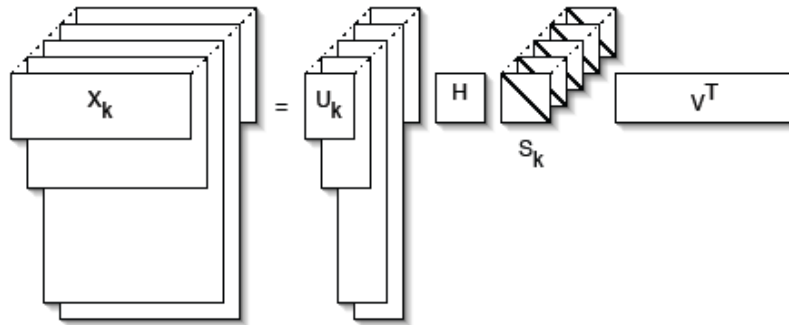
LSI Matrix (though terms are mixed)





# PARAFAC2 Model

Step 1: Compute **PARAFAC2** on Parallel Corpus for training. Each “document” consists of all its translations.

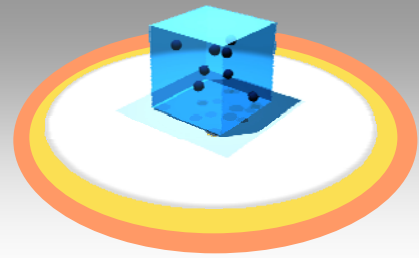


Step 2: Map test documents to concept space. Each document is only a single translation.

$$\hat{Y}_k = U_k Y_k$$

Minor  
Drawback

Need to know  
language of test  
document.



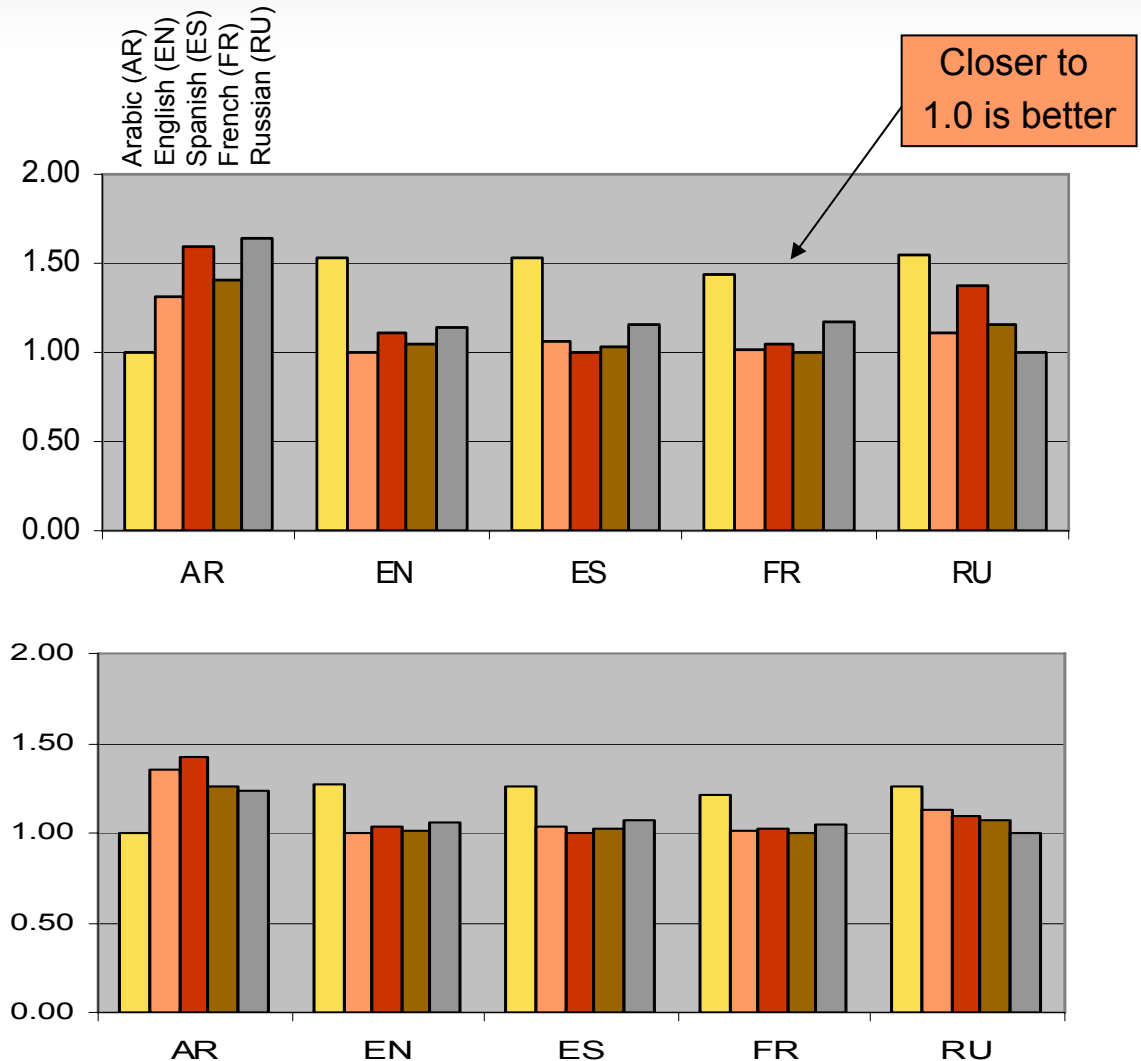
# Results Comparison

Trained on Bible.  
Tested on Quran.

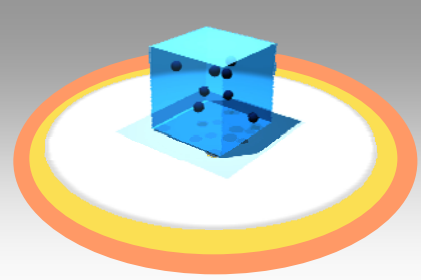
SVD  
Rank-300

For each document in each language on the vertical axis, we ranked documents in each of the other languages. The bar represents the average rank of the correct document. Rank 1 is ideal.

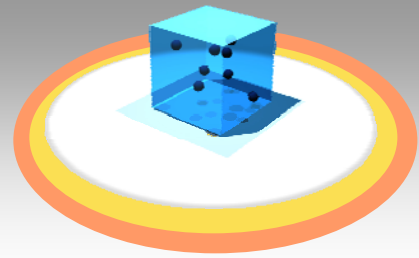
PARAFAC2  
Rank-240







# Software



# A Brief History of Tensors in MATLAB

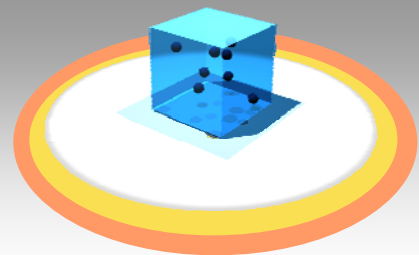
## Tensor Toolbox

for MATLAB™

- **MATLAB** (~1997)
  - Version 5.0 adds support for multidimensional arrays (MDAs)
- **N-way Toolbox** (<1997)
  - Extensive collection of functions and algorithms for analyzing multiway data
    - Handles constraints
    - Handles missing data
    - Etc.
  - Andersson & Bro, 2000

*Few tools exist in  
other languages.*

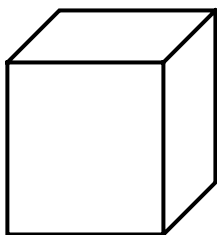
- **Tensor Toolbox V1** (2005)
  - MATLAB classes for dense tensors, etc.
  - Extends MDA capabilities to include multiplication, matricization, etc.
- **Tensor Toolbox V2** (2006)
  - Adds support for sparse and structured tensors
  - Performance enhancements
  - 1000+ registered users



# Tensor Toolbox V2.0

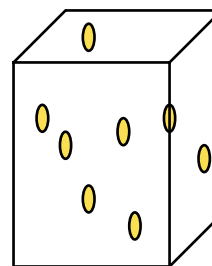
## supports 4 types of tensors

### Dense Tensors **tensor**



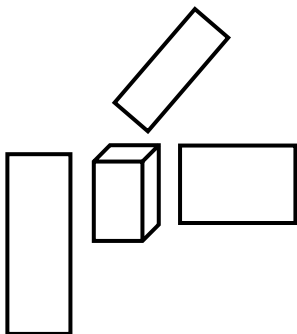
- Extends MATLAB's native MDA capabilities
- Can be converted to a matrix and vice versa

### Sparse Tensors **sptensor**



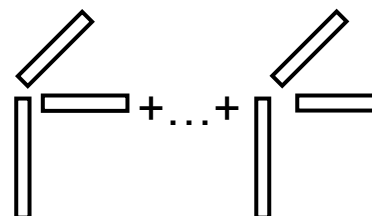
- Unique to Tensor Toolbox
- Can be converted to a (sparse) matrix and vice versa
- Effort to choose suitable representation
- Efficient functions for computation

### Tucker Tensors **ttensor**

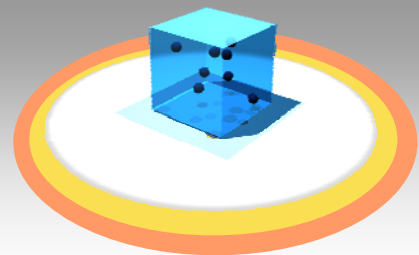


- Stores a tensor in decomposed form
- A different way to store a large-scale dense tensor
- Can do many operations in factored form

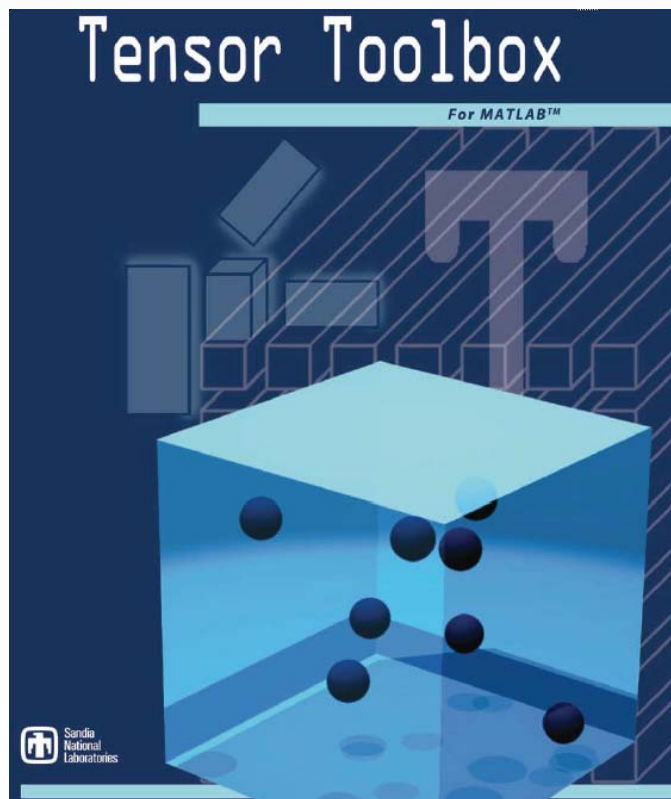
### Kruskal Tensors **ktensor**



- Stores a tensor as sum of rank-1 tensors
- A different way to store a large-scale dense tensor
- Can do many operations in factored form

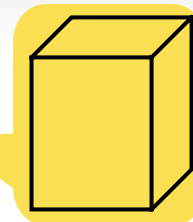


# Tensor Toolbox Classes

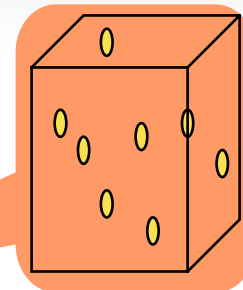


Available online.  
Free for research and  
evaluation purposes.

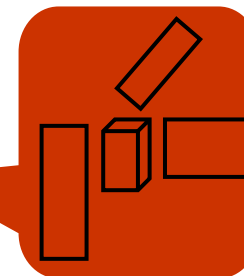
- **tensor**



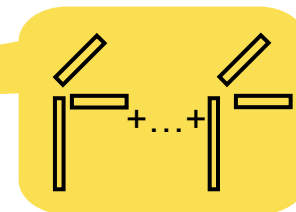
- **sptensor**



- **ttensor**

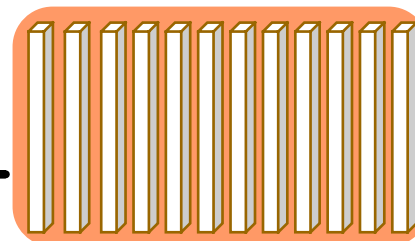
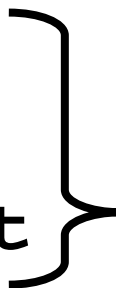


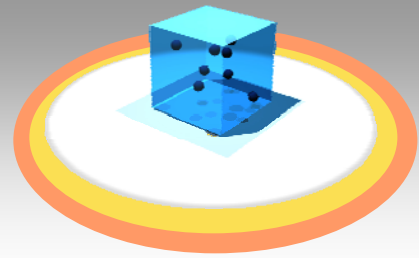
- **ktensor**



- **tenmat**

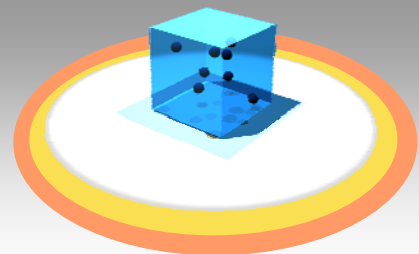
- **sptenmat**





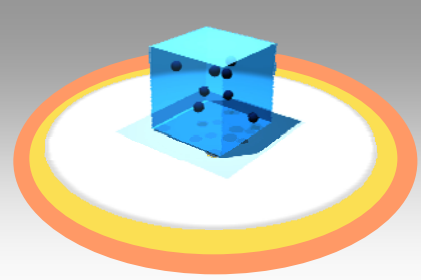
# Examples of Other Work on Data Mining with Tensors

- **Chatroom analysis** using Tucker and CP - Acar et al., 2005 & 2006
- **Handwritten digit analysis** - Elden and Savas, (check date)
- **Window-based tensor analysis (WTA)** on streaming data - Sun, Papadimitriou, and Yu, 2006
- **Dynamic tensor analysis (DTA)** - Sun, Tao, and Papadimitriou, 2006
- **Multi-way clustering on relational graphs** - Banerjee, Basu, and Merugu, 2007
- PARAFAC and NN-PARAFAC for **Enron email analysis** - Bader, Berry, Browne, 2007
- All of the above used the Tensor Toolbox, but there are many other papers in this area starting in 2005.
- Related applications date back much further: chemometrics, EEG analysis, signal processing, etc.



# Acknowledgements/References

- Survey papers on tensors
  - TGK and **Brett W. Bader**. **Tensor decompositions and applications**. Submitted, Aug 2007.
  - TGK. **Multilinear operators for higher-order decompositions**. Tech. Rep., Apr 2006.
- Tensor Toolbox
  - **Brett W. Bader** and TGK. **Efficient MATLAB computations with sparse and factored tensors**. *SIAM J. Scientific Computing*, to appear.
  - Brett W. Bader and TGK. **Algorithm 862: MATLAB tensor classes for fast algorithm prototyping**. *ACM Trans. Mathematical Software*, Dec 2006.
- TOPHITS
  - TGK, **Brett W. Bader**, and **Joseph P. Kenny**. **Higher-order web link analysis using multilinear algebra**. In *ICDM 2005*.
  - TGK and **Brett Bader**. **The TOPHITS model for higher-order web link analysis**. In *Workshop on Link Analysis, Counterterrorism and Security*, 2006.
- Cross-Language IR with PARAFAC2
  - **Peter A. Chew**, **Brett W. Bader**, TGK, and **Ahmed Abdelali**. **Cross-language information retrieval using PARAFAC2**. In *KDD '07*
- Tutorial
  - **Christos Faloutsos**, TGK, **Jimeng Sun**, **Mining Large Time-evolving Data Using Matrix and Tensor Tools** at SDM07, SIGMOD07, ICML07, KDD07.



**Thank you.  
Questions?**

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[tgkolda@sandia.gov](mailto:tgkolda@sandia.gov)