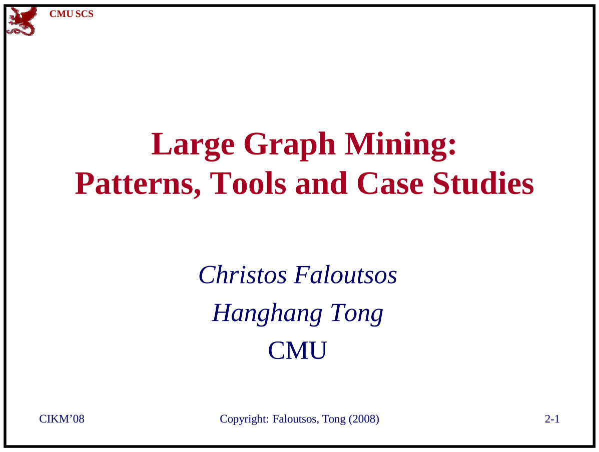

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# Large Graph Mining: Patterns, Tools and Case Studies

*Christos Faloutsos*

*Hanghang Tong*

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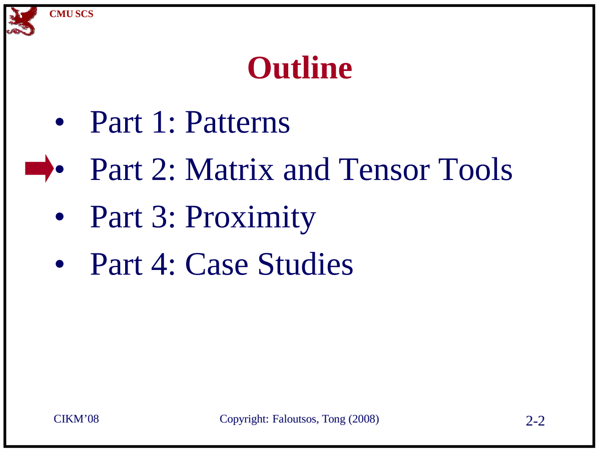

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## Outline

- Part 1: Patterns
- ➡ Part 2: Matrix and Tensor Tools
- Part 3: Proximity
- Part 4: Case Studies

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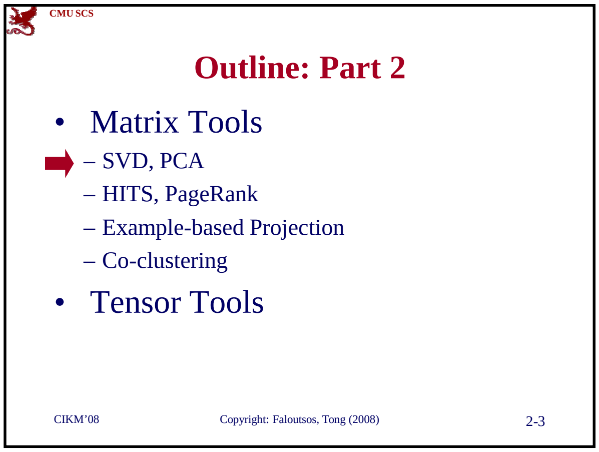

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## Outline: Part 2

- Matrix Tools
  - ➡ SVD, PCA
  - HITS, PageRank
  - Example-based Projection
  - Co-clustering
- Tensor Tools

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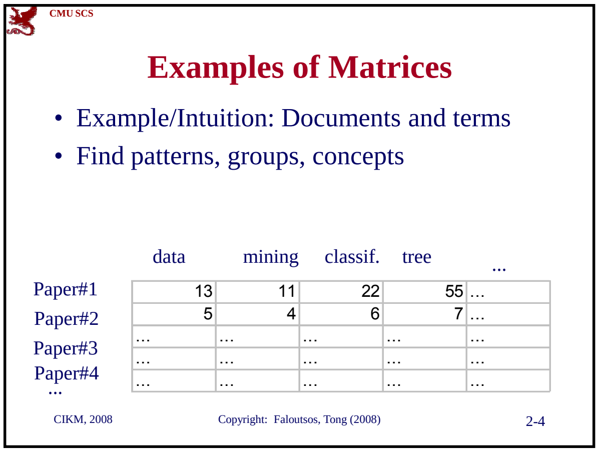

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## Examples of Matrices

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

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

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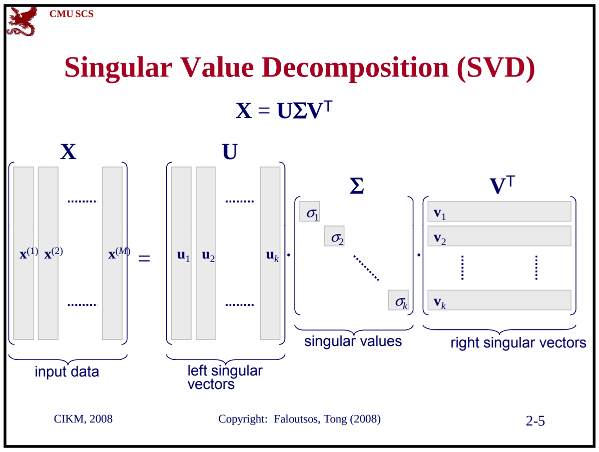

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## Singular Value Decomposition (SVD)

$$\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^{\mathrm{T}}$$

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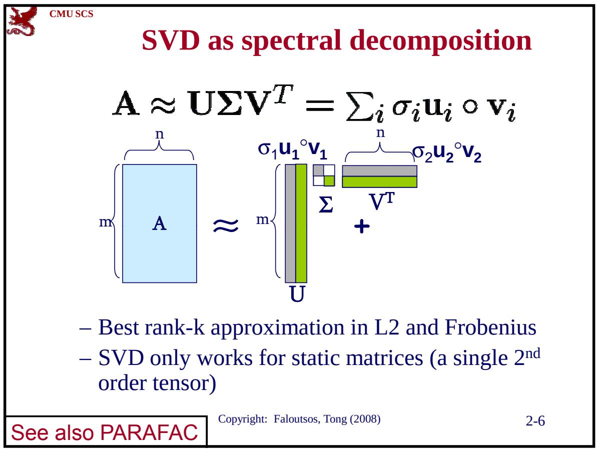

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## SVD as spectral decomposition

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

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

See also PARAFAC

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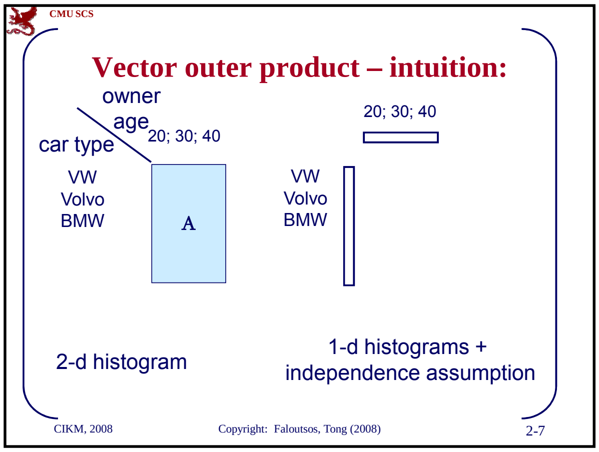

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## Vector outer product – intuition:

2-d histogram

1-d histograms + independence assumption

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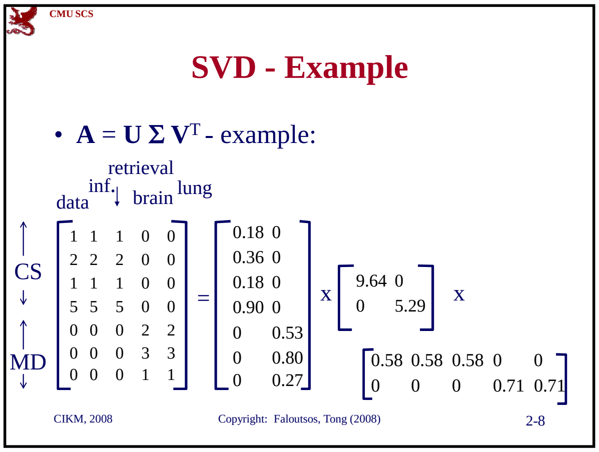

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## SVD - Example

- **A** = **U** **Σ** **V**$^T$ - example:

$$\begin{array}{cccccc} & \text{data} & \text{inf.} & \text{retrieval} & \text{brain} & \text{lung} \\ \text{CS} & 1 & 1 & 1 & 0 & 0 \\ & 2 & 2 & 2 & 0 & 0 \\ & 1 & 1 & 1 & 0 & 0 \\ & 5 & 5 & 5 & 0 & 0 \\ \text{MD} & 0 & 0 & 0 & 2 & 2 \\ & 0 & 0 & 0 & 3 & 3 \\ & 0 & 0 & 0 & 1 & 1 \end{array} = \begin{bmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.27 \end{bmatrix} \text{x} \begin{bmatrix} 9.64 & 0 \\ 0 & 5.29 \end{bmatrix} \text{x} \begin{bmatrix} 0.58 & 0.58 & 0.58 & 0 & 0 \\ 0 & 0 & 0 & 0.71 & 0.71 \end{bmatrix}$$

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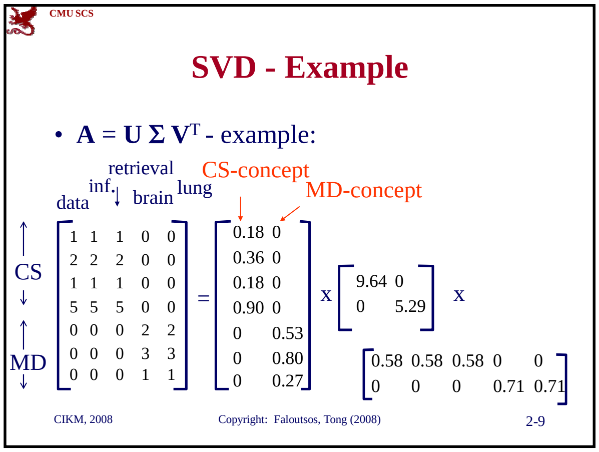

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## SVD - Example

- **A** = **U** **Σ** **V**$^T$ - example:

$$\begin{array}{cccccc} & \text{data} & \text{inf.} & \text{retrieval} & \text{brain} & \text{lung} \\ \text{CS} & 1 & 1 & 1 & 0 & 0 \\ & 2 & 2 & 2 & 0 & 0 \\ & 1 & 1 & 1 & 0 & 0 \\ & 5 & 5 & 5 & 0 & 0 \\ \text{MD} & 0 & 0 & 0 & 2 & 2 \\ & 0 & 0 & 0 & 3 & 3 \\ & 0 & 0 & 0 & 1 & 1 \end{array} = \begin{bmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.27 \end{bmatrix} \text{x} \begin{bmatrix} 9.64 & 0 \\ 0 & 5.29 \end{bmatrix} \text{x} \begin{bmatrix} 0.58 & 0.58 & 0.58 & 0 & 0 \\ 0 & 0 & 0 & 0.71 & 0.71 \end{bmatrix}$$

CS-concept

MD-concept

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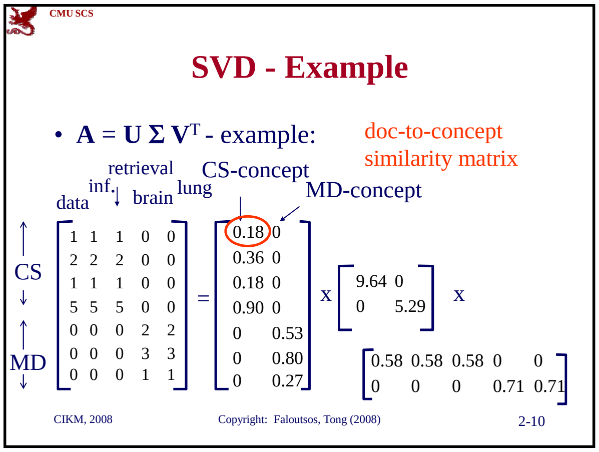

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## SVD - Example

- **A** = **U** **Σ** **V**$^T$ - example:

doc-to-concept similarity matrix

$$\begin{array}{cccccc} & \text{data} & \text{inf.} & \text{retrieval} & \text{brain} & \text{lung} \\ \text{CS} & 1 & 1 & 1 & 0 & 0 \\ & 2 & 2 & 2 & 0 & 0 \\ & 1 & 1 & 1 & 0 & 0 \\ & 5 & 5 & 5 & 0 & 0 \\ \text{MD} & 0 & 0 & 0 & 2 & 2 \\ & 0 & 0 & 0 & 3 & 3 \\ & 0 & 0 & 0 & 1 & 1 \end{array} = \begin{bmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.27 \end{bmatrix} \text{x} \begin{bmatrix} 9.64 & 0 \\ 0 & 5.29 \end{bmatrix} \text{x} \begin{bmatrix} 0.58 & 0.58 & 0.58 & 0 & 0 \\ 0 & 0 & 0 & 0.71 & 0.71 \end{bmatrix}$$

CS-concept

MD-concept

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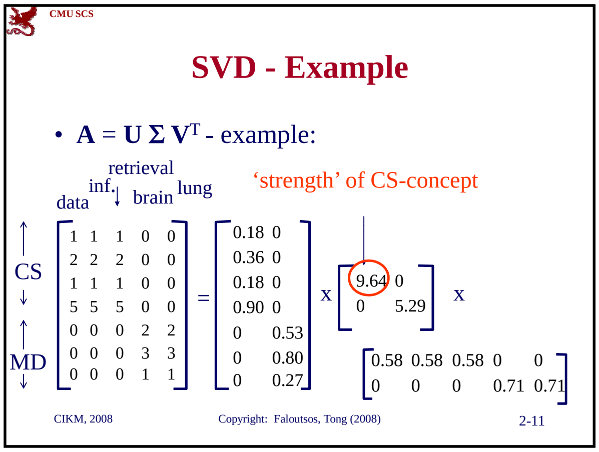

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## SVD - Example

- **A** = **U** **Σ** **V**$^T$ - example:

'strength' of CS-concept

$$\begin{array}{cccccc} & \text{data} & \text{inf.} & \text{retrieval} & \text{brain} & \text{lung} \\ \text{CS} & 1 & 1 & 1 & 0 & 0 \\ & 2 & 2 & 2 & 0 & 0 \\ & 1 & 1 & 1 & 0 & 0 \\ & 5 & 5 & 5 & 0 & 0 \\ \text{MD} & 0 & 0 & 0 & 2 & 2 \\ & 0 & 0 & 0 & 3 & 3 \\ & 0 & 0 & 0 & 1 & 1 \end{array} = \begin{bmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.27 \end{bmatrix} \text{x} \begin{bmatrix} 9.64 & 0 \\ 0 & 5.29 \end{bmatrix} \text{x} \begin{bmatrix} 0.58 & 0.58 & 0.58 & 0 & 0 \\ 0 & 0 & 0 & 0.71 & 0.71 \end{bmatrix}$$

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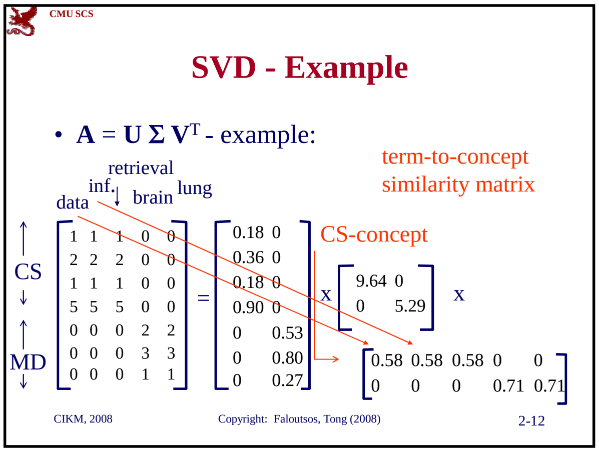

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## SVD - Example

- **A** = **U** **Σ** **V**$^T$ - example:

term-to-concept similarity matrix

$$\begin{array}{cccccc} & \text{data} & \text{inf.} & \text{retrieval} & \text{brain} & \text{lung} \\ \text{CS} & 1 & 1 & 1 & 0 & 0 \\ & 2 & 2 & 2 & 0 & 0 \\ & 1 & 1 & 1 & 0 & 0 \\ & 5 & 5 & 5 & 0 & 0 \\ \text{MD} & 0 & 0 & 0 & 2 & 2 \\ & 0 & 0 & 0 & 3 & 3 \\ & 0 & 0 & 0 & 1 & 1 \end{array} = \begin{bmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.27 \end{bmatrix} \text{x} \begin{bmatrix} 9.64 & 0 \\ 0 & 5.29 \end{bmatrix} \text{x} \begin{bmatrix} 0.58 & 0.58 & 0.58 & 0 & 0 \\ 0 & 0 & 0 & 0.71 & 0.71 \end{bmatrix}$$

CS-concept

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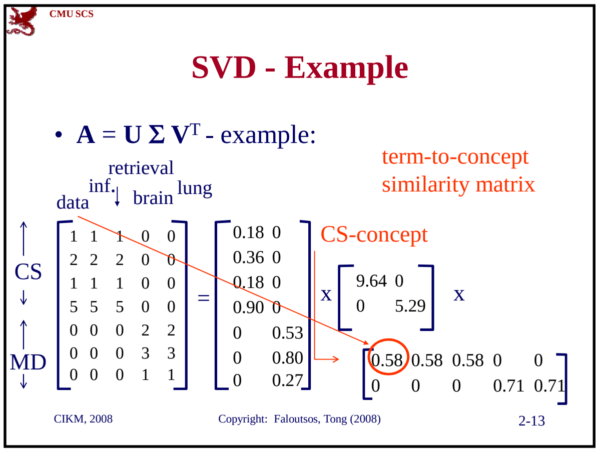

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## SVD - Example

- $\mathbf{A} = \mathbf{U}\,\boldsymbol{\Sigma}\,\mathbf{V}^T$ - example:

term-to-concept similarity matrix

CS-concept

$$\begin{array}{c|ccccc} & \text{data} & \text{inf.} & \text{retrieval} & \text{brain} & \text{lung} \\ \hline \text{CS} & 1 & 1 & 1 & 0 & 0 \\ & 2 & 2 & 2 & 0 & 0 \\ & 1 & 1 & 1 & 0 & 0 \\ & 5 & 5 & 5 & 0 & 0 \\ \text{MD} & 0 & 0 & 0 & 2 & 2 \\ & 0 & 0 & 0 & 3 & 3 \\ & 0 & 0 & 0 & 1 & 1 \end{array} = \begin{bmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.27 \end{bmatrix} \times \begin{bmatrix} 9.64 & 0 \\ 0 & 5.29 \end{bmatrix} \times \begin{bmatrix} 0.58 & 0.58 & 0.58 & 0 & 0 \\ 0 & 0 & 0 & 0.71 & 0.71 \end{bmatrix}$$

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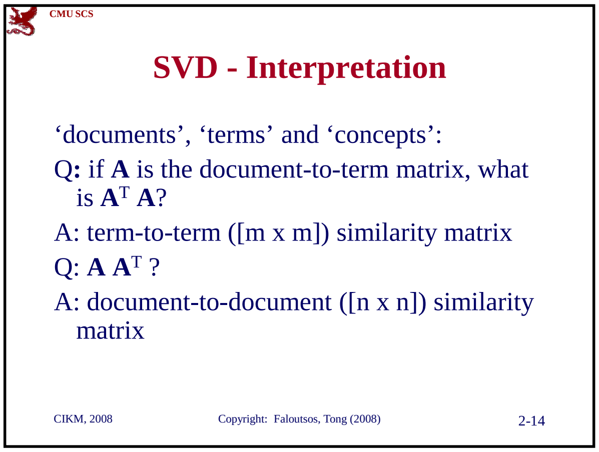

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## SVD - Interpretation

'documents', 'terms' and 'concepts':

Q: if **A** is the document-to-term matrix, what is $\mathbf{A}^T\,\mathbf{A}$?

A: term-to-term ([m x m]) similarity matrix

Q: $\mathbf{A}\,\mathbf{A}^T$ ?

A: document-to-document ([n x n]) similarity matrix

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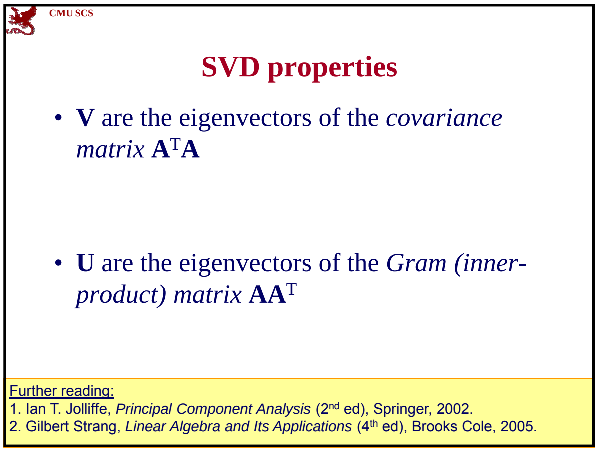

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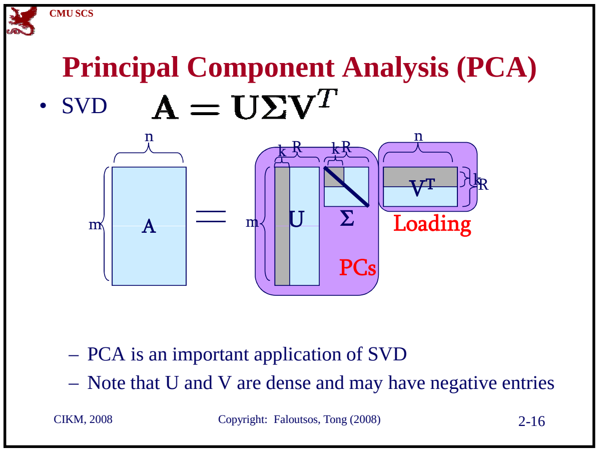
## SVD properties

- **V** are the eigenvectors of the *covariance matrix* $\mathbf{A}^T\mathbf{A}$
- **U** are the eigenvectors of the *Gram (inner-product) matrix* $\mathbf{A}\mathbf{A}^T$

Further reading:
1. Ian T. Jolliffe, *Principal Component Analysis* (2nd ed), Springer, 2002.
2. Gilbert Strang, *Linear Algebra and Its Applications* (4th ed), Brooks Cole, 2005.



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## Principal Component Analysis (PCA)

- SVD $\mathbf{A} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$

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

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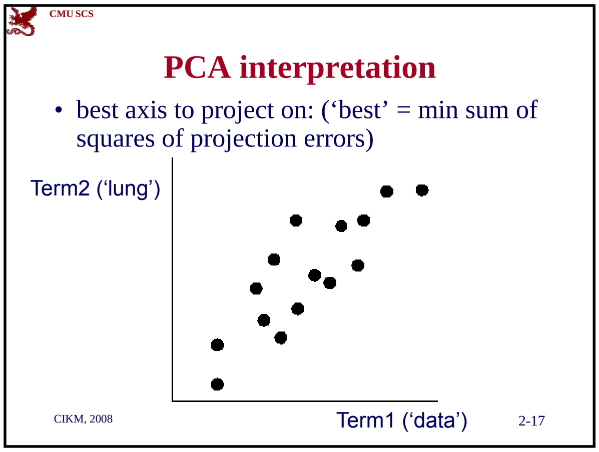

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## PCA interpretation

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

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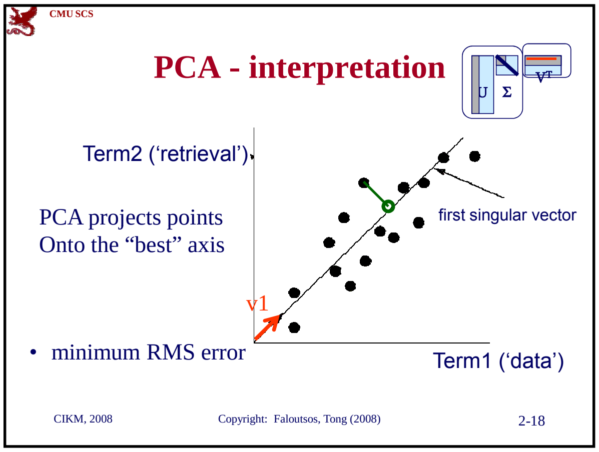

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## PCA - interpretation

PCA projects points Onto the "best" axis

- minimum RMS error

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## Outline: Part 2

- Matrix Tools
  - – SVD, PCA
  - ➡ – HITS, PageRank
  - – Example-based Projection
  - – Co-clustering
- Tensor Tools

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## Kleinberg's algorithm HITS

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

Step 0: find all pages containing the query terms

Step 1: expand by one move forward and backward

Further reading:

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

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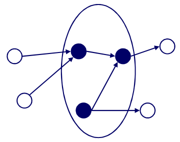
## Kleinberg's algorithm HITS

- Step 1: expand by one move forward and backward



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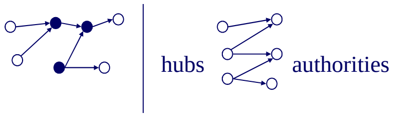
## Kleinberg's algorithm HITS

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



hubs authorities

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## Kleinberg's algorithm HITS

observations

- recursive definition!
- each node (say, '$i$'-th node) has both an authoritativeness score $a_i$ and a hubness score $h_i$

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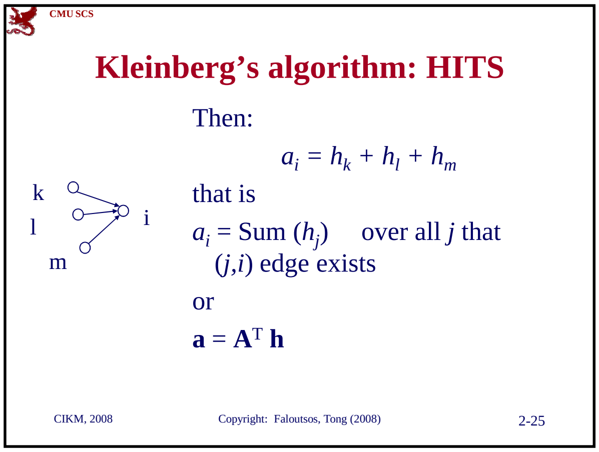
## Kleinberg's algorithm: HITS

Let **A** be the adjacency matrix:

the ($i$,$j$) entry is 1 if the edge from $i$ to $j$ exists

Let **h** and **a** be [n x 1] vectors with the 'hubness' and 'authoritativiness' scores.

Then:



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## Kleinberg's algorithm: HITS

Then:

$$a_i = h_k + h_l + h_m$$

that is

$a_i$ = Sum ($h_j$) over all $j$ that ($j$,$i$) edge exists

or

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

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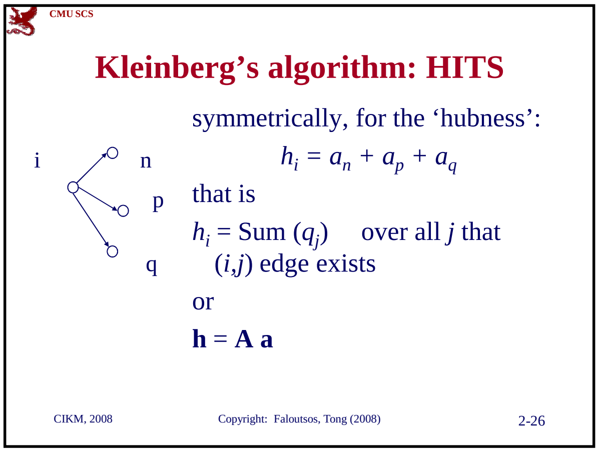

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## Kleinberg's algorithm: HITS

symmetrically, for the 'hubness':

$$h_i = a_n + a_p + a_q$$

that is

$h_i$ = Sum ($q_j$) over all $j$ that ($i$,$j$) edge exists

or

$\mathbf{h} = \mathbf{A}\ \mathbf{a}$

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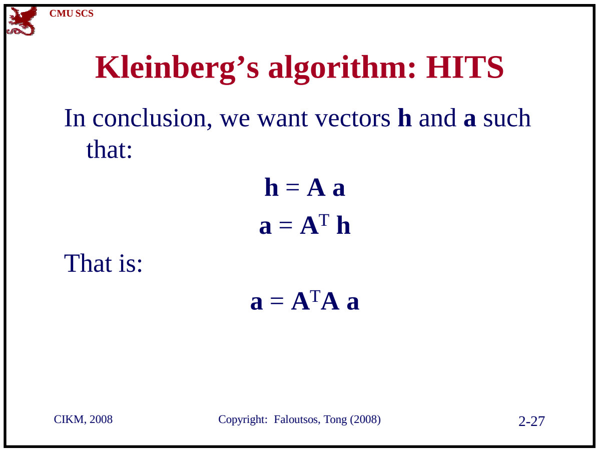

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## Kleinberg's algorithm: HITS

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

$$\mathbf{h} = \mathbf{A}\ \mathbf{a}$$

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

That is:

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

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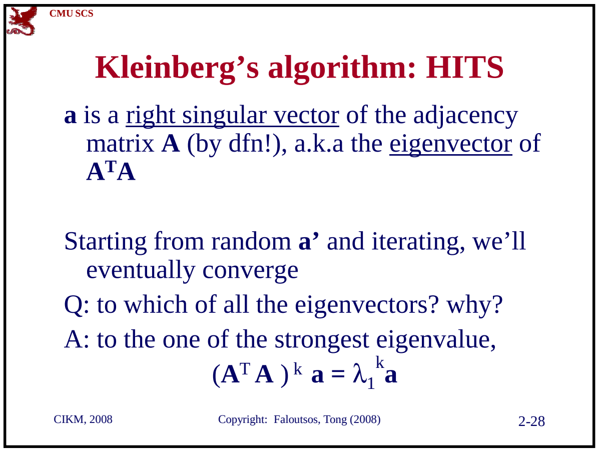

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## Kleinberg's algorithm: HITS

**a** is a right singular vector of the adjacency matrix **A** (by dfn!), a.k.a the eigenvector of $\mathbf{A}^T\mathbf{A}$

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

Q: to which of all the eigenvectors? why?

A: to the one of the strongest eigenvalue,

$$(\mathbf{A}^T \mathbf{A})^k\ \mathbf{a} = \lambda_1^{\ k} \mathbf{a}$$

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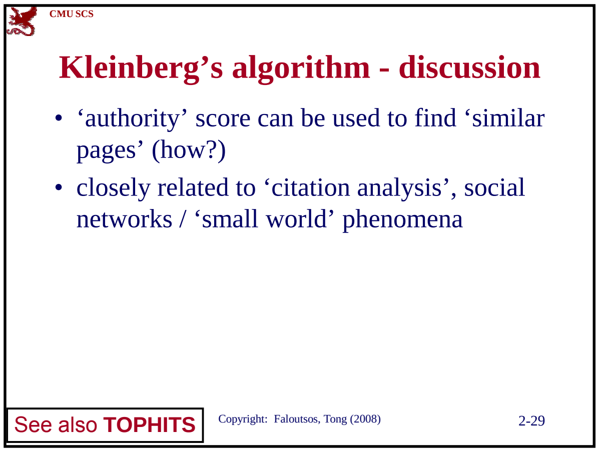

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## Kleinberg's algorithm - discussion

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

See also TOPHITS

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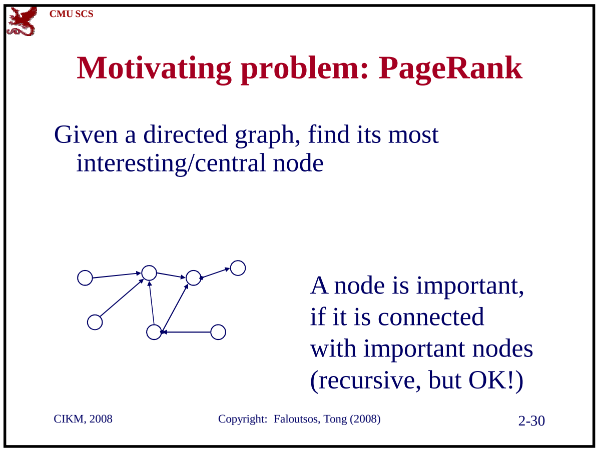

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## Motivating problem: PageRank

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

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

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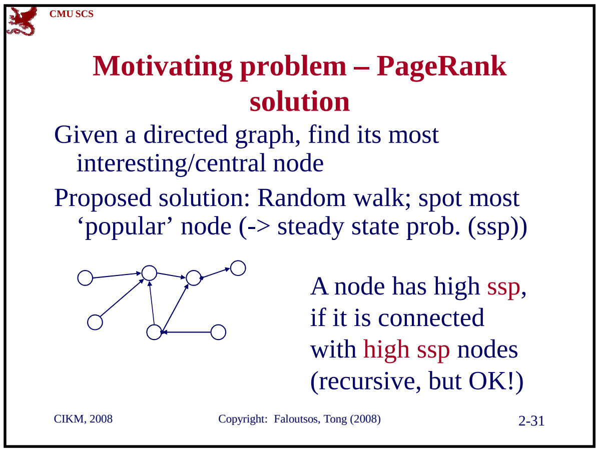
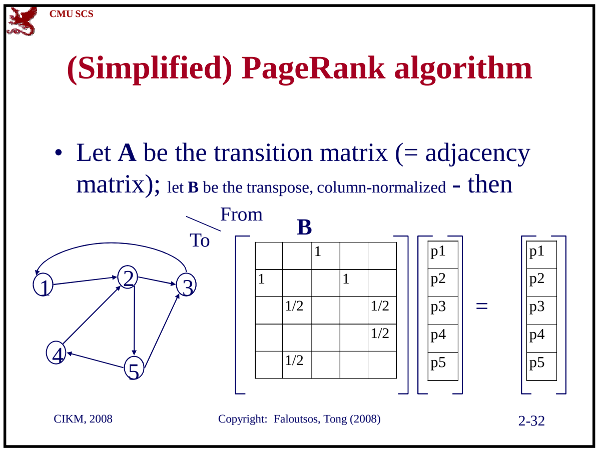


## Motivating problem – PageRank solution

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

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

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

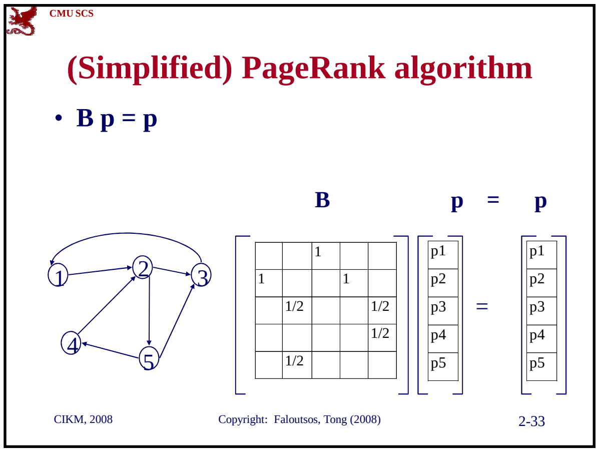


## (Simplified) PageRank algorithm

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

**B**

$$\begin{array}{c|ccccc} \text{To} \backslash \text{From} & & & & & \\ \hline & & & 1 & & \\ & 1 & & & 1 & \\ & & 1/2 & & & 1/2 \\ & & & & & 1/2 \\ & & 1/2 & & & \end{array} \begin{bmatrix} p1 \\ p2 \\ p3 \\ p4 \\ p5 \end{bmatrix} = \begin{bmatrix} p1 \\ p2 \\ p3 \\ p4 \\ p5 \end{bmatrix}$$

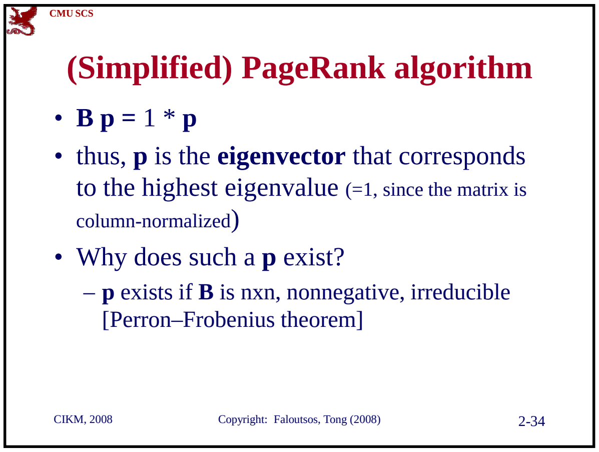


## (Simplified) PageRank algorithm

- **B p = p**

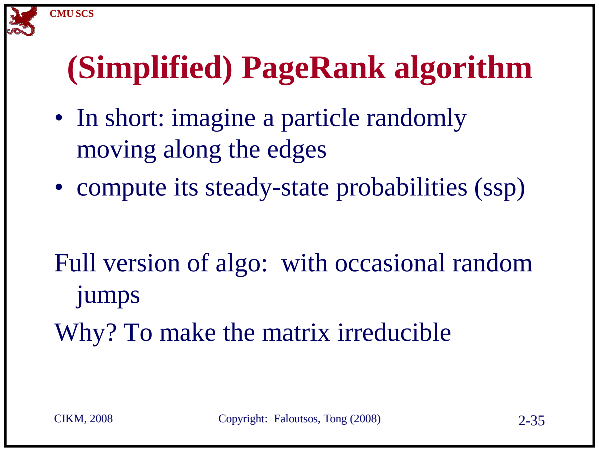
**B** **p** = **p**

$$\begin{bmatrix} & & 1 & & \\ 1 & & & 1 & \\ & 1/2 & & & 1/2 \\ & & & & 1/2 \\ & 1/2 & & & \end{bmatrix} \begin{bmatrix} p1 \\ p2 \\ p3 \\ p4 \\ p5 \end{bmatrix} = \begin{bmatrix} p1 \\ p2 \\ p3 \\ p4 \\ p5 \end{bmatrix}$$



## (Simplified) PageRank algorithm

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

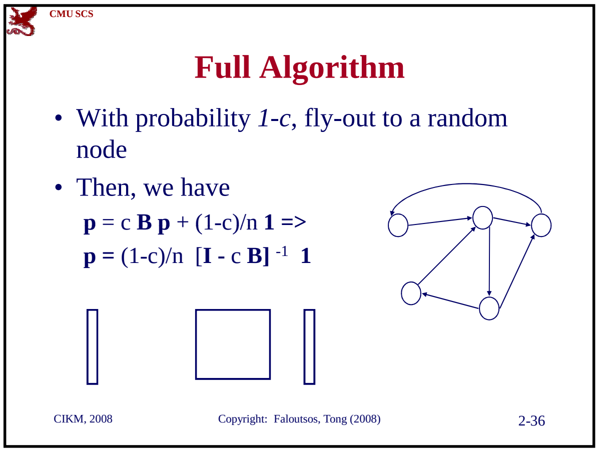


## (Simplified) PageRank algorithm

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

Full version of algo: with occasional random jumps

Why? To make the matrix irreducible



## Full Algorithm

- With probability *1-c*, fly-out to a random node
- Then, we have

$\mathbf{p}$ = c $\mathbf{B}\,\mathbf{p}$ + (1-c)/n $\mathbf{1}$ =>

$\mathbf{p}$ = (1-c)/n $[\mathbf{I} - c\,\mathbf{B}]^{-1}$ $\mathbf{1}$

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## Outline: Part 2

- Matrix Tools
  - – SVD, PCA
  - – HITS, PageRank
  - ➡ – Example-based Projection
  - – Co-clustering
- Tensor Tools

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## Motivation

(Example-Based Low-Rank Approximation (LRA))

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

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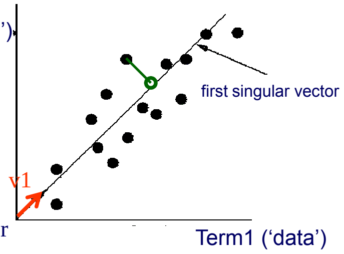
## PCA - interpretation



PCA projects points Onto the "best" axis

- minimum RMS error

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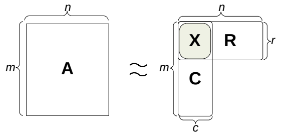
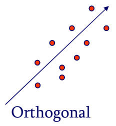
## CUR

- Example-based projection: use actual rows and columns to specify the subspace
- Given a matrix $A \in R^{m \times n}$, find three matrices $C \in R^{m \times c}$, $U \in R^{c \times r}$, $R \in R^{r \times n}$, such that $\|A-CUR\|$ is small



U is the pseudo-inverse of X



Orthogonal projection

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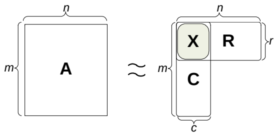
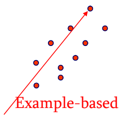
## CUR

- Example-based projection: use actual rows and columns to specify the subspace
- Given a matrix $A \in R^{m \times n}$, find three matrices $C \in R^{m \times c}$, $U \in R^{c \times r}$, $R \in R^{r \times n}$, such that $\|A-CUR\|$ is small





Example-based

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

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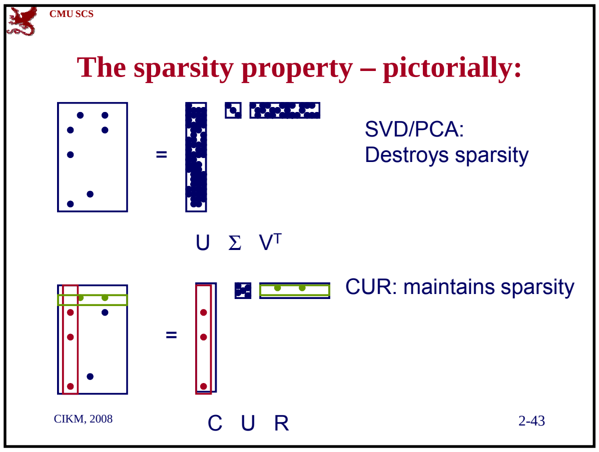
## CUR (cont.)

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

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



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## The sparsity property – pictorially:

SVD/PCA:
Destroys sparsity

CUR: maintains sparsity

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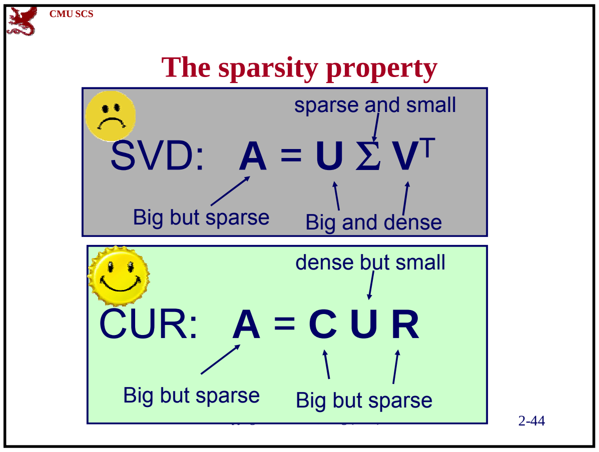

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## The sparsity property

SVD: **A = U Σ V$^T$**

sparse and small

Big but sparse

Big and dense

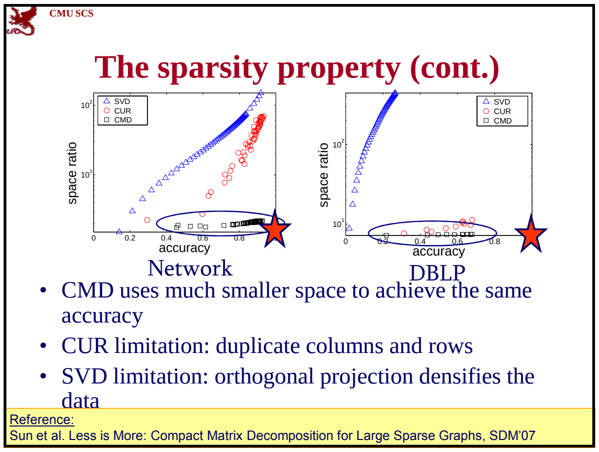
CUR: **A = C U R**

dense but small

Big but sparse

Big but sparse

2-44



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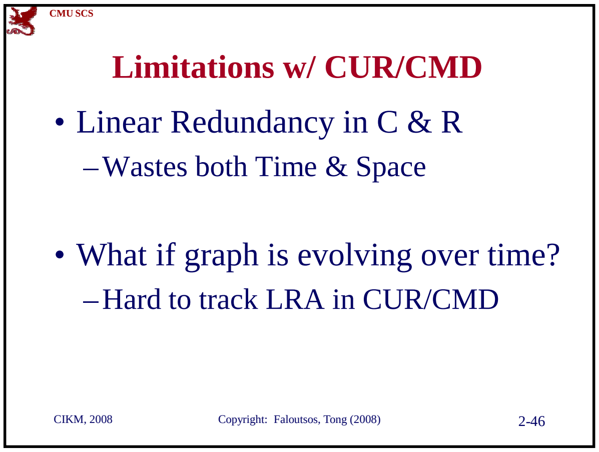
## The sparsity property (cont.)

Network

DBLP

- CMD uses much smaller space to achieve the same accuracy
- CUR limitation: duplicate columns and rows
- SVD limitation: orthogonal projection densifies the data

Reference:
Sun et al. Less is More: Compact Matrix Decomposition for Large Sparse Graphs, SDM'07



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## Limitations w/ CUR/CMD

- Linear Redundancy in C & R
  - Wastes both Time & Space
- What if graph is evolving over time?
  - Hard to track LRA in CUR/CMD

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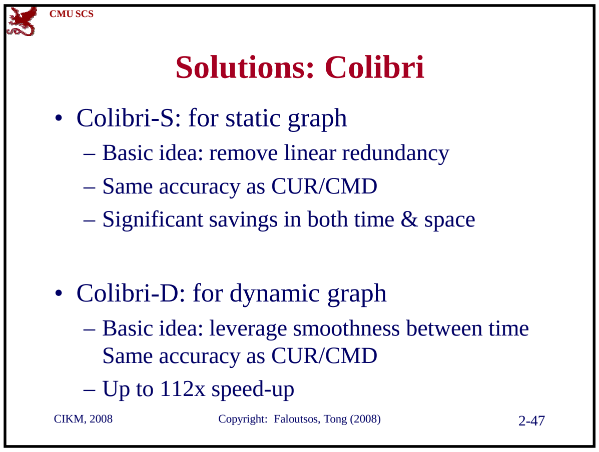

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## Solutions: Colibri

- Colibri-S: for static graph
  - Basic idea: remove linear redundancy
  - Same accuracy as CUR/CMD
  - Significant savings in both time & space
- Colibri-D: for dynamic graph
  - Basic idea: leverage smoothness between time Same accuracy as CUR/CMD
  - Up to 112x speed-up

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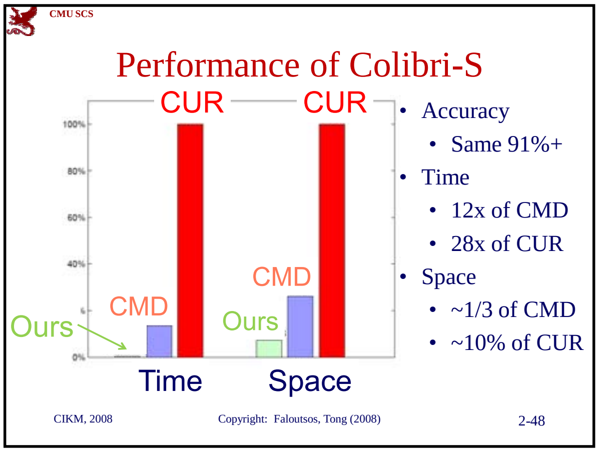

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## Performance of Colibri-S

- Accuracy
  - Same 91%+
- Time
  - 12x of CMD
  - 28x of CUR
- Space
  - ~1/3 of CMD
  - ~10% of CUR

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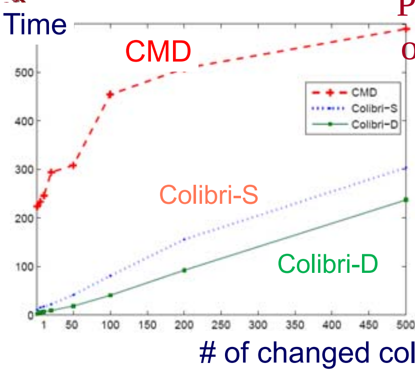
## Performance of Colibri-D



Colibri-D achieves up to 112x speedups

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## Outline: Part 2

- Matrix Tools
  - SVD, PCA
  - HITS, PageRank
  - Example-based Projection
  - ➡ Co-clustering
- Tensor Tools

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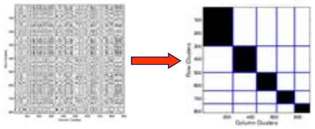
## Co-clustering

- Given data matrix and the number of row and column groups $k$ and $l$
- Simultaneously
  - Cluster rows of $p(X, Y)$ into $k$ disjoint groups
  - Cluster columns of $p(X, Y)$ into $l$ disjoint groups



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## Co-clustering

- Let $X$ and $Y$ be discrete random variables
  - $X$ and $Y$ take values in $\{1, 2, \ldots, m\}$ and $\{1, 2, \ldots, n\}$
  - $p(X, Y)$ denotes the joint probability distribution—if not known, it is often estimated based on co-occurrence data
  - Application areas: text mining, market-basket analysis, analysis of browsing behavior, etc.
- Key Obstacles in Clustering Contingency Tables
  - High Dimensionality, Sparsity, Noise
  - Need for robust and scalable algorithms

Reference:
1. Dhillon et al. Information-Theoretic Co-clustering, KDD'03

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$$\begin{array}{cc} & n \\ m & \begin{bmatrix} .05&.05&.05&0&0&0\\ .05&.05&.05&0&0&0\\ 0&0&0&.05&.05&.05\\ 0&0&0&.05&.05&.05\\ .04&.04&0&.04&.04&.04\\ .04&.04&.04&0&.04&.04 \end{bmatrix} \end{array}$$

eg, terms x documents

$$\begin{array}{cc} & k \\ m & \begin{bmatrix} .5&0&0\\ .5&0&0\\ 0&.5&0\\ 0&.5&0\\ 0&0&.5\\ 0&0&.5 \end{bmatrix} \end{array} \begin{array}{cc} & l \\ k & \begin{bmatrix} .3&0\\ 0&.3\\ .2&.2 \end{bmatrix} \end{array} \begin{array}{cc} & n \\ l & \begin{bmatrix} .36&.36&.28&0&0&0\\ 0&0&0&.28&.36&.36 \end{bmatrix} \end{array} = \left[\begin{array}{ccc|ccc} .054&.054&.042&0&0&0\\ .054&.054&.042&0&0&0\\ \hline 0&0&0&.042&.054&.054\\ 0&0&0&.042&.054&.054\\ \hline .036&.036&028&.028&.036&.036\\ .036&.036&.028&.028&.036&.036 \end{array}\right]$$

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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

$$\begin{bmatrix} .5&0&0\\ .5&0&0\\ 0&.5&0\\ 0&.5&0\\ 0&0&.5\\ 0&0&.5 \end{bmatrix} \begin{bmatrix} .3&0\\ 0&.3\\ .2&.2 \end{bmatrix} \begin{bmatrix} .36&.36&.28&0&0&0\\ 0&0&0&.28&.36&.36 \end{bmatrix} = \left[\begin{array}{ccc|ccc} .054&.054&.042&0&0&0\\ .054&.054&.042&0&0&0\\ \hline 0&0&0&.042&.054&.054\\ 0&0&0&.042&.054&.054\\ \hline .036&.036&028&.028&.036&.036\\ .036&.036&.028&.028&.036&.036 \end{array}\right]$$

doc x doc group

term x term-group

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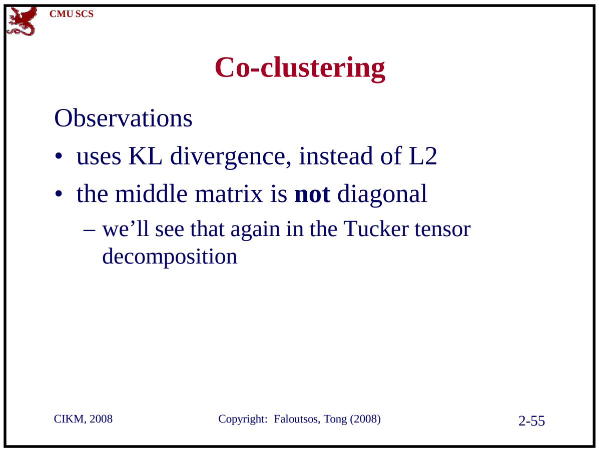

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## Co-clustering

Observations

- uses KL divergence, instead of L2
- the middle matrix is **not** diagonal
  - we'll see that again in the Tucker tensor decomposition

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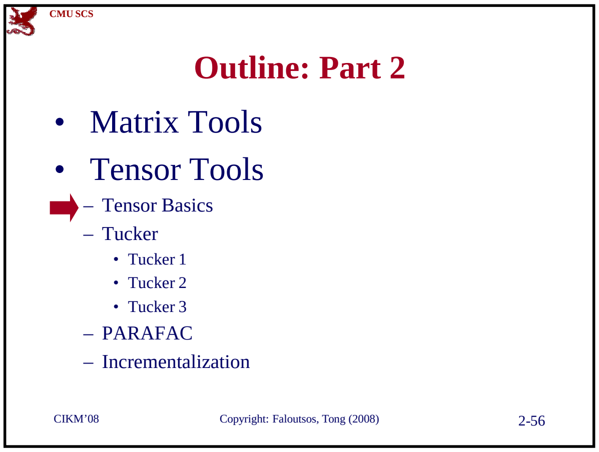

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## Outline: Part 2

- Matrix Tools
- Tensor Tools
  - Tensor Basics
  - Tucker
    - Tucker 1
    - Tucker 2
    - Tucker 3
  - PARAFAC
  - Incrementalization

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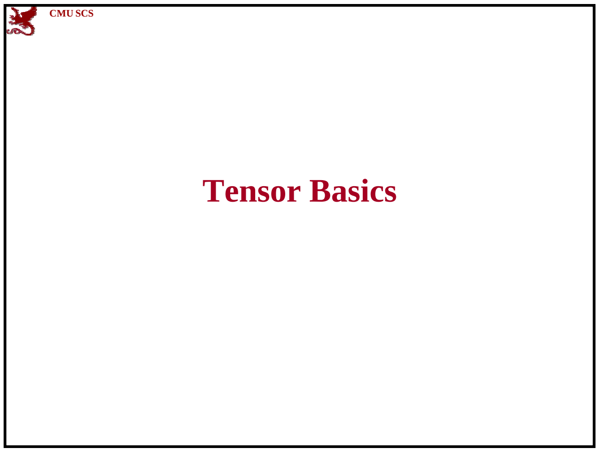

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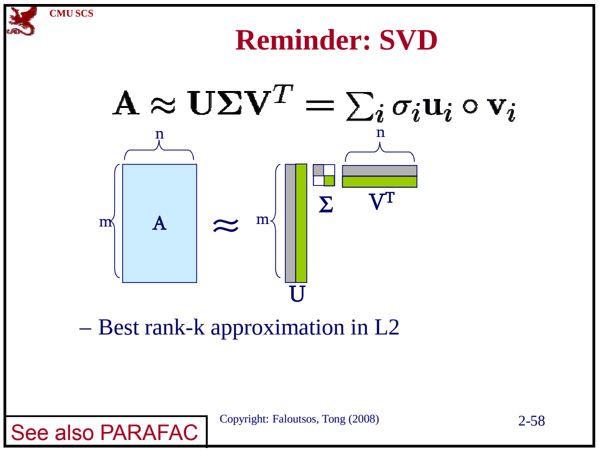
## Tensor Basics



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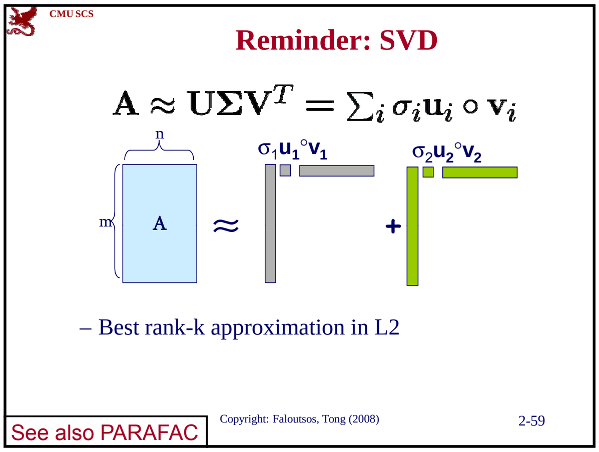
## Reminder: SVD

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

- Best rank-k approximation in L2

See also PARAFAC Copyright: Faloutsos, Tong (2008) 2-58



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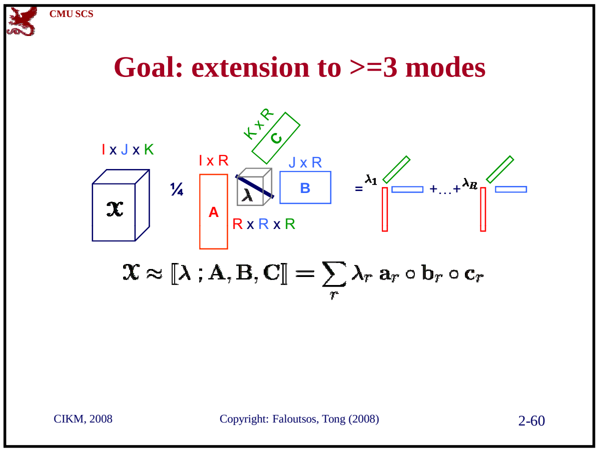
## Reminder: SVD

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

- Best rank-k approximation in L2

See also PARAFAC Copyright: Faloutsos, Tong (2008) 2-59



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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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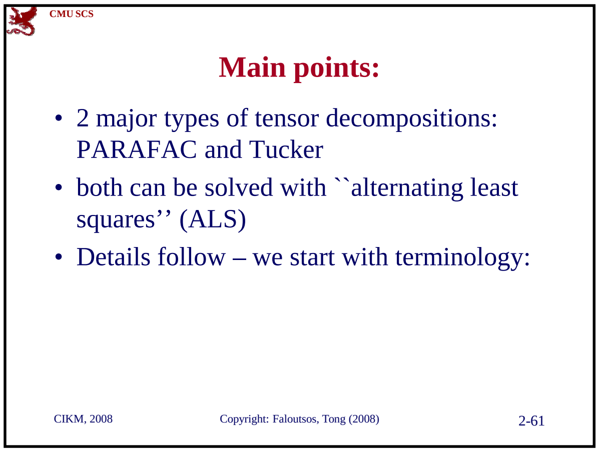

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## Main points:

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

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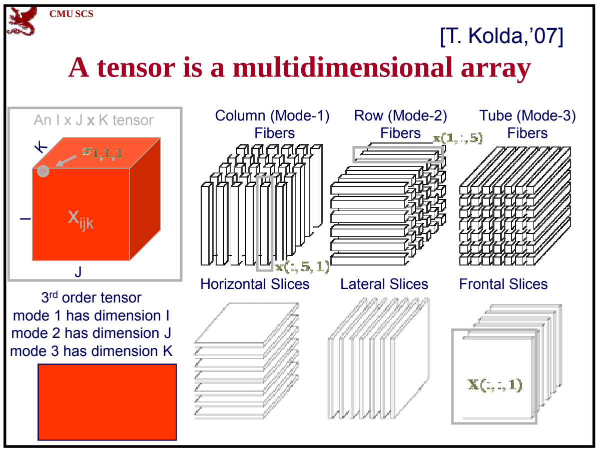

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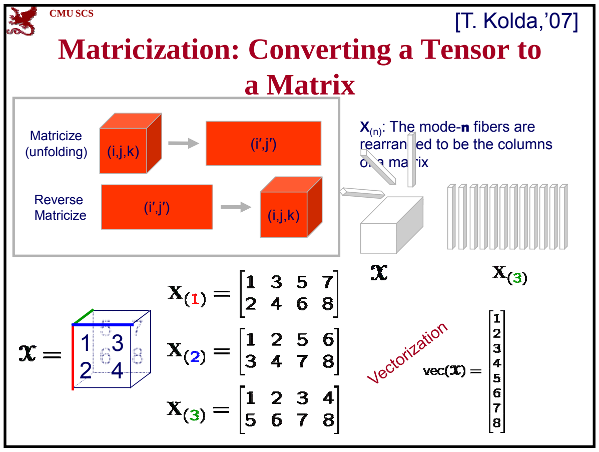
[T. Kolda,'07]

## A tensor is a multidimensional array

3rd order tensor
mode 1 has dimension I
mode 2 has dimension J
mode 3 has dimension K



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[T. Kolda,'07]

## Matricization: Converting a Tensor to a Matrix

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

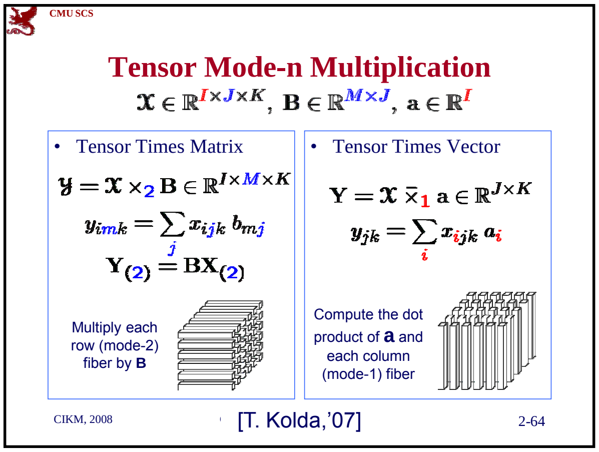
$$\mathcal{X} = $$

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

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

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

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



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## 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 row (mode-2) fiber by **B**

- Tensor Times Vector

$$\mathbf{Y} = \mathcal{X} \ \bar{\times}_1 \ \mathbf{a} \in \mathbb{R}^{J \times K}$$

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

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

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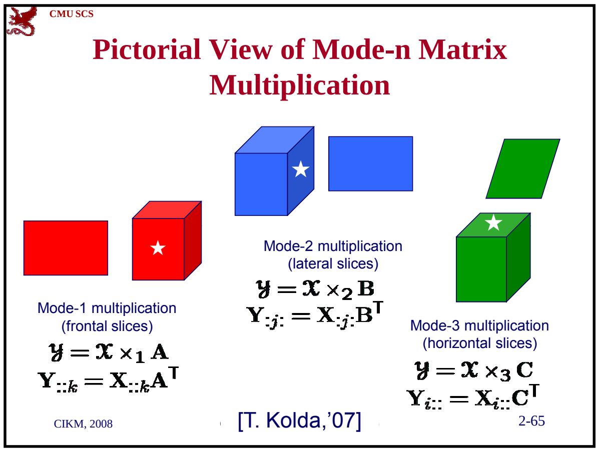

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## Pictorial View of Mode-n Matrix Multiplication

Mode-1 multiplication (frontal slices)

$$\mathcal{Y} = \mathcal{X} \times_1 \mathbf{A}$$

$$\mathbf{Y}_{::k} = \mathbf{X}_{::k}\mathbf{A}^{\mathsf{T}}$$

Mode-2 multiplication (lateral slices)

$$\mathcal{Y} = \mathcal{X} \times_2 \mathbf{B}$$

$$\mathbf{Y}_{:j:} = \mathbf{X}_{:j:}\mathbf{B}^{\mathsf{T}}$$

Mode-3 multiplication (horizontal slices)

$$\mathcal{Y} = \mathcal{X} \times_3 \mathbf{C}$$

$$\mathbf{Y}_{i::} = \mathbf{X}_{i::}\mathbf{C}^{\mathsf{T}}$$

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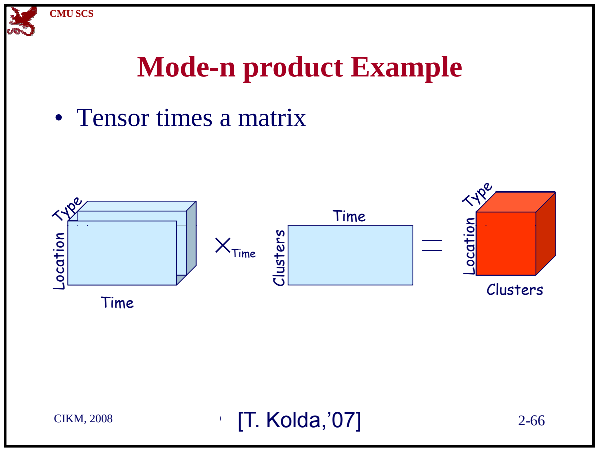

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## Mode-n product Example

- Tensor times a matrix

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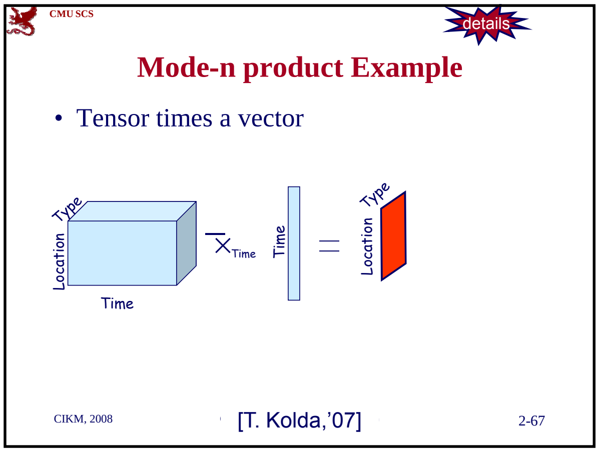

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details

## Mode-n product Example

- Tensor times a vector

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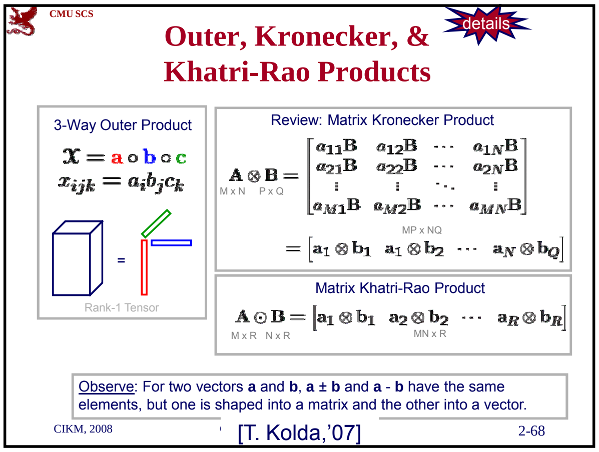

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## Outer, Kronecker, & Khatri-Rao Products

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

Review: Matrix Kronecker Product

$$\underset{M \times N}{\mathbf{A}} \otimes \underset{P \times Q}{\mathbf{B}} = \underset{MP \times NQ}{\begin{bmatrix} a_{11}\mathbf{B} & a_{12}\mathbf{B} & \cdots & a_{1N}\mathbf{B} \\ a_{21}\mathbf{B} & a_{22}\mathbf{B} & \cdots & a_{2N}\mathbf{B} \\ \vdots & \vdots & \ddots & \vdots \\ a_{M1}\mathbf{B} & a_{M2}\mathbf{B} & \cdots & a_{MN}\mathbf{B} \end{bmatrix}}$$

$$= \begin{bmatrix} \mathbf{a}_1 \otimes \mathbf{b}_1 & \mathbf{a}_1 \otimes \mathbf{b}_2 & \cdots & \mathbf{a}_N \otimes \mathbf{b}_Q \end{bmatrix}$$

Matrix Khatri-Rao Product

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

Observe: For two vectors **a** and **b**, **a** ± **b** and **a** - **b** have the same elements, but one is shaped into a matrix and the other into a vector.

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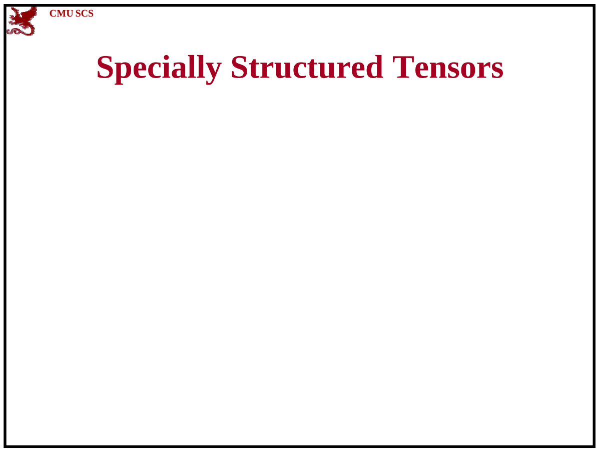

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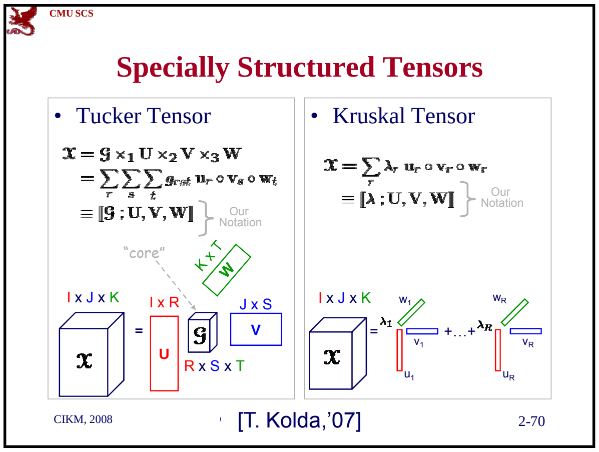
## Specially Structured Tensors



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## Specially Structured Tensors

- Tucker Tensor

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

- Kruskal Tensor

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

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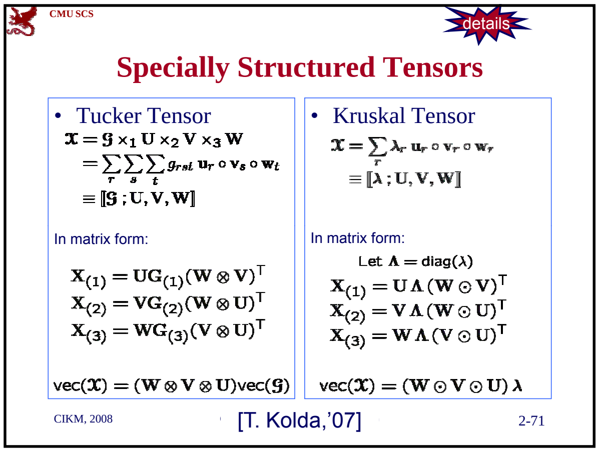

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details

## 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

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

In matrix form:

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

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

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

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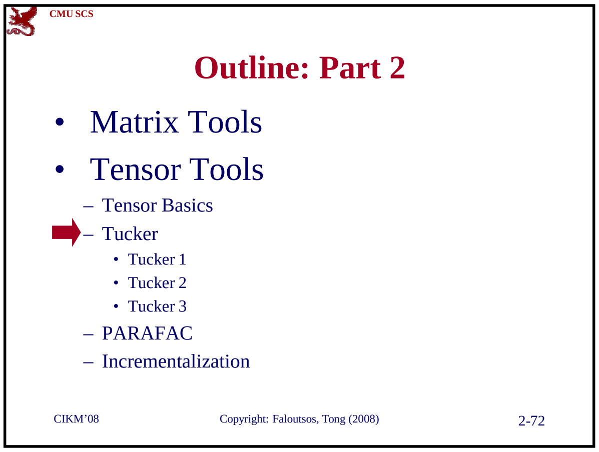

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## Outline: Part 2

- Matrix Tools
- Tensor Tools
  - Tensor Basics
  - ➡ Tucker
    - Tucker 1
    - Tucker 2
    - Tucker 3
  - PARAFAC
  - Incrementalization

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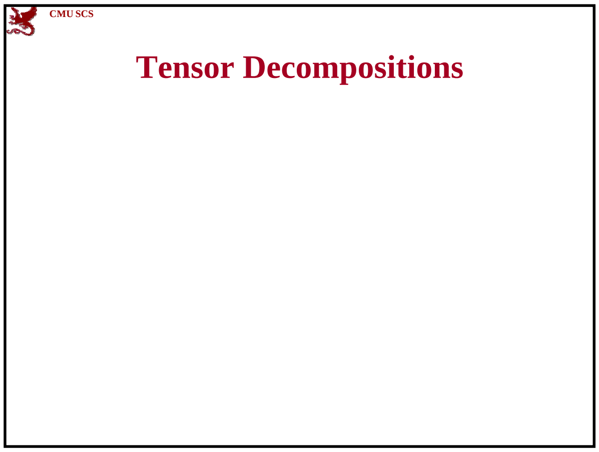

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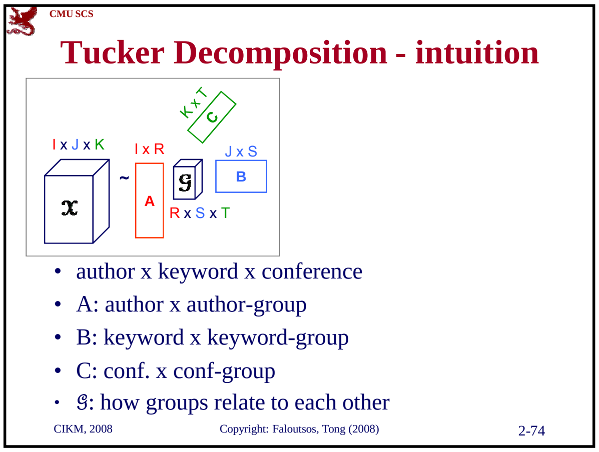
# Tensor Decompositions



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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

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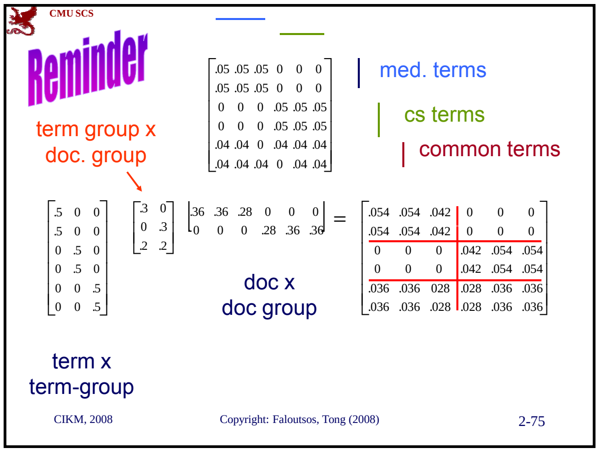

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## Reminder

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

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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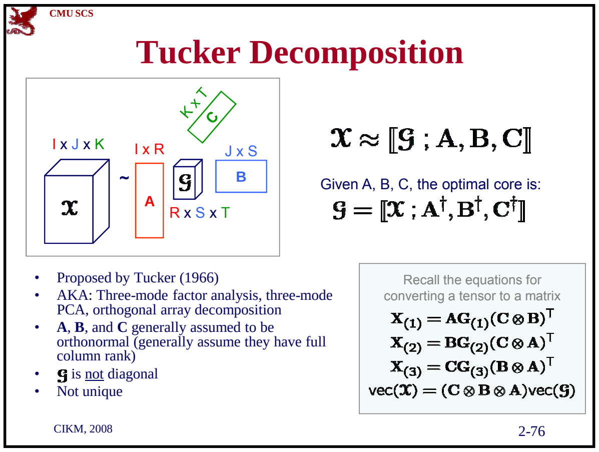

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# Tucker Decomposition

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

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 not diagonal
- Not unique

Recall the equations for converting a tensor to a matrix

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

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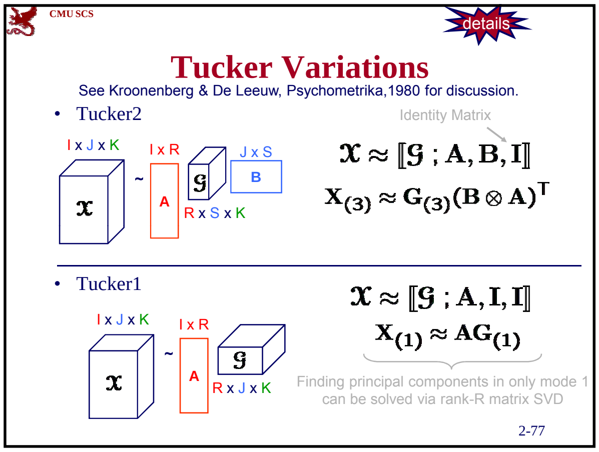

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# Tucker Variations

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

- Tucker2

Identity Matrix

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

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

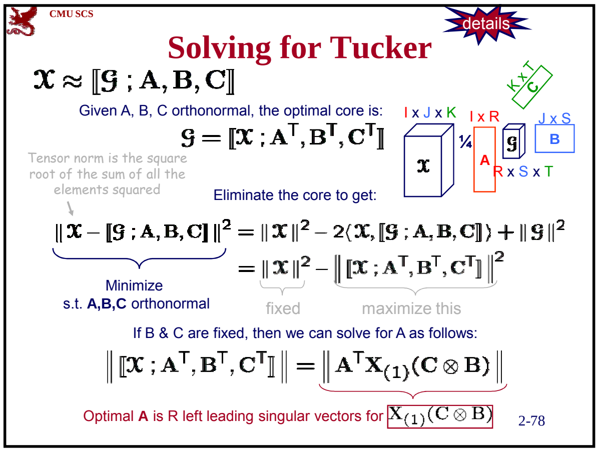
- Tucker1

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

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

Finding principal components in only mode 1 can be solved via rank-R matrix SVD

2-77



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# Solving for Tucker

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

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

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

Tensor norm is the square root of the sum of all the elements squared

Eliminate the core to get:

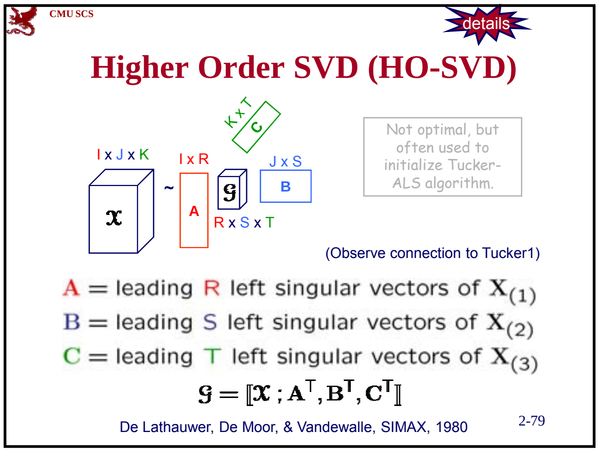
$$\underbrace{\| \mathcal{X} - [\![ \mathcal{G} \,; \mathbf{A}, \mathbf{B}, \mathbf{C} ]\!] \|^2}_{\substack{\text{Minimize} \\ \text{s.t. } \mathbf{A,B,C} \text{ orthonormal}}} = \| \mathcal{X} \|^2 - 2\langle \mathcal{X}, [\![ \mathcal{G} \,; \mathbf{A}, \mathbf{B}, \mathbf{C} ]\!] \rangle + \| \mathcal{G} \|^2$$
$$= \underbrace{\| \mathcal{X} \|^2}_{\text{fixed}} - \underbrace{\left\| [\![ \mathcal{X} \,; \mathbf{A}^{\mathsf{T}}, \mathbf{B}^{\mathsf{T}}, \mathbf{C}^{\mathsf{T}} ]\!] \right\|^2}_{\text{maximize this}}$$

If B & C are fixed, then we can solve for A as follows:

$$\left\| [\![ \mathcal{X} \,; \mathbf{A}^{\mathsf{T}}, \mathbf{B}^{\mathsf{T}}, \mathbf{C}^{\mathsf{T}} ]\!] \right\| = \underbrace{\left\| \mathbf{A}^{\mathsf{T}} \mathbf{X}_{(1)} (\mathbf{C} \otimes \mathbf{B}) \right\|}_{}$$

Optimal **A** is R left leading singular vectors for $\boxed{\mathbf{X}_{(1)}(\mathbf{C} \otimes \mathbf{B})}$

2-78



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## Higher Order SVD (HO-SVD)

Not optimal, but often used to initialize Tucker-ALS algorithm.

(Observe connection to Tucker1)

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

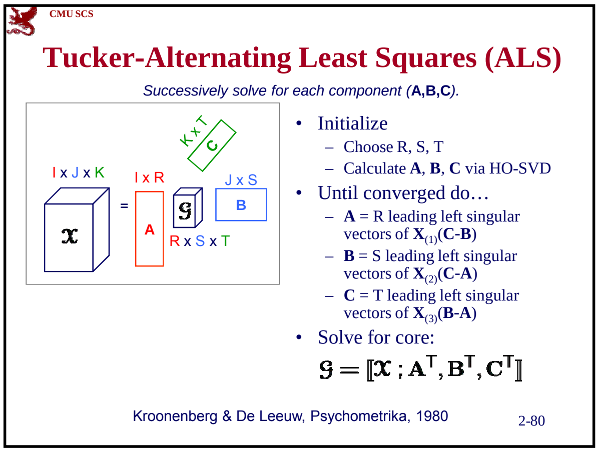
$$\mathbf{B} = \text{leading } S \text{ left singular vectors of } \mathbf{X}_{(2)}$$

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

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

De Lathauwer, De Moor, & Vandewalle, SIMAX, 1980

2-79



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## Tucker-Alternating Least Squares (ALS)

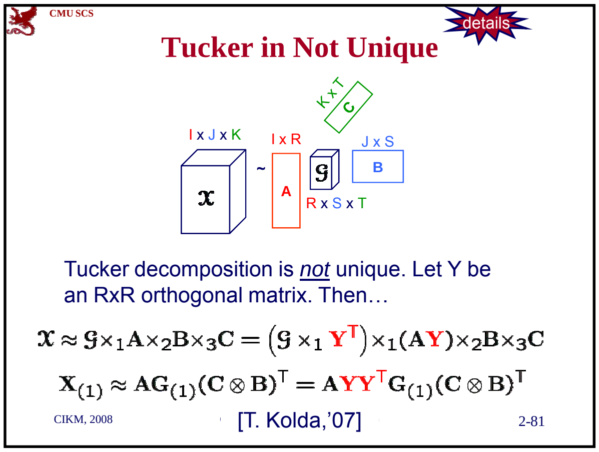
*Successively solve for each component (**A**,**B**,**C**).*

- Initialize
  - Choose R, S, T
  - Calculate **A**, **B**, **C** via HO-SVD
- Until converged do…
  - **A** = R leading left singular vectors of $\mathbf{X}_{(1)}(\mathbf{C}\text{-}\mathbf{B})$
  - **B** = S leading left singular vectors of $\mathbf{X}_{(2)}(\mathbf{C}\text{-}\mathbf{A})$
  - **C** = T leading left singular vectors of $\mathbf{X}_{(3)}(\mathbf{B}\text{-}\mathbf{A})$
- Solve for core:

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

Kroonenberg & De Leeuw, Psychometrika, 1980

2-80



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## Tucker in Not Unique

Tucker decomposition is *not* unique. Let Y be an RxR orthogonal matrix. Then…

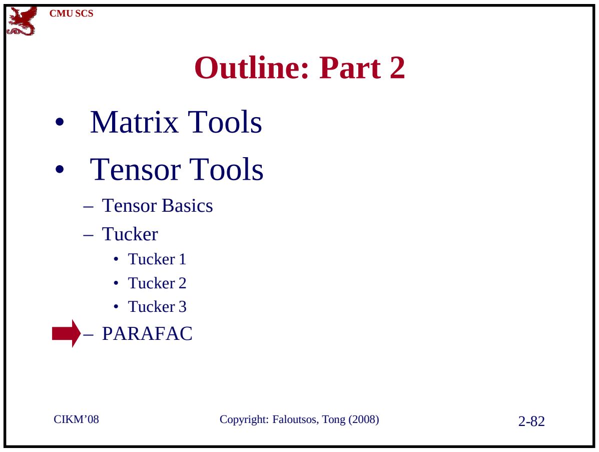
$$\mathcal{X} \approx \mathcal{G} \times_1 \mathbf{A} \times_2 \mathbf{B} \times_3 \mathbf{C} = \left( \mathcal{G} \times_1 \mathbf{Y}^\mathsf{T} \right) \times_1 (\mathbf{A}\mathbf{Y}) \times_2 \mathbf{B} \times_3 \mathbf{C}$$

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

CIKM, 2008

[T. Kolda,’07]

2-81



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## Outline: Part 2

- Matrix Tools
- Tensor Tools
  - Tensor Basics
  - Tucker
    - Tucker 1
    - Tucker 2
    - Tucker 3
  - ➡ PARAFAC

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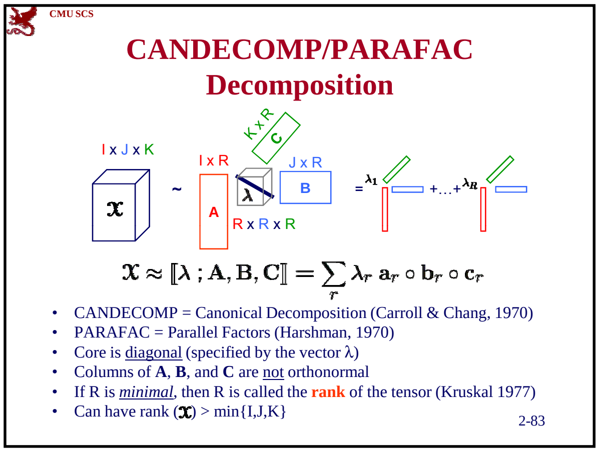

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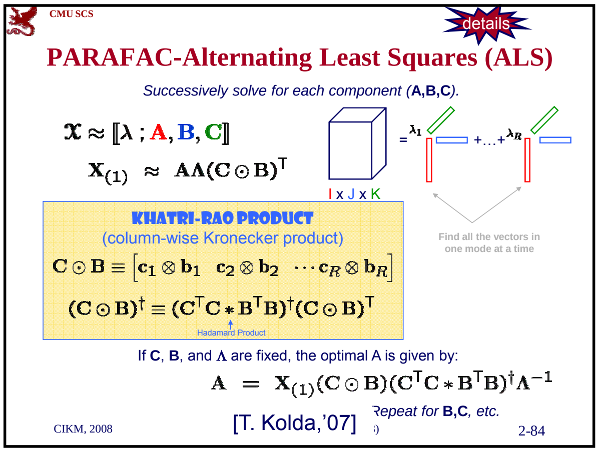
## CANDECOMP/PARAFAC Decomposition

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

- CANDECOMP = Canonical Decomposition (Carroll & Chang, 1970)
- PARAFAC = Parallel Factors (Harshman, 1970)
- Core is diagonal (specified by the vector $\lambda$)
- 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}

2-83



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## PARAFAC-Alternating Least Squares (ALS)

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

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

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

Find all the vectors in one mode at a time

**KHATRI-RAO PRODUCT**

(column-wise Kronecker product)

$$\mathbf{C} \odot \mathbf{B} \equiv \left[ \mathbf{c}_1 \otimes \mathbf{b}_1 \quad \mathbf{c}_2 \otimes \mathbf{b}_2 \quad \cdots \mathbf{c}_R \otimes \mathbf{b}_R \right]$$

$$(\mathbf{C} \odot \mathbf{B})^\dagger \equiv (\mathbf{C}^\mathsf{T}\mathbf{C} \underset{\uparrow}{*} \mathbf{B}^\mathsf{T}\mathbf{B})^\dagger (\mathbf{C} \odot \mathbf{B})^\mathsf{T}$$

Hadamard Product

If **C**, **B**, and $\Lambda$ are fixed, the optimal A is given by:

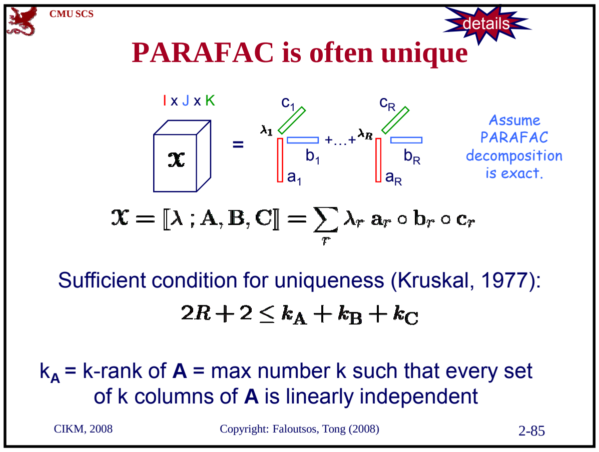
$$\mathbf{A} = \mathbf{X}_{(1)}(\mathbf{C} \odot \mathbf{B})(\mathbf{C}^\mathsf{T}\mathbf{C} * \mathbf{B}^\mathsf{T}\mathbf{B})^\dagger \mathbf{\Lambda}^{-1}$$

*Repeat for **B**,**C**, etc.*

CIKM, 2008

[T. Kolda,’07]

2-84



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## PARAFAC is often unique

I x J x K
$\mathcal{X}$
=
$\lambda_1$
c1
b1
a1
+…+
$\lambda_R$
cR
bR
aR

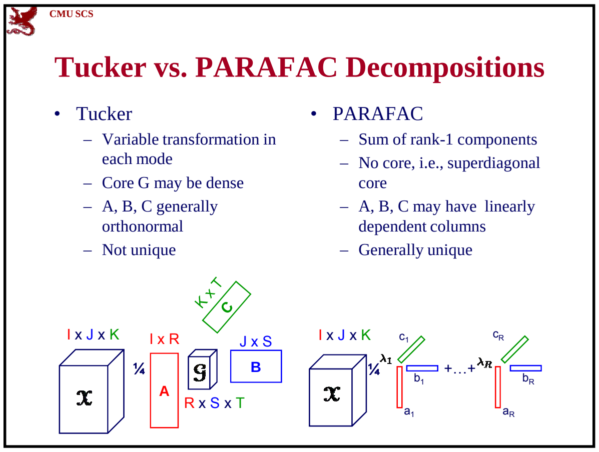
Assume PARAFAC decomposition is exact.

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

Sufficient condition for uniqueness (Kruskal, 1977):

$$2R + 2 \le k_\mathbf{A} + k_\mathbf{B} + k_\mathbf{C}$$

$k_A$ = k-rank of **A** = max number k such that every set of k columns of **A** is linearly independent



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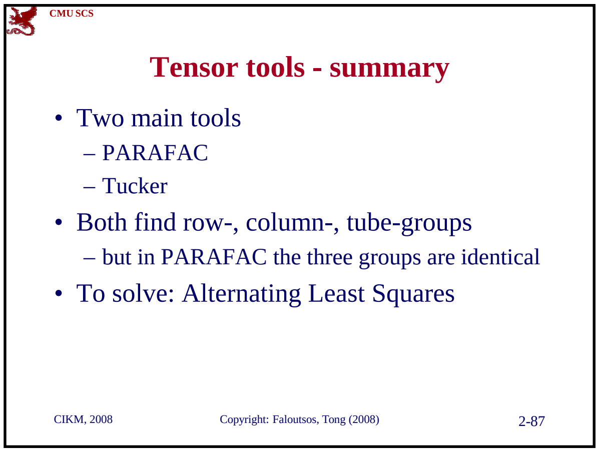
## Tucker vs. PARAFAC Decompositions

- 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

I x J x K
$\mathcal{X}$
¼
I x R
A
K x T
C
$\mathcal{G}$
J x S
B
R x S x T
I x J x K
$\mathcal{X}$
¼
$\lambda_1$
c1
b1
a1
+…+
$\lambda_R$
cR
bR
aR



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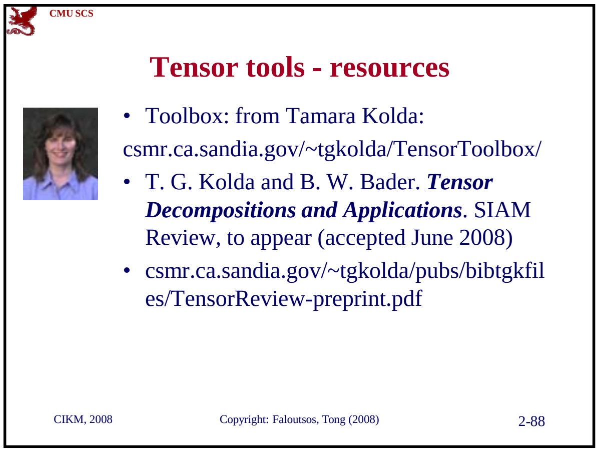
## Tensor tools - summary

- Two main tools
  - PARAFAC
  - Tucker
- Both find row-, column-, tube-groups
  - but in PARAFAC the three groups are identical
- To solve: Alternating Least Squares



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## Tensor tools - resources

- Toolbox: from Tamara Kolda:
csmr.ca.sandia.gov/~tgkolda/TensorToolbox/
- T. G. Kolda and B. W. Bader. ***Tensor Decompositions and Applications***. SIAM Review, to appear (accepted June 2008)
- csmr.ca.sandia.gov/~tgkolda/pubs/bibtgkfiles/TensorReview-preprint.pdf