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


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| $\quad$ Motivating Applications |
| :--- |
| - Why matrices are important? |
| - Why tensors are useful? |
| - P1: social networks |
| - P2: web mining |
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## 35 ${ }^{\text {cmuscs }}$ <br> P1: Social network analysis

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



## P2: Web graph mining

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


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Best rank-k approximation in L2

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## Main points:

- 2 major types of tensor decompositions: PARAFAC and Tucker
- both can be solved with ` ${ }^{\text {alternating least }}$ squares'" (ALS)
- Details follow - we start with terminology:



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- Tensor times a matrix

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- Tensor times a vector
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Observe: For two vectors $\mathbf{a}$ and $\mathbf{b}, \mathbf{a} \pm \mathbf{b}$ and $\mathbf{a}-\mathbf{b}$ have the same elements, but one is shaped into a matrix and the other into a vector. 35 $\qquad$

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| - Tucker Tensor $\begin{aligned} \mathcal{X} & =\mathcal{G} \times \times_{1} \mathbf{U} \times_{2} \mathbf{V} \times{ }_{3} \mathbf{W} \\ & =\sum_{r} \sum_{s} \sum_{t} g_{r s t} \mathbf{u}_{r} \circ \mathbf{v}_{s} \circ \mathbf{w}_{t} \\ & \equiv \llbracket \mathcal{G} ; \mathbf{U}, \mathbf{V}, \mathbf{W} \rrbracket \end{aligned}$ | - Kruskal Tensor $\begin{aligned} x & =\sum_{r} \lambda_{r} \mathbf{u}_{r} \circ \mathbf{v}_{r} \circ \mathbf{w}_{r} \\ & \equiv \llbracket \lambda ; \mathbf{U}, \mathbf{V}, \mathbf{W} \rrbracket \end{aligned}$ |
| :---: | :---: |
| In matrix form: | In matrix form: |
| $\mathrm{X}_{(1)}=\mathrm{UG}_{(1)}(\mathbf{W} \otimes \mathrm{V})^{\top}$ | $\begin{gathered} \text { Let } \boldsymbol{\Lambda}=\operatorname{diag}(\lambda) \\ \mathbf{X}_{(1)}=\mathbf{U} \boldsymbol{\Lambda}(\mathbf{W} \odot \mathbf{V})^{\top} \end{gathered}$ |
| $\mathrm{X}_{(2)}=\mathrm{VG}_{(2)}(\mathbf{W} \otimes \mathrm{U})^{\top}$ | $\mathbf{X}_{(2)}=\mathbf{V} \boldsymbol{\Lambda}(\mathbf{W} \odot \mathbf{U})^{\top}$ |
| $\mathrm{X}_{(3)}=\mathrm{WG}_{(3)}(\mathbf{V} \otimes \mathbf{U})^{\top}$ | $\mathrm{X}_{(3)}=\mathbf{W} \boldsymbol{\Lambda}(\mathrm{V} \odot \mathbf{U})^{\top}$ |
| $\operatorname{vec}(\boldsymbol{X})=(\mathbf{W} \otimes \mathbf{V} \otimes \mathbf{U}) \operatorname{vec}(\mathcal{G})$ | $\operatorname{vec}(\boldsymbol{X})=\mathbf{W}$ ( $\odot \mathbf{V} \odot \mathbf{U}) \lambda$ |

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## Tucker Decomposition - intuition

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term x
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$x \approx \llbracket \mathcal{G} ; \mathrm{A}, \mathrm{B}, \mathrm{C} \rrbracket$
Given A, B, C orthonormal, the optimal core is:

root of the sum of all the
elements squared
Eliminate the core to get:


$$
\|\mathcal{X}-\llbracket \mathcal{G} ; \mathbf{A}, \mathbf{B}, \mathbf{C} \rrbracket\|^{2}=\|\mathcal{X}\|^{2}-2\langle\mathcal{X}, \llbracket \mathcal{G} ; \mathbf{A}, \mathbf{B}, \mathbf{C} \rrbracket\rangle+\|\mathcal{G}\|^{2}
$$

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Higher Order SVD (HO-SVD)


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

(Observe connection to Tucker1)
$A=$ leading $R$ left singular vectors of $\mathbf{X}_{(1)}$
$B=$ leading $S$ left singular vectors of $X_{(2)}$
$C=$ leading $T$ left singular vectors of $\mathbf{X}_{(3)}$

$$
\mathcal{G}=\llbracket \boldsymbol{X} ; \mathbf{A}^{\top}, \mathbf{B}^{\top}, \mathbf{C}^{\top} \rrbracket
$$

De Lathauwer, De Moor, \& Vandewalle, SIMAX, 198045
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Tucker-Alternating Least Squares (ALS)

- Initialize
- Choose R, S, T

Calculate A, B, C via HO-SVD
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- Until converged do
$-\mathbf{A}=\mathrm{R}$ leading left singular vectors of $\mathbf{X}_{(1)}(\mathbf{C} \otimes \mathbf{B})$
- $\mathbf{B}=\mathrm{S}$ leading left singular vectors of $\mathbf{X}_{(2)}(\mathbf{C} \otimes \mathbf{A})$
- $\mathbf{C}=\mathrm{T}$ leading left singular vectors of $\mathbf{X}_{(3)}(\mathbf{B} \otimes \mathbf{A})$
- Solve for core:
$\mathcal{G}=\llbracket \mathcal{X} ; \mathbf{A}^{\top}, \mathbf{B}^{\top}, \mathbf{C}^{\top} \rrbracket$
Kroonenberg \& De Leeuw, Psychometrika, 1980

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$$
X \approx \llbracket \lambda ; \mathbf{A}, \mathbf{B}, \mathbf{C} \rrbracket=\sum_{r} \lambda_{r} \mathbf{a}_{r} \circ \mathbf{b}_{r} \circ \mathbf{c}_{r}
$$

- CANDECOMP = Canonical Decomposition (Carroll \& Chang, 1970)
- PARAFAC = Parallel Factors (Harshman, 1970)
- Core is diagonal (specified by the vector $\lambda$ )
- Columns of $\mathbf{A}, \mathbf{B}$, and $\mathbf{C}$ are not orthonormal
- If R is minimal, then R is called the rank of the tensor (Kruskal 1977)
- Can have $\operatorname{rank}(X)>\min \{\mathrm{I}, \mathrm{J}, \mathrm{K}\}$
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PARAFAC-Alternating Least Squares (ALS)
Successively solve for each component (A,B,C).

$$
\begin{aligned}
& x \approx \llbracket \lambda ; \mathrm{A}, \mathrm{~B}, \mathrm{C} \rrbracket \\
& \mathrm{X}_{(1)} \approx \mathrm{A} \Lambda(\mathrm{C} \odot \mathrm{~B})^{\top}
\end{aligned}
$$


Khatri-Rao Product (column-wise Kronecker product)

$C \cdot \mathbf{B} \equiv\left[\begin{array}{llll}\mathbf{c}_{1} \otimes \mathbf{b}_{1} & \mathbf{c}_{2} \otimes \mathbf{b}_{2} & \cdots \mathbf{c}_{R} \otimes \mathbf{b}_{R}\end{array}\right]$
$(\mathbf{C} \odot \mathbf{B})^{\dagger} \equiv\left(\mathbf{C}^{\top} \mathbf{C} * \mathbf{B}^{\top} \mathbf{B}\right)^{\dagger}(\mathbf{C} \odot B)^{\top}$
Hadamad Product
If $\mathbf{C}, \mathbf{B}$, and $\boldsymbol{\Lambda}$ are fixed, the optimal $A$ is given by:

$$
\begin{gathered}
\mathbf{A}=\mathbf{X}_{(1)}(\mathbf{C} \odot \mathbf{B})\left(\mathbf{C}^{\top} \mathbf{C} * \mathbf{B}^{\top} \mathbf{B}\right)^{\dagger} \boldsymbol{\Lambda}^{-1} \\
\text { Repeat for } \mathbf{B}, \mathbf{C}, \text { etc. }
\end{gathered}
$$

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$$
x=\llbracket \lambda ; \mathbf{A}, \mathbf{B}, \mathbf{C} \rrbracket=\sum_{r} \lambda_{r} \mathbf{a}_{r} \circ \mathbf{b}_{r} \circ \mathbf{c}_{r}
$$

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Sufficient condition for uniqueness (Kruskal, 1977):

$$
2 R+2 \leq k_{\mathrm{A}}+k_{\mathrm{B}}+k_{\mathrm{C}}
$$

$\mathrm{k}_{\mathrm{A}}=\mathrm{k}$-rank of $\mathbf{A}=$ max number $k$ such that every set of $k$ columns of $\mathbf{A}$ is linearly independent

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## Tensor tools - summary

- Two main tools
- PARAFAC
- Tucker
- Both find row-, column-, tube-groups
- but in PARAFAC the three groups are identical
- To solve: Alternating Least Squares
- Toolbox: from Tamara Kolda:
http://csmr.ca.sandia.gov/~tgkolda/TensorToolbox/

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- Two groups are correctly identified: Databases and Data mining
- People and concepts are drifting over time

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$\begin{array}{ll}3 \mathrm{~J}^{\text {cmuscs }} & \\ & \text { Topical HITS (TOPHITS) }\end{array}$
Main Idea: Extend the idea behind the HITS model to incorporate term (i.e., topical) information.

$$
\boldsymbol{X} \approx \sum_{r=1}^{R} \lambda_{r} \mathbf{h}_{r} \circ \mathbf{a}_{r}
$$


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