Tensors in Data Analysis

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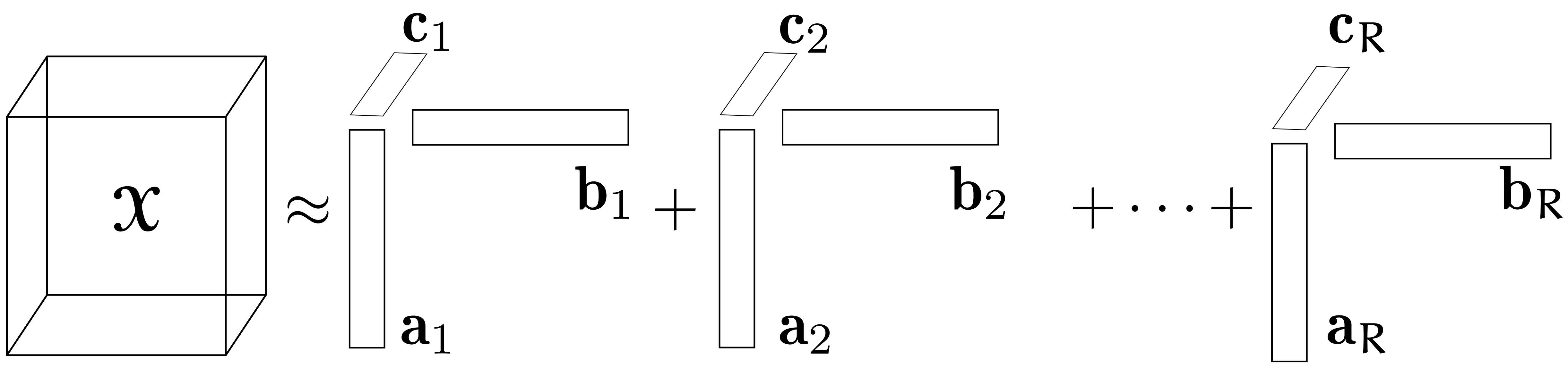
Tensors in Data Analysis

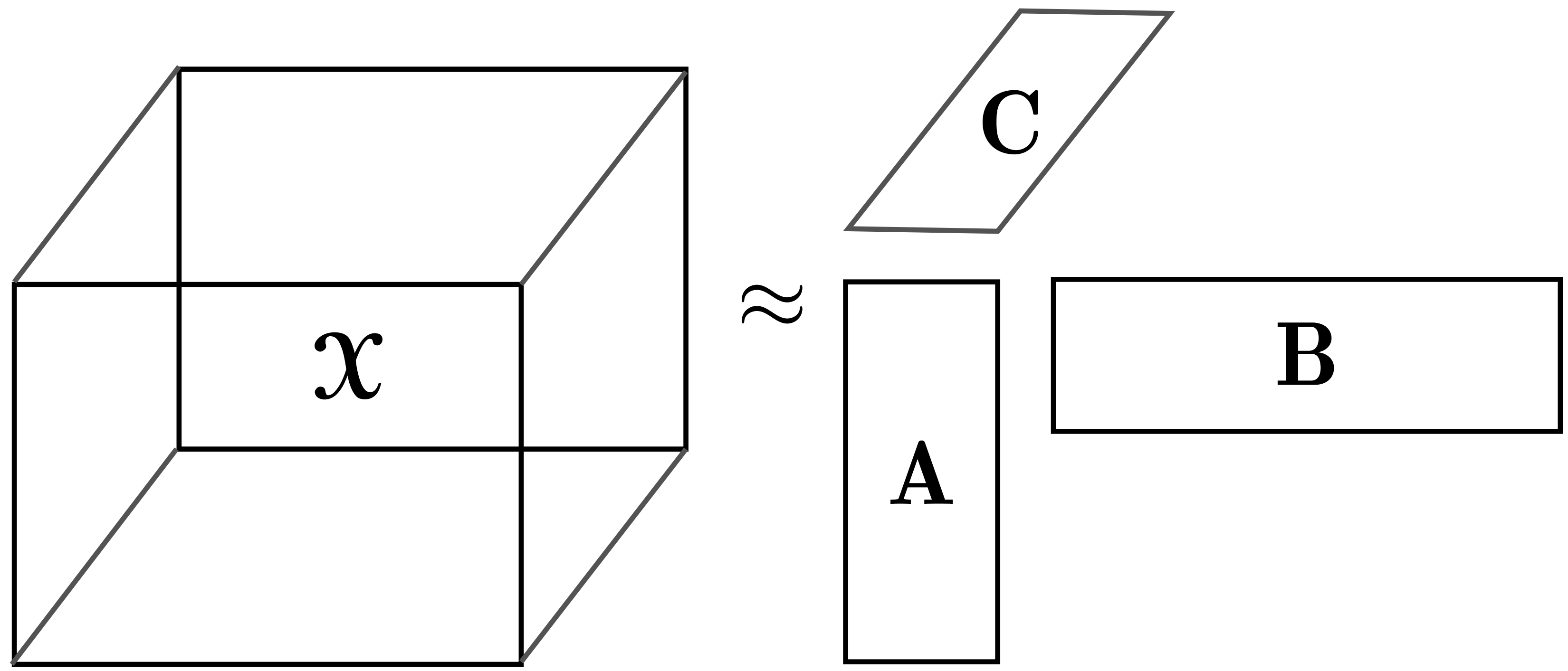
1. CP and INDSCAL and some applications
2. The Tucker tensor decompositions
3. HOSVD, RESCAL, and DEDICOM
4. The non-negative variants

CP Recap (Rank-1 View)



$$x_{ijk} \approx \sum_{r=1}^{R} a_{ir} b_{jr} c_{kr}$$

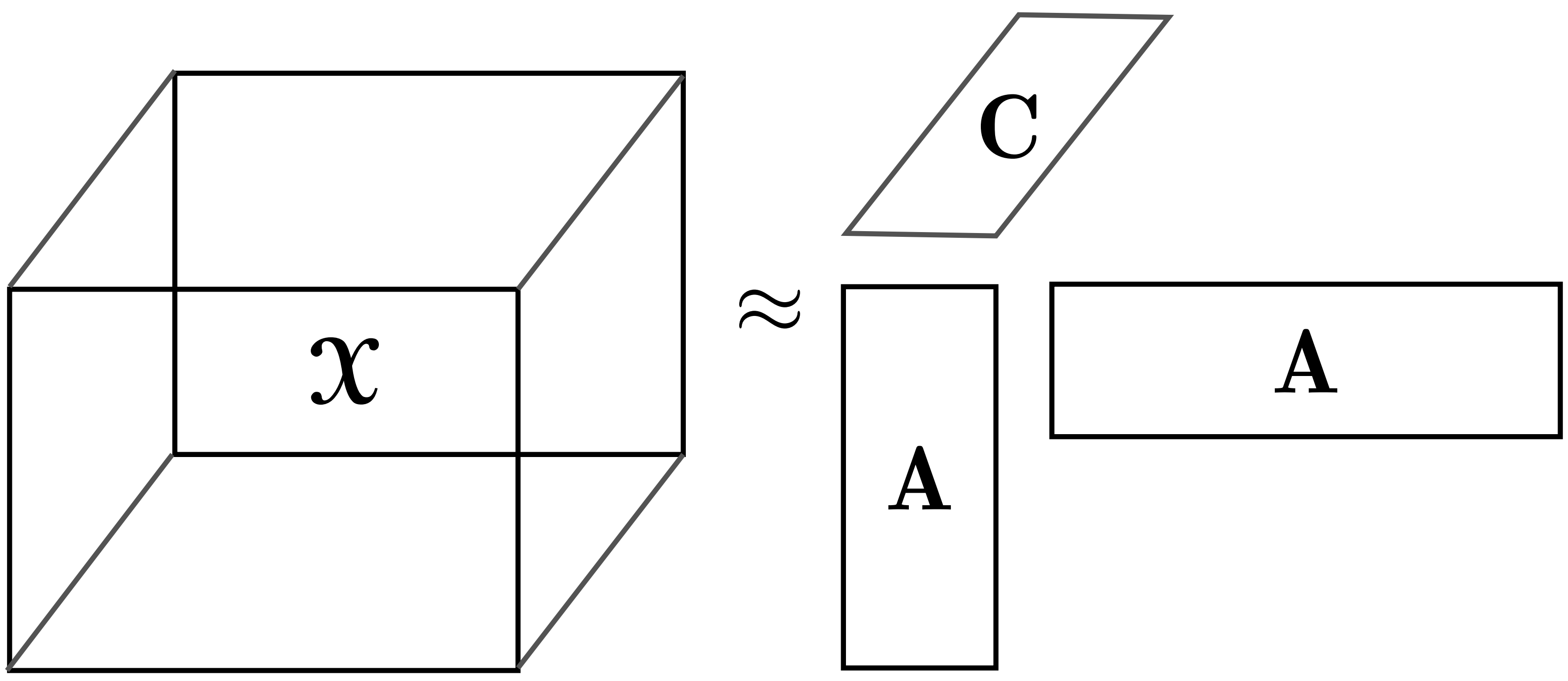
CP Recap (Matrix View)



$$x_{ijk} \approx \sum_{r=1}^{R} a_{ir} b_{jr} c_{kr}$$

The INDSCAL Decomposition

- The **INDSCAL decomposition** decomposes a 3-way tensor $\mathcal{X}$ into **two** factor matrices ***A*** and ***C***



$$x_{ijk} \approx \sum_{r=1}^{R} a_{ir} a_{jr} c_{kr}$$

More on INDSCAL

- First two modes of $\mathcal{X}$ are expect to be symmetric
  - Not mandatory, but must have same dimensions
- Commonly computed by solving CP and hoping ***A*** and ***B*** merge
  - End by forcing ***A*** and ***B*** the same and update ***C***

Why INDSCAL

- INDSCAL keeps the symmetry of the modes
- Stands for Individual Differences in Scaling
  - Assume K subjects ranked the similarity of N objects
  - Assume each subject is influenced by the same factors, but with different weights
  - $\boldsymbol{A}$ contains the factors, $\boldsymbol{C}$ gives the weights

INDSCAL Example

- Carroll and Chang (1970) proposed to use INDSCAL and CANDECOMP (CP) to analyse psychological data
  - PCA has long history in psychology
- Example: 20 subjects rate the similarity of countries
  - Multi-way data

Carroll, J.D. & Chan, J.-J., 1970. Analysis of individual differences in multidimensional scaling via an n-way generalization of ”Eckart–Young” decomposition. Psychometrika 35(3), pp. 283–319

Countries in Carroll & Chan (1970) [1]

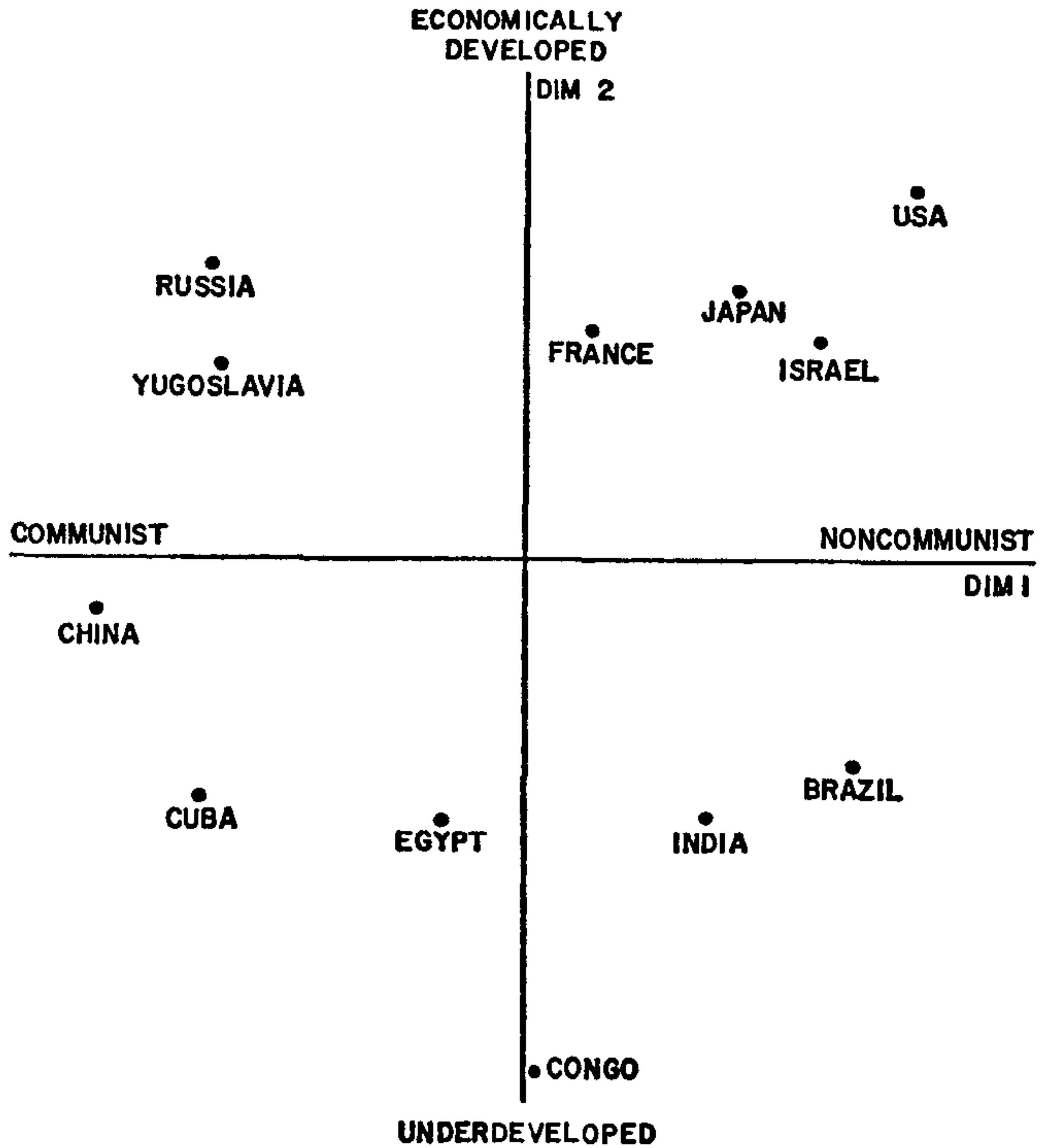


FIGURE 11

Countries in Carroll & Chan (1970) [2]

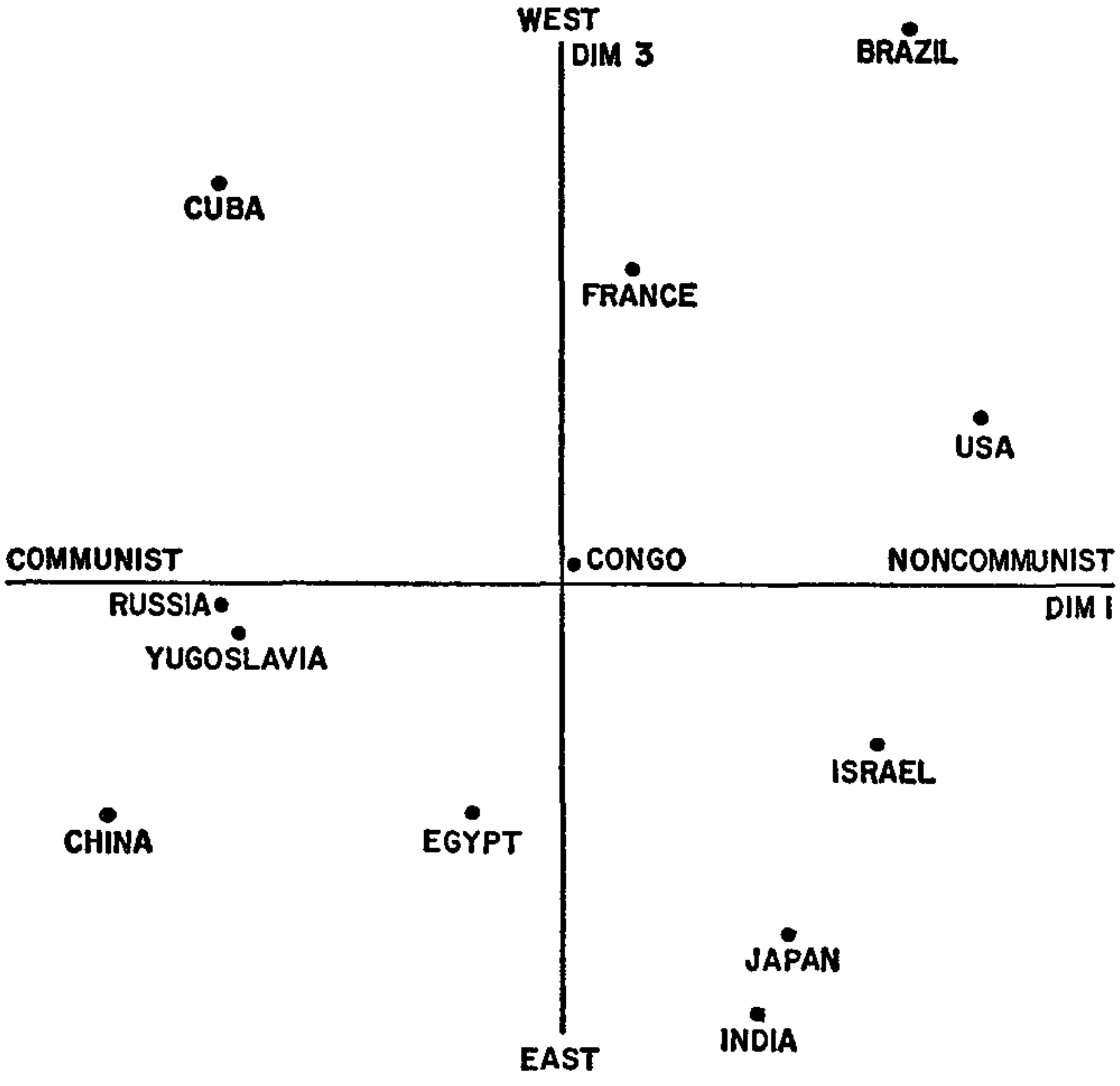


FIGURE 12

Countries in Carroll & Chan (1970) [3]

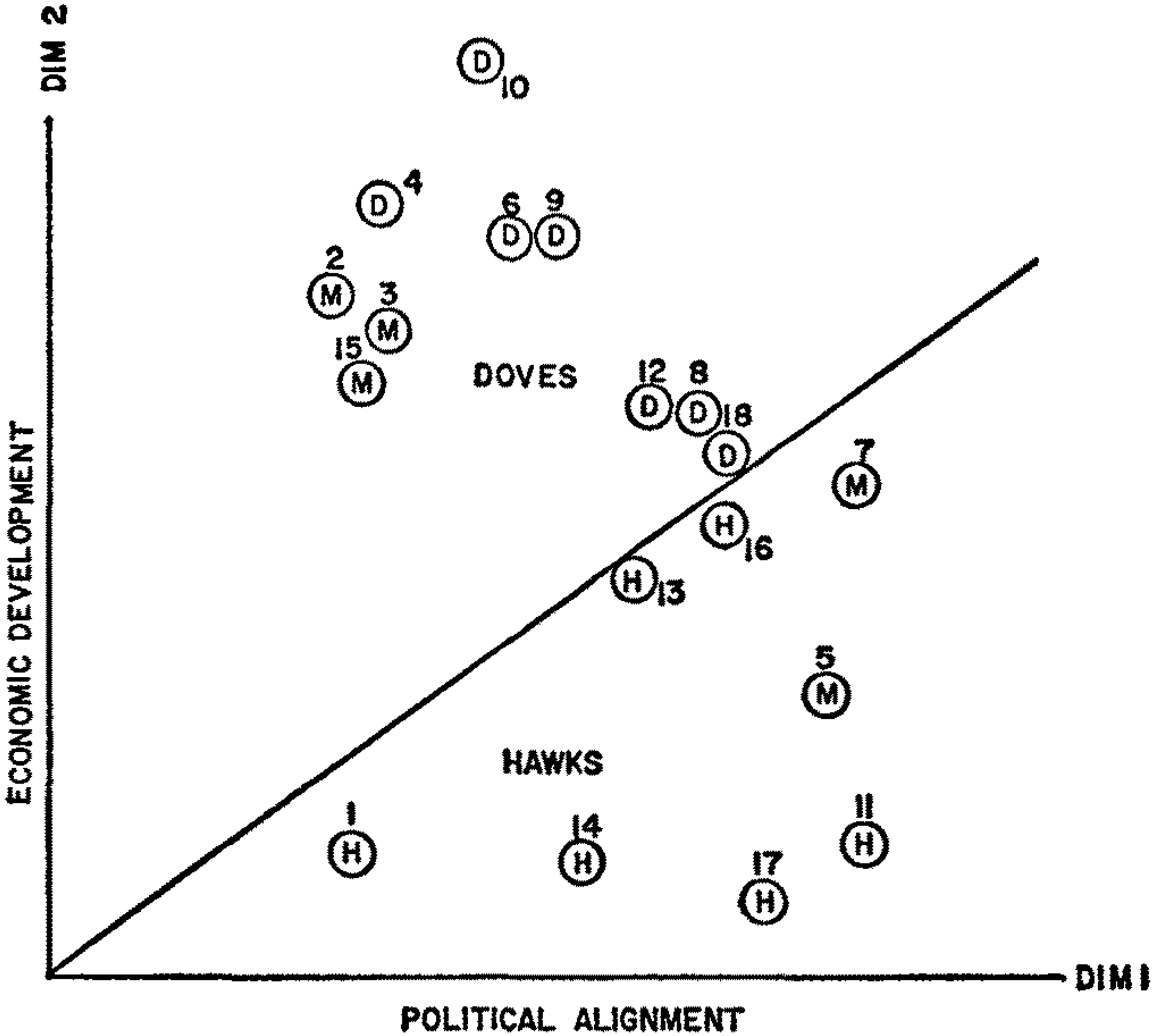


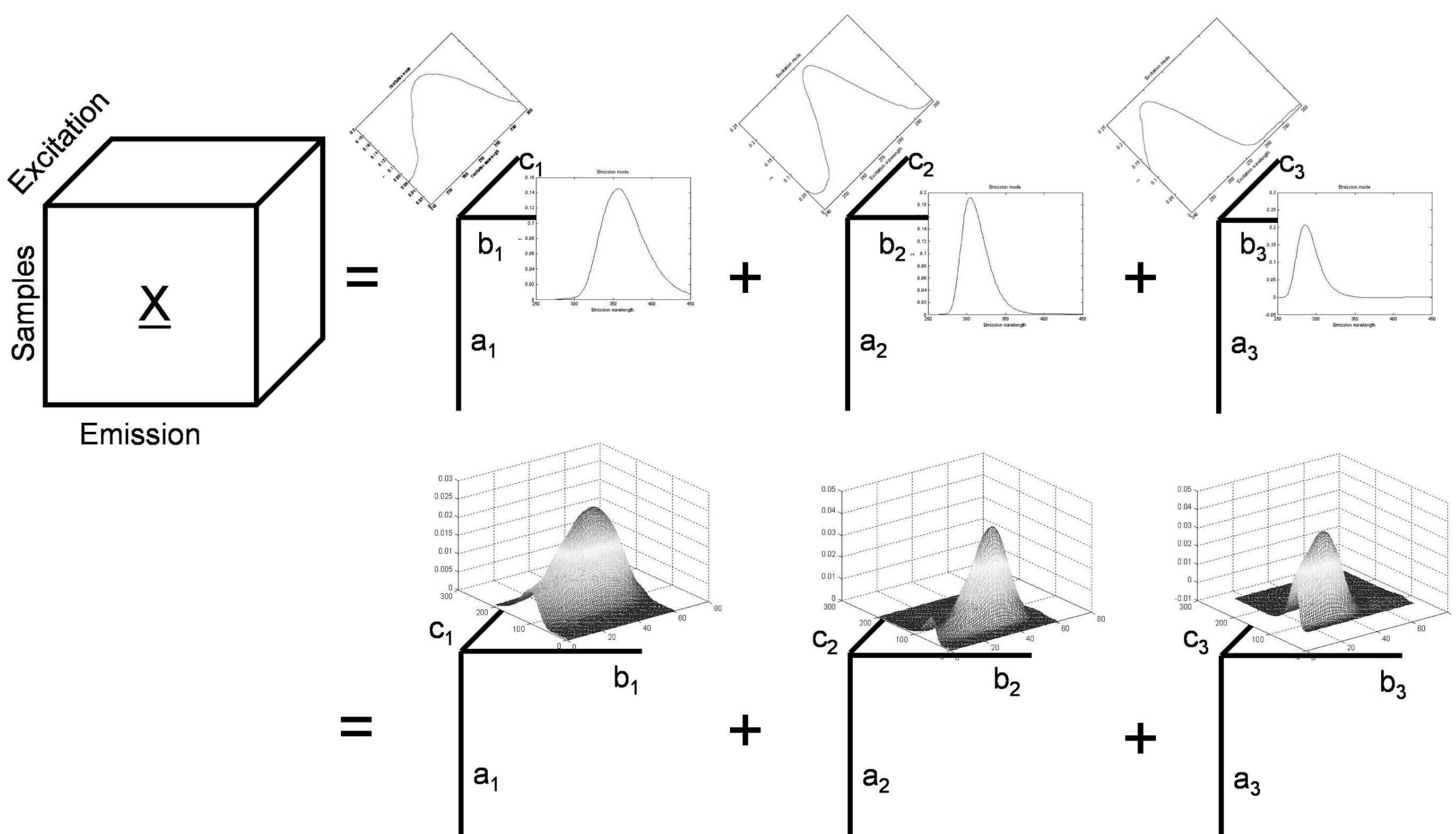
FIGURE 13

Fluorescence Excitation–Emission Analysis

- Fluorescence spectroscopy analyses (typically) organic compounds
  - A beam of (UV) light excites electrons in molecules
  - The excited electrons release a photon, which is measured
  - A **fluorescence landscape** of a compound is a rank-1 matrix that maps the exciter’s wavelength to the emitted photon’s wavelength
    - Lets us to identify the compounds

CP for Fluorescence Analysis

- Samples-by-excitation wavelengths-by-emission wavelengths tensor $\mathcal{X}$
  - Matrix $\boldsymbol{b}_i\boldsymbol{c}_i^T$ is the landscape for the *i*th component
  - Vector $\boldsymbol{a}_i$ gives the weights of landscapes in each sample



Acar, Evrim, and B Yener. 2009. “Unsupervised Multiway Data Analysis: a Literature Survey.” IEEE Transactions on Knowledge and Data Engineering 21(1). pp. 6–20.

TOPHITS for IR

- Three-way pages-by-pages-by-anchor text tensor $\mathcal{T}$
  - Element t_{ijk} = max{1+log(x_{ijk}), 0} where x_{ijk} is the number of times page *i* links to page *j* using term *k*
- The CP decomposition of $\mathcal{T}$ behaves akin to HITS
  - Each rank-1 component is one topic
  - ***A*** and ***B*** give the authority and hub scores, ***C*** gives the weights for terms

Kolda, Tamara G, Brett W Bader, and J P Kenny 2005. “Higher-Order Web Link Analysis Using Multilinear Algebra.” In ICDM '05, 242–49. IEEE. doi:10.1109/ICDM.2005.77.

The Tucker Decompositions

- The CP decomposition requires the factors to have the same number of columns
- In Tucker decompositions, different number of columns can be mixed using a **core tensor**
  - This enables very different looking decompositions

Tensor–Vector Multiplication

- Vectors can be multiplied with tensors along specific modes
  - For *n*-th mode multiplication, the tensor's dimensionality in mode *n* must agree with the vector's dimensions
- The *n*-mode vector product is denoted $\mathcal{X} \bar{\times}_n \boldsymbol{v}$
  - The result is of order *N*–1
  - $(\mathcal{X} \bar{\times}_n \boldsymbol{v})_{i_1 \cdots i_{n-1} i_{n+1} \cdots i_N} = \sum_{i_n=1}^{I_n} x_{i_1 i_2 \cdots i_N} v_{i_n}$
    - Inner product between mode-*n* fibres and vector $\boldsymbol{v}$

Tensor-Vector Multiplication Example

Given tensor $\mathcal{T}$ and vector $\boldsymbol{v}$,

$$\boldsymbol{T}_1 = \begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix} \quad \boldsymbol{T}_2 = \begin{pmatrix} 5 & 7 \\ 6 & 8 \end{pmatrix} \qquad \boldsymbol{v} = \begin{pmatrix} 2 & 1 \end{pmatrix}$$

Computing $\mathcal{Y} = \mathcal{T} \bar{\times}_3 \boldsymbol{v}$ gives

$$\mathcal{Y} = \begin{pmatrix} 7 & 13 \\ 10 & 16 \end{pmatrix}$$

Tensor–Matrix Multiplication

- Let $\mathcal{X}$ be an N-way tensor of size $I_1 \times I_2 \times \ldots \times I_N$, and let $\boldsymbol{U}$ be a matrix of size $J \times I_n$
  - The n-mode matrix product of $\mathcal{X}$ with $\boldsymbol{U}$, $\mathcal{X} \times_n \boldsymbol{U}$ is of size $I_1 \times I_2 \times \ldots \times I_{n-1} \times J \times I_{n+1} \times \ldots \times I_N$
  - $(\mathcal{X} \times_n \boldsymbol{U})_{i_1 \cdots i_{n-1} j i_{n+1} \cdots i_N} = \sum_{i_n=1}^{I_n} x_{i_1 i_2 \cdots i_N} u_{j i_n}$
    - Each mode-n fibre is multiplied by the matrix $\boldsymbol{U}$
  - In terms of unfold tensors:

$$\mathcal{Y} = \mathcal{X} \times_n \boldsymbol{U} \iff \boldsymbol{Y}_{(n)} = \boldsymbol{U}\boldsymbol{X}_{(n)}$$

Tensor-Matrix Multiplication Example

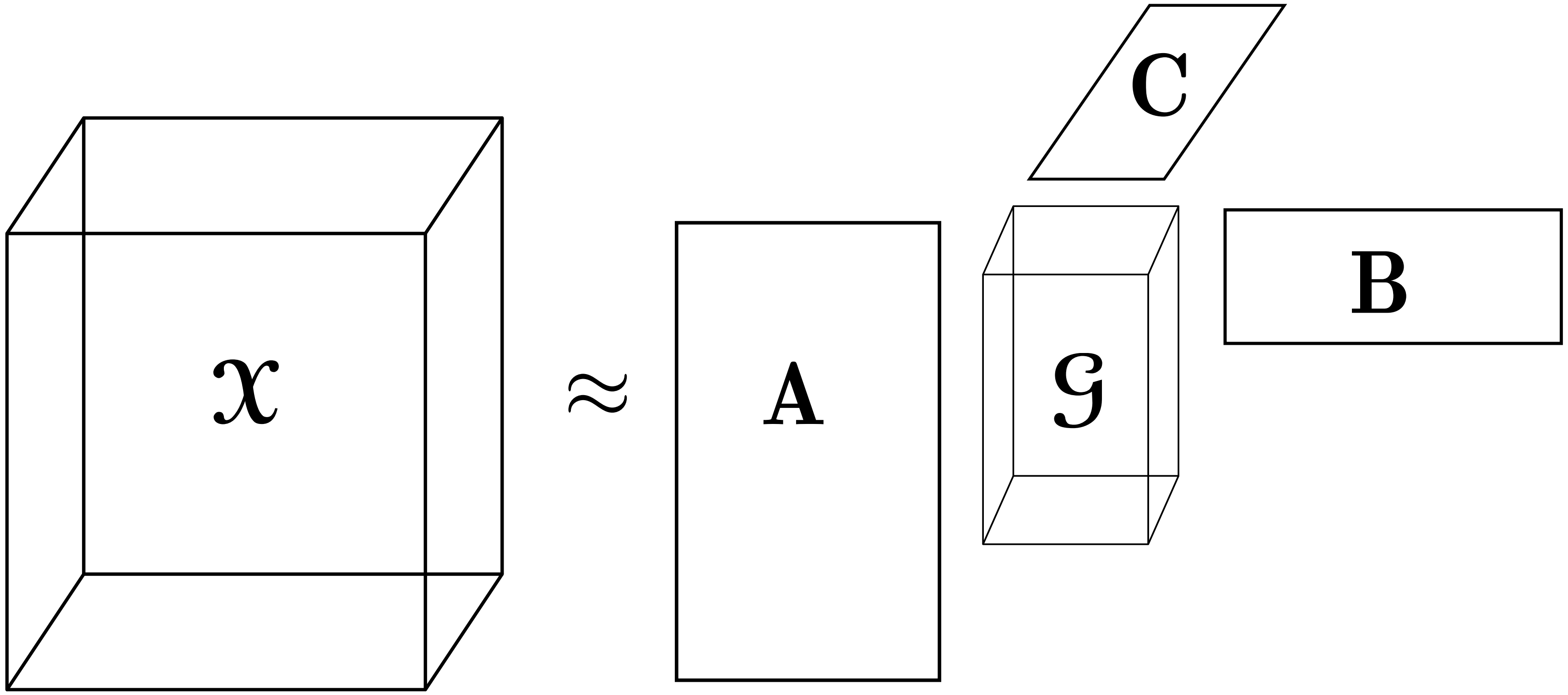
Given tensor $\mathcal{T}$ and matrix $\boldsymbol{M}$,

$$\boldsymbol{T}_1 = \begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix} \quad \boldsymbol{T}_2 = \begin{pmatrix} 5 & 7 \\ 6 & 8 \end{pmatrix} \qquad \boldsymbol{M} = \begin{pmatrix} 10 & 0 \\ 0 & 100 \\ 1 & 1 \end{pmatrix}$$

Computing $\mathcal{Y} = \mathcal{T} \times_1 \boldsymbol{M}$ gives

$$\boldsymbol{Y}_1 = \begin{pmatrix} 10 & 30 \\ 200 & 400 \\ 3 & 7 \end{pmatrix} \qquad \boldsymbol{Y}_2 = \begin{pmatrix} 50 & 60 \\ 600 & 800 \\ 11 & 15 \end{pmatrix}$$

The Tucker3 Tensor Decomposition



$$x_{ijk} \approx \sum_{p=1}^{P} \sum_{q=1}^{Q} \sum_{r=1}^{R} g_{pqr} a_{ip} b_{jq} c_{kr}$$

Tucker3 Decomposition

- The **Tucker3 tensor decomposition** decomposes the tensor into three **factor matrices** $\boldsymbol{A}$, $\boldsymbol{B}$, and $\boldsymbol{C}$, and a **core tensor** $\mathcal{G}$
    - $\boldsymbol{A}$ has P, $\boldsymbol{B}$ has Q, and $\boldsymbol{C}$ has R columns and $\mathcal{G}$ is P-by-Q-by-R
- Many degrees of freedom: often $\boldsymbol{A}$, $\boldsymbol{B}$, and $\boldsymbol{C}$ are required to be orthogonal
- If $P=Q=R$ and core tensor $\mathcal{G}$ is **hyper-diagonal**, then Tucker3 decomposition reduces to CP decomposition

Solving Tucker3

- ALS-style methods are typically used
  - The matricized forms are

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

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

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

- If factor matrices are orthogonal, we can get $\mathcal{G}$ as $\mathcal{G} = \mathcal{X} \times_1 \boldsymbol{A}^T \times_2 \boldsymbol{B}^T \times_3 \boldsymbol{C}^T$

HOSVD, Tucker2, RESCAL, and DEDICOM

- There are many tensor decompositions that are based on or similar to Tucker3
  - Or merge Tucker3 and CP
- Here are few, but the list is by no means exhaustive

Higher-Order SVD (HOSVD)

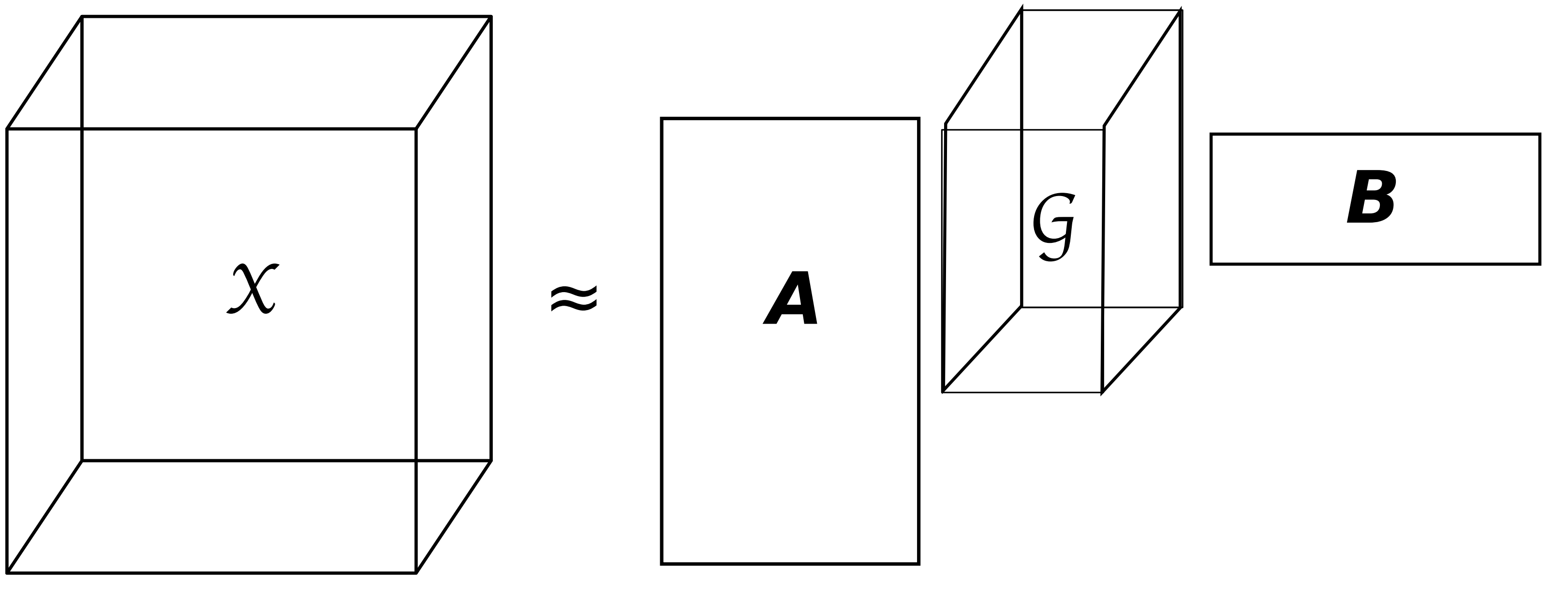
- One method to compute the Tucker3 decomposition
  - Set $\boldsymbol{A}$ as the leading P left singular vectors of $\boldsymbol{X}_{(1)}$
  - Set $\boldsymbol{B}$ as the leading Q left singular vectors of $\boldsymbol{X}_{(2)}$
  - Set $\boldsymbol{C}$ as the leading R left singular vectors of $\boldsymbol{X}_{(3)}$
  - Set tensor $\mathcal{G}$ as $\mathcal{X} \times_1 \boldsymbol{A}^T \times_2 \boldsymbol{B}^T \times_3 \boldsymbol{C}^T$

Why HOSVD?

- Can be used as is for data analysis
  - E.g. TensorFaces
- Can be used to initialize other Tucker3 algorithms
  - Instead of random $\boldsymbol{A}$, $\boldsymbol{B}$, and $\boldsymbol{C}$

Tucker2 Decomposition

- The Tucker2 decomposition decomposes a 3-way tensor into a core tensor and two factor matrices
  - Or, third factor matrix is forced to be an identity matrix
  - Core keeps that mode's dimensionality



Tucker2 Sliced and Matricized

- The slice-wise Tucker2: $\boldsymbol{X}_k = \boldsymbol{A}\boldsymbol{G}_k\boldsymbol{B}^T$ for each k
- Matricized forms replace $\boldsymbol{C}$ with identity matrix $\boldsymbol{I}$: $\boldsymbol{X}_{(1)} = \boldsymbol{A}\boldsymbol{G}_{(1)}(\boldsymbol{I} \otimes \boldsymbol{B})^T$ etc.
- To compute Tucker2:
  - Solve $\boldsymbol{A}$ and $\boldsymbol{B}$ using the matricized forms
  - Update each frontal slice of $\mathcal{G}$ separately

Why Tucker2?

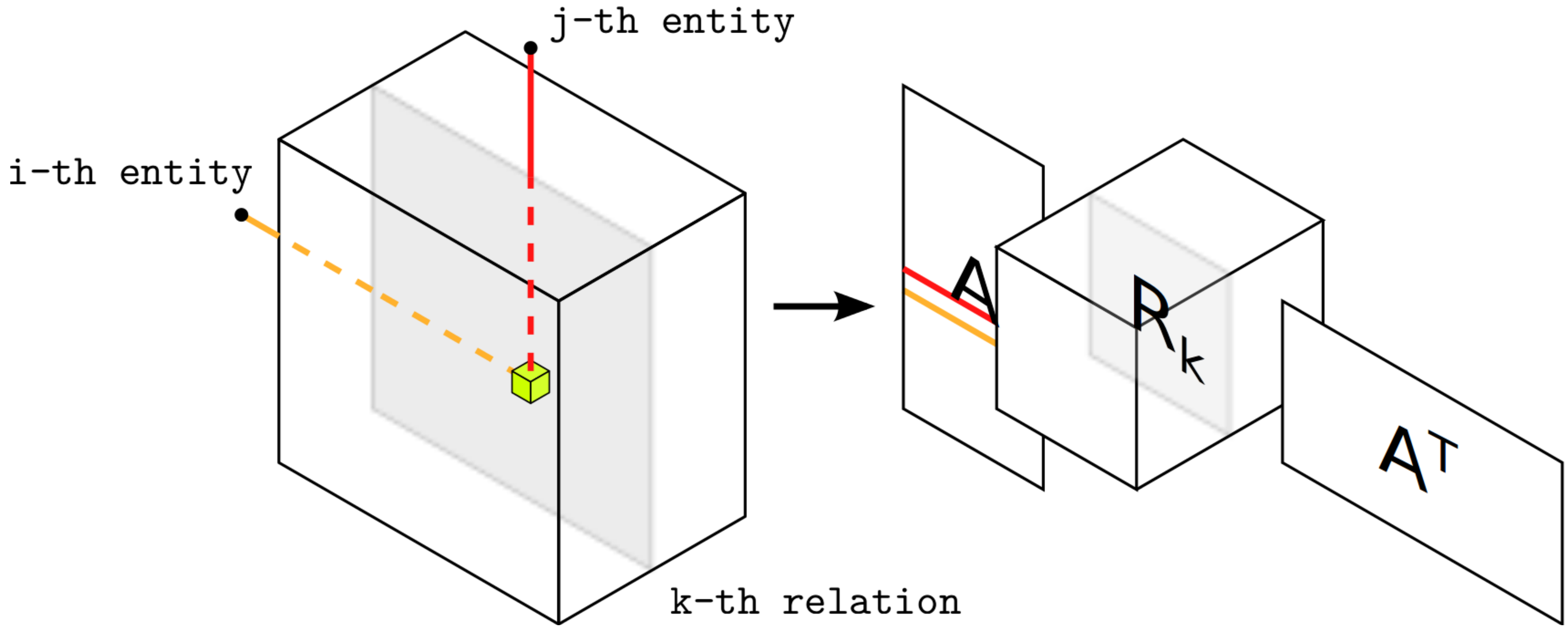
- Use Tucker2 if you don’t want to factorize one mode
  - Too small dimension (e.g. 500-by-300-by-3)
  - This mode requires separate handling
    - E.g. if third mode is time, first Tucker2 and then time-series analysis on third mode
- Tucker2 is slightly simpler than Tucker3

The RESCAL Decomposition

- The **RESCAL decomposition** merges Tucker2 and INDSCAL
- Tensor $\mathcal{X}$ is factored into one factor matrix $\boldsymbol{A}$ and one core tensor $\boldsymbol{R}$
  - $\boldsymbol{X}_k = \boldsymbol{A}\boldsymbol{R}_k\boldsymbol{A}^T$
- Tensor $\mathcal{X}$ might not be symmetric on first two modes

Nickel, M., Tresp, V., & Kriegel, H.-P. (2011). A Three-Way Model for Collective Learning on Multi-Relational Data (pp. 809–816). Presented at the 28th International Conference on Machine Learning.

RESCAL in Picture



Nickel, M., Tresp, V., & Kriegel, H.-P. (2011). A Three-Way Model for Collective Learning on Multi-Relational Data (pp. 809–816). Presented at the 28th International Conference on Machine Learning.

Computing RESCAL (1)

- Mode-1 matricization of RESCAL is $\boldsymbol{X}_{(1)} = \boldsymbol{A}\boldsymbol{R}_{(1)}(\boldsymbol{I} \otimes \boldsymbol{A})^T$
  - This is hard as $\boldsymbol{A}$ is both left and right
  - Simplify: place pairs $(\boldsymbol{X}_k\ \boldsymbol{X}_k^T)$ side-by-side and consider the right $\boldsymbol{A}$ fixed
    - The $\boldsymbol{X}_k^T$ guide $\boldsymbol{A}$ to fit well also in RHS

Computing RESCAL (2)

- To minimize the error, we minimize $||\boldsymbol{Y} - \boldsymbol{AH}(\boldsymbol{I}_{2K} \otimes \boldsymbol{A}^T)||_F$
  - $\boldsymbol{Y} = [\boldsymbol{X}_1\ \boldsymbol{X}_1{}^T\ \boldsymbol{X}_2\ \boldsymbol{X}_2{}^T \ldots \boldsymbol{X}_K\ \boldsymbol{X}_K{}^T]$
  - $\boldsymbol{H} = [\boldsymbol{R}_1\ \boldsymbol{R}_1{}^T\ \boldsymbol{R}_2\ \boldsymbol{R}_2{}^T \ldots \boldsymbol{R}_K\ \boldsymbol{R}_K{}^T]$
- For fixed $\boldsymbol{A}^T$ and $\mathcal{R}$, the update rule for $\boldsymbol{A}$ is

$$\boldsymbol{A} = \left(\sum_{k=1}^{K}(\boldsymbol{X}_k\boldsymbol{R}_k^T + \boldsymbol{X}_k^T\boldsymbol{A}\boldsymbol{R}_k)\right)\left(\sum_{k=1}^{K}(\boldsymbol{B}_k + \boldsymbol{C}_k)\right)^{-1}$$

- Here, $\boldsymbol{B}_k = \boldsymbol{R}_k\boldsymbol{A}^T\boldsymbol{A}\boldsymbol{R}_k{}^T$ and $\boldsymbol{C}_k = \boldsymbol{R}_k{}^T\boldsymbol{A}^T\boldsymbol{A}\boldsymbol{R}_k$

Computing RESCAL (3)

- Each slice $\boldsymbol{R}_k$ can be updated separately
  - Minimize $||\text{vec}(\boldsymbol{X}_k) - (\boldsymbol{A} \otimes \boldsymbol{A})\text{vec}(\boldsymbol{R}_k)||$
    - Linear regression, set $\text{vec}(\boldsymbol{R}_k) = (\boldsymbol{A} \otimes \boldsymbol{A})^{+}\text{vec}(\boldsymbol{X}_k)$
  - To avoid computing the pseudo-inverse of big $\boldsymbol{A} \otimes \boldsymbol{A}$, compute the skinny QR decomposition of $\boldsymbol{A}$
    - $\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{U}$, $\boldsymbol{Q}$ column-orthogonal, $\boldsymbol{U}$ upper-triangular
    - Now: $||\boldsymbol{X}_k - \boldsymbol{A}\boldsymbol{R}_k\boldsymbol{A}^T|| = ||\boldsymbol{X}_k - \boldsymbol{Q}\boldsymbol{U}\boldsymbol{R}_k\boldsymbol{U}^T\boldsymbol{Q}^T||$ $= ||\boldsymbol{Q}^T\boldsymbol{X}_k\boldsymbol{Q} - \boldsymbol{U}\boldsymbol{R}_k\boldsymbol{U}^T||$ and update rule as $(\boldsymbol{U} \otimes \boldsymbol{U})$ which is only R^2-by-R^2

Why RESCAL

- No factorization of the third mode
  - Same as in Tucker2
- Only one factor matrix
  - We assume some kind of symmetry (INDSCAL)
    - E.g. subjects and objects
  - Provides ”information flow” between the modes
- Each frontal slice has a separate ”mixing matrix” for the interactions between factors

The DEDICOM Decomposition: Matrix Version

- The **DEDICOM decomposition** is a matrix decomposition for an asymmetric relation between entities
  - What is the value of export from country *i* to country *j*?
  - How many emails person *i* sent to person *j*?
- $\boldsymbol{X} = \boldsymbol{A}\boldsymbol{R}\boldsymbol{A}^T$
  - $\boldsymbol{A}$ factors the entities
  - $\boldsymbol{R}$ explains the asymmetric relation

The DEDICOM Decomposition: Tensor Version

- The **three-way DEDICOM** adds weights for each factor's participation in each position in the third mode
  - E.g. how much country factor r acts as a seller or buyer at time k?
- $\boldsymbol{X}_k = \boldsymbol{A}\boldsymbol{D}_k\boldsymbol{R}\boldsymbol{D}_k\boldsymbol{A}^T$
  - $\boldsymbol{A}$ and $\boldsymbol{R}$ as before, $\mathcal{D}$ is R-by-R-by-K tensor such that each frontal slice $\boldsymbol{D}_k$ is diagonal
  - $(\boldsymbol{D}_k)_{rr}$ is the weight for factor r at time k

DEDICOM in Picture

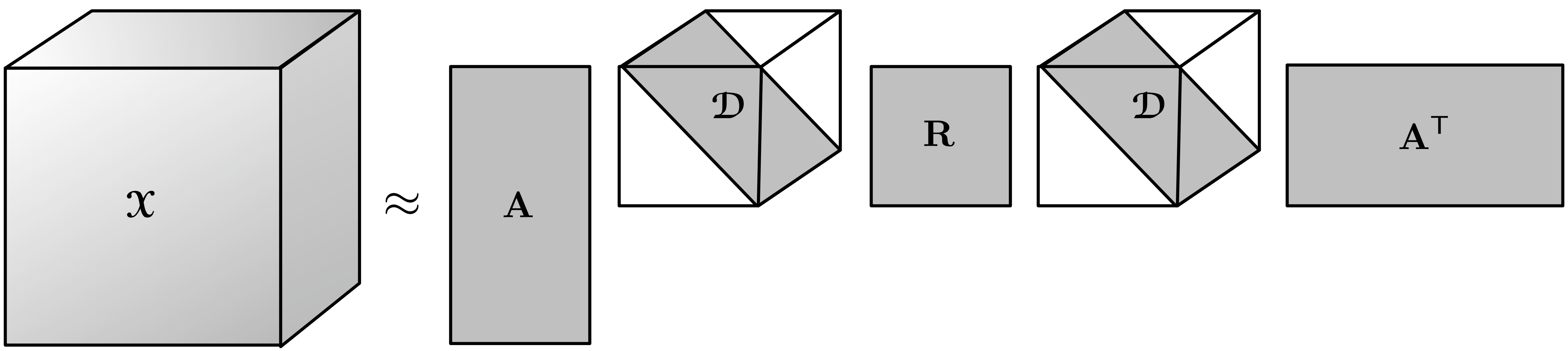


Fig. 5.2: Three-way DEDICOM model.

Kolda, T. G., & Bader, B. W. (2009). Tensor decompositions and applications. SIAM Review, 51(3), 455–500.

Computing DEDICOM: ASALSAN (1)

- We want to minimize $\sum_k ||\boldsymbol{X}_k - \boldsymbol{A}\boldsymbol{D}_k\boldsymbol{R}\boldsymbol{D}_k\boldsymbol{A}^T||$
- ASALSAN (Alternating Simultaneous Approximation, Least Squares, and Newton) is one way
  - Stack pairs ($\boldsymbol{X}_k$ $\boldsymbol{X}_k^T$): $\boldsymbol{Y}$=[$\boldsymbol{X}_1$ $\boldsymbol{X}_1^T$ … $\boldsymbol{X}_K\boldsymbol{X}_K^T$]
  - We get $||\boldsymbol{Y} - \boldsymbol{A}\boldsymbol{H}(\boldsymbol{I}_{2K} \otimes \boldsymbol{A}^T)||$ with $\boldsymbol{H} = [\boldsymbol{D}_1\boldsymbol{R}\boldsymbol{D}_1\ \boldsymbol{D}_1\boldsymbol{R}^T\boldsymbol{D}_1 \ldots \boldsymbol{D}_K\boldsymbol{R}\boldsymbol{D}_K\ \boldsymbol{D}_K\boldsymbol{R}^T\boldsymbol{D}_K]$

Bader, B. W., Harshman, R. A., & Kolda, T. G. (2007). Temporal Analysis of Semantic Graphs Using ASALSAN (pp. 33–42). Presented at the 7th IEEE International Conference on Data Mining, IEEE. doi:10.1109/ICDM.2007.54

Computing DEDICOM: ASALSAN (2)

- To update $\boldsymbol{A}$, fix right $\boldsymbol{A}$ and update the left
  $\boldsymbol{A} = \left(\sum_{k=1}^{K} (\boldsymbol{X}_k \boldsymbol{A} \boldsymbol{D}_k \boldsymbol{R}^T \boldsymbol{D}_k + \boldsymbol{X}_k^T \boldsymbol{A} \boldsymbol{D}_k \boldsymbol{R} \boldsymbol{D}_k)\right) \left(\sum_{k=1}^{K} (\boldsymbol{B}_k + \boldsymbol{C}_k)\right)^{-1}$
  - $\boldsymbol{B}_k = \boldsymbol{D}_k \boldsymbol{R} \boldsymbol{D}_k (\boldsymbol{A}^T \boldsymbol{A}) \boldsymbol{D}_k \boldsymbol{R}^T \boldsymbol{D}_k$ and $\boldsymbol{C}_k = \boldsymbol{D}_k \boldsymbol{R}^T \boldsymbol{D}_k (\boldsymbol{A}^T \boldsymbol{A}) \boldsymbol{D}_k \boldsymbol{R} \boldsymbol{D}_k$
- To update R, we use vectors:

$$\min_{\boldsymbol{R}} \left\| \begin{pmatrix} \mathrm{vec}(\boldsymbol{X}_1) \\ \vdots \\ \mathrm{vec}(\boldsymbol{X}_K) \end{pmatrix} - \begin{pmatrix} \boldsymbol{A}\boldsymbol{D}_1 \otimes \boldsymbol{A}\boldsymbol{D}_1 \\ \vdots \\ \boldsymbol{A}\boldsymbol{D}_K \otimes \boldsymbol{A}\boldsymbol{D}_K \end{pmatrix} \mathrm{vec}(\boldsymbol{R}) \right\|$$

- To update $\mathcal{D}$, use Newton's method for each slice $\boldsymbol{D}_k$

DEDICOM vs. RESCAL vs. INDSCAL vs. Tucker2

- RESCAL is a relaxed version of DEDICOM
  - Mixing matrix $\boldsymbol{R}$ is different for each slice
  - Easier to compute as there's no tensor $\mathcal{D}$
    - Algorithm similar to ASALSAN, but simpler
- RESCAL is to Tucker2 what INDSCAL is to CP
  - Share's INDSCAL's equal factor matrix
  - Uses Tucker2's core

The Non-Negative Variants

- Sometimes having non-negative factors is beneficial for data analysis
  - Improved interpretability
    - E.g. physical measurements
  - Sparsity
- All of the discussed methods can be cast into non-negative variants

Non-Negative CP

- The simplest way to compute non-negative CP is to use non-negative least-squares solver with the matricized equations
  - $\min_{\boldsymbol{A} \in \mathbb{R}_{+}^{N \times R}} \left\| \boldsymbol{X}_{(1)} - \boldsymbol{A}(\boldsymbol{C} \odot \boldsymbol{B})^T \right\|$
- Also multiplicative updates are possible
  - $a_{ir} = a_{ir} \frac{(\boldsymbol{X}_{(1)}\boldsymbol{Z})_{ir}}{(\boldsymbol{A}\boldsymbol{Z}^T\boldsymbol{Z})_{ir}}$ with $\boldsymbol{Z} = (\boldsymbol{C} \odot \boldsymbol{B})$
- Also other methods exist

Non-Negative Others

- Also non-negative Tucker[2|3] can be solved using multiplicative update rules
- Non-negative ASALSAN yields non-negative DEDICOM
  - Similar algorithm will work for RESCAL

Summary

- Many, many different tensor decomposition
  - User's responsibility to choose the correct one
    - How do the results look like?
    - What's the time complexity?
- Most algorithms are geared towards dense data
  - But many data analysis data are sparse

Suggested Reading

- In addition to those from last time:
- Acar, E., & Yener, B. (2009). Unsupervised Multiway Data Analysis: A Literature Survey. *IEEE Transactions on Knowledge and Data Engineering*, 21(1), 6–20. doi:10.1109/TKDE.2008.112
    - Shorter and more focused on applications than Kolda & Bader (2009)