Simplicity transformations for three-way arrays with symmetric slices

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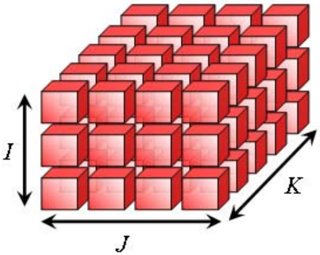
Outline

Definition



Idea

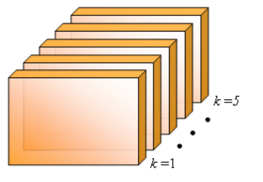
- three-way arrays: generalize matrix structure to 3D
- loaf-of-bread structure

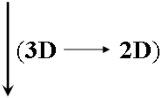
Examples of three-way data

- different anxiety measures, different circumstances, various subjects
- sales of different products, in different shops, in different weeks
- job requirements for various jobs, according to various job analysts

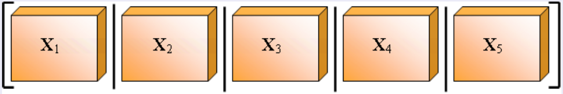
Unfolding a three-way array

Frontal slices ($\mathbf{X}_k$)





Matricizing $\underline{\mathbf{X}}$



Notation: $\underline{\mathbf{X}} = [\mathbf{X}_1 | \cdots | \mathbf{X}_K]$

PCA

X : matrix of order $I \times J$ (I=subjects, J=variables)
Goal: representation of variables in low-space dimension.

$$x_{ij} = \sum_{r=1}^{R} a_{ir} b_{jr} + e_{ij}$$

▸ ...

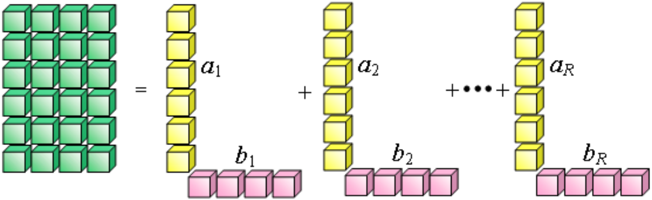
- x_{ij} = score of subject i on variable j
- a_{ir} = score of subject i on component r
- b_{jr} = loading of variable j on component r
- e_{ij} = residual error

PCA – other formulation

$$\mathbf{X} = \sum_{r=1}^{R} (\mathbf{a}_r \circ \mathbf{b}_r) + \mathbf{E}$$

▸ ...

- $\mathbf{a}_r \circ \mathbf{b}_r$: rank-1 matrix
- PCA decomposes $\mathbf{X}$ as a sum of rank-1 matrices
- rank($\mathbf{X}$): minimum R such that $\mathbf{E} \equiv \mathbf{0}$



CANDECOMP/PARAFAC (CP)

<u>X</u> : array of order $I \times J \times K$ (I=subjects, J=variables, K=situations)
<u>Goal</u>: find components for subjects, variables and situations.

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

▸ PCA

▸ ...

- x_{ijk} = score of subject i on variable j on situation k
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CP – other formulation

$$\underline{\mathbf{X}} = \sum_{r=1}^{R} (\mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r) + \underline{\mathbf{E}}$$

PCA
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- $\mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r$: rank-1 array
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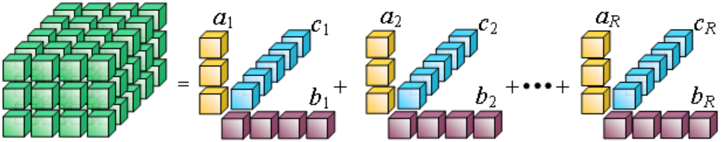

Tucker3

X : array of order $I \times J \times K$ (I=subjects, J=variables, K=situations)
Goal: find components for subjects, variables and situations.

$$x_{ijk} = \sum_{p=1}^{P}\sum_{q=1}^{Q}\sum_{r=1}^{R} g_{pqr}\left(a_{ip}b_{jq}c_{kr}\right) + e_{ijk},$$

CP

- x_{ijk} = score of subject i on variable j on situation k
- a_{ip} = score of subject i on component p
- b_{jq} = loading of variable j on component q
- c_{kr} = loading of situation k on component r
- g_{pqr} = weight (core array **G**, order $P \times Q \times R$)
- e_{ijk} = residual error

Tucker3 – other formulations

$$\underline{\mathbf{X}} = \sum_{p=1}^{P}\sum_{q=1}^{Q}\sum_{r=1}^{R} g_{pqr}\left(\mathbf{a}_p \circ \mathbf{b}_q \circ \mathbf{c}_r\right) + \underline{\mathbf{E}}$$

CP

- $\mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r$: rank-1 array
- Tucker3 decomposes $\underline{\mathbf{X}}$ as a sum of rank-1 arrays
- rank($\underline{\mathbf{X}}$)$\leqslant PQR$ (usually rank($\underline{\mathbf{X}}$) $\ll PQR$)

Formula using unfolded notation

$$\underline{\mathbf{X}}\ (I \times J \times K) \longrightarrow \mathbf{X} = [\mathbf{X}_1|\mathbf{X}_2|\cdots|\mathbf{X}_K]\ \text{(fitted part)}$$

$$\underline{\mathbf{G}}\ (P \times Q \times R) \longrightarrow \mathbf{G} = [\mathbf{G}_1|\mathbf{G}_2|\cdots|\mathbf{G}_R]$$

$$\mathbf{X} = \mathbf{AG}(\mathbf{C}' \otimes \mathbf{B}')$$

Tucker3 – seeing CP as particular situation

- Tucker3 reduces to Candecomp/Parafac when the core array has a super-diagonal form:

$$\underline{\mathbf{G}} = \left[\begin{array}{cccc|cccc|c|cccc} 1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & & 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 & 0 & 1 & \cdots & 0 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & & 0 & 0 & \cdots & 1 \end{array}\right]$$

- only interactions between corresponding components are accounted for in CP

Tucker3 – freedom of rotation

PCA's freedom of rotation (motivation)

S nonsingular

$$\begin{aligned} \mathbf{X} &= \mathbf{A}\mathbf{B}' \\ &= (\mathbf{A}\mathbf{S})(\mathbf{S}^{-1}\mathbf{B}') \end{aligned}$$

Tucker3's freedom of rotation

S, **T**, **U** nonsingular

$$\begin{aligned} \mathbf{A} &\longrightarrow \mathbf{A}(\mathbf{S}')^{-1} \\ \mathbf{B} &\longrightarrow \mathbf{B}(\mathbf{T}')^{-1} \\ \mathbf{C} &\longrightarrow \mathbf{C}(\mathbf{U}')^{-1} \\ \mathbf{G}_a = [\mathbf{G}_1 | \cdots | \mathbf{G}_R] &\longrightarrow \mathbf{S}'\mathbf{G}_a(\mathbf{U} \otimes \mathbf{T}) \end{aligned}$$

Tucker transformation

Simplifying three-way arrays

Goal

Find suitable linear combinations of frontal (and/or lateral and/or horizontal) slices that allow transforming $\underline{\mathbf{X}}$ into an "equivalent" array with many zero entries.

Formally: **S**, **T**, **U**=?: $\qquad \mathbf{H} = \mathbf{SX}(\mathbf{U} \otimes \mathbf{T})$

$\downarrow$

- many zero entries = few nonzero entries
- weight of $\underline{\mathbf{H}}$ = # nonzero entries of $\underline{\mathbf{H}}$

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Simplifying three-way arrays

Why?

1. Facilitate interpretation of 3PCA decompositions

   Example: rotate $\underline{\mathbf{G}}$ so that several entries become zero

   ↓

   less interactions of components to account for during interpretion of 3PCA

2. Constrained 3PCA: distinguish between tautologies and non-trivial models

3. Mathematical applications: typical rank, maximal rank

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Some examples (I-III)

- Cohen (1974, 1975), MacCallum (1976), Kroonenberg (1983): "diagonalize" frontal slices of $\underline{\mathbf{G}}$ ($P = Q$)
- Kiers (1992): "super-diagonalize" $\underline{\mathbf{G}}$ ($P = Q = R$)
- Kiers (1998): SIMPLIMAX
  $\underline{\mathbf{G}} \longrightarrow$ minimize ssq (m smallest elements)

$\underline{\mathbf{X}}$ of order $P \times Q \times R$, $P = QR$

Example: $\underline{\mathbf{X}}$ of order $6 \times 3 \times 2$

$$\underline{\mathbf{X}} \longrightarrow \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right] = \mathbf{X}^{-1}\mathbf{X}(\mathbf{I}_2 \otimes \mathbf{I}_3)$$

Some examples (II-III)

$\underline{\mathbf{X}}$ of order $P \times Q \times R$, $P = QR - 1$

Murakami, Ten Berge & Kiers (1998)
Example: $\underline{\mathbf{X}}$ of order $5 \times 3 \times 2$

$$\underline{\mathbf{X}} \longrightarrow \left[\begin{array}{ccc|ccc} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ \mu_1 & 0 & 0 & 0 & \mu_2 & 0 \end{array}\right]$$

Some examples (III-III)

$\underline{\mathbf{X}}$ of order $P \times Q \times 2$

- $P > Q$: Ten Berge & Kiers (1999)

$$\underline{\mathbf{X}} \longrightarrow \left[\begin{array}{c|c} \mathbf{I}_Q & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{I}_Q \end{array} \right]$$

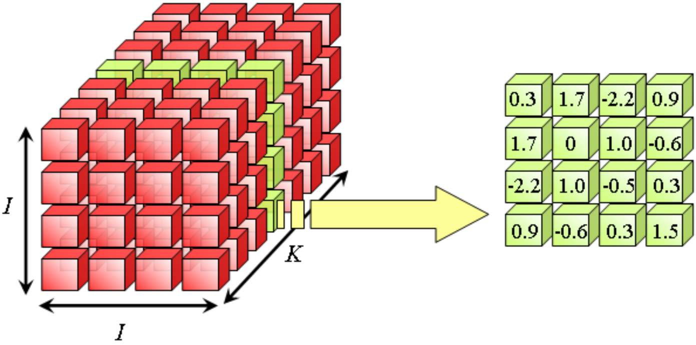
- $P = Q$: Rocci & Ten Berge (2002)
  Example: $\underline{\mathbf{X}} = [\mathbf{X}_1 | \mathbf{X}_2]$ of order $3 \times 3 \times 2$

$$\left[\begin{array}{ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & \mu_1 & 0 & 0 & \mu_2 \end{array} \right] \quad \text{or} \quad \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & \mu \\ 0 & 0 & 1 & 0 & -\mu & 0 \end{array} \right]$$

($\mathbf{X}_1^{-1}\mathbf{X}_2$ has real eigs.) ($\mathbf{X}_1^{-1}\mathbf{X}_2$ has complex eigs.)

Our goal: simplifying arrays with SYMMETRIC slices

Example: set of similarity matrices over time



Symmetric-slice arrays

- $\underline{\mathbf{X}} = [\mathbf{X}_1 | \cdots | \mathbf{X}_K]$: order $I \times I \times K$
  - assume: $\underline{\mathbf{X}}$ is randomly sampled from a continuous distribution with symmetry constraint ($\mathbf{X}_k$ symmetric, $\forall k$)
  - slices $\mathbf{X}_k$ linearly independent
  - number of slices: $K = 1, 2, \ldots, \underbrace{\frac{I(I+1)}{2}}_{K_{\max}}$
- symmetry-preserving transformation of $\underline{\mathbf{X}}$
  - $\mathbf{S}_{I \times I}$, $\mathbf{U}_{K \times K}$ nonsingular

$$\mathbf{H}_l = \mathbf{S}' \left(\sum_k u_{kl} \mathbf{X}_k \right) \mathbf{S}, \quad l = 1, 2, \ldots, K$$

  - GOAL: introduce as many zeros in $\underline{\mathbf{H}}$ as possible
- Orthogonal Complement Method: "symmetric" version

Symmetric slice $I \times I \times K_{max}$ arrays

- $\{$frontal slices$\}$ = basis for the space of symmetric $I \times I$ matrices
- simple basis for the same space (Rocci & Ten Berge(1994)): (notation: $\mathbf{e}_i$= column i of $\mathbf{I}_I$)

$$\mathbf{e}_i\mathbf{e}_i', \quad i = 1, \ldots, I$$
$$\mathbf{e}_i\mathbf{e}_j' + \mathbf{e}_j\mathbf{e}_i', \quad 1 \leqslant i < j \leqslant I$$

Example: $I = 3$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

- frontal slice mix suffices

Symmetric slice $3 \times 3 \times K$ arrays

- $K_{max} = 6$, so $K = 1, 2, 3, 4, 5, 6$
- $3 \times 3 \times 6$: done (K_{max} situation)
- $3 \times 3 \times 1$: use EVD

$$\underline{\mathbf{X}} \longrightarrow \begin{bmatrix} d_1 & 0 & 0 \\ 0 & d_2 & 0 \\ 0 & 0 & d_3 \end{bmatrix} ; \text{ if } d_2 d_3 < 0 : \begin{bmatrix} d_1 & 0 & 0 \\ 0 & 0 & 2d_2 \\ 0 & 2d_2 & 0 \end{bmatrix}$$

- $3 \times 3 \times 5$ = orthogonal complement of $3 \times 3 \times 1$

$$\underline{\mathbf{X}} \longrightarrow \left[\begin{array}{ccc|ccc|ccc|ccc|ccc} 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & \alpha & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & \beta & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \end{array}\right]$$

$$\left[\begin{array}{ccc|ccc|ccc|ccc|ccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & \alpha & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \end{array}\right]$$

Conclusion for $3 \times 3 \times 5$:

- weight 10 is always possible
- if $\underline{\mathbf{X}}^c$ has eigenvalues of both signs then weight 9 is possible

Symmetric slice $3 \times 3 \times K$ arrays

- $3 \times 3 \times 2$: see EVD($\mathbf{X}_1^{-1}\mathbf{X}_2$)
  - real eigenvalues

$$\underline{\mathbf{X}} \longrightarrow \left[\begin{array}{ccc|ccc} 0 & 0 & 0 & \beta & 0 & 0 \\ 0 & \alpha & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \end{array}\right]; \text{ also: } \left[\begin{array}{ccc|ccc} -\alpha & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 \end{array}\right]$$

  - complex eigenvalues

$$\underline{\mathbf{X}} \longrightarrow \left[\begin{array}{ccc|ccc} -\alpha & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 & 1 & 0 \end{array}\right]$$

Conclusion for $3 \times 3 \times 2$:

- weight 5 is always possible
- if $\mathbf{X}_1^{-1}\mathbf{X}_2$ has real eigenvalues then weight 4 is possible

Symmetric slice $3 \times 3 \times K$ arrays

- $3 \times 3 \times 4$ = orthogonal complement of $3 \times 3 \times 2$

$$\left[\begin{array}{ccc|ccc|ccc|ccc} 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & \alpha & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \delta\alpha & 0 & 0 & 0 & 1 & 0 & 0 \end{array}\right]$$

▸ . . .

($\delta = 1/-1$ in real/complex case)

Conclusion for $3 \times 3 \times 4$:
  - weight 8 is always possible

- $3 \times 3 \times 3$: still open!
  - when a $3 \times 3 \times 3$ array has an orthogonal complement, it is also $3 \times 3 \times 3$...
  - simulation: a weight 9 pattern seems to be possible almost 90% of the times
  - to be continued (...)

Symmetric slice $4 \times 4 \times K$ arrays

- $K_{\text{max}} = 10$, so $K = 1, 2, \cdots, 8, 9, 10$
- $4 \times 4 \times 10$: done (K_{max} situation)
- $4 \times 4 \times 1$: use EVD

$$\text{in general: } \underline{\mathbf{X}} \longrightarrow \begin{bmatrix} d_1 & 0 & 0 & 0 \\ 0 & d_2 & 0 & 0 \\ 0 & 0 & d_3 & 0 \\ 0 & 0 & 0 & d_4 \end{bmatrix}$$

$$\begin{aligned} \text{if } d_1, d_2, d_3 &> 0 \\ d_4 &< 0 \end{aligned} \longrightarrow \begin{bmatrix} d_1 & 0 & 0 & 0 \\ 0 & d_2 & 0 & 0 \\ 0 & 0 & 0 & 2d_3 \\ 0 & 0 & 2d_3 & 0 \end{bmatrix}$$

$$\begin{aligned} \text{if } d_1, d_3 &> 0 \\ d_2, d_4 &< 0 \end{aligned} \longrightarrow \begin{bmatrix} 0 & 2d_1 & 0 & 0 \\ 2d_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2d_3 \\ 0 & 0 & 2d_3 & 0 \end{bmatrix}$$

- $4 \times 4 \times 9$ = orthogonal complement of $4 \times 4 \times 1$
  - weight 18 is always possible
  - depending on the signs of eigs($\underline{\mathbf{X}}^c$) we can have weight 17 or 16

Symmetric slice $4 \times 4 \times K$ arrays

- $4 \times 4 \times 2$: see EVD($\mathbf{X}_1^{-1}\mathbf{X}_2$)
  - real eigenvalues: weight 6

$$\left[\begin{array}{cccc|cccc} 0 & 0 & 0 & 0 & \gamma & 0 & 0 & 0 \\ 0 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \beta & 0 & 0 & 0 & \delta & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \end{array}\right]$$

  - one pair of complex eigenvalues: weight 7

$$\left[\begin{array}{cccc|cccc} \alpha & 0 & 0 & 0 & \gamma & 0 & 0 & 0 \\ 0 & \beta & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 \end{array}\right]$$

  - two pairs of complex eigenvalues: weight 8

$$\left[\begin{array}{cccc|cccc} 1 & 0 & 0 & 0 & 0 & \gamma & 0 & 0 \\ 0 & -1 & 0 & 0 & \gamma & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 \end{array}\right]$$

Symmetric slice $4 \times 4 \times K$ arrays

- $4 \times 4 \times 8$ = orthogonal complement of $4 \times 4 \times 2$
  - any symmetric slice $4 \times 4 \times 8$ array can almost surely be simplified into one out of two weight 18 arrays

Example: one of the targets

$$\left[\begin{array}{cccc|cccc|cccc|cccc|}
\star & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \star & 0 & 0 \\
0 & \star & 0 & 0 & 0 & \star & 0 & 0 & 0 & \star & 0 & 0 & \star & 0 & 0 & 0 \\
0 & 0 & 0 & \star & 0 & 0 & \star & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \star & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \star & 0 & 0 & 0 & 0
\end{array}\right.$$

$$\left.\begin{array}{cccc|cccc|cccc|cccc}
0 & 0 & \star & 0 & 0 & 0 & 0 & \star & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \star & 0 & 0 & 0 & 0 & \star \\
\star & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \star & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \star & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \star & 0 & 0
\end{array}\right]$$

Maximal simplicity

<u>Question</u>: can simpler targets be found for the cases previously presented?

<u>Answer</u>:

- $3 \times 3 \times K$ for $K = 1, 2, 4, 5, 6$: NO (proved)
- $4 \times 4 \times K$ for $K = 8, 9$: NO(?) (simulation)

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Example of application: typical rank

- $\underline{\mathbf{X}}$: symmetric slice $3 \times 3 \times 4$ array
- Ten Berge et al. (2004)

  typical rank ($\underline{\mathbf{X}}$)= $\{4, 5\}$

- rank=4?, rank=5?

  Check if roots of a certain fourth degree polynomial are real and distinct.

Using ▸ $3 \times 3 \times 4$ simple form, and applying the same reasoning as in Ten Berge et al. (2004), we conclude that:

- rank ($\underline{\mathbf{X}}$)=4 iif $\delta = 1$ and $\alpha > 0$ (and rank is 5 otherwise)
- a CP decomposition is now straightforward

Example: rank=4

$$\mathbf{A} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 0 & \sqrt{\alpha} & -\sqrt{\alpha} \\ \sqrt{\alpha} & -\sqrt{\alpha} & 0 & 0 \end{bmatrix}, \mathbf{C} = \begin{bmatrix} 0 & 0 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0 & 0 \\ 0 & 0 & 0.5\sqrt{\alpha^{-1}} & -0.5\sqrt{\alpha^{-1}} \\ 0.5\sqrt{\alpha^{-1}} & -0.5\sqrt{\alpha^{-1}} & 0 & 0 \end{bmatrix}$$

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Conclusions. Considerations. Developments

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- simplification achieved for some types of arrays with symmetric frontal slices; closed form rotation matrices available
- maximal simplicity achieved (mathematically proved or empirically verified via SIMPLIMAX)
- typical rank considerations come as nice follow-ups

Considerations

- 3PCA core arrays are not “randomly sampled from a continuous distribution”, but do behave as if they were
- valid contribution for Matrix Theory: simultaneous reduction of more than a pair of matrices to sparse forms is scarce

Developments

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- address issues like: maximal simplicity, typical rank

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