Simplicity transformations for three-way arrays with symmetric slices

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Definitions. Concepts. Notation

- $\underline{\mathbf{X}}$: $I \times J \times K$ three-way array
  $\mathbf{X}_1, ..., \mathbf{X}_K$: $I \times J$ frontal slices

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

- 3PCA: find $\mathbf{A}_{I\times P}$, $\mathbf{B}_{J\times Q}$, $\mathbf{C}_{K\times R}$, $\underline{\mathbf{G}}_{P\times Q\times R}$ to minimize $\sum_k \mathrm{tr}(\mathbf{E}_k'\mathbf{E}_k)$

$$\boxed{\underline{\mathbf{X}} = \sum_p \sum_q \sum_r g_{pqr} \left(\mathbf{a}_p \circ \mathbf{b}_q \circ \mathbf{c}_r\right) + \underline{\mathbf{E}}}$$

- CP: constrained 3PCA ($P = Q = R$, $\underline{\mathbf{G}}$ superunit diagonal)

$$\boxed{\underline{\mathbf{X}} = \sum_r \left(\mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r\right) + \underline{\mathbf{E}}}$$

- Typical rank: minimal number of components R that allow a perfect CP decomposition

Definitions. Concepts. Notation

- Weight of an array = # nonzero entries
- 3PCA is not unique: for any nonsingular $\mathbf{S}_{P\times P}$, $\mathbf{T}_{Q\times Q}$, $\mathbf{U}_{R\times R}$

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

Tucker transformation

Why?

Challenge: given $\underline{\mathbf{X}}$, find suitable $\mathbf{S}$, $\mathbf{T}$, $\mathbf{U}$ such that $\mathbf{S}\underline{\mathbf{X}}(\mathbf{U} \otimes \mathbf{T})$ has many zero entries (small weight)

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

Results available so far (I)

- 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)
- Murakami et al. (1998)

  $P = QR - 1$

  Example: $P = 5, Q = 3, R = 2$

$$\mathbf{G}_a = [\mathbf{G}_1 | \mathbf{G}_2] \longrightarrow \left[\begin{array}{ccc|ccc} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ \mu_1 & 0 & 0 & 0 & \mu_2 & 0 \end{array}\right]$$

Results available so far (II)

- Ten Berge & Kiers (1999)
  $P \times Q \times 2$, $P > Q$
  $$\mathbf{G}_a = [\mathbf{G}_1|\mathbf{G}_2] \longrightarrow \left[\begin{array}{c|c} \mathbf{I}_Q & \mathbf{0} \\ \mathbf{0} & \mathbf{I}_Q \end{array}\right]$$
- Ten Berge et al. (2000): Multiple orthonormality
- Rocci & Ten Berge (2002)
  - $P \times P \times 2$
    Example: $P = 3$
    $$\mathbf{G}_a = \longrightarrow \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & a & 0 & 0 & b \end{array}\right] \text{ or } \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & a \\ 0 & 0 & 1 & 0 & -a & 0 \end{array}\right]$$
  - Orthogonal Complement Algorithm

What about symmetric slice arrays?

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 $2 \times 2 \times K$ arrays

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

$$\underline{\mathbf{X}} \longrightarrow \begin{bmatrix} 1 & 0 \\ 0 & \alpha \end{bmatrix};\ \text{if } \alpha < 0 : \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

- $2 \times 2 \times 2$ = orthogonal complement of $2 \times 2 \times 1$

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

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

- weight 4 is always possible
- if $\underline{\mathbf{X}}^c$ has eigenvalues of both signs then weight 2 is possible

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 $3 \times 3 \times 1$

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

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

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

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

<u>Conclusion for $3 \times 3 \times 2$:</u>

- 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 $3 \times 3 \times 2$

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

▸ $3 \times 3 \times 4$

($\delta = 1/-1$ 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 $3 \times 3 \times 3 \ldots$
  - 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

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

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

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

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

- $4 \times 4 \times 9$ = 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

Question: can simpler targets be found for the cases previously presented?

Answer:

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

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

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

Conclusions. Considerations. Developments

Conclusions

- 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

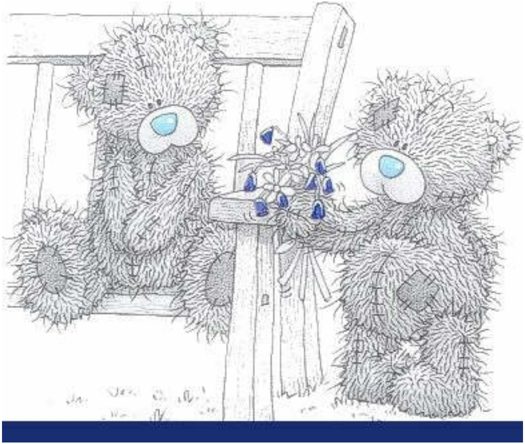
Considerations

- 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

- extend results to other orders
- address issues like: maximal simplicity, typical rank

Muchas gracias!



QUESTIONS?