university of groningen

Candecomp / Parafac

from diverging components to a decomposition in block terms

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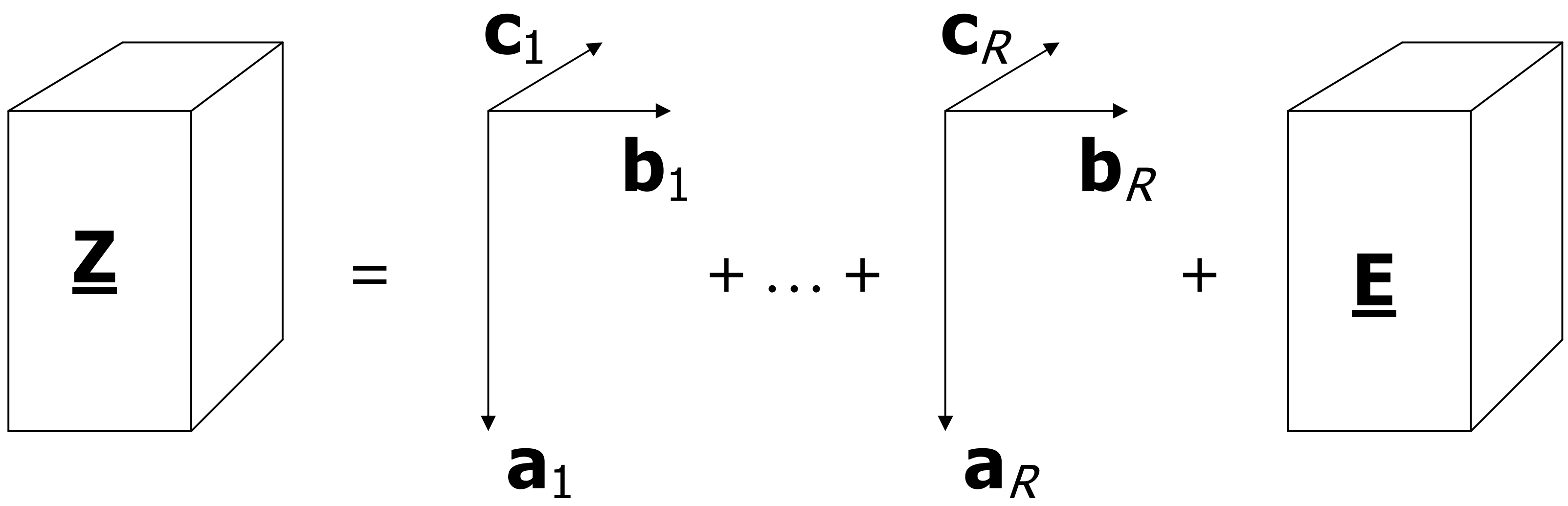
Candecomp / Parafac (CP) model

$$\underline{\underline{\mathbf{Z}}} = \mathbf{a}_1 \circ \mathbf{b}_1 \circ \mathbf{c}_1 + \ldots + \mathbf{a}_R \circ \mathbf{b}_R \circ \mathbf{c}_R + \underline{\underline{\mathbf{E}}}$$

$\mathbf{Z}_k = \mathbf{A} \ \mathbf{C}_k \ \mathbf{B}^{\mathrm{T}} + \mathbf{E}_k$ frontal slice k

$\mathbf{C}_k$ = diag(row k of $\mathbf{C}$)



$\text{rank}(\underline{\underline{\mathbf{Z}}}) = \min \{R : \underline{\underline{\mathbf{Z}}} = \mathbf{a}_1 \circ \mathbf{b}_1 \circ \mathbf{c}_1 + \ldots + \mathbf{a}_R \circ \mathbf{b}_R \circ \mathbf{c}_R \}$

$\text{rank}(\mathbf{a} \circ \mathbf{b} \circ \mathbf{c}) = 1$

<u>Computation of CP solution</u>

minimize ssq($\underline{\underline{\mathbf{E}}}$) over ($\mathbf{A}$,$\mathbf{B}$,$\mathbf{C}$)

optimal $\underline{\underline{\mathbf{X}}}$ = ($\mathbf{A}$,$\mathbf{B}$,$\mathbf{C}$) is a best rank-R approximation of $\underline{\underline{\mathbf{Z}}}$

computation ($\mathbf{A}$,$\mathbf{B}$,$\mathbf{C}$) by iterative algorithm

The Candecomp / Parafac problem

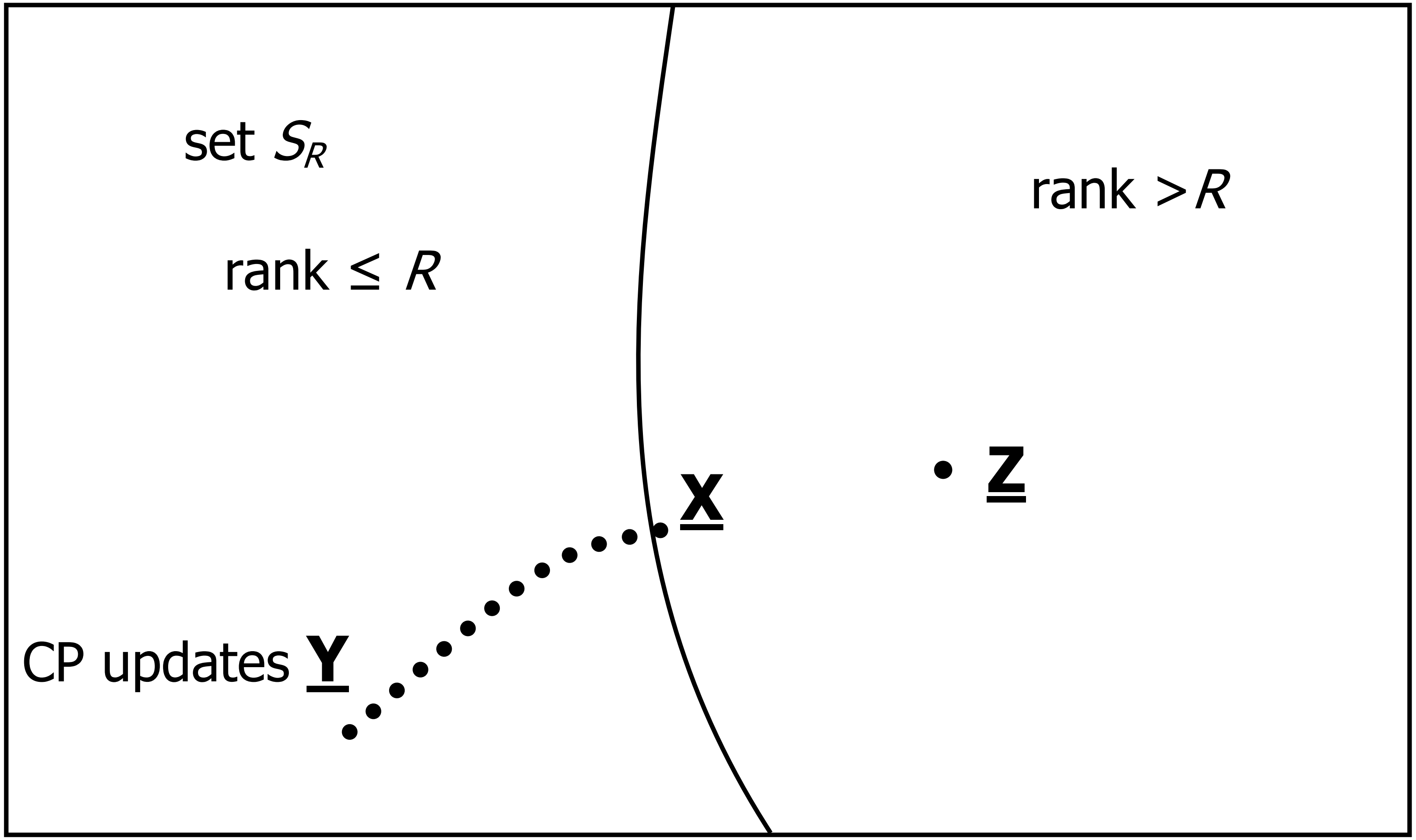
Minimize	$\text{ssq}(\underline{\mathbf{Z}} - \underline{\mathbf{Y}})$
over	$S_R = \{\ \underline{\mathbf{Y}}$ with rank $\leq R\ \}$

➔ if $\underline{\mathbf{Z}} \notin S_R$, then an optimal solution $\underline{\mathbf{X}}$ (if it exists) will be a boundary point of S_R

But: the set S_R is not closed for $R \geq 2$

Bini et al. (1979), Paatero (2000), Lim (2004)
De Silva & Lim (2008)

A misleading picture



Suppose $\underline{\mathbf{Y}} = (\mathbf{A},\mathbf{B},\mathbf{C}) \longrightarrow$ optimal $\underline{\mathbf{X}}$ and $\underline{\mathbf{X}} \notin S_R$

Then, some rank-1 terms $\mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r$ converge to

linear dependency and **infinite norm**

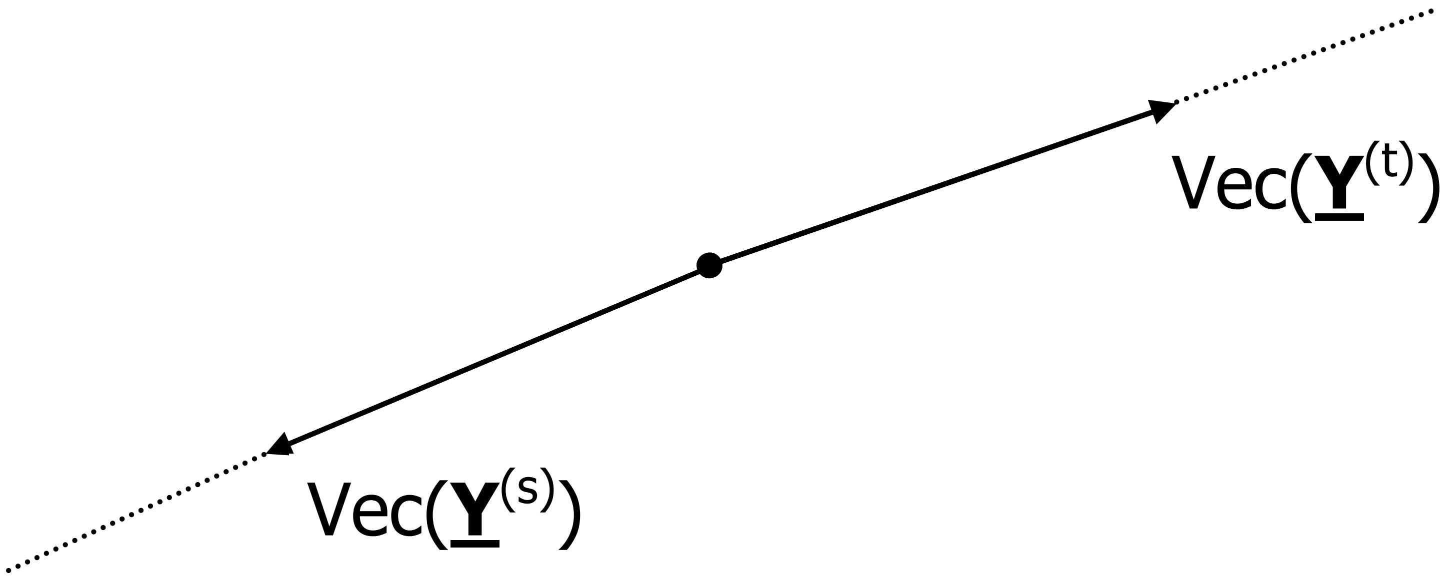
➔ diverging components ("degeneracy")

In practice also: slow convergence of CP algorithm ("swamp")

Kruskal et al. (1989), Krijnen et al. (2008)

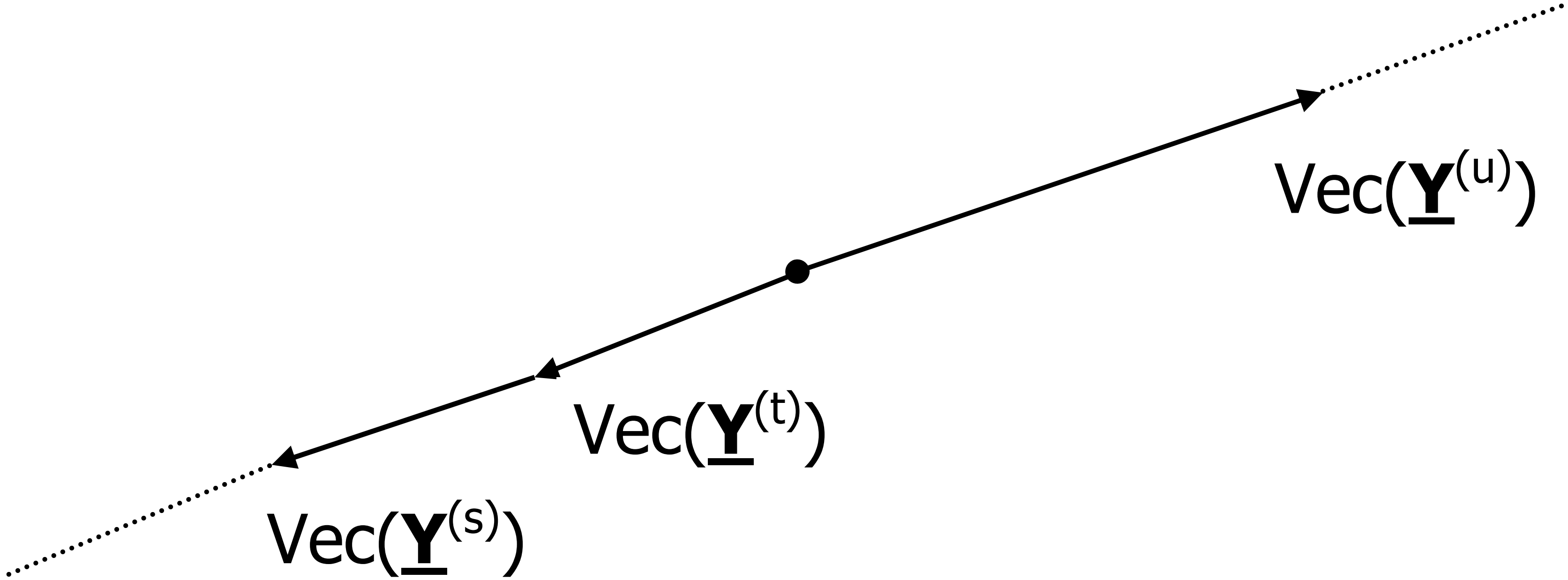
Two diverging components

$\underline{\mathbf{Y}}^{(s)} = \mathbf{a}_s \circ \mathbf{b}_s \circ \mathbf{c}_s$ $\qquad$ $\underline{\mathbf{Y}}^{(t)} = \mathbf{a}_t \circ \mathbf{b}_t \circ \mathbf{c}_t$



$\underline{\mathbf{Y}}^{(s)} + \underline{\mathbf{Y}}^{(t)}$ remains "small" and contributes to a better CP fit

Three diverging components



$\underline{\mathbf{Y}}^{(s)} + \underline{\mathbf{Y}}^{(t)} + \underline{\mathbf{Y}}^{(u)}$ remains “small” and contributes to a better CP fit

Example: $3\times3\times2$ with $R = 3$

$$\mathbf{A} = \begin{bmatrix} 0.48 & 0.46 & -0.47 \\ -0.66 & -0.65 & 0.66 \\ -0.57 & -0.60 & 0.58 \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} 0.72 & -0.69 & 0.71 \\ 0.61 & -0.65 & 0.63 \\ 0.33 & -0.31 & 0.32 \end{bmatrix}$$

$$\mathbf{C} = \begin{bmatrix} 653 & -625 & 1278 \\ 2162 & -2239 & 4398 \end{bmatrix}$$

$$\underline{\mathbf{Y}}^{(1)} \approx \underline{\mathbf{Y}}^{(2)} \approx -2\ \underline{\mathbf{Y}}^{(3)}$$

How often do diverging components occur ?

array $\underline{\underline{\mathbf{Z}}}$	rank($\underline{\underline{\mathbf{Z}}}$)	R	diverging components?
$2 \times 2 \times 2$	3	$R = 2$	always *
$I \times I \times 2$	$I+1$	$R = I$	always +
$I \times I \times 2$	I or $I+1$	$R < I$	sometimes +
$I \times J \times 2$, $I > J$	$\min(I, 2J)$	$R \leq J$	sometimes +

* any $\underline{\underline{\mathbf{Z}}}$; proven by De Silva & Lim (2008)

+ random $\underline{\underline{\mathbf{Z}}}$; conjectured/partial proof by Stegeman (2008)
see Stegeman (2007) for several $I \times J \times 3$ cases

Some remarks

1. If the CP problem does not have an optimal solution, then **any** CP algorithm trying to minimize ssq($\underline{\mathbf{Z}}$ – $\underline{\mathbf{Y}}$) will terminate with diverging components.

(Krijnen et al., 2008)

2. We do **not** consider cases of diverging components where an optimal CP solution exists, but the CP algorithm gets slow or stuck near the boundary.

(Mitchell & Burdick, 1994; Paatero, 2000; Stegeman, 2009)

How to avoid diverging components (1)

➔ make sure CP has an optimal solution

By imposing restrictions in CP:

- **A**, **B** or **C** is restricted to have orthogonal columns (Krijnen et al., 2008)
- **Z̲** is nonnegative and **A**, **B** and **C** are restricted to be nonnegative (Lim, 2005; Lim & Comon, 2009)

How to avoid diverging components (2)

➔ change the CP problem into: (De Silva & Lim, 2008)

Minimize	ssq(**Z** – **Y**)
over	closure of S_R

What is needed?

➔ Complete characterization of boundary points

➔ Algorithm to find an optimal boundary point

Tucker3 model and block decomposition

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

$\underline{\mathbf{Z}} = (\mathbf{A},\mathbf{B},\mathbf{C}) \cdot \underline{\mathbf{G}} + \underline{\mathbf{E}}$ with $\underline{\mathbf{G}}$: $R \times P \times Q$ core array

(Tucker, 1966)

$\underline{\mathbf{Z}} = \sum_{d} (\mathbf{A}_d, \mathbf{B}_d, \mathbf{C}_d) \cdot \underline{\mathbf{G}}_d$ decomposition in block terms

(De Lathauwer, 2008)

$I \times J \times 2$ with $R \leq \min(I,J)$

$\underline{\mathbf{Y}}$ in closure of S_R satisfies $\underline{\mathbf{Y}} = (\mathbf{S},\mathbf{T},\mathbf{I}_2)\cdot\underline{\mathbf{H}}$

with $\mathbf{S}^{\mathsf{T}}\mathbf{S} = \mathbf{T}^{\mathsf{T}}\mathbf{T} = \mathbf{I}_R$ and

$\underline{\mathbf{H}}$ ($R \times R \times 2$) in closure of $S_R{}'$

$\mathrm{rank}(\underline{\mathbf{Y}}) = \mathrm{rank}(\underline{\mathbf{H}})$

$\underline{\mathbf{Y}}$ boundary point of S_R $\Leftrightarrow$ $\underline{\mathbf{H}}$ boundary point of $S_R{}'$

De Silva & Lim (2008)

Classification of $R \times R \times 2$ arrays w.r.t. S_R'

$\underline{\mathbf{H}} = [\mathbf{H}_1 \mid \mathbf{H}_2]$ with nonsingular $\mathbf{H}_1$

Interior of S_R' : $\mathbf{H}_2(\mathbf{H}_1)^{-1}$ has R real distinct eigenvalues
Boundary S_R' : $\mathbf{H}_2(\mathbf{H}_1)^{-1}$ has R real eigenvalues, not all distinct rank($\underline{\mathbf{H}}$) = R if $\mathbf{H}_2(\mathbf{H}_1)^{-1}$ diagonalizable rank($\underline{\mathbf{H}}$) > R if $\mathbf{H}_2(\mathbf{H}_1)^{-1}$ not diag.
Exterior of S_R' : $\mathbf{H}_2(\mathbf{H}_1)^{-1}$ has some complex eigenvalues

$\underline{\mathbf{H}} = [\mathbf{H}_1 \mid \mathbf{H}_2]$ with singular $\mathbf{H}_1$

$\underline{\mathbf{G}} = (\mathbf{I}_R, \mathbf{I}_R, \mathbf{U}) \cdot \underline{\mathbf{H}}$ with some $\mathbf{U}$ (2×2) nonsingular

- Interior / boundary / exterior same for $\underline{\mathbf{G}}$ and $\underline{\mathbf{H}}$
- If $\mathbf{G}_1$ nonsingular, then classification as above
- If $\mathbf{G}_1$ singular for all $\mathbf{U}$, then boundary point

Ja' Ja' (1979), Ten Berge (1991), Ten Berge & Kiers (1999)
Stegeman (2006,2010)

Generalized Schur Decomposition ($I \times J \times 2$)

$\mathbf{Z}_k = \mathbf{Q}_a \, \mathbf{R}_k \, \mathbf{Q}_b^T + \mathbf{E}_k$ slice $k = 1,2$

with $\mathbf{Q}_a^T \mathbf{Q}_a = \mathbf{Q}_b^T \mathbf{Q}_b = \mathbf{I}_R$, $\mathbf{R}_k$ ($R \times R$) upper triangular

$\underline{\underline{\mathbf{Z}}} = (\mathbf{Q}_a, \mathbf{Q}_b, \mathbf{I}_2) \cdot \underline{\mathbf{R}} + \underline{\underline{\mathbf{E}}}$ with $\underline{\mathbf{R}} = [\mathbf{R}_1 \mid \mathbf{R}_2]$

closure of S_R equals $\{ \underline{\mathbf{Y}} : \underline{\mathbf{Y}} = (\mathbf{Q}_a, \mathbf{Q}_b, \mathbf{I}_2) \cdot \underline{\mathbf{R}} \}$

Stegeman & De Lathauwer (2009), Stegeman (2010)

- Jacobi-type algorithm fits GSD to $\underline{\underline{\mathbf{Z}}}$ (fast!) and obtains optimal solution $\underline{\underline{\mathbf{X}}}$ with GSD $(\mathbf{Q}_a, \mathbf{Q}_b, \mathbf{R}_1, \mathbf{R}_2)$

- Jordan form $\mathbf{R}_2(\mathbf{R}_1)^{-1} = \mathbf{P}\,\mathbf{J}\,\mathbf{P}^{-1}$ gives decomp. of $\underline{\underline{\mathbf{X}}}$

$$\mathbf{X}_1 = \mathbf{Q}_a\,\mathbf{R}_1\,\mathbf{Q}_b^T = (\mathbf{Q}_a\,\mathbf{P})\ \mathbf{I}_R\ (\mathbf{P}^{-1}\,\mathbf{R}_1\,\mathbf{Q}_b^T)$$

$$\mathbf{X}_2 = \mathbf{Q}_a\,\mathbf{R}_2\,\mathbf{Q}_b^T = (\mathbf{Q}_a\,\mathbf{P})\ \mathbf{J}\ (\mathbf{P}^{-1}\,\mathbf{R}_1\,\mathbf{Q}_b^T)$$

1×1 Jordan block $\Leftrightarrow$ nondiverging component

$m\times m$ Jordan block $\Leftrightarrow$ limit of m diverging comp.

Stegeman & De Lathauwer (2009)

Alternative representation :

$$\underline{\mathbf{X}} = (\mathbf{A},\mathbf{B},\mathbf{C}) + \sum_{d} (\mathbf{K}_d,\mathbf{L}_d,\mathbf{M}_d)\cdot\underline{\mathbf{G}}_d$$

$(\mathbf{A},\mathbf{B},\mathbf{C})$: CP part of nondiverging components

$(\mathbf{K}_d,\mathbf{L}_d,\mathbf{M}_d)\cdot\underline{\mathbf{G}}_d$: Tucker3 limit of m diverging comp.

$$\text{with } \underline{\mathbf{G}}_d \ (m\times m\times 2) = \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{array}\right] \quad \text{for } m=3$$

Stegeman & De Lathauwer (2009)

Proposal for $I \times J \times K$ with $R \leq \min(I,J,K)$

(I) First try CP algorithm. If diverging components occur:

(II) Write each group of m div. comp. as $(\mathbf{S}_d,\mathbf{T}_d,\mathbf{U}_d)\cdot\underline{\mathbf{H}}_d$ with $(\mathbf{S}_d,\mathbf{T}_d,\mathbf{U}_d)$ orthonormal columns and $\underline{\mathbf{H}}_d$ $(m \times m \times m)$ upper triangular slices

(III) Using $(\mathbf{S}_d,\mathbf{T}_d,\mathbf{U}_d)\cdot\underline{\mathbf{H}}_d$ as initial values, fit model:

$$\underline{\underline{\mathbf{Z}}} = \sum_d (\mathbf{K}_d,\mathbf{L}_d,\mathbf{M}_d)\cdot\underline{\mathbf{G}}_d + \underline{\underline{\mathbf{E}}}$$

with $\underline{\mathbf{G}}_d$ in canonical form (using Tucker3 ALS)

Stegeman (2010)

<u>Step (II)</u>

Let $\underline{\mathbf{Y}} = (\mathbf{A},\mathbf{B},\mathbf{C})$ form a group of m diverging comp.

$\mathbf{A} = \mathbf{S}\,\mathbf{R}_a$ QR-decomp: $\mathbf{S}^T\mathbf{S} = \mathbf{I}_m$, $\mathbf{R}_a$ upper triangular
$\mathbf{B} = \mathbf{T}\,\mathbf{L}_b$ QL-decomp: $\mathbf{T}^T\mathbf{T} = \mathbf{I}_m$, $\mathbf{L}_b$ lower triangular

➔ $\mathbf{Y}_k = \mathbf{S}\,(\mathbf{R}_a\,\mathbf{C}_k\,\mathbf{L}_b^T)\,\mathbf{T}^T$ slice k

We can find $\mathbf{U}$ such that $\mathbf{U}^T\mathbf{U} = \mathbf{I}_m$ and

$\underline{\mathbf{Y}} = (\mathbf{S},\mathbf{T},\mathbf{U})\cdot\underline{\mathbf{H}}$ with $\underline{\mathbf{H}}$ $(m\times m\times m)$
upper triangular slices

Step (III)

Assume $\underline{\mathbf{Y}} = (\mathbf{A},\mathbf{B},\mathbf{C})$ $\longrightarrow$ boundary point $\underline{\mathbf{X}}$ of S_m m diverging comp. and $\underline{\mathbf{X}} \notin S_m$

For m=2 : $\underline{\mathbf{X}} = (\mathbf{K},\mathbf{L},\mathbf{M}) \cdot \underline{\mathbf{G}}$ with $\mathbf{K},\mathbf{L},\mathbf{M}$ of rank 2

$$\underline{\mathbf{G}} = \left[\begin{array}{cc|cc} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{array}\right] \quad \text{with} \quad \text{rank}(\underline{\mathbf{G}}) = 3$$

De Silva & Lim (2008)

For m=3 : $\underline{\mathbf{X}} = (\mathbf{K},\mathbf{L},\mathbf{M}) \cdot \underline{\mathbf{G}}$ with **K**,**L**,**M** of rank 3

$$\underline{\mathbf{G}} = \left[\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & 0 & \delta & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & \varepsilon & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right]$$

with rank($\underline{\mathbf{G}}$) = 5

For nondiverging components (m=1), we take $\underline{\mathbf{G}}$ = 1

Stegeman (2010), Paatero (2000) for case δ=0, ε=1

$$\underline{\mathbf{X}} = \sum_{d} (\mathbf{K}_d, \mathbf{L}_d, \mathbf{M}_d) \cdot \underline{\mathbf{G}}_d$$

sets $\{\mathbf{K}_d\}$ $\{\mathbf{L}_d\}$ $\{\mathbf{M}_d\}$ all have rank R

$m \geq 3$ at most once, $\max(m) \geq 2$

$\Downarrow$

$\underline{\mathbf{X}}$ is boundary point of S_R

$$\text{rank}(\underline{\mathbf{X}}) = \sum_{d} \text{rank}(\underline{\mathbf{G}}_d) > \text{R}$$

Ja' Ja' & Takche (1986), Stegeman (2010)

Numerical Example 1: 5×5×5 and R=3

CP ALS with tolerance 1e-9 terminates after 11.100 iters

$\underline{\mathbf{Y}} = (\mathbf{A},\mathbf{B},\mathbf{C})$ has 2 diverging components

$\text{ssq}(\underline{\mathbf{Z}} - \underline{\mathbf{Y}}) = 61.971147$

fit model $\underline{\mathbf{Z}} = (\mathbf{k}_1,\mathbf{l}_1,\mathbf{m}_1) + (\mathbf{K}_2,\mathbf{L}_2,\mathbf{M}_2)\cdot\underline{\mathbf{G}}_2 + \underline{\mathbf{E}}$

$\text{ssq}(\underline{\mathbf{Z}} - \underline{\mathbf{X}}) = 61.970457$, tolerance 1e-12, 38 iters

condition numbers of $[\mathbf{k}_1\ \mathbf{K}_2]$, $[\mathbf{l}_1\ \mathbf{L}_2]$, $[\mathbf{m}_1\ \mathbf{M}_2]$ are:

5.66 1.62 7.18

Numerical Example 2: $3\times3\times3$ and $R=3$

CP ALS with tolerance 1e-9 terminates after 20.913 iters

$\underline{\mathbf{Y}} = (\mathbf{A},\mathbf{B},\mathbf{C})$ has 3 diverging components

$\text{ssq}(\underline{\mathbf{Z}} - \underline{\mathbf{Y}}) = 0.779692$

fit model $\underline{\mathbf{Z}} = (\mathbf{K}_1,\mathbf{L}_1,\mathbf{M}_1)\cdot\underline{\mathbf{G}}_1 + \underline{\mathbf{E}}$

$\text{ssq}(\underline{\mathbf{Z}} - \underline{\mathbf{X}}) = 0.779379$, tolerance 1e-12, 98 iters

condition numbers of $\mathbf{K}_1$, $\mathbf{L}_1$, $\mathbf{M}_1$ are: 98.5, 1.1, 43.3

Concluding Remarks

- For $I \times J \times K$ and $R=2$ a Tucker3 model exists that equals closure of S_2 Rocci & Giordani (2010)
- For $I \times J \times 2$ and for $R=2$, much faster algorithms exist than any CP algorithm !
- Harshman (2004) has been confirmed:

  diverging components are due to

  "Parafac trying to model Tucker variation"

- for $I \times J \times 2$ and $I \times J \times K$: rank($\underline{\mathbf{X}}$) = # rank-1 terms

  if max(m)≤2

- Uniqueness of decomposition of $\underline{\mathbf{X}}$:

<u>for $I \times J \times 2$</u> : uniqueness given Jordan form decomp.

not unique in rank-1 terms within blocks

<u>for $I \times J \times K$</u> : uniqueness given block decomp. form

(proven for max(m)≤2)

not unique in rank-1 terms within blocks

Post-doc vacancy

2 years full-time, starting 2010 or 2011

University of Groningen, The Netherlands

uniqueness or existence of tensor decompositions

required: PhD in relevant field

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