



university of
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Candecom / Parafac

from diverging components to a decomposition
in block terms

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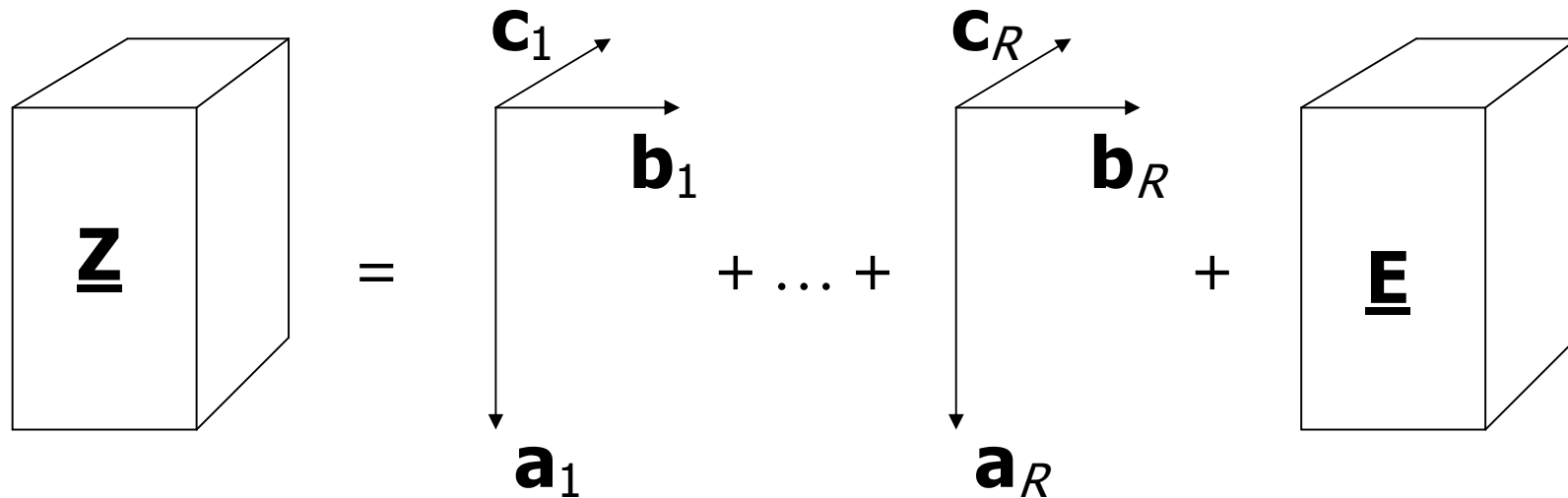
Candecomp / Parafac (CP) model

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

$$\mathbf{Z}_k = \mathbf{A} \mathbf{C}_k \mathbf{B}^T + \mathbf{E}_k$$

frontal slice k

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



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

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

Computation of CP solution

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

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

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

The Candecomp / Parafac problem

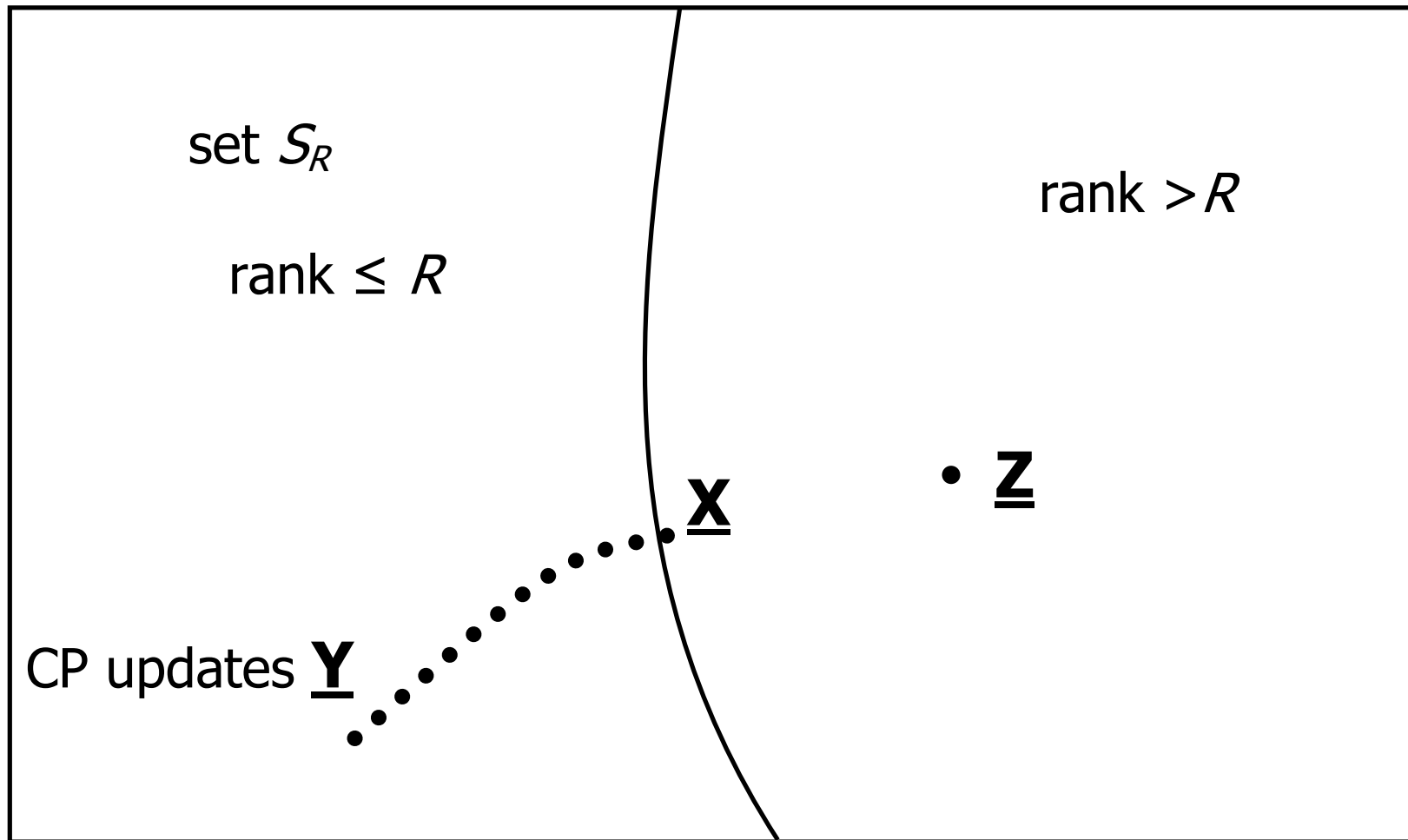
$$\begin{array}{ll} \text{Minimize} & \text{ssq}(\underline{\mathbf{Z}} - \underline{\mathbf{Y}}) \\ \text{over} & S_R = \{ \underline{\mathbf{Y}} \text{ with rank} \leq R \} \end{array}$$

→ 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”)

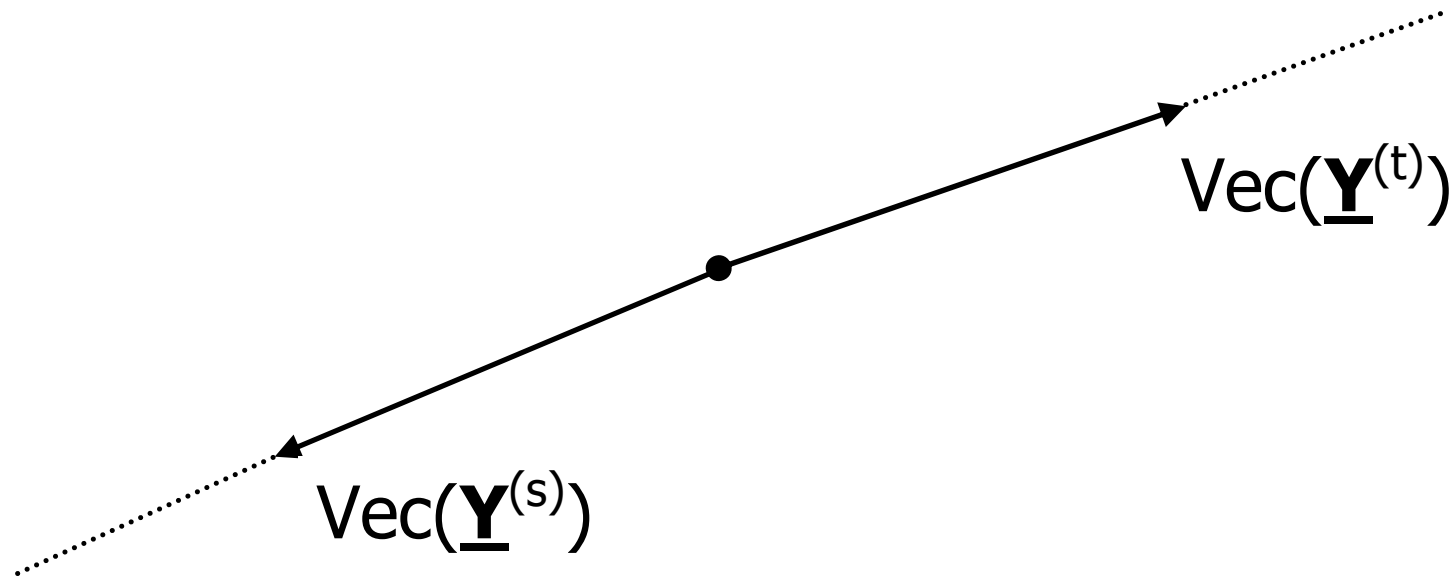
In practice also: slow convergence of CP algorithm
 (“swamp”)

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

Two diverging components

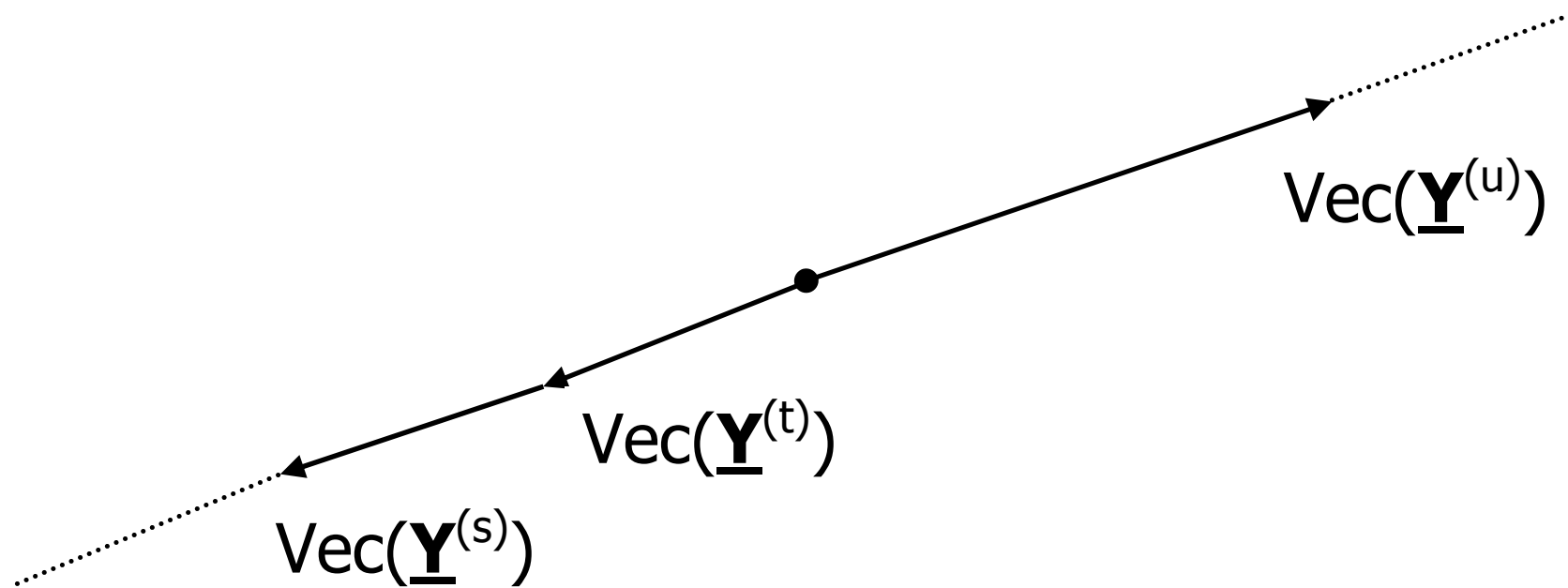
$$\underline{\mathbf{Y}}^{(s)} = \mathbf{a}_s \circ \mathbf{b}_s \circ \mathbf{c}_s$$

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



$\underline{\mathbf{Y}}^{(s)} + \underline{\mathbf{Y}}^{(t)}$ 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: 3×3×2 with $R = 3$

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

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

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

How often do diverging components occur ?

array $\underline{\mathbf{z}}$	rank($\underline{\mathbf{z}}$)	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 $\underline{\mathbf{z}}$; proven by De Silva & Lim (2008)

+ random $\underline{\mathbf{z}}$; 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 $\text{ssq}(\underline{\mathbf{Z}} - \underline{\mathbf{Y}})$ 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)
- **Z** 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)

$$\begin{array}{ll} \text{Minimize} & \text{ssq}(\underline{\mathbf{Z}} - \underline{\mathbf{Y}}) \\ & \text{over closure of } S_R \end{array}$$

What is needed?

- Complete characterization of boundary points
- Algorithm to find an optimal boundary point

Tucker3 model and block decomposition

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

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

(Tucker, 1966)

$$\underline{\mathbf{Z}} = \sum_d (\mathbf{A}_{d_l} \mathbf{B}_{d_l} \mathbf{C}_d) \cdot \underline{\mathbf{G}}_d \quad \text{decomposition in block terms}$$

(De Lathauwer, 2008)

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

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

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

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

$\text{rank}(\mathbf{Y}) = \text{rank}(\mathbf{H})$

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

De Silva & Lim (2008)

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

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

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

$\text{rank}(\underline{\mathbf{H}}) = R$ if $\mathbf{H}_2(\mathbf{H}_1)^{-1}$ diagonalizable

$\text{rank}(\underline{\mathbf{H}}) > R$ 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

$\underline{\mathbf{G}} = (\mathbf{I}_{R_f} \mathbf{I}_{R_f} \mathbf{U}) \cdot \underline{\mathbf{H}}$ 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 ($I \times J \times 2$)

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

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

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

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 $\underline{\mathbf{Z}}$ (fast!) and obtains optimal solution $\underline{\mathbf{X}}$ 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 $\underline{\mathbf{X}}$

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

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

1×1 Jordan block \iff nondiverging component
 $m \times m$ Jordan block \iff limit of m diverging comp.

Stegeman & De Lathauwer (2009)

Alternative representation :

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

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

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

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

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 $(\mathbf{S}_{d_r} \mathbf{T}_{d_r} \mathbf{U}_d) \cdot \underline{\mathbf{H}}_d$ with $(\mathbf{S}_{d_r} \mathbf{T}_{d_r} \mathbf{U}_d)$ orthonormal columns and $\underline{\mathbf{H}}_d$ ($m \times m \times m$) upper triangular slices
- (III) Using $(\mathbf{S}_{d_r} \mathbf{T}_{d_r} \mathbf{U}_d) \cdot \underline{\mathbf{H}}_d$ as initial values, fit model:

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

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

Stegeman (2010)

Step (II)

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

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

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

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

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

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

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

De Silva & Lim (2008)

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

$$\underline{\mathbf{G}} = \left[\begin{array}{ccc|ccc|cc} 1 & 0 & 0 & 0 & \delta & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & \varepsilon & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right] \text{ with } \text{rank}(\underline{\mathbf{G}}) = 5$$

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

Stegeman (2010), Paatero (2000) for case $\delta=0$, $\varepsilon=1$

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

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

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



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

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

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: $3 \times 3 \times 3$ 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 $\underline{\mathbf{Z}} = (\mathbf{K}_1, \mathbf{L}_1, \mathbf{M}_1) \cdot \underline{\mathbf{G}}_1 + \underline{\mathbf{E}}$

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

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 $I \times J \times K$: $\text{rank}(\underline{\mathbf{X}}) = \# \text{ rank-1 terms}$
if $\max(m) \leq 2$

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

for $I \times J \times 2$: uniqueness given Jordan form decomp.
not unique in rank-1 terms within blocks

for $I \times J \times K$: uniqueness given block decomp. form
(proven for $\max(m) \leq 2$)
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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