university of groningen

A solution for diverging components in 3-way Candecomp/Parafac

Alwin Stegeman

a.w.stegeman@rug.nl www.gmw.rug.nl/~stegeman

Summarizing Data in Simple Patterns

Information Technology ➔ collection of huge data sets, often multi-way data $z(i,j,k,\ldots)$

Approximation: Multi-way data ≈ simple patterns

- data interpretation (psychometrics, neuro-imaging, data mining)
- separation of chemical compounds (chemometrics)
- separation of mixed signals (signal processing)
- faster calculations (algebraic complexity theory, scientific computing)

Simple structure = rank 1

2-way array = matrix $\mathbf{Z}$ $(I \times J)$ with entries z(i,j)

rank 1: $\mathbf{Z} = \mathbf{a}\,\mathbf{b}^T = \mathbf{a} \circ \mathbf{b}$ ⇐⇒ $z(i,j) = a(i) \cdot b(j)$

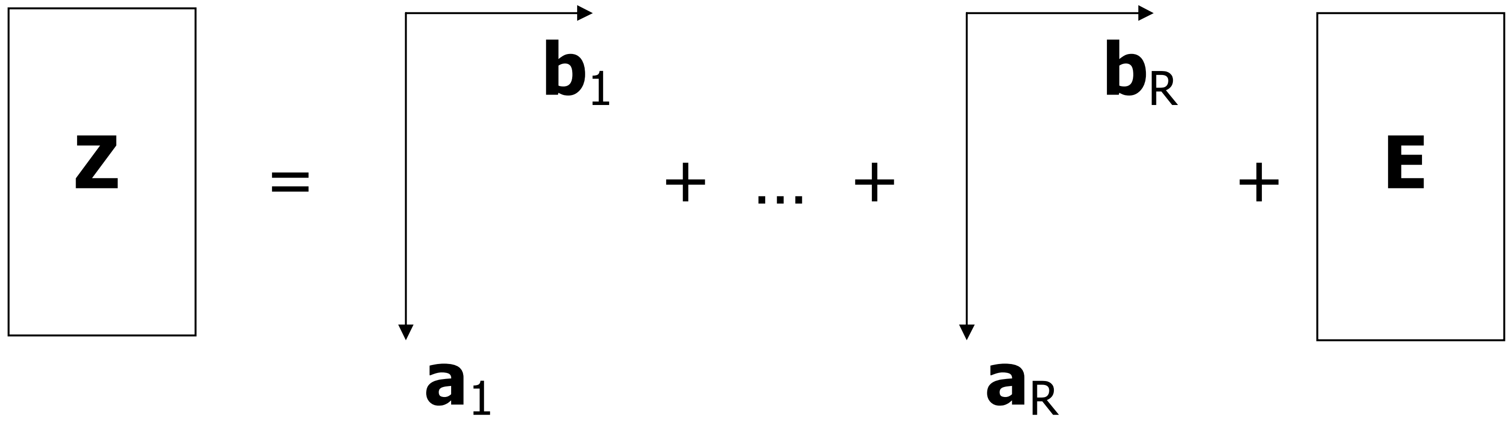
$\text{rank}(\mathbf{Z}) = \min \{R : \mathbf{Z} = \mathbf{a}_1 \circ \mathbf{b}_1 + \ldots + \mathbf{a}_R \circ \mathbf{b}_R\}$

3-way array $\underline{\underline{\mathbf{Z}}}$ $(I \times J \times K)$ with entries z(i,j,k)

rank 1: $\underline{\underline{\mathbf{Z}}} = \mathbf{a} \circ \mathbf{b} \circ \mathbf{c}$ ⇐⇒ $z(i,j,k) = a(i) \cdot b(j) \cdot c(k)$

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

2-way (PCA) decomposition

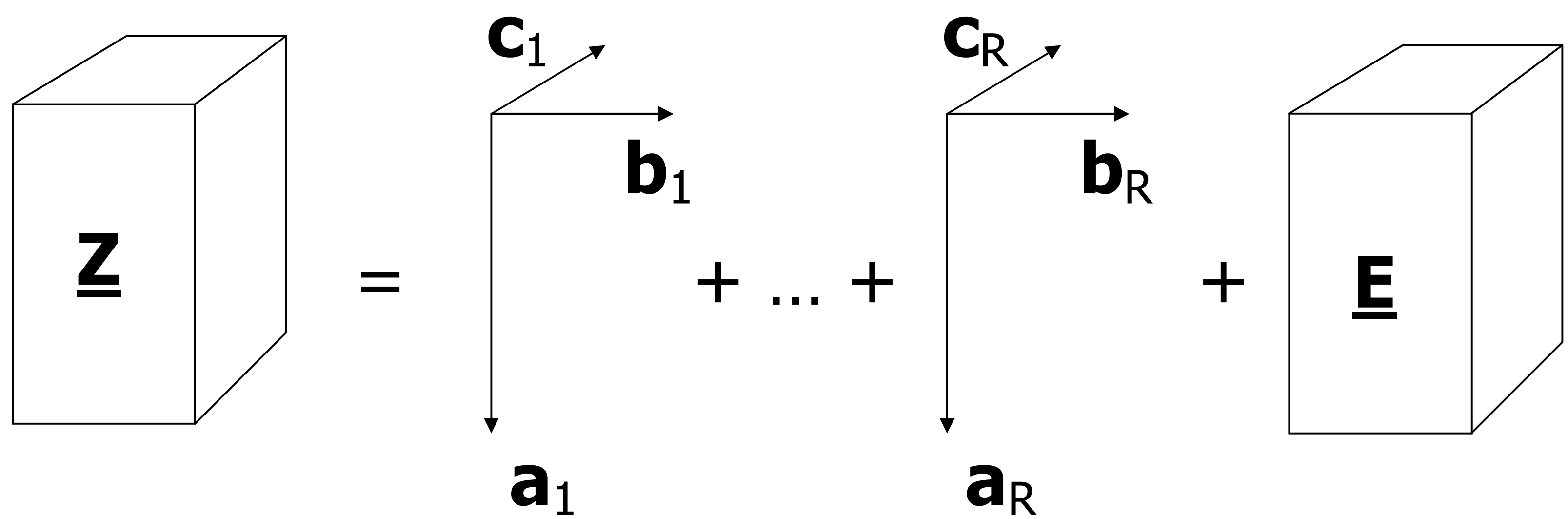


$$\mathbf{Z} = \mathbf{a}_1 \circ \mathbf{b}_1 + \ldots + \mathbf{a}_R \circ \mathbf{b}_R + \mathbf{E}$$

$$= \mathbf{A}\,\mathbf{B}^T + \mathbf{E} \qquad \text{with} \qquad \mathbf{A} = [\mathbf{a}_1 \ldots \mathbf{a}_R], \quad \mathbf{B} = [\mathbf{b}_1 \ldots \mathbf{b}_R]$$

Goal: Find (**A**,**B**) that minimize ssq(**E**)

3-way Candecomp/Parafac (CP)



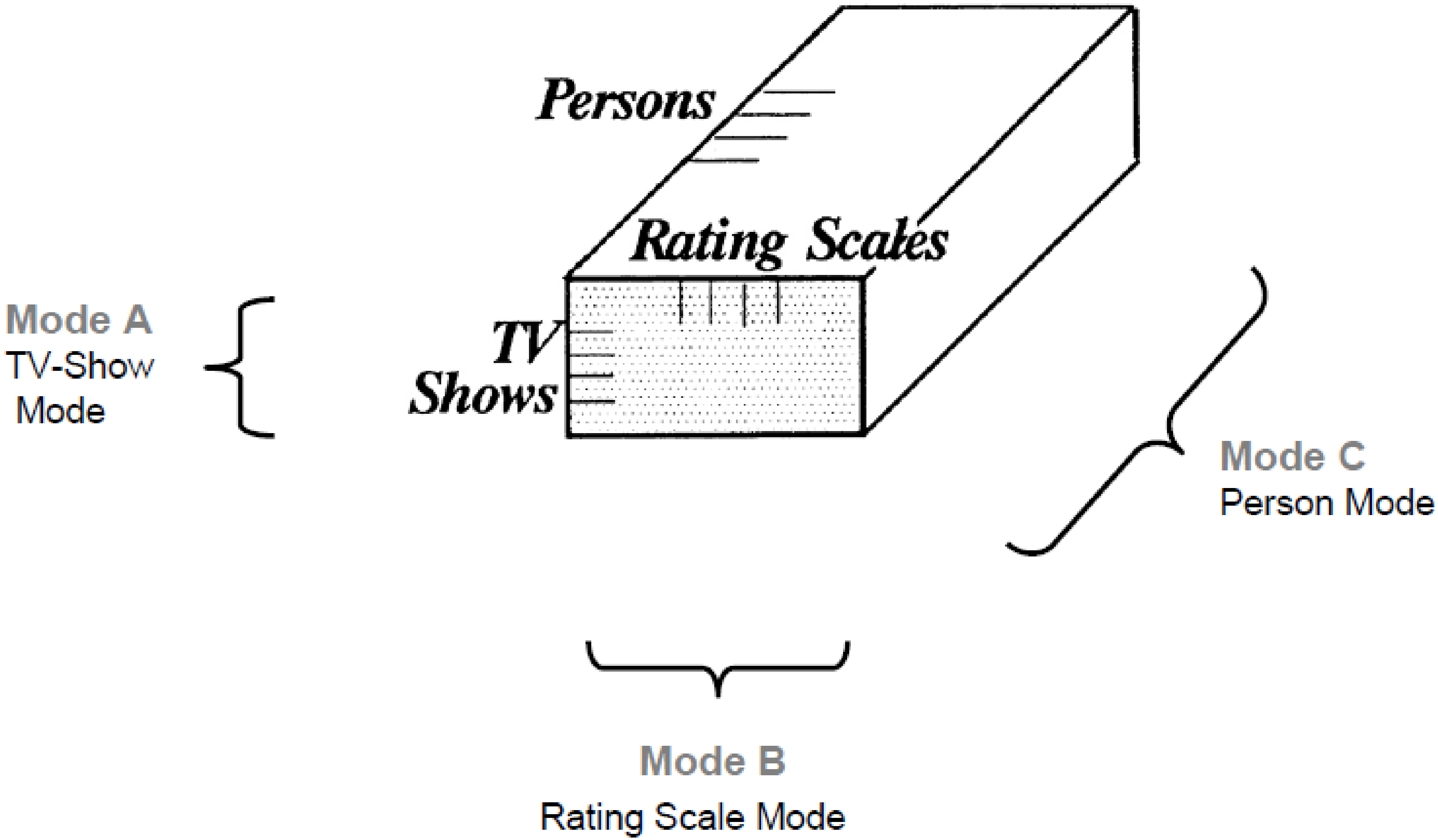
$$\underline{\mathbf{Z}} = \mathbf{a}_1 \circ \mathbf{b}_1 \circ \mathbf{c}_1 + \ldots + \mathbf{a}_R \circ \mathbf{b}_R \circ \mathbf{c}_R + \underline{\mathbf{E}}$$

Goal: Find $(\mathbf{A},\mathbf{B},\mathbf{C})$ that minimize $\mathrm{ssq}(\underline{\mathbf{E}})$

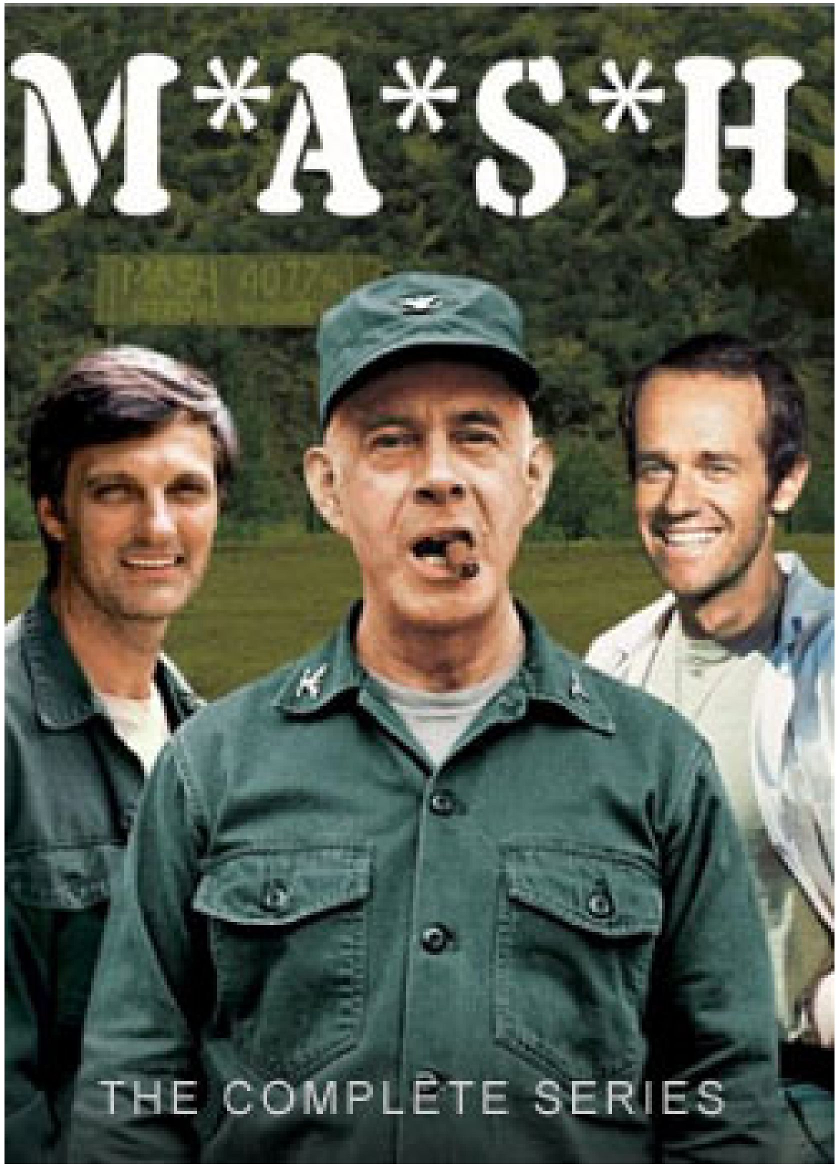
with $\mathbf{C} = [\mathbf{c}_1 \ldots \mathbf{c}_R]$

	3-way CP	2-way decomp
computation	iterative algorithm	SVD
best rank-R approximation	yes	yes
rotational uniqueness	under mild conditions	no
existence for R < rank(data)	not guaranteed	yes

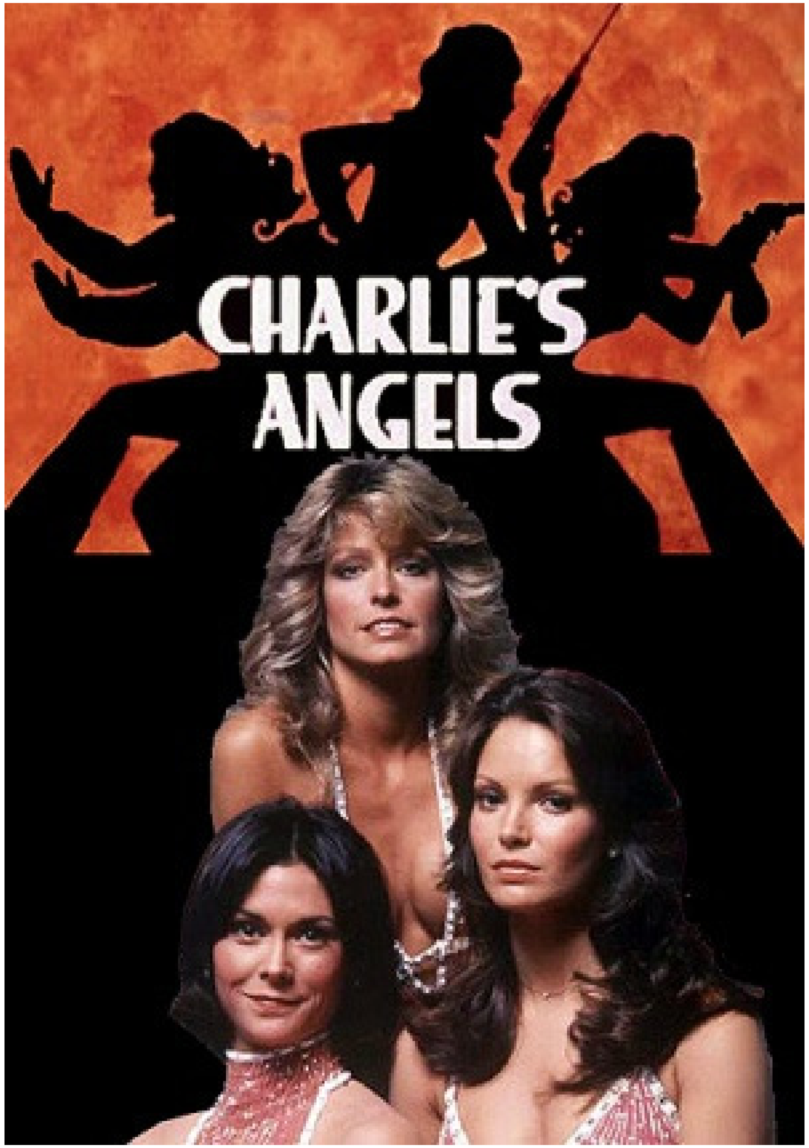
CP analysis of 3-way TV-ratings data



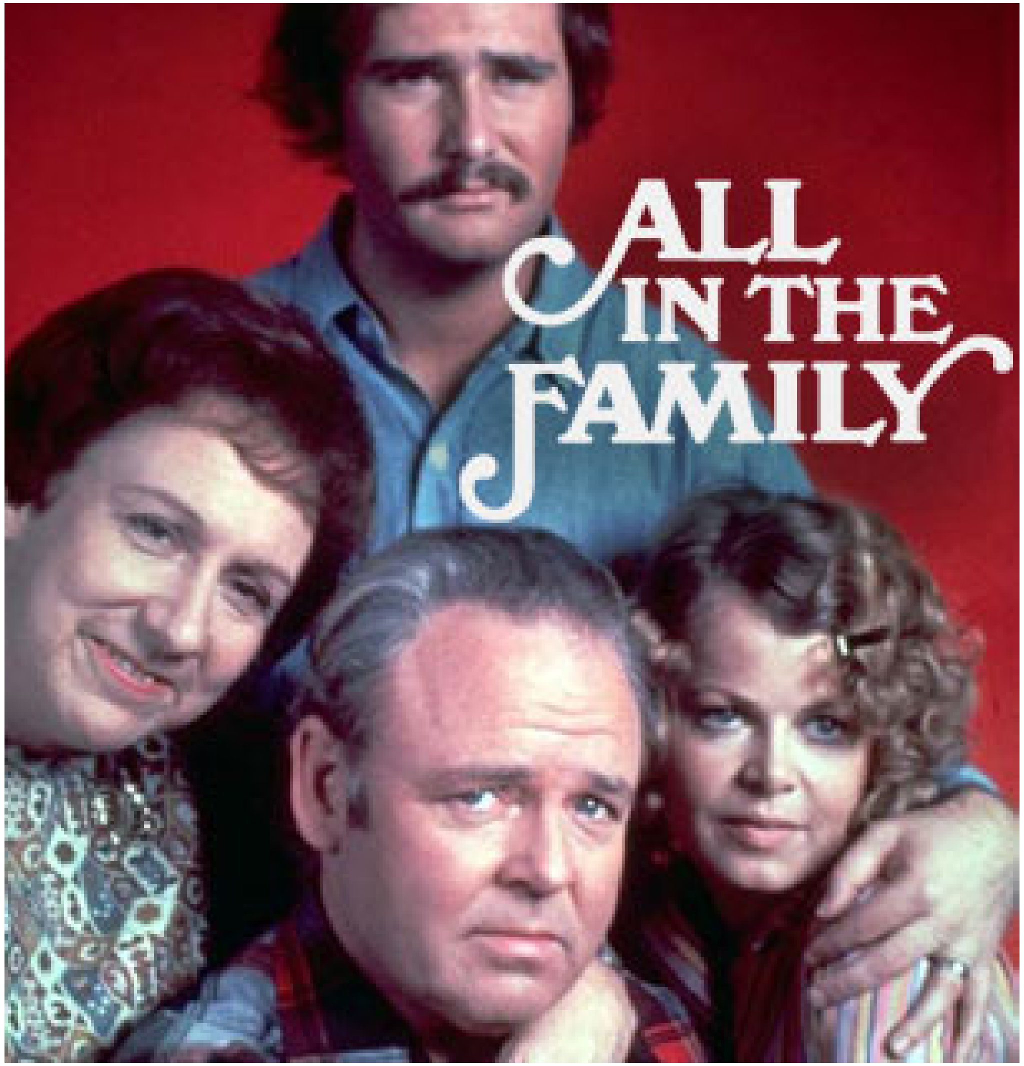
TV show 1 – Mash



TV show 2 – Charlie's Angels



TV show 3 – All in the Family



TV show 4 – 60 Minutes

TV show 5 – The Tonight Show

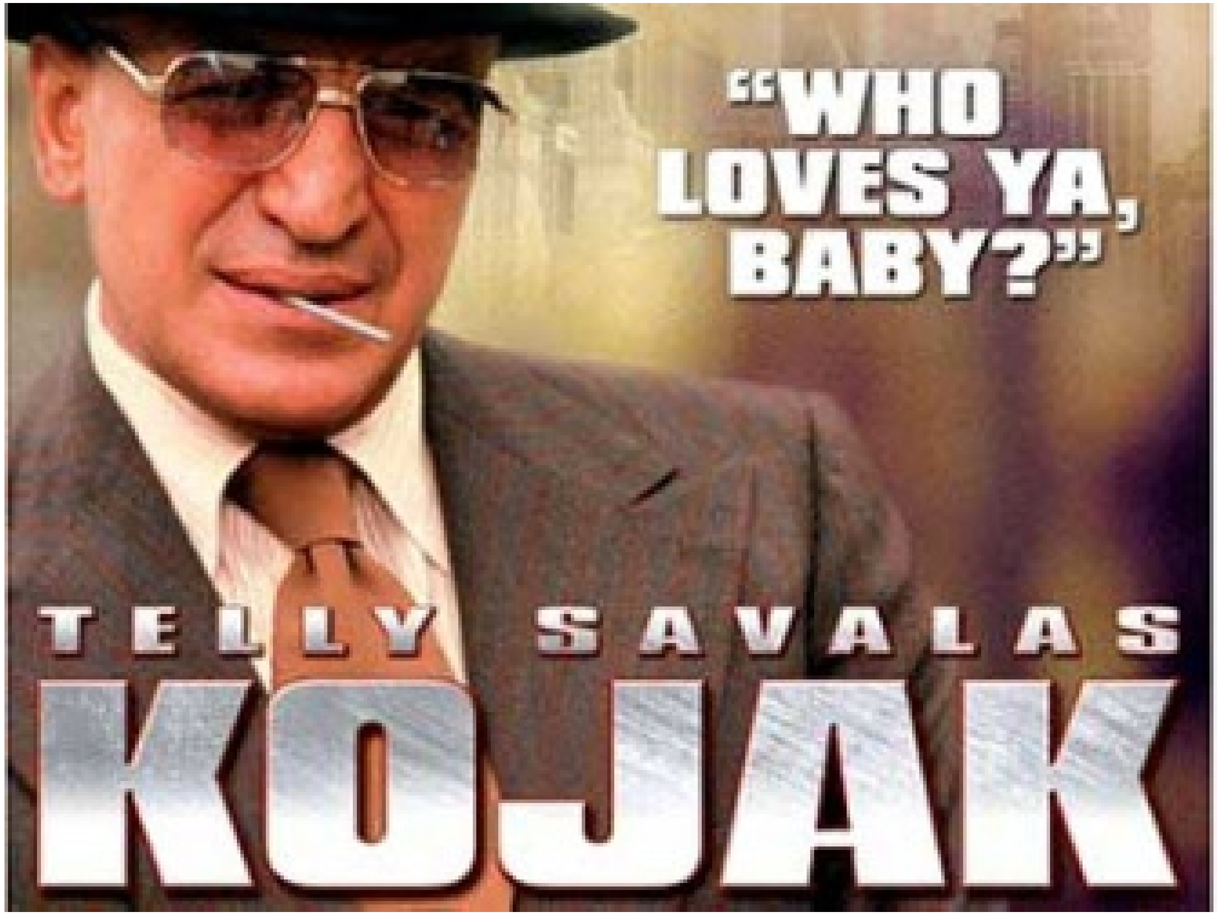
TV show 6 – Let's Make a Deal

TV show 7 – The Waltons

TV show 8 – Saturday Night Live

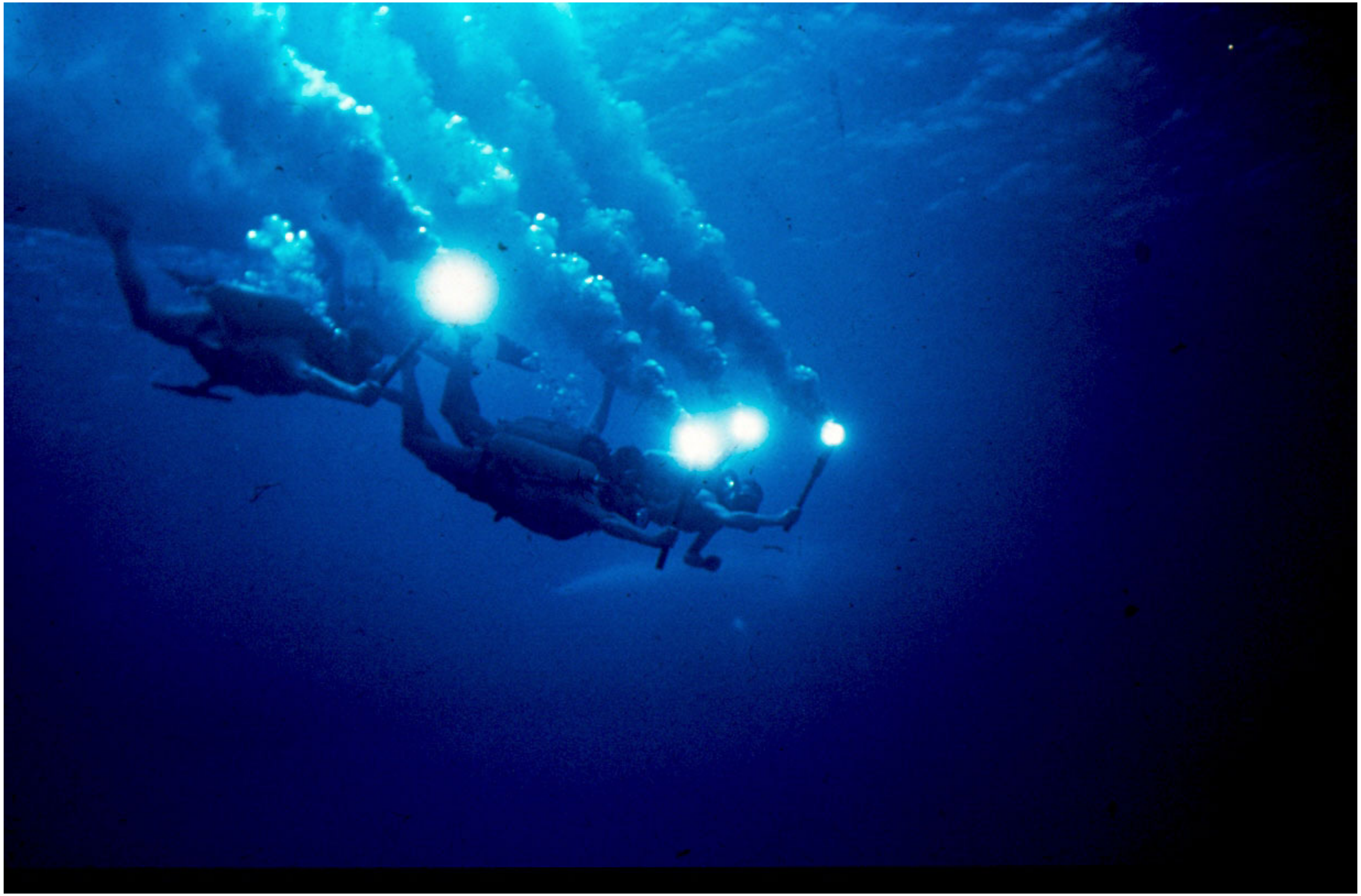
TV show 9 – News

TV show 10 – Kojak



TV show 11 – Mork and Mindy

TV show 12 – Jacques Cousteau



TV show 13 – Football

TV show 14 – Little House on the Prairie

TV show 15 – Wild Kingdom

Rating Scales 1-8

-6, -5, …, -1 , 0, 1, …, 5, 6

1. Thrilling . . . . Boring
2. Intelligent . . . Idiotic
3. Erotic . . . . . Not Erotic
4. Sensitive . . . . Insensitive
5. Interesting . . Uninteresting
6. Fast . . . . Slow
7. Intellectually Stimulating . . . Intellectually Dull
8. Violent . . . . Peaceful

Rating Scales 9-16

-6, -5, …, -1, 0, 1, …, 5, 6

9. Caring . . . . . Callous
10. Satirical . . . . Not Satirical
11. Informative . . Uninformative
12. Touching . . . "Leaves Me Cold"
13. Deep . . . . . . Shallow
14. Tasteful . . . . Crude
15. Real . . . . . . Fantasy
16. Funny . . . . . Not Funny

TV-ratings data

30 persons have rated 15 TV shows on 16 rating scales

Preprocessing:

- Centering across rating scales
- Centering across TV shows
- Normalizing within persons

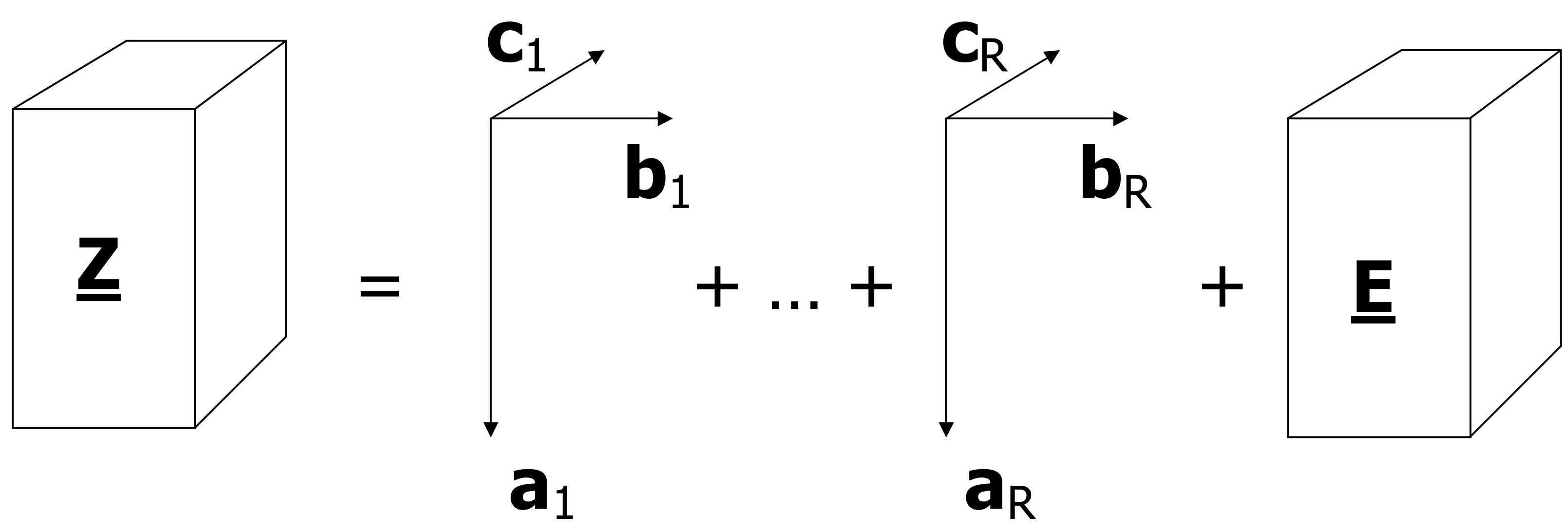
TV data also analyzed by Lundy et al. (1989) and Harshman (2004)

Output of the CP analysis with R components

Matrix **A** (15×R): columns are TV show components

Matrix **B** (16×R): columns are rating scales loadings

Matrix **C** (30×R): columns are person loadings



Scaling the CP solution

Column of **A**: mean squared component score = 1

Column of **B**: mean squared loading = 1

Column of **C**: sum of squared loadings = 4

$$\underline{\mathbf{Z}} = g_1 (\mathbf{a}_1 \circ \mathbf{b}_1 \circ \mathbf{c}_1) + \ldots + g_R (\mathbf{a}_R \circ \mathbf{b}_R \circ \mathbf{c}_R) + \underline{\mathbf{E}}$$

weight g_r indicates strength of component r

columns are sign changed such that **C** has positive loadings

Fit of the CP solution

Fit % = 100 – 100 ssq($\underline{\mathbf{E}}$) / ssq($\underline{\mathbf{Z}}$) (range 0 to 100)

Congruence coefficient of two components

$$cc_A(1,2) = \frac{\mathbf{a}_1^T \mathbf{a}_2}{\sqrt{\mathrm{ssq}(\mathbf{a}_1)}\sqrt{\mathrm{ssq}(\mathbf{a}_2)}}$$ (range -1 to +1)

$$cc(1,2) = cc_A(1,2)\, cc_B(1,2)\, cc_C(1,2)$$

The CP solution with 2 components

Overall:	fit = 41.96 %	cc(1,2) = 0.002
Component 1:	fit = 28.46 %	$g_1 = 1.46$
Component 2:	fit = 13.59 %	$g_2 = 1.01$

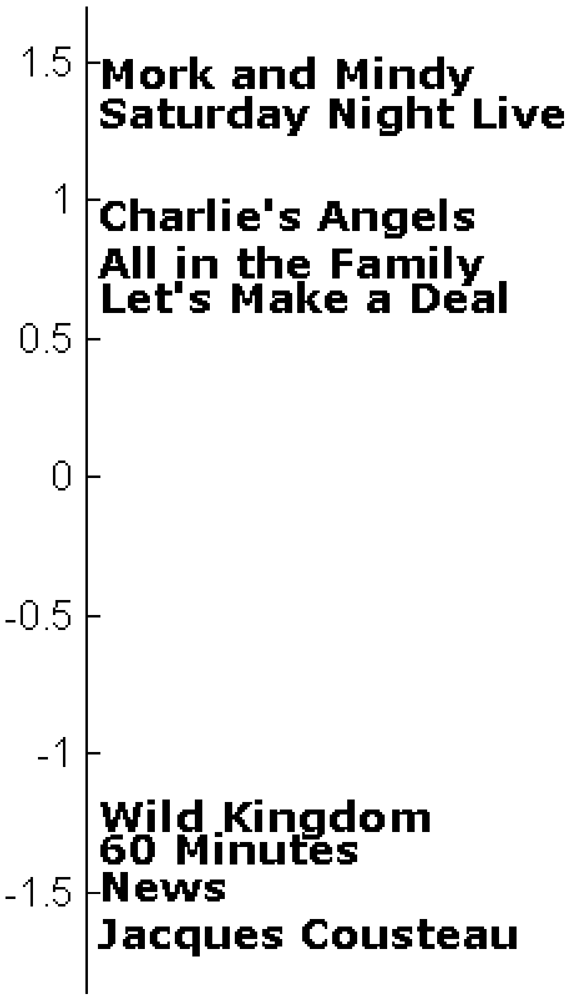
Interpretation:

Component 1 = “Humor”

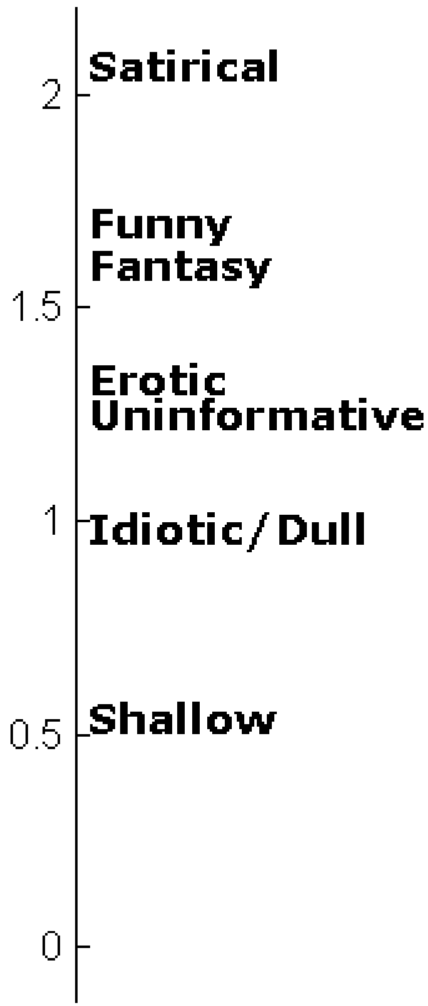
Component 2 = “Sensitivity”

Component 1 = "Humor"

TV shows mode

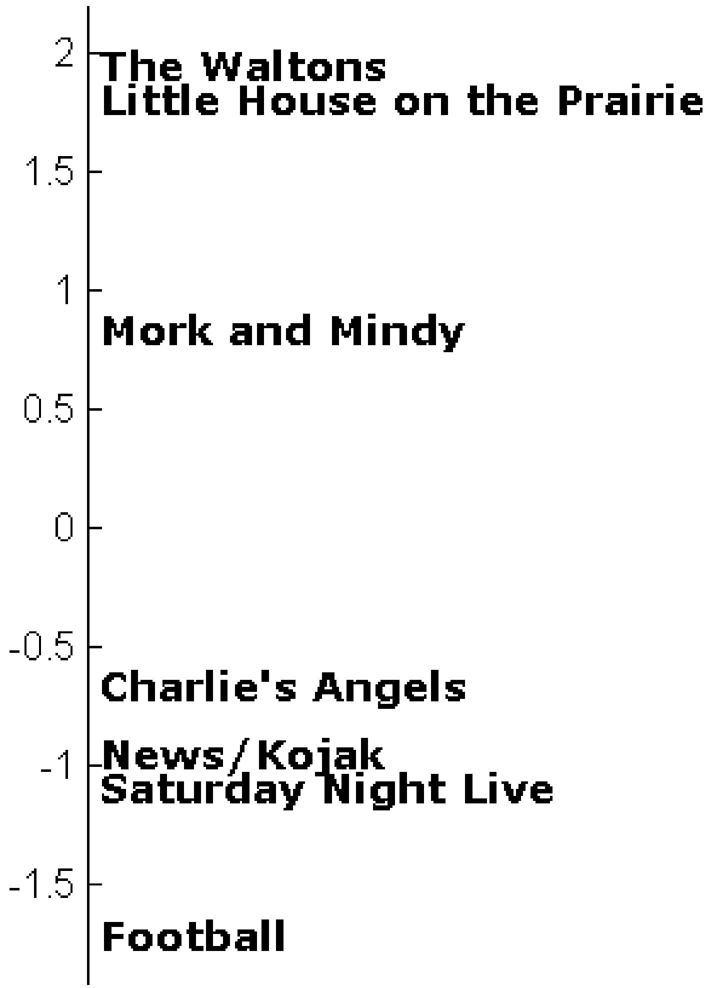


Scales mode

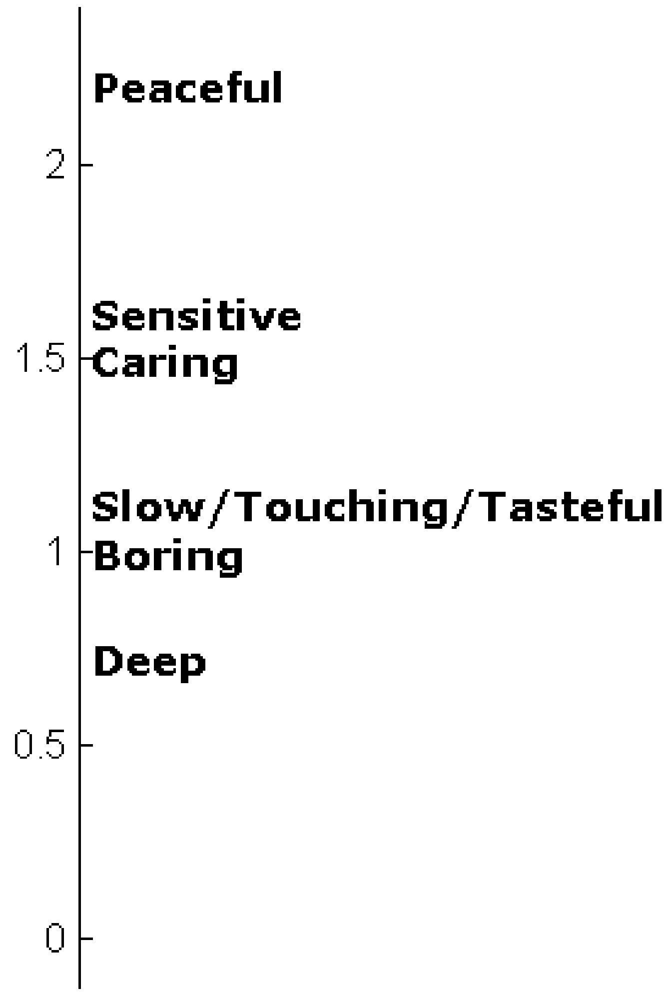


Component 2 = "Sensitivity"

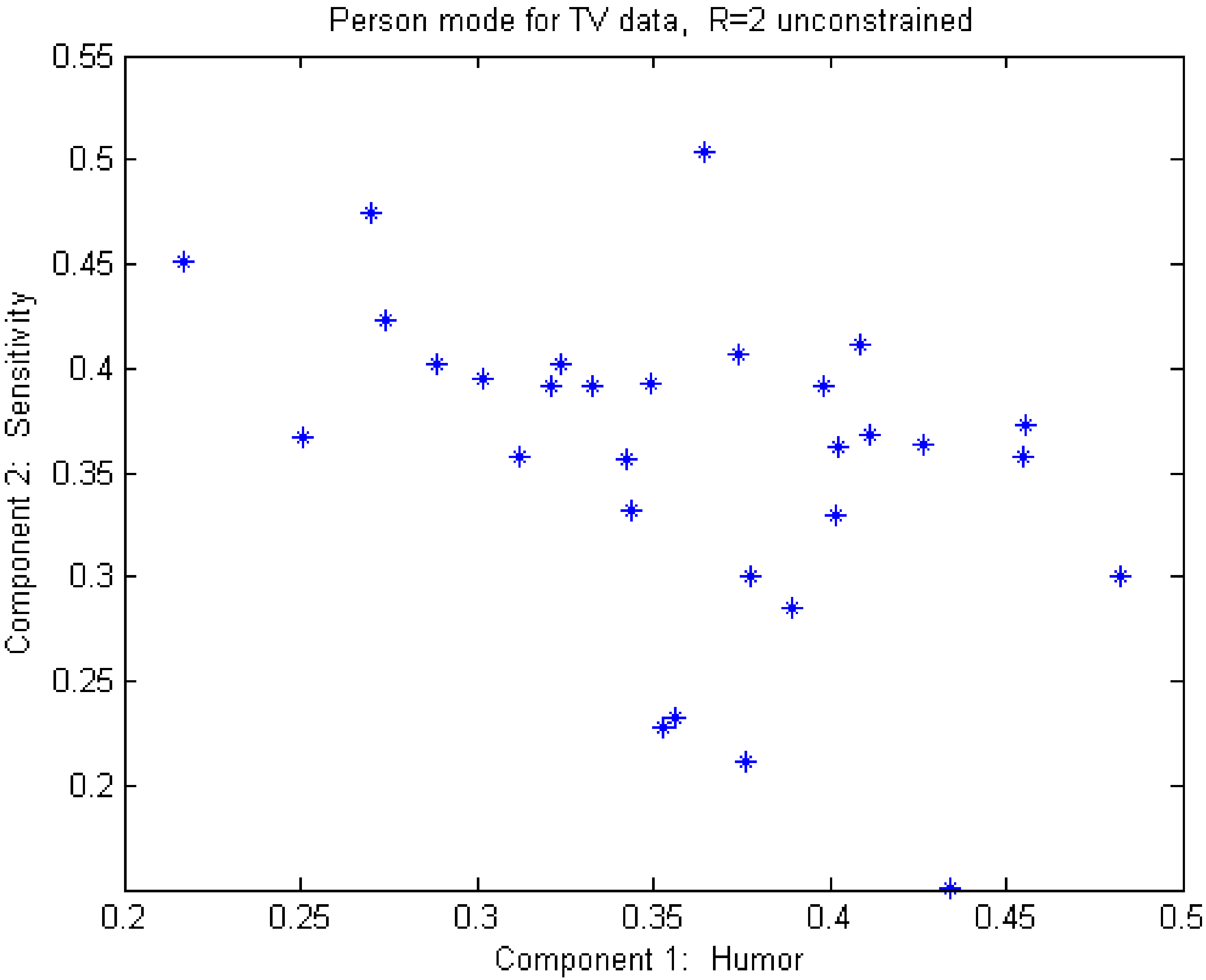
TV shows mode



Scales mode



Components 1 and 2 – persons plot



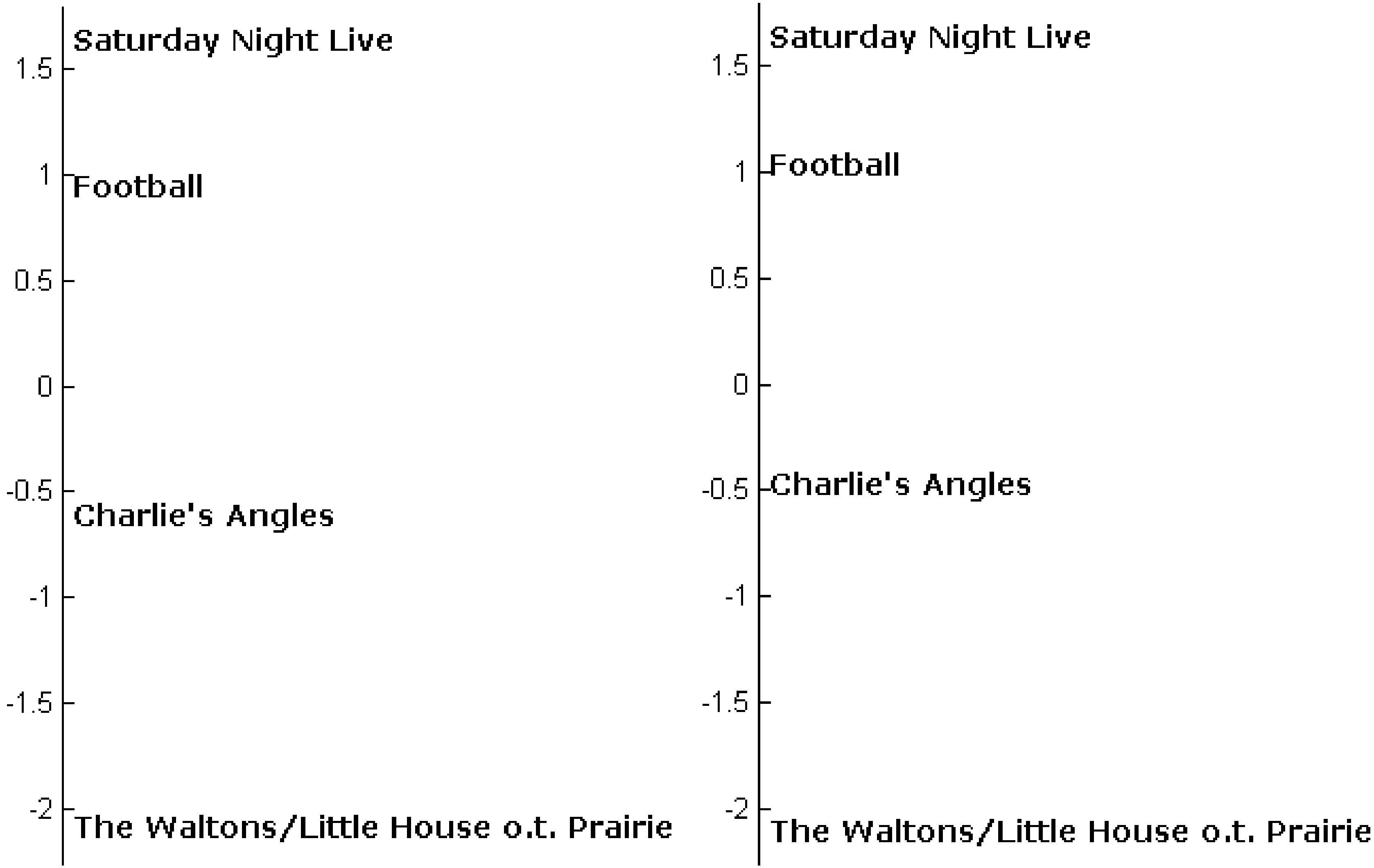
The CP solution with 3 components

Overall:	fit = 50.76 %	cc(1,2) = -0.996
		cc(1,3) = -0.13
		cc(2,3) = 0.12
Comps. 1+2:	fit = 20.11 %	g_1 = 15.23
		g_2 = 15.39
Component 3:	fit = 24.38 %	g_3 = 1.52

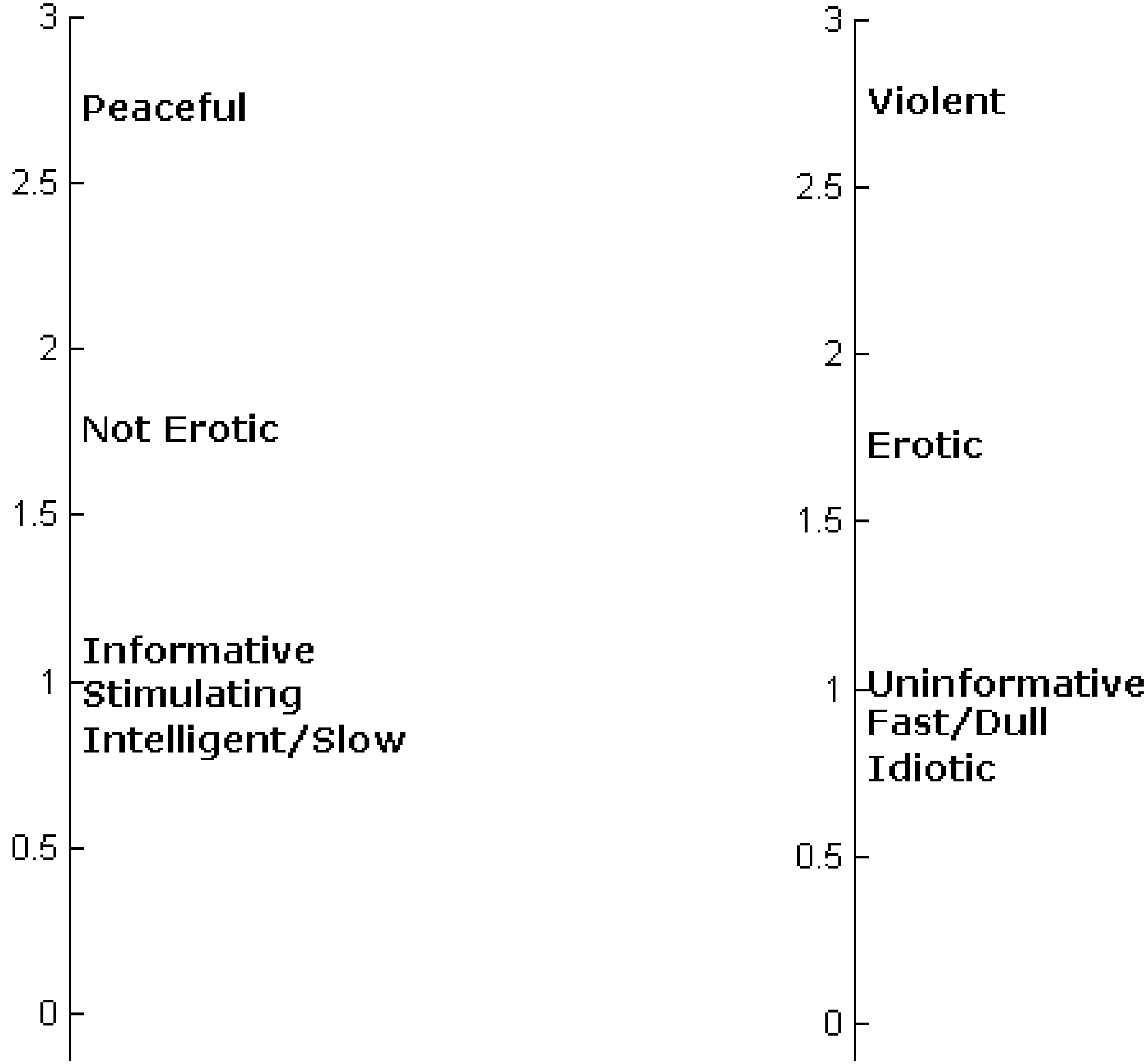
<u>Interpretation</u>: Components 1 & 2 = ???

Component 3 = “Humor”

Components 1 and 2 – TV shows mode



Components 1 and 2 – Scales mode



Comparing the solutions for R=2 and R=3

congruence coefficients of R=2 components (columns) and R=3 components (rows):

	"Humor"	"Sensitivity"
Comp. 1	-0.15	-0.41
Comp. 2	0.15	0.46
"Humor"	0.93	0.01

Some Theory

- Diverging components occur when CP does not have an optimal solution (Krijnen et al., 2008; De Silva & Lim, 2008)
- CP has an optimal solution if the columns of **A** (or **B** or **C**) are restricted to be orthogonal (Harshman & Lundy, 1984; Krijnen et al., 2008)
- CP has an optimal solution if the data is nonnegative and **A**,**B**,**C** are restricted to be nonnegative (Lim, 2005; Lim & Comon, 2009)

R=3 components and orthogonal TV shows mode

Overall:	fit = 50.22 %	cc(r,t) = 0
Component 1:	fit = 27.19 %	$g_1 = 1.43$
Component 2:	fit = 13.04 %	$g_2 = 0.99$
Component 3:	fit = 9.99 %	$g_3 = 0.87$

Interpretation:

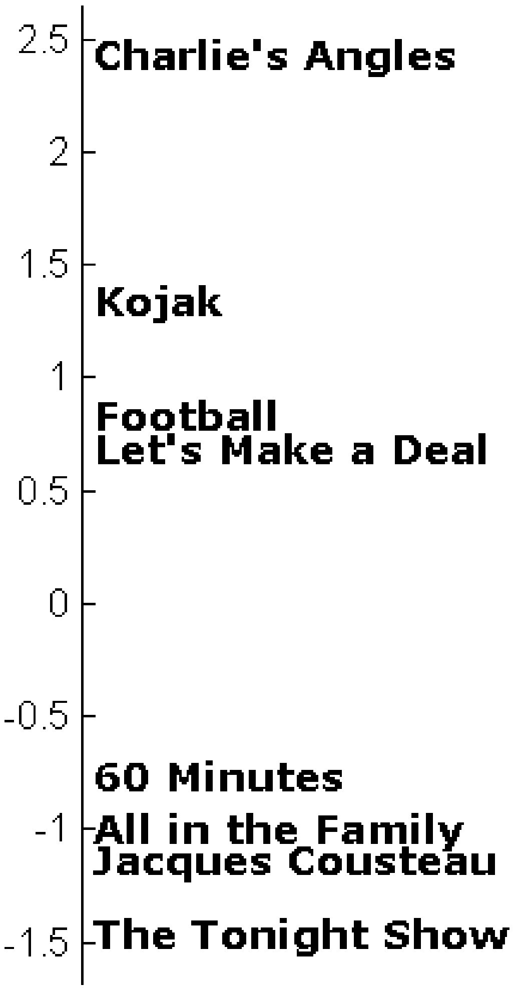
Component 1 = "Humor"

Component 2 = "Sensitivity"

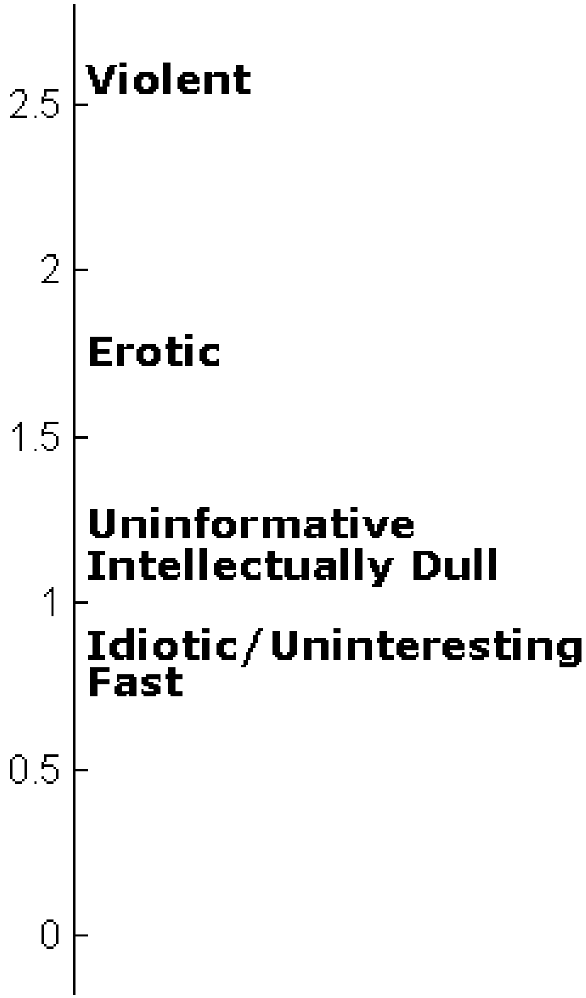
Component 3 = "Violence"

Component 3 = "Violence"

TV shows mode



Scales mode

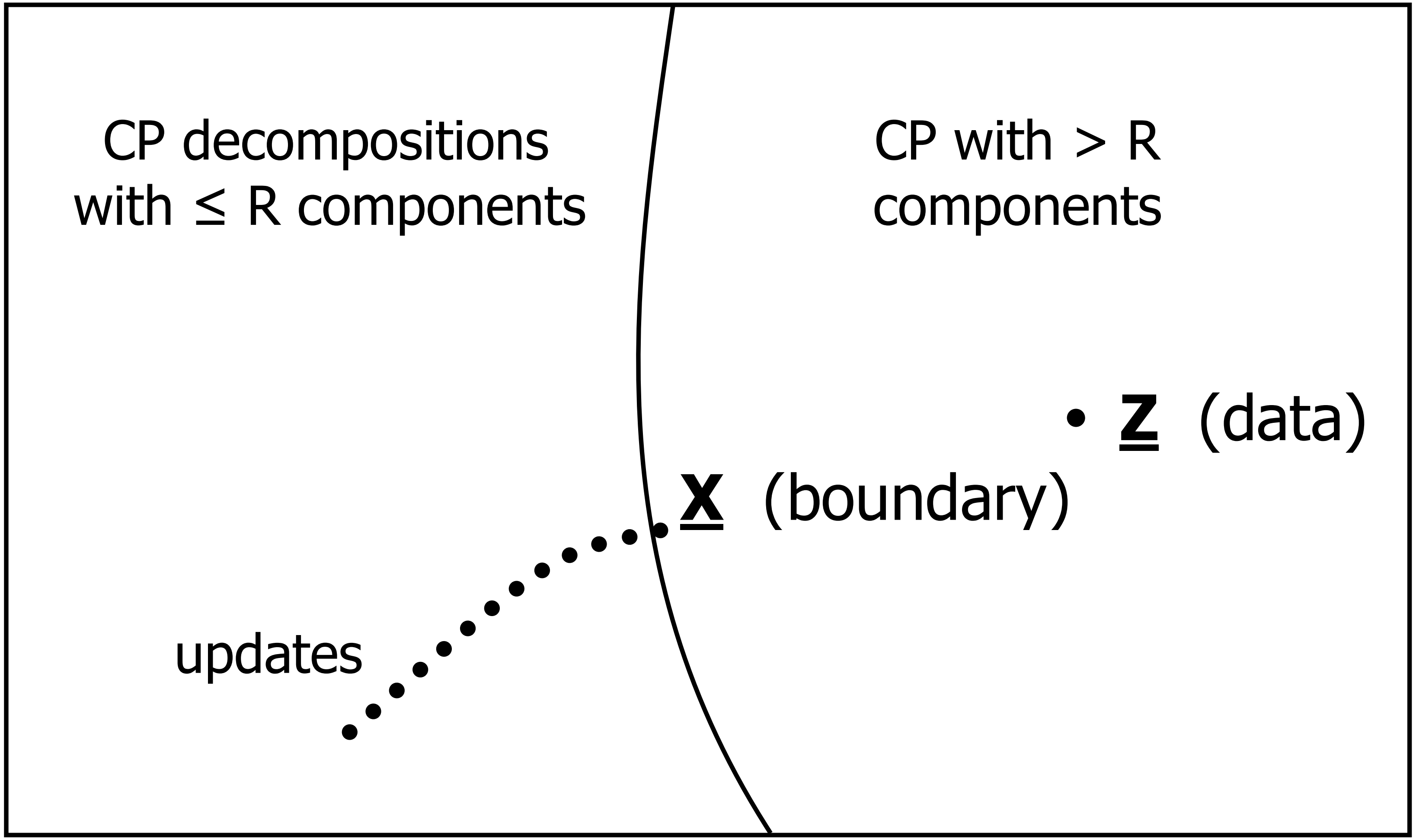


Comparing the solutions obtained so far

	R=2		R=3		
R=3 orth.	"H"	"S"	Comp.1	Comp.2	"H"
"Humor"	0.96	0.00	-0.20	0.19	0.95
"Sensitivity"	0.00	0.94	-0.30	0.36	0.03
"Violence"	0.11	0.08	0.30	-0.24	-0.03
"H" (R=2)			-0.15	0.15	0.93
"S" (R=2)			-0.41	0.46	0.01

➔ the two diverging components relate to "S" and "V"

Some more Theory



- CP does not have an optimal solution if optimal boundary point $\underline{\mathbf{X}}$ does not have a CP decomposition with ≤ R components

- In that case, the decomposition of $\underline{\mathbf{X}}$ contains one or more interaction terms, e.g., $\mathbf{s}_1 \circ \mathbf{t}_2 \circ \mathbf{u}_2$

➔ How to find $\underline{\mathbf{X}}$ and its decomposition?

<u>Algorithms exist for</u>:

- I×J×2 arrays and R ≤ min(I,J)
  (Stegeman & De Lathauwer, 2009)

- I×J×K arrays and R=2
  (Rocci & Giordani, 2010)

Two-stage method for I×J×K arrays and general R

First fit CP. In case of diverging components, do this:

- For combinations of nondiverging and groups of 2,3,4 diverging components, the form of the decomposition of the limit point **X** has been proven (Stegeman, 2012,2013)
- This form of decomposition is fitted to the data **Z** with initial values obtained from the diverging CP decomposition (Stegeman, 2012,2013)
- This yields **X** and its decomposition with interaction terms (Stegeman, 2012,2013)

The form of the limit of two diverging components is:

$$g_{111}\,(\mathbf{s}_1 \circ \mathbf{t}_1 \circ \mathbf{u}_1) + g_{221}\,(\mathbf{s}_2 \circ \mathbf{t}_2 \circ \mathbf{u}_1) + g_{122}\,(\mathbf{s}_1 \circ \mathbf{t}_2 \circ \mathbf{u}_2)$$

For the TV data with R=3, we fit the decomposition:

$$g_{111}\,(\mathbf{s}_1 \circ \mathbf{t}_1 \circ \mathbf{u}_1) + g_{221}\,(\mathbf{s}_2 \circ \mathbf{t}_2 \circ \mathbf{u}_1) + g_{122}\,(\mathbf{s}_1 \circ \mathbf{t}_2 \circ \mathbf{u}_2)$$

$$+\, g_{333}\,(\mathbf{s}_3 \circ \mathbf{t}_3 \circ \mathbf{u}_3)$$

Decomposition of the limit point in 4 terms

Overall:	fit = 50.7571 %	(50.7569 for R=3)
g_{111} ($\mathbf{s}_1 \circ \mathbf{t}_1 \circ \mathbf{u}_1$):	fit = 7.62 %	g_{111} = 0.99
g_{221} ($\mathbf{s}_2 \circ \mathbf{t}_2 \circ \mathbf{u}_1$):	fit = 10.75 %	g_{221} = 0.95
g_{122} ($\mathbf{s}_1 \circ \mathbf{t}_2 \circ \mathbf{u}_2$):	fit = 1.55 %	g_{122} = -0.33
g_{333} ($\mathbf{s}_3 \circ \mathbf{t}_3 \circ \mathbf{u}_3$):	fit = 24.37 %	g_{333} = 1.52

Interpretation: $\mathbf{s}_1$ and $\mathbf{t}_1$ = “Violence”

$\mathbf{s}_2$ and $\mathbf{t}_2$ = “Sensitivity”

$\mathbf{s}_3$ and $\mathbf{t}_3$ = “Humor”

Comparison to R=3 solution with orth. TV shows

	"Humor"	"Sensitivity"	"Violence"
g_{111} ($\mathbf{s}_1 \circ \mathbf{t}_1 \circ \mathbf{u}_1$)	-0.07	0.13	0.86
g_{221} ($\mathbf{s}_2 \circ \mathbf{t}_2 \circ \mathbf{u}_1$)	0.05	0.81	0.02
g_{122} ($\mathbf{s}_1 \circ \mathbf{t}_2 \circ \mathbf{u}_2$)	-0.03	-0.02	-0.03
g_{333} ($\mathbf{s}_3 \circ \mathbf{t}_3 \circ \mathbf{u}_3$)	0.95	0.04	-0.03

Interpretation of the decomposition in 4 terms

$\mathbf{s}_r$ = TV show component r
$\mathbf{t}_r$ = Rating scale loadings r
$\mathbf{u}_r$ = Idealized person r

	TV shows	scales	id. person	weight g
$(\mathbf{s}_1 \circ \mathbf{t}_1 \circ \mathbf{u}_1)$	Violent	Violence	1	0.99
$(\mathbf{s}_2 \circ \mathbf{t}_2 \circ \mathbf{u}_1)$	Sensitive	Sensitivity	1	0.95
$(\mathbf{s}_1 \circ \mathbf{t}_2 \circ \mathbf{u}_2)$	Violent	Sensitivity	2	-0.33
$(\mathbf{s}_3 \circ \mathbf{t}_3 \circ \mathbf{u}_3)$	Humorous	Humor	3	1.52

Remarks

The decomposition of the limit point resembles the R=3 CP solution with orthogonal scales.

However, orthogonality between "Sensitivity" and "Violence" is not intuitive.

The negative interaction term between "Violent" TV shows and "Sensitivity" scales is more intuitive.

Lundy et al. (1989) use R=3 orth. CP solution and fit full 3×3×3 weights array: interactions between "Humor" scales and "Sensitive" and "Violent" TV shows.

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