TRICAP 2006

Chania

Typical rank when arrays have symmetric slices, and the Carroll & Chang conjecture of equal CP components

Jos ten Berge

Research with Henk Kiers, Nikos Sidiropoulos, Roberto Rocci, and Alwin Stegeman.

1. *Typical rank of three-way arrays:*
   What changes when slices are symmetric?

2. *Best known application:*
   INDSCAL-related fitting problem, based on Carroll & Chang conjecture that CP produces **A**=**B***.*

3. *Evaluation of conjecture in low-rank approximation cases*

4. *Evaluation of conjecture in full rank decomposition cases*
   - *How to find* **A** ≠ **B** *for* 4×3×3 *arrays of rank 5.*
   - *How to fix the problem.*

Definition:

The rank of a three-way array is smallest number of rank-one arrays (outer products of three vectors) that have the array as their sum.

Equivalent definition:

The rank of a three-way array is the smallest number of components that admits perfect fit in CP.

When $\underline{\mathbf{X}}$ is $I \times J \times K$ array of rank r, r is smallest number of components admitting decomposition

$$\mathbf{X}_k = \mathbf{A}\mathbf{C}_k\mathbf{B}',$$

with $\mathbf{A}$ $I \times r$, $\mathbf{B}$ $J \times r$, *and* $\mathbf{C}_k$ $r \times r$ (diagonal), $k=1,\ldots,K$.

Array formats have maximal and typical rank:

Example: $2\times4\times4$ array. Slices $\mathbf{X}_1$ and $\mathbf{X}_2$.

When 4 eigenvalues of $\mathbf{X}_1^{-1}\mathbf{X}_2$ complex,

array can be transformed to

$$\mathbf{Y}_1=\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \text{ and } \mathbf{Y}_2=\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & b \\ 0 & 0 & b & 0 \end{bmatrix},$$

with $b \neq 0$ (Rocci & Ten Berge, 2002).

Result: Rank is 5 when $b^2 \neq 1$, and 6 otherwise.

Also: When 4 eigenvalues real, rank is 4;

when 2 real, rank is 5.

Conclusion: $2\times4\times4$ array has typical rank {4, 5},

and maximal rank 6.

Focus on *typical* rank

Theory: Basic fact about three-way arrays.
Practice: Hybrid models in between CP and Tucker-3-way PCA: Simple core with rank less than typical rank is model instead of tautology (Ten Berge, 2004)

What do we know of typical ranks?

Typical rank results for arrays with K=2 and K=3

	K=2				K=3		
	J=2	J=3	J=4		J=3	J=4	J=5
I=2	{2,3}	3	4				
I=3	3	{3,4}	4	I=3	5	?	{5,6}
I=4	4	4	{4,5}	I=4	{5,?}	?	?
I=5	4	5	5	I=5	{5,6}	?	?
I=6	4	6	6	I=6	6	?	?
I=7	4	6	7	I=7	7	?	?
I=8	4	6	8	I=8	8	{8,9}	?
I=9	4	6	8	I=9	9	9	?
I=10	4	6	8	I=10	9	10	10
I=11	4	6	8	I=11	9	11	11
I=12	4	6	8	I=12	9	12	12

Based on random sampling from continuous distribution of *all* elements of the array.

What if slices are sampled to be symmetric?

Typical ranks, unconstrained $I \times J \times J$ arrays

Ten Berge & Stegeman (2006)

	J=2	J=3	J=4	J=5
I=2	{2,3}	{3,4}	{4,5}	{5,6}
I=3	3	5	$6 \leq r$	$7 \leq r$
I=4	4	$5 \leq r \leq 6$	$6 \leq r$	$7 \leq r$
I=5	4	{5,6}	$6 \leq r$	$7 \leq r$
I=6	4	6	$6 \leq r$	$7 \leq r$
I=7	4	7	$7 \leq r$	$7 \leq r$
I=8	4	8	$8 \leq r$	$8 \leq r$

Typical ranks, symmetric slice $I \times J \times J$ arrays

Ten Berge, Sidiropoulos & Rocci (2004)

	J=2	J=3	J=4	J=5
I=2	{2,3}	{3,4}	{4,5}	{5,6}
I=3	3	4	?	?
I=4	3	{4,5}	?	?
I=5	3	{5,6}	?	?
I=6	3	6	?	?
I=7	3	6	?	?
I=8	3	6	?	?

Partial explanation of equal values.

Which array formats admit rank-preserving transformations to symmetry (of slices)?

(Ten Berge & Stegeman, 2006).

Example $I\times4\times4$ array: We want $\mathbf{SX}_i$ symmetric.

$$\mathbf{X}_i=[\mathbf{x}_{i1}|\mathbf{x}_{i2}|\mathbf{x}_{i3}|\mathbf{x}_{i4}],\ \mathbf{S}=\begin{bmatrix} \mathbf{s}_1' \\ \hline \mathbf{s}_2' \\ \hline \mathbf{s}_3' \\ \hline \mathbf{s}_4' \end{bmatrix}.$$

Symmetry means $\mathbf{s}_j'\mathbf{x}_{ik} = \mathbf{s}_k'\mathbf{x}_{ij}$. Find $[\mathbf{s}_1'|\mathbf{s}_2'|\mathbf{s}_3'|\mathbf{s}_4']$ orthogonal to columns of

$$\mathbf{H}_i=\begin{bmatrix} -\mathbf{x}_{i2} & -\mathbf{x}_{i3} & -\mathbf{x}_{i4} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{x}_{i1} & \mathbf{0} & \mathbf{0} & -\mathbf{x}_{i3} & -\mathbf{x}_{i4} & \mathbf{0} \\ \mathbf{0} & \mathbf{x}_{i1} & \mathbf{0} & \mathbf{x}_{i2} & \mathbf{0} & -\mathbf{x}_{i4} \\ \mathbf{0} & \mathbf{0} & \mathbf{x}_{i1} & \mathbf{0} & \mathbf{x}_{i2} & \mathbf{x}_{i3} \end{bmatrix}$$

Result: Solution with $\mathbf{S}$ nonsingular exists almost surely when there are two slices, or when there are three 2×2 slices.

Sometimes symmetric slices entail *lower* typical rank

Example $4\times2\times2$ array

Asymmetric slices are linear comb of

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

Symmetric slices are linear comb of

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

Typical ranks 4 and 3, respectively.

No cases found where symmetric slice arrays have *higher* typical rank than asymmetric counterparts.

Application of results on symmetric slices: INDSCAL-related scalar product fitting problem (Carroll & Chang, 1970). We need constrained CP-decomposition for symmetric slices

$$\mathbf{X}_i = \mathbf{A}\mathbf{C}_i\mathbf{A}' + \mathbf{E}_i \qquad (1)$$

CP can only fit $\mathbf{X}_i = \mathbf{A}\mathbf{C}_i\mathbf{B}' + \mathbf{E}_i$, with $\mathbf{A}$ and $\mathbf{B}$ $J \times r$, $\mathbf{C}_i$ $r \times r$ (diagonal), $i=1,\ldots,K$.

C&C conjecture: Upon convergence of CP, **A** and **B** proportional columnwise. When conjecture false, CP unsuitable to fit (1).

In most applications, conjecture seems correct. But there are exceptions, where $\mathbf{A} \neq \mathbf{B}$.

- When precisely do exceptions occur?
- Do these cases admit alternative CP solution which does have $\mathbf{A}=\mathbf{B}$?
- If so, how do we find the alternative solution?

C & C conjecture in low rank approximations

Ten Berge & Kiers (1991).

$$\mathbf{X}_1 = \begin{bmatrix} 3 & 1 & 0 \\ 1 & 3 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \mathbf{X}_2 = \begin{bmatrix} 3 & -1 & 0 \\ -1 & 3 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Non-optimal stationary value 39 when

$$\mathbf{A} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \mathbf{B} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \text{and } \mathbf{C} = \begin{bmatrix} 1 \\ -1 \end{bmatrix}.$$

First order derivatives vanish, but **A** and **B** differ. Can only happen (r=1) with *asymmetric* estimates $\mathbf{AC}_1\mathbf{B}'$ and $\mathbf{AC}_2\mathbf{B}'$.

Global minimum 21 of CP function for

$$\mathbf{A} = \mathbf{B} = \begin{bmatrix} \sqrt{.5} \\ \sqrt{.5} \\ 0 \end{bmatrix}, \text{and } \mathbf{C} = \begin{bmatrix} 4 \\ 2 \end{bmatrix}.$$

Possibility: Under random sampling of the data from a continuous distribution, asymmetric estimates at stationary points of the least squares CP loss function arise with probability zero at global minima of the CP function.

If true, then always **A**=**B** in low rank approximation cases at global minima.

C & C conjecture in perfect fit situation

Ten Berge, Sidiropoulos and Rocci (2004) investigated when **A**=**B** is guaranteed in perfect fit situation

- When CP decomposition is unique, **A**=**B**.
- When number of slices $I \geq r$, almost all solutions have **A** = **B**.

  Example: when 5×3×3 array has rank 5, all solutions have **A** = **B** almost surely.
- When k-rank of **C** satisfies $k_{\mathbf{C}} \geq r-J+2$, we have **A** = **B** almost surely .

  (k_C *= largest number of columns of* **C** *that are linearly independent, no matter how we pick those columns)*

To find cases with **A** ≠ **B**, we need cases with $I < r$, and $k_C < r-J+2$

Example: $4 \times 3 \times 3$ array (symmetric slices) has typical rank {4,5}.

When it has rank 4, $I = r$, and **A**=**B**.

When it has rank 5, and $k_C < 4$, we may have **A** $\neq$ **B**.

Does $k_C < 4$ ever arise?

Numerical experiment (Ten Berge & Stegeman, 2007)

Generate random $4 \times 3 \times 3$ array, symmetric slices. Typical rank {4,5}. Check if rank is 5. Then run CP to convergence.

Find null of **C** (4×5).

- **o** If it has no zeroes, $k_C = 4$ so **A** = **B**. Run CP again.
- **o** Else, look if **A** and **B** differ.

Result: Low k-rank for **C** with **A**$\neq$**B** does occur with positive probability.

Random 4$\times$3$\times$3 array of rank 5

1.1346	0.1630	1.8262
0.1630	0.1299	1.9809
1.8262	1.9809	2.1604
-2.1353	-0.2361	1.2687
-0.2361	2.3622	0.0724
1.2687	0.0724	0.9238
2.0254	-0.3567	0.1805
-0.3567	2.2626	0.5967
0.1805	0.5967	0.2767
3.4732	-0.2749	-0.9870
-0.2749	-0.4460	1.1702
-0.9870	1.1702	5.1791

	.5601	.2075	.0717	–.1597	.9106
A	.4775	.2568	.1646	.9832	–.0684
	.6770	.9439	.9838	–.0880	–.4077
	.3798	**.7954**	**.3549**	–.1597	.9106
B	**.1659**	**.5854**	**.3529**	.9832	–.0684
	–.9101	**.1570**	**.8657**	–.0880	–.4077
null(**C**)	.7040	.6594	.2636	**.0000**	**.0000**

Why two columns equal? Premultiply **C** by inverse of columns 2-3-4-5. This yields

–.9366	1.0000	.0000	.0000	.0000
–.3744	.0000	1.0000	.0000	.0000
.0000	.0000	.0000	1.0000	.0000
.0000	.0000	.0000	.0000	1.0000

Now slice 3 is $\mathbf{a}_4\mathbf{b}_4'$, slice 4 is $\mathbf{a}_5\mathbf{b}_5'$.

So $[\mathbf{a}_4\ \mathbf{a}_5] = [\mathbf{b}_4\ \mathbf{b}_5]$.

To see which other low k-ranks for **C** occur are possible with random arrays, we ran CP with constraint of low k_C to see if it fits perfectly. (Paatero's multilinear engine (1999) and home-made alternative).

What happened?

- We never found $k_C = 1$ as a possibility
- We found $k_C = 2$ now and then, with **A** and **B** sometimes different
- We found $k_C=3$ now and then, but then always **A**=**B**.

Explanation

Rank criterion of Ten Berge-Sidiropoulos-Rocci (2004) for $4\times3\times3$ arrays.

If rank is 4, **C** can be transformed to $\mathbf{I}_4$ by slice mixing. So slices can be mixed to be of rank 1 in four independent ways, which correspond to 4 real roots of 4-th degree polynomial.

Because real roots come in pairs, we have these possibilities

1. Four real roots; rank 4.
2. Two real roots; rank 5. The array admits two slice mixes of rank 1, with $k_C = 2$.

$$\mathbf{C}^{+} = \begin{bmatrix} x & 1 & 0 & 0 & 0 \\ y & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

3. No real roots; array rank 5. Low k-rank for **C** impossible. Hence **A** = **B**.

What did our simulations show?

- We never found $k_C = 1$. OK, because 3 roots real implies 4 roots real, so rank = 4.
- We found $k_C = 2$ now and then, with **A** and **B** often different
- We found $k_C=3$ now and then, but then always with **A**=**B**.

Why **A**=**B** when $k_C=3$? There is slice mix with

$$\mathbf{C}^{+} = \begin{bmatrix} 1 & 0 & 0 & 0 & x \\ 0 & 1 & 0 & 0 & y \\ 0 & 0 & 1 & 0 & z \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

Leave out slice 4, which has a unique factoring $\mathbf{a}_4\mathbf{b}_4'$. What remains is 3×3×3 with r=4 and $k_C = 3 \geq r - J + 2$. **A**=**B** guaranteed.

Question 1:

Does array admit a CP solution with low k_C?

Question 2:

Do slices admit linear combinations of rank one?

The more rank-one mixes are possible, the smaller k_C *can get.*

Back to $4 \times 3 \times 3$ array:

no real roots $\Rightarrow k_C = 4$

two real roots $\Rightarrow k_C = 2, 3$ possible

four real roots $\Rightarrow k_C = 0, 1$ possible $\Rightarrow r = 4$

How to fix a solution with **A** $\neq$ **B**, k_C=2.

	.5601	.2075	.0717	–.1597	.9106
A	.4775	.2568	.1646	.9832	–.0684
	.6770	.9439	.9838	–.0880	–.4077
	.3798	**.7954**	**.3549**	–.1597	.9106
B	**.1659**	**.5854**	**.3529**	.9832	–.0684
	–**.9101**	**.1570**	**.8657**	–.0880	–.4077
null(**C**)	.7040	.6594	.2636	**.0000**	**.0000**

New **C** after slice mixing:

–.9366	1.0000	.0000	.0000	.0000
–.3744	.0000	1.0000	.0000	.0000
.0000	.0000	.0000	1.0000	.0000
.0000	.0000	.0000	.0000	1.0000

Leave out the two common components and last two slices. What remains is $2\times3\times3$ with

$$\mathbf{S}_1=\mathbf{AC}_1\mathbf{B}' \quad \mathbf{S}_2=\mathbf{AC}_2\mathbf{B}',$$

A and **B** square, r=3, k_C=2. When **A** and **B** nonsingular, $k_A=k_B=3$, so $k_A+k_B+k_C=8$ (unique). Hence **A**=**B**. Contradiction. So **A** (or **B**) has rank < 3.

Let **n** be orthogonal to **A**. Construct orthonormal **N** with **n** as column 3. Then $\mathbf{Y}_1=\mathbf{N}'\mathbf{S}_1\mathbf{N}$ and $\mathbf{Y}_2=\mathbf{N}'\mathbf{S}_2\mathbf{N}$ has vanishing third row and third column. What remains is $2\times2\times2$ which has $\mathbf{A}^+ = \mathbf{B}^+$. So $\mathbf{S}_i = \mathbf{NY}_i\mathbf{N}'$ can be factored in components $\mathbf{NA}^+=\mathbf{NB}^+$, i=1, 2.

Easier recipe: Set **B** = **A** and recompute **C**.

Bottom line: Even when $\mathbf{A} \neq \mathbf{B}$, we can fix the problem. Also in other cases.

Missing general result: Whenever CP solution has **A** ≠ **B**, an alternative solution exists which does have **A** = **B**.

References

Carroll, J.D. & Chang, J.J. (1970). Analysis of individual differences in multidimensional scaling via an *n*-way generalization of Eckart-Young decomposition. *Psychometrika, 35,* 283-319.

Paatero, P. (1999). The multilinear engine - A table-driven least squares program for solving multilinear programs, including the n-way parallel factor analysis model. *Journal of Computational and Graphical Statistics, 8,* 845-888.

Rocci, R. & Ten Berge, J.M.F. (2002). Transforming three-way arrays to maximal simplicity. *Psychometrika*, *67*, 351-365.

Ten Berge, J.M.F. (2004). Simplicity and typical rank of three-way arrays, with applications to TUCKER-3 analysis with simple cores. *J. Chemometrics*, *18*, 17-21

Ten Berge, J.M.F. & Kiers, H.A.L. (1991). Some clarifications of the Candecomp algorithm applied to INDSCAL. *Psychometrika*, *56*, 317-326.

Ten Berge, J.M.F., Sidiropoulos, N.D. & Rocci, R. (2004). Typical rank and INDSCAL dimensionality for symmetric 3-way arrays of order $I\times 2\times 2$ and $I\times 3\times 3$. *Linear Algebra & Applications*, *388*, 363-377.

Ten Berge, J.M.F. & Stegeman, A. (2006). Symmetry transformations for square sliced three-way arrays, with applications to their typical rank. *Linear Algebra & Applications,* (in press).

Ten Berge, J.M.F. & Stegeman, A. (2007). *From partial to full equivalence when CP gives perfect fit. A complete treatment of $I\times 3\times 3$ arrays with symmetric slices.* (In preparation).