Khatri-Rao Products and Conditions for the Uniqueness of PARAFAC Solutions for IxJxK Arrays

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Outline

- Column and Orthogonal Complement (OC) Spaces
- Uniqueness questions and OC Spaces
- Results from OC Spaces

Uniqueness

- ***X*** is a 3-way array of order IxJxK
- PARAFAC decomposes the slices of the array as $\mathbf{X_k = A C_k B^t + E_k}$
  - $\mathbf{A_{IxR}}$; $\mathbf{B_{JxR}}$; $\mathbf{C_{KxR}}$
- Suppose there exists another decomposition $\mathbf{X_k = G D_k H^t + E_k}$
  - $\mathbf{G_{IxR}}$; $\mathbf{H_{JxR}}$; $\mathbf{D_{KxR}}$
- The decomposition is unique if every alternative satisfies: $\mathbf{G = A \Pi \Lambda_1}$; $\mathbf{H = B \Pi \Lambda_2}$; $\mathbf{D = C \Pi \Lambda_3}$
  - Π is a permutation matrix and Λ_i is diagonal and $\Lambda_1 \Lambda_2 \Lambda_3 = \mathbf{I_R}$

Bro 1998, McDonald 1980, Rao & Mitra 1971

KR Products

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & 0 & a_1 \\ 0 & 1 & 0 & a_2 \\ 0 & 0 & 1 & a_3 \end{pmatrix}$$

$$\mathbf{B} = \begin{pmatrix} 1 & 0 & 0 & b_1 \\ 0 & 1 & 0 & b_2 \\ 0 & 0 & 1 & b_3 \end{pmatrix}$$

$$\xrightarrow{\mathbf{A} \circ \mathbf{B}} \begin{pmatrix} 1 & 0 & 0 & a_1 b_1 \\ 0 & 0 & 0 & a_1 b_2 \\ 0 & 0 & 0 & a_1 b_3 \\ 0 & 0 & 0 & a_2 b_1 \\ 0 & 1 & 0 & a_2 b_2 \\ 0 & 0 & 0 & a_2 b_3 \\ 0 & 0 & 0 & a_3 b_1 \\ 0 & 0 & 0 & a_3 b_2 \\ 0 & 0 & 1 & a_3 b_3 \end{pmatrix}$$

ten Berge, J.M. and Sidiropoulos, N.D. 2002. On uniqueness in CANDECOMP/PARAFAC. *Psychometrika* 67: 399-409.

Summary

- The decomposition is considered without error

$$\boldsymbol{X} = (\mathbf{A} \circ \mathbf{B})\mathbf{C}^t$$

- KR products are full column rank (Liu and Sidiropoulos, 2001)
- The KR product is a basis for the column space
- Is the KR product $(\mathbf{A} \circ \mathbf{B})$ the only KR product that generates the columns of $\boldsymbol{X}$?
- The alternative is assumed to be $\boldsymbol{X} = (\mathbf{G} \circ \mathbf{H})\mathbf{D}^t$
- The component matrices are investigated in reduced form (characterizing the k-rank and rank)

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Column Spaces

$$\boldsymbol{X} = (\mathbf{A} \circ \mathbf{B})\mathbf{C}'$$

- The KR product representation of the PARAFAC suggests that the columns of ***X*** are linear combinations of the columns of the KR product

$$\boldsymbol{X} = \left[(\mathbf{A} \circ \mathbf{B})\mathbf{c}_1^t \quad (\mathbf{A} \circ \mathbf{B})\mathbf{c}_2^t \quad \cdots \quad (\mathbf{A} \circ \mathbf{B})\mathbf{c}_k^t \right]_{IJxK}$$

- So...the columns of ***X*** are generated from the columns of the KR product (**A**∘**B**)

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Investigating Column Spaces

- Replacement
  - Used when the elements can be switched without changing the column space
- Transformation
  - Used when one of the loading matrices has full-column rank

- Finding a non-trivial alternative basis for the column space implies a non-unique decomposition
  - Once one is found, all decompositions with that KR product can also be considered non-unique

ten Berge, J.M. and Sidiropoulos, N.D. 2002. On uniqueness in CANDECOMP/PARAFAC. *Psychometrika* 67: 399-409.

Reduced Forms

Instead of considering loading matrices of the form

$$\begin{pmatrix} \alpha_1 & \beta_1 & \gamma_1 & a\alpha_1 + b\beta_1 \\ \alpha_2 & \beta_2 & \gamma_2 & a\alpha_2 + b\beta_2 \\ \alpha_3 & \beta_3 & \gamma_3 & a\alpha_3 + b\beta_3 \\ & & & \end{pmatrix}$$

loading matrices in reduced form were considered

$$\begin{pmatrix} 1 & 0 & 0 & a \\ 0 & 1 & 0 & b \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

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Key Elements Learned

- The KR product allows us to talk about decompositions in column space language
- The properties of symmetry that applied for the “slab” notation also apply
- Matrices and the resulting KR products can be considered in “reduced form”.
- More to uniqueness than k-rank?

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When k-rank didn't give the full story

- R = 4
- $\mathbf{M_1}$: rank = 3 and k-rank = 2
- $\mathbf{M_2}$: rank = 3 and k-rank = 2
- $\mathbf{M_3}$: full column rank (rank = k-rank = 4)

$$\begin{pmatrix} 1 & 0 & 0 & x \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & z \end{pmatrix} \quad \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & y \\ 0 & 0 & 1 & z \end{pmatrix} \quad \begin{pmatrix} 1 & 0 & 0 & x \\ 0 & 1 & 0 & y \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

ten Berge, J.M. and Sidiropoulos, N.D. 2002. On uniqueness in CANDECOMP/PARAFAC. *Psychometrika* 67: 399-409.

When k-rank didn't give the full story

$$\begin{pmatrix} 1 & 0 & 0 & X \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & X \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & X \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & X \end{pmatrix}$$

Same position

$$\begin{pmatrix} 1 & 0 & 0 & X \\ 0 & 0 & 0 & X \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & X \\ 0 & 0 & 0 & X \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

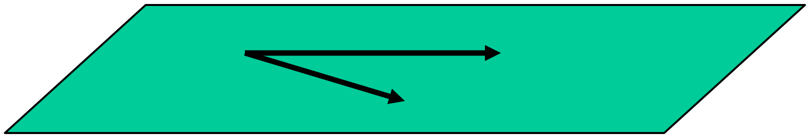
Different position

Orthogonal Complement Spaces (OCS)

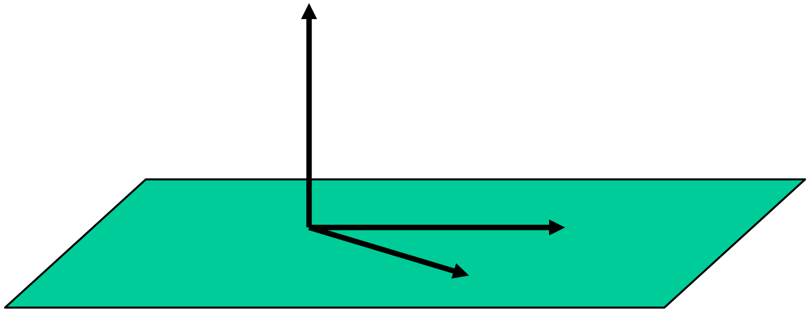
What’s different about an OCS approach?

Column Spaces and Orthogonal Complement Spaces

Column Space Approach



Orthogonal Complement Space Approach



Finding OC Constraints: The Steps

1. Suppose you have **A**^{o}**B**
2. Assume that an alternative **A**^{o}**B** exists, represented by **G**^{o}**H**
3. Find basis vectors for the null space of (**A**^{o}**B**)^{t}
4. Take the inner product of the columns of the **G**^{o}**H** and the null space basis vectors
5. Set equal to 0 (orthogonal) and solve

The constraints that result will determine if non-trivial alternatives are possible

OCSA: Finding Constraints

$$M_1 = \begin{pmatrix} 1 & 0 & 0 & a_1 \\ 0 & 1 & 0 & a_2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$M_2 = \begin{pmatrix} 1 & 0 & 0 & b_1 \\ 0 & 1 & 0 & b_2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\xrightarrow{M_1 \circ M_2} \begin{pmatrix} 1 & 0 & 0 & a_1b_1 \\ 0 & 0 & 0 & a_1b_2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & a_2b_1 \\ 0 & 1 & 0 & a_2b_2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

OCSA: Finding Constraints

$$\left[\begin{bmatrix} 0 \\ -\dfrac{b_1 a_2}{b_2 a_1} \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}\right] \longrightarrow \frac{h_2 g_1}{h_1 g_2} = \frac{b_2 a_1}{b_1 a_2}$$

OCSA: Finding Constraints

$$\mathbf{M_1} = \begin{pmatrix} 1 & 0 & 0 & a_1 \\ 0 & 1 & 0 & a_2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\mathbf{M_2} = \begin{pmatrix} 1 & 0 & 0 & b_1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & b_3 \end{pmatrix}$$

$$\xrightarrow{\mathbf{M_1 \circ M_2}} \begin{pmatrix} 1 & 0 & 0 & a_1b_1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & a_1b_3 \\ 0 & 0 & 0 & a_2b_1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & a_2b_3 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

OCSA: Finding Constraints

$$\left[\begin{bmatrix}0\\0\\-\frac{b_1a_2}{b_3a_1}\\1\\0\\0\\0\\0\\0\end{bmatrix},\begin{bmatrix}0\\0\\-\frac{a_2}{a_1}\\0\\0\\1\\0\\0\\0\end{bmatrix},\begin{bmatrix}0\\0\\0\\0\\0\\0\\1\\0\\0\end{bmatrix},\begin{bmatrix}0\\0\\1\\0\\0\\0\\0\\0\\0\end{bmatrix},\begin{bmatrix}0\\0\\0\\0\\0\\1\\0\\0\\0\end{bmatrix}\right] \longrightarrow \begin{array}{c}\dfrac{g_1}{g_2}=\dfrac{a_1}{a_2}\\ \dfrac{h_1}{h_3}=\dfrac{b_1}{b_3}\end{array}$$

OCSA: OC Constraints

Non-Separable Constraints

$$\frac{h_2 g_1}{h_1 g_2} = \frac{b_2 a_1}{b_1 a_2}$$

Non-trivial transformations

Separable Constraints

$$\frac{g_1}{g_2} = \frac{a_1}{a_2},$$

$$\frac{h_1}{h_3} = \frac{b_1}{b_3}$$

Trivial transformations

OCSA: Utilizing Symmetry

- If an alternative KR product can be found that is non-trivial transformation, then all PARAFAC decompositions with that KR product are non-unique
- A PARAFAC decomposition is unique if every alternative KR product can only be a trivial transformation.

OCSA: When R = 4

k-rank (M_1)	k-rank (M_2)	rank(M_1)	rank(M_2)	P/S Only?
2	2	2	2	No
2	2	2	3	No
2	2	3	3	Yes/No
2	3	2	3	No
2	3	3	3	Yes
2	4	2	4	Yes
2	4	3	4	Yes
3	3	3	3	Yes*
3	4	3	4	Yes

k-rank (M_1)	rank(M_1)	k-rank (M_2)	rank(M_2)	k-rank (M_3)	rank(M_3)	Uniqueness?
2	2	2	2	2	2	No
2	2	4	4	2	2	No
2	3	4	4	2	2	No
3	3	3	3	2	2	No
3	3	4	4	2	2	No
2	2	2	3	2	2	No
2	2	3	3	2	2	No
2	2	3	3	4	4	No
2	3	2	3	2	2	No
2	3	3	3	2	2	No
2	3	2	3	2	3	No/Yes
2	3	3	3	2	3	No/Yes
2	3	4	4	2	3	No/Yes
3	3	3	3	2	3	Yes
3	3	3	3	3	3	Yes*
3	3	4	4	2	3	Yes

OCSA: Conclusions for R = 4

- Necessary and Sufficient Conditions for uniqueness (when k-rank=rank)
  - A PARAFAC decomposition is unique if and only if $r(\mathbf{M}_i) + r(\mathbf{M}_j) \geq R + 2$, for all $i \neq j$

- Conditions for uniqueness
  - If two of the matrices have k-rank < rank, you will need to look at the number of OC constraints
  - Otherwise, A PARAFAC decomposition is unique if and only if $r(\mathbf{M}_i) + r(\mathbf{M}_j) \geq R + 2$, for all $i \neq j$

OCSA: Conclusions

- The OCSA provided a method for determining if alternative KR products could have non-trivial transformations
- The OC constraints offered an explanation of uniqueness when k-rank couldn’t.
- Based on the OC constraints, it was possible to determine if PARAFAC decompositions were unique
- Being able to “look” at decomposition uniqueness provided necessary and sufficient conditions for uniqueness for R = 4, 5, and 6 (k-rank = rank)

Discussion

- The tools we have…
  - KR products allow the use of linear algebra
  - Simplification allows for a better “view” of the decomposition
  - The OCSA provides a straightforward approach for determining if decompositions are unique for any R
- We need…
  - A better “tool” for determining which alternatives are truly alternatives
  - With more information on the decompositions that are unique, it will be possible to provide further empirical evidence for what causes uniqueness
- It looks like the key to defining necessary and sufficient conditions could rest with orthogonal complement spaces

Selected References

- Harshman, R.A. 1972. Determination and proof of minimum uniqueness conditions for PARAFAC1. *UCLA Working Papers in Phonetics* 22: 111-117.
- Kruskal, J.B. 1977. Three-way arrays: Rank and uniqueness of trilinear decompositions with application to arithmetic complexity and statistics. *Linear Algebra Appl.* 18: 95-138.
- Bro, R. 1998. Multi-way Analysis in the Food Industry. Models, algorithms and Applications, Ph.D. Thesis, University of Amsterdam, The Netherlands.
- ten Berge, J.M. and Sidiropoulos, N.D. 2002. On uniqueness in CANDECOMP/PARAFAC. *Psychometrika* 67: 399-409.

Extra Slides

OC Spaces and Column Spaces

- Column Space of : $\mathcal{C}(\mathbf{A}^{o}\mathbf{B})$
- Null Space of $(\mathbf{A}^{o}\mathbf{B})^{t}$: $\mathcal{N}((\mathbf{A}^{o}\mathbf{B})^{t})$
- $\mathcal{C}(\mathbf{A}^{o}\mathbf{B}) = [\mathcal{N}((\mathbf{A}^{o}\mathbf{B})^{t})]^{\perp}$

- All vectors orthogonal to $[\mathcal{N}((\mathbf{A}^{o}\mathbf{B})^{t})]$ are elements of $\mathcal{C}(\mathbf{A}^{o}\mathbf{B})$
- So...we need to find an alternative KR product that has columns that are orthogonal to $[\mathcal{N}((\mathbf{A}^{o}\mathbf{B})^{t})]$

Sample MAPLE Code

```
with(LinearAlgebra):

A:=Matrix(3,4,[[1,0,0,a[1]],[0,1,0,0],[0,0,1,a[3]]]);
B:=Matrix(3,4,[[1,0,0,b[1]],[0,1,0,0],[0,0,1,b[3]]]);

AB:=Matrix(9,4,[convert((OuterProductMatrix(B[1..3,1],A[1..3,1])),Vector),convert((OuterProductMatrix(B[1..3,2],A[1..3,
    2])),Vector),convert((OuterProductMatrix(B[1..3,3],A[1..3,3])),Vector),convert((OuterProductMatrix(B[1..3,4],A[1..3,
    4])),Vector)]);

G:=Matrix(3,4,[[1,0,0,g[1]],[0,1,0,g[2]],[0,0,1,g[3]]]);
H:=Matrix(3,4,[[1,0,0,h[1]],[0,1,0,h[2]],[0,0,1,h[3]]]);

GH:=Matrix(9,4,[convert((OuterProductMatrix(H[1..3,1],G[1..3,1])),Vector),convert((OuterProductMatrix(H[1..3,2],G[1..3,
    2])),Vector),convert((OuterProductMatrix(H[1..3,3],G[1..3,3])),Vector),convert((OuterProductMatrix(H[1..3,4],G[1..3,
    4])),Vector)]);

NAB:=NullSpace(Transpose(AB));

eqns:={Multiply(Transpose(NAB[1]),GH[1..9,4])=0,Multiply(Transpose(NAB[2]),GH[1..9,4])=0,Multiply(Transpose(NAB[
    3]),GH[1..9,4])=0,Multiply(Transpose(NAB[4]),GH[1..9,4])=0,Multiply(Transpose(NAB[5]),GH[1..9,4])=0,a[1]<>0,a[2]
    <>0,a[3]<>0,b[1]<>0,b[2]<>0,b[3]<>0};

solve(eqns);
```

OCSA: When R = 5 (k-rank = rank)

k-rank (M1)	k-rank (M2)	rank(M1)	rank(M2)	P/S Only?
2	2	2	2	No
2	3	2	3	No
2	4	2	4	No
2	5	2	5	Yes
3	3	3	3	No
3	4	3	4	Yes
3	5	3	5	Yes
4	4	4	4	Yes
4	5	4	5	Yes

k-rank (M1)	rank(M1)	k-rank (M2)	rank(M2)	k-rank (M3)	rank(M3)	Uniqueness?
2	2	2	2	2	2	No
2	2	3	3	2	2	No
2	2	4	4	2	2	No
2	2	5	5	2	2	No
3	3	3	3	2	2	No
3	3	4	4	2	2	No
3	3	5	5	2	2	No
4	4	4	4	2	2	No
4	4	5	5	2	2	No
2	2	5	5	3	3	No
3	3	3	3	3	3	No
3	3	4	4	3	3	No
3	3	5	5	3	3	No
4	4	4	4	3	3	Yes

OCSA: When R = 6 (k-rank = rank)

k-rank (M1)	k-rank (M2)	rank(M1)	rank(M2)	P/S Only?
2	2	2	2	No
2	3	2	3	No
2	4	2	4	No
2	5	2	5	No
2	6	2	6	Yes
3	3	3	3	No
3	4	3	4	No
3	5	3	5	Yes
3	6	3	6	Yes
4	4	4	4	Yes
4	5	4	5	Yes
4	6	4	6	Yes
5	5	5	5	Yes
5	6	5	6	Yes

k-rank (M1)	rank(M1)	k-rank (M2)	rank(M2)	k-rank (M3)	rank(M3)	Uniqueness?
2	2	2	2	2	2	N
2	2	3	3	2	2	N
2	2	4	4	2	2	N
2	2	5	5	2	2	N
2	2	6	6	2	2	N
3	3	3	3	2	2	N
3	3	4	4	2	2	N
3	3	5	5	2	2	N
3	3	6	6	2	2	N
4	4	4	4	2	2	N
4	4	5	5	2	2	N
4	4	6	6	2	2	N
5	5	5	5	2	2	N
5	5	6	6	2	2	N
3	3	3	3	3	3	N
3	3	4	4	3	3	N
3	3	5	5	3	3	N
3	3	6	6	3	3	N
4	4	4	4	3	3	N
4	4	5	5	3	3	N
4	4	6	6	3	3	N
5	5	5	5	3	3	Y
4	4	4	4	4	4	Y
4	4	5	5	4	4	Y

Kruskal and Pairwise Combinations

- $k_A + k_B + k_C \geq 2R + 2$
- $k_C \leq R$

$$
\begin{aligned}
k_A + k_B &\geq 2R + 2 - k_C \\
&\geq 2R + 2 - R \\
&= R + 2
\end{aligned}
$$

$$r_A + r_B \geq 2R + 2$$