From blind source separation to tensor decomposition: an algebraic algorithm

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joint work with Ignat Domanov and Lieven De Lathauwer

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Overview

The Blind Source Separation

Deterministic uniqueness

Generic uniqueness

The Canonical Polyadic Decomposition From the theorem to the algorithm Algorithm outline Computational challenges **Q** construction Intersection shrinking Symmetric CPD Conclusion













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Constraints for uniqueness

Let \boldsymbol{X} be a matrix

Definition: a *deterministic condition of* \mathbf{X} is a particular matrix property which is always true.

Definition: a generic condition of **X** depends on a parameter $z \in \Omega$ and holds almost everywhere, i.e., if Σ is the set of z values for which the condition doesn't hold, then $\mu(\Sigma) = 0$ where μ is a measure absolute continuous w.r.t. the Lebesgue one.

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General case



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Uniqueness isn't guaranteed!

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- each $\mathbf{s}_r(\mathbf{z})$ depends on ℓ independent parameters, entries of $\boldsymbol{\xi}_r \in \mathbb{R}^{\ell}$;
- each $\mathbf{s}_r(\boldsymbol{\xi}_r)$ has the structure

$$\mathbf{s}(\boldsymbol{\xi}_r) = \begin{bmatrix} \frac{p_1}{q_1} \circ \mathbf{f}(\boldsymbol{\xi}_r) & \dots & \frac{p_N}{q_N} \circ \mathbf{f}(\boldsymbol{\xi}_r) \end{bmatrix}$$

with p_h, q_h polynomials and $\mathbf{f} = [f_1, \ldots, f_\ell]$ a vectorial function.



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A cookbook recipe for generic uniqueness

[Domanov and De Lathauwer 2016]

Let
$$\mathbf{t}(\mathbf{x}) = \begin{bmatrix} \frac{p_1}{q_1}(\mathbf{x}) & \dots & \frac{p_N}{q_N}(\mathbf{x}) \end{bmatrix}^T$$
 for $\mathbf{x} \in \Theta = \{\mathbf{x} \in \mathbb{C}^\ell : q_1(\mathbf{x}) \cdots q_N(\mathbf{x}) \neq 0\}$, if

- 1. rank $\mathbf{M}(z) = R$ for a generic choice of \mathbf{z} ;
- 2. each f_h is the ratio of two analytical functions on \mathbb{C}^{ℓ} ;
- 3. there exists $\boldsymbol{\xi}_0 \in \mathbb{C}^\ell$ s.t. det $J(\boldsymbol{f}, \boldsymbol{\xi}_0) \neq 0$;
- 4. the dimension of the span of $\mathbf{t}(\mathbf{x})$ for $\mathbf{x} \in \Theta$ is at least \hat{N} ;
- 5. rank $\mathbf{J}(\mathbf{t}, \mathbf{x}) > \hat{\ell}$ for a generic choice of \mathbf{z} ; 6. $R \leq \hat{N} - \hat{\ell}$;

then

$$\mathbf{X} = \sum_{r=1}^{R} \mathbf{m}_r(\mathbf{z}) \otimes \mathbf{s}(\boldsymbol{\xi}_r)$$

is generically unique.

Remarks for BSS

It is assumed that the columns of $\boldsymbol{\mathsf{S}}$ are values of the rational function

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$$\mathcal{V} = \Big\{(z_1,\ldots,z_N) \in \mathbb{C}^N : P_k(z_1,\ldots,z_N) = 0\Big\}.$$

Composed with the function \boldsymbol{f}

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Link with the CPD

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then
$$\mathbf{X}^{(3)} = (\mathbf{a}_1 \otimes_{\mathrm{K}} \mathbf{b}_1) \otimes \mathbf{c}_1^T + \ldots + (\mathbf{a}_R \otimes_{\mathrm{K}} \mathbf{b}_R) \otimes \mathbf{c}_R^T$$

 $\mathbf{X}^{(3)} = \begin{bmatrix} \mathbf{c}_1 \\ \mathbf{c}_1 \\ \mathbf{a}_1 \otimes_{\mathrm{K}} \mathbf{b}_1 \end{bmatrix} + \cdots + \begin{bmatrix} \mathbf{c}_R \\ \mathbf{a}_R \otimes_{\mathrm{K}} \mathbf{b}_R \end{bmatrix}$

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 $(\mathbf{a}_r \otimes_{\mathrm{K}} \mathbf{b}_r) \in \mathcal{V} = \left\{ \operatorname{vec}(\mathbf{Z}) : \begin{vmatrix} z_{i_1 j_1} & z_{i_1 j_2} \\ z_{i_2 j_1} & z_{i_2 j_2} \end{vmatrix} = 0 \right\}$

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Algebraic algorithm: high view

Let \mathcal{X} be a $(I \times J \times R)$ tensor, then

$$\mathbf{X}^{(3)} = \sum_{r=1}^{R} (\mathbf{a}_r \otimes_{\mathrm{K}} \mathbf{b}_r) \otimes \mathbf{c}_r^{\mathsf{T}} = (\mathbf{A} \odot \mathbf{B}) \mathbf{C}^{\mathsf{T}}.$$

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- 4. compute **C** by solving $(\mathbf{A} \odot \mathbf{B})\mathbf{C} = \mathbf{X}$.

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where $P_k^{\otimes}(\mathbf{x}_1^T, \dots, \mathbf{x}_N^T)$ is the vector obtained by formal substitution of (z_1, \dots, z_N) by $\mathbf{x}_1^T, \dots, \mathbf{x}_N^T$ and the scalar multiplication by the tensor product.

c is a column of **C**⁻¹ if and only if **X**^T**c** is equal to a column of **A** \odot **B** $P_{\nu}^{\otimes}(\mathbf{x}_{1}^{T}, \dots, \mathbf{x}_{N}^{T})(\mathbf{c} \otimes \dots \otimes \mathbf{c}) = 0$ for $k = 1, \dots, K$

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The columns of \mathbf{C}^{-1} belong to the intersection of \mathbf{Q} kernel and $\operatorname{vec}(\operatorname{Sym}_R^N)$ the subspace of vectorized order N symmetric tensors, i.e., $\mathbf{c} \in \operatorname{null}(\mathbf{Q}) \cap \operatorname{vec}(\operatorname{Sym}_R^d).$

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$$\mathcal{E}_{h+1} = (\mathbb{K} \otimes \mathcal{E}_h) \cap \mathsf{vec}(\mathsf{Sym}_R^{d+h})$$

until dim $\mathcal{E}_{h+1} = R^{h+1}$ and go to step 1.2.1;



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- 2. compute $(\mathbf{A} \odot \mathbf{B})$ as $\mathbf{C}^{-1}\mathbf{X}$ transposed;
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 ${\bf Q}$ for CPD

[Domanov and De Lathauwer 2013]

Let \mathcal{X} be an order-3 tensor of dimension $(I \times J \times R)$, then



Definition: **Q** is a $C_I^2 C_J^2 \times C_{R+1}^2$ matrix whose k-th column can be written as $\mathbf{Q}(\cdot, k) = \operatorname{vec}(\mathcal{C}_2(\mathbf{X}_{k_1} + \mathbf{X}_{k_2}) - \mathcal{C}_2(\mathbf{X}_{k_1}) - \mathcal{C}_2(\mathbf{X}_{k_2}))$

where

•
$$(k_1, k_2)$$
 is the *k*-th element of $Q_R^2 = \{(k_1, k_2) : 1 \le k_1 \le k_2 \le R\};$

- C_N^2 is the binomial of N over 2;
- $C_2(\mathbf{X}_h)$ is the matrix with the determinants of every 2 × 2 minors of \mathbf{X}_h .

Let \mathcal{X} be an order-3 tensor of dimension $(I \times 3 \times 2)$ such that

$$\mathbf{X}_1 = \begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \mathbf{a}_3 \end{bmatrix}$$
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The matrix $\mathbf{Q} = \begin{bmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \mathbf{q}_3 \end{bmatrix}$ associated with \mathcal{X} slices is such that $\mathbf{q}_1 = \operatorname{vec}(\mathcal{C}_2(\mathbf{X}_1 + \mathbf{X}_1) - \mathcal{C}_2(\mathbf{X}_1) - \mathcal{C}_2(\mathbf{X}_1)) = 2\operatorname{vec}(\mathcal{C}_2(\mathbf{X}_1));$

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- **q**₂ = vec($C_2(X_1 + X_2) C_2(X_1) C_2(X_2)$);

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The compound matrices are

$$\square \qquad \mathbf{Q} = \begin{bmatrix} 2\alpha_1 & \gamma_1 - (\alpha_1 + \beta_1) & 2\beta_1 \\ 2\alpha_2 & \gamma_2 - (\alpha_2 + \beta_2) & 2\beta_2 \\ 2\alpha_3 & \gamma_3 - (\alpha_3 + \beta_3) & 2\beta_3 \end{bmatrix}$$

■ *Ignore structure* and compute **Q** by its definition;

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All options present limitations!

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Structure highlight

Example

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We can remark that

- the entries of α_1 appears[†] in $\mathbf{a}_1 \mathbf{a}_2^T \mathbf{a}_2 \mathbf{a}_1^T$
- the entries of β_1 appears[†] in $\mathbf{b}_1 \mathbf{b}_2^T \mathbf{b}_2 \mathbf{b}_1^T$
- the entries of $\gamma_1 (\alpha_1 + \beta_1)$ appears[†] in $\mathbf{a}_1 \mathbf{b}_2^T + \mathbf{b}_1 \mathbf{a}_2^T \mathbf{b}_2^T \mathbf{a}_1 \mathbf{a}_2 \mathbf{b}_1^T$

Exterior algebra and \mathcal{C}_2

Definition: The exterior product $\wedge : \mathbb{R}^{I} \times \mathbb{R}^{J} \to \mathbb{R}^{I \times J}$ is defined as

$$\mathbf{a} \wedge \mathbf{b} = \mathbf{a} \mathbf{b}^T - \mathbf{b} \mathbf{a}^T$$
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Example Let $\mathbf{a}^T = \begin{bmatrix} a & b & c \end{bmatrix}$ and $\mathbf{b}^T = \begin{bmatrix} d & e & f \end{bmatrix}$ be two vectors, then $\mathbf{a} \wedge \mathbf{b} = \begin{bmatrix} 0 & ae - bd & af - cd \\ -ae + bd & 0 & bf - ce \\ -af + cd & -bf + ce & 0 \end{bmatrix}$.

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The matrix $\mathbf{a} \wedge \mathbf{b}$ has the properties:

- the diagonal entries are zeros;
- it is skew-symmetric;
- the elements highlighted are the entries of $C_2([\mathbf{a} \ \mathbf{b}])$.

$$\begin{array}{l} \mbox{Property: } \left< \mbox{vec}(\mathcal{C}_2([\mathbf{a} \quad \mathbf{b}])), \mbox{vec}(\mathcal{C}_2([\mathbf{a} \quad \mathbf{b}])) \right> = 2 \left< \mbox{vec}(\mathbf{a} \wedge \mathbf{b}), \mbox{vec}(\mathbf{a} \wedge \mathbf{b}) \right> \\ = 4 ||\mathbf{a}||^2 ||\mathbf{b}||^2 - \langle \mathbf{a}, \mathbf{b} \rangle^2 \end{array}$$

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Idea: Using the exterior and exploiting the structure.

 \blacksquare ${\bf Q}$ is not explicitly constructed

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- **Q** is not explicitly constructed
- $\langle \mathbf{q}_k, \mathbf{q}_h \rangle = \langle \operatorname{vec}(\mathcal{C}_2(\mathbf{Y})), \operatorname{vec}(\mathcal{C}_2(\mathbf{Z})) \rangle$ with \mathbf{Y}, \mathbf{Z} slices or a linear combination of slices of the input tensor \mathcal{X} .

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$$\langle \mathbf{q}_k, \mathbf{q}_h
angle = \mathsf{tr}(\mathbf{A}_{h_1k_1})\mathsf{tr}(\mathbf{A}_{h_2k_2}) + \mathsf{tr}(\mathbf{A}_{h_1k_2})\mathsf{tr}(\mathbf{A}_{h_2k_1}) - \mathsf{tr}(\mathbf{A}_{h_1k_1}^{\mathsf{T}}\mathbf{A}_{h_1k_2}) - \mathsf{tr}(\mathbf{A}_{h_1k_2}^{\mathsf{T}}\mathbf{A}_{h_2k_1})$$

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where
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 for $h_i \leq k_j$.

Let \mathcal{X} be a $(I \times J \times R)$ tensor of rank R

Direct construction: the matrix **Q** has size $(C_I^2 C_J^2 \times C_{R+1}^2)$

- each entry requires two multiplications;
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assuming that $R \sim IJ$, then the computational complexity is $R^4/4$.

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 be a vector of length J^2 , then
 $\mathbf{I}_{\mathbf{x}} = \operatorname{tr}(\mathbf{A}_{h_i,k_j}^T \mathbf{A}_{k_\ell,h_m}) = \mathbf{a}_{h_i,k_\ell}^T \mathbf{a}_{k_\ell,h_m};$

• compute $\mathbf{a}_{h_i,k_i}^T \mathbf{a}_{k_\ell,h_m}$ require J^2 multiplications;

• the total number of inner product to compute is C_{N+1}^2 with $N = C_{R+1}^2$;

assuming that $J\sim \sqrt{R}$, then the computational complexity is $R^5/8$.

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Given an input random tensor \mathcal{X} of dimensions $(I \times I \times R)$ such that its rank is

$$R = (I-1)^2$$

Size	Q		$\mathbf{O}^{T}\mathbf{O}$
	det	recursive	~~~
(11, 11, 100)	1.364e+01	1.556e+00	7.373e-01
(12, 12, 121)	2.876e+01	3.613e+00	1.621e+00
(13, 13, 144)	5.814e+01	6.353e+00	3.477e+00
(14, 14, 169)	1.071e+02	1.130e+01	6.928e+00
(15, 15, 196)	1.937e+02	1.956e+01	8.954e+01
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Table: Time estimates in seconds for computing \mathbf{Q} and its Gram matrix.

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Given an input random tensor \mathcal{X} of dimensions $(I \times I \times R)$ such that its rank is

$$R = (I-1)^2$$

Size	Q		$\mathbf{O}^{T}\mathbf{O}$
	det	recursive	<u>v</u> vv
(11, 11, 100)	1.364e+01	1.556e+00	7.373e-01
(12, 12, 121)	2.876e+01	3.613e+00	1.621e+00
(13, 13, 144)	5.814e+01	6.353e+00	3.477e+00
(14, 14, 169)	1.071e+02	1.130e+01	6.928e+00
(15, 15, 196)	1.937e+02	1.956e+01	8.954e+01
(16, 16, 225)	3.298e+02	3.291e+01	9.325e+02

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Combining the two approaches

constructing Q

benefiting from **Q** structure

develop^{\dagger} a more convenient matrix-vector product, using **Q** structure.

[†] possibly based on the exterior product

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Intersection shrinking

Once \mathbf{Q}^{\dagger} is computed, the intersection subspace

 $\mathcal{E}_0 = \mathsf{null}(\mathbf{Q}) \cap \mathsf{vec}(\mathsf{Sym}_R^N)$

has to be computed, cheking its dimension:

- if dim $\mathcal{E}_0 = R$, then the algorithm proceed;
- if dim $\mathcal{E}_0 > R$, then the intersection is shrinked, computing \mathcal{E}_{h+1} such that

$${\mathcal E}_{h+1} = ({\mathbb K}^R \otimes {\mathcal E}_h) \cap {\sf vec}({\sf Sym}_R^{N+h})$$

until dim $\mathcal{E}_{h+1} = R^{h+1}$ and then proceed.

or its Gram matrix $\mathbf{Q}^T \mathbf{Q}$.

\mathcal{E}_0 basis

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- 3. define the basis of null(Q) as $\mathbf{F}_0 = [\mathbf{v}_{m+1}, \dots, \mathbf{v}_N]$ with \mathbf{v}_ℓ the ℓ -th column of V

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 - 5.1 if \hat{R} is equal to R, then reshape \mathbf{E}_0 as a $(R \times R \times R)$ and compute its CPD; 5.2 if \hat{R} is *not* equal to R, then shrink the intersection until $\hat{R} = R^{h+1}$.

If the matrix \mathbf{E}_0 of size $(R^2 \times \hat{R})$ span the intersection subspace \mathcal{E}_0 with $\hat{R} > R$ until \hat{R} is equal to R^{h+1} , set h = 0 and repeat

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$$\mathcal{F}_{h+1} = \mathbb{K}^R \otimes \mathcal{E}_h$$

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- 3. orthogonalize \mathbf{E}_{h+1} ;
- 4. check how many of \mathbf{E}_{h+1} columns satisfy the symmetric conditions, updating \hat{R} .

Currently to avoid forming \mathbf{F}_{h+1} and the symmetrizer matrix \mathbf{G}_{h+1}

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Study theoretically the enlargement-shrinking process to estimate m a priori and orthogonalize just once[†]

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Let \mathbf{E}_{h+1} the basis of \mathcal{E}_{h+1} has size $(R^{h+1} \times R)$, then 1. reshape \mathbf{E}_{h+1} as a $(R^h \times R^2)$ matrix;

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- 4. reshape **R** as a tensor \mathcal{R} of size $(R \times R \times R)$;
- 5. compute the CPD of \mathcal{R} getting the factor **C** of size $(R \times R)$.



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- use an optimization based CPD algorithm;
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- try to preserve (partially)-symmetric properties and tune CPD algorithm.

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Current state

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Summary

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- using matrix structure in the computation of Q;
 - exterior algebra could be a tool
 - Gram matrix doesn't seem to be beneficial
- estimate the order of the symmetric tensor to product an auxiliary tensor of proper size;
- using the (partially)-symmetric structure into CPD of the auxiliary tensor.

Thank you for the attention! Questions? Advice?

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