Canonical Polyadic Decomposition of Incomplete Tensors: an Algebraic Study

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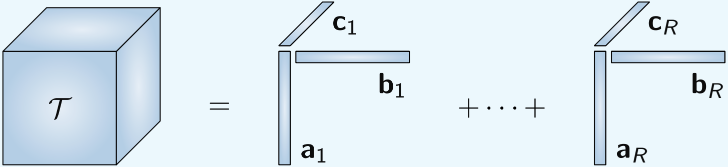
Workshop Low-rank Optimization and Applications
MPI MiS Leipzig, April 1-5, 2019

Canonical Polyadic Decomposition

Canonical Polyadic Decomposition (CPD):
decomposition in minimal number of rank-1 terms

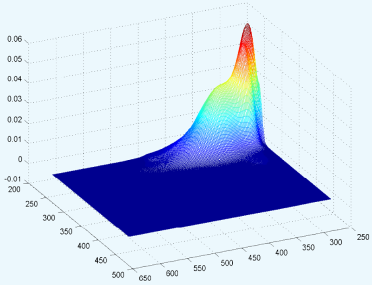


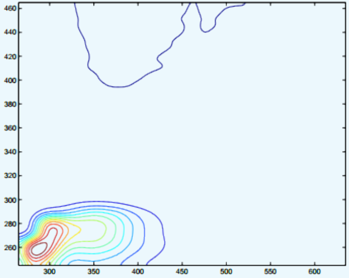
[Hitchcock, 1927; Harshman, 1970; Carroll and Chang, 1970]

- Unique under mild conditions on number of terms and differences between terms
- Orthogonality (triangularity, ...) not required (but may be imposed)
- Fundamental tool for signal separation

Application example

Excitation-emission spectroscopy





Excitation-emission spectroscopy: matrix approach fails

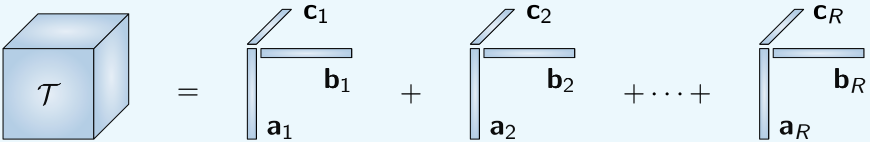
row vector $\sim$ excitation spectrum
column vector $\sim$ emission spectrum
coefficients $\sim$ concentrations

$$\mathbf{M} = \mathbf{a}_1 \mathbf{b}_1 + \mathbf{a}_2 \mathbf{b}_2 + \cdots + \mathbf{a}_R \mathbf{b}_R$$

Spectra are nonnegative (and not orthogonal)
Nonnegative Matrix Factorization (NMF) not unique in general

Excitation-emission spectroscopy: tensor approach

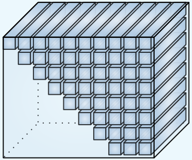
row vector $\sim$ excitation spectrum
column vector $\sim$ emission spectrum
coefficients $\sim$ concentrations



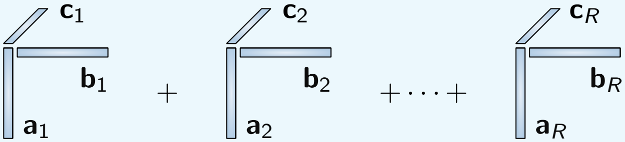
[Smilde et al., 2004]

Tensor approach: incomplete tensor

row vector $\sim$ excitation spectrum
column vector $\sim$ emission spectrum
coefficients $\sim$ concentrations



$$= \quad \mathbf{a}_1, \mathbf{b}_1, \mathbf{c}_1 \quad + \quad \mathbf{a}_2, \mathbf{b}_2, \mathbf{c}_2 \quad + \cdots + \quad \mathbf{a}_R, \mathbf{b}_R, \mathbf{c}_R$$



No emission below excitation

[Smilde et al., 2004]

Incomplete tensors

entries given	$\leftrightarrow$	entries to be sampled
CPD	$\leftrightarrow$	MLSVD/TT/hT
maximization fit	$\leftrightarrow$	minimization rank

(very) large-scale

This talk: fibers $\leftrightarrow$ entries

Optimization for CPD with missing entries

- Optimization problem:

$$\min_{\mathbf{A}^{(1)},\mathbf{A}^{(2)},\ldots,\mathbf{A}^{(N)}} \frac{1}{2} \left\| \mathcal{W} * \left(\mathcal{T} - \left[\!\left[\mathbf{A}^{(1)}, \mathbf{A}^{(2)}, \ldots, \mathbf{A}^{(N)} \right]\!\right] \right) \right\|_{\mathsf{F}}^{2}$$

- Algorithms
  - CPWOPT [Acar et al., 2011]
    Nonlinear Conjugate Gradients
  - INDAFAC [Tomasi and Bro, 2005]
    Gauss–Newton
  - CPD/SDF [Sorber et al., 2015]
    Quasi-Newton and (approximate) inexact Gauss–Newton
    Tensorlab: `cpd_nls`, `sdf_nls`
  - CPD(L)I [Vervliet et al., 2016a,c]
    Inexact Gauss–Newton with possible linear constraints
    Tensorlab: `cpd_nls` with `UseCPDI` option, `cpdli_nls`
  - Randomized block sampling, stochastic gradient [Vervliet and De Lathauwer, 2016]

Exploiting low multilinear/TT/hT rank for tensor decompositions

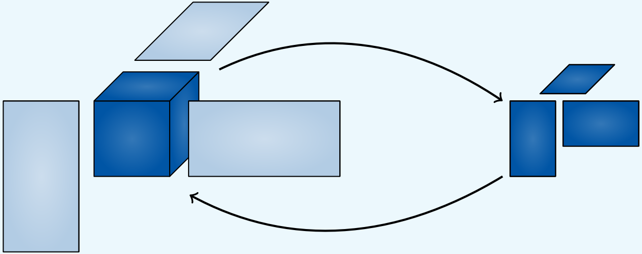
Strategy without constraints:

1| Compress tensor useing MLSVD, TT, hT
- randomized NLA [Mahoney et al., 2008; Vervliet et al., 2016b]
- cross approximation [Oseledets and Tyrtyshnikov, 2010; Caiafa and Cichocki, 2010; Bebendorf, 2000]

2| Compute CPD of core tensor

3| Expand CPD using factor matrices of compression

4| Refine result if necessary

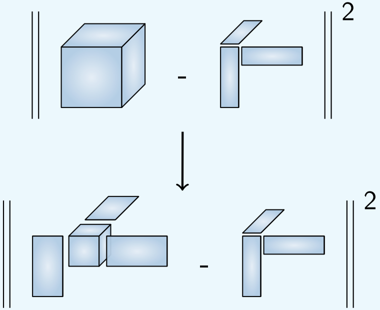


Orthogonal factor matrices preserve length and distance

Exploiting low multilinear/hT/TT rank for tensor decompositions

Strategy with constraints: [Vervliet et al., 2016b]

1. Compute LMLRA, TT, hT
2. Decompose while exploiting structure



Many combinations of structures and decompositions possible

Nuclear norm minimization

Matrix:

$$\begin{aligned} &\text{minimize } \|\hat{\mathbf{M}}\|_* && (\Leftarrow \text{minimize rank}(\hat{\mathbf{M}})) \\ &\text{subject to } \|\mathbf{W} * (\mathbf{M} - \hat{\mathbf{M}})\| \leqslant \delta \\ &\quad\updownarrow \\ &\text{minimize } \|\mathbf{M} - \hat{\mathbf{M}}\| \\ &\text{subject to } \quad \text{rank}(\hat{\mathbf{M}}) = R \end{aligned}$$

Tensor:

$$\|\mathcal{T}\|_* = \min\Big(\sum_r \|\mathbf{a}_r \otimes \mathbf{b}_r \otimes \mathbf{c}_r\|\Big)$$

$$\text{subject to} \quad \mathcal{T} = \sum_r \mathbf{a}_r \otimes \mathbf{b}_r \otimes \mathbf{c}_r$$

[Derksen, 2016]

CPD uniqueness: several cases

Some intuition

Two factor matrices have f.c.r.

One factor matrix has f.c.r.

No factor matrix has f.c.r.

Uniqueness: two factor matrices have f.c.r.

Deterministic bound: Uniqueness if:

- columns of **A**: linearly independent
- columns of **B**: linearly independent
- columns of **C**: no proportional pair

Generic version:

$$I \geqslant R \qquad J \geqslant R \qquad K \geqslant 2$$

one matrix $\rightarrow$ two (or more) matrices $\rightarrow$ uniqueness!

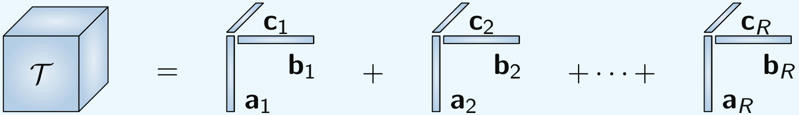
Computation: via matrix EVD

[Sanchez and Kowalski, 1990; Leurgans et al., 1993; Faber et al., 1994]

Tensorlab: `cpd_gevd`

Pencil-based computation: two factor matrices have f.c.r

CPD :



Slices :

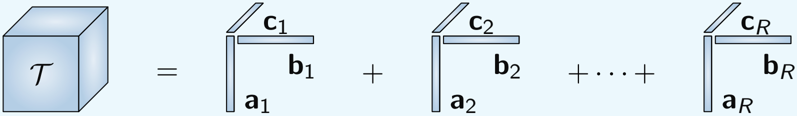
$$\mathcal{T}_{(:,:,1)} = \begin{bmatrix}\mathbf{a}_1 & \mathbf{a}_2 \cdots \mathbf{a}_R\end{bmatrix} \begin{bmatrix} c_{11} & & & \\ & c_{12} & & \\ & & \ddots & \\ & & & c_{1R}\end{bmatrix} \begin{bmatrix}\mathbf{b}_1 & \mathbf{b}_2 \cdots \mathbf{b}_R\end{bmatrix}^{\mathsf{T}}$$

$$\mathcal{T}_{(:,:,2)} = \begin{bmatrix}\mathbf{a}_1 & \mathbf{a}_2 \cdots \mathbf{a}_R\end{bmatrix} \begin{bmatrix} c_{21} & & & \\ & c_{22} & & \\ & & \ddots & \\ & & & c_{2R}\end{bmatrix} \begin{bmatrix}\mathbf{b}_1 & \mathbf{b}_2 \cdots \mathbf{b}_R\end{bmatrix}^{\mathsf{T}}$$

$$(G)EVD: \mathcal{T}_{(:,:,1)} \cdot \mathcal{T}_{(:,:,2)}^{-1} = \begin{bmatrix}\mathbf{a}_1 & \mathbf{a}_2 \cdots \mathbf{a}_R\end{bmatrix} \begin{bmatrix} c_{11}/c_{21} & & & \\ & c_{12}/c_{22} & & \\ & & \ddots & \\ & & & c_{1R}/c_{2R}\end{bmatrix} \begin{bmatrix}\mathbf{a}_1 & \mathbf{a}_2 \cdots \mathbf{a}_R\end{bmatrix}^{-1}$$

Pencil-based computation: numerical implication

CPD:



(G)EVD: $$\mathcal{T}_{(:,:,1)} \cdot \mathcal{T}_{(:,:,2)}^{-1} = \begin{bmatrix}\mathbf{a}_1 & \mathbf{a}_2 \cdots \mathbf{a}_R\end{bmatrix} \begin{bmatrix} c_{11}/c_{21} & & & \\ & c_{12}/c_{22} & & \\ & & \ddots & \\ & & & c_{1R}/c_{2R} \end{bmatrix} \begin{bmatrix}\mathbf{a}_1 & \mathbf{a}_2 \cdots \mathbf{a}_R\end{bmatrix}^{-1}$$

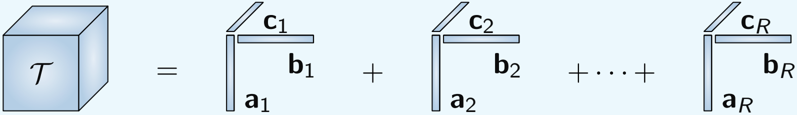
Algebraically equivalent but computational differences

- init optimization algorithm
- quantization noise $\rightarrow$ condition number [Beltrán et al., 2019]

CPD structure is collapsed into matrix pencil

Pencil-based computation: combination of partial results

CPD:



(G)EVD: $$\mathcal{T}_{(:,:,1)} \cdot \mathcal{T}_{(:,:,2)}^{-1} = \begin{bmatrix}\mathbf{a}_1 & \mathbf{a}_2 \cdots \mathbf{a}_R\end{bmatrix} \begin{bmatrix} c_{11}/c_{21} & & & \\ & c_{12}/c_{22} & & \\ & & \ddots & \\ & & & c_{1R}/c_{2R} \end{bmatrix} \begin{bmatrix}\mathbf{a}_1 & \mathbf{a}_2 \cdots \mathbf{a}_R\end{bmatrix}^{-1}$$

Use several pencils instead of just one

Use pencil for “safe splitting”

Eigenspaces $\rightarrow$ eigenvectors

Computation: from **C** to **A** and **B**

Assumption: **C** has full column rank

Rank-revealing factorization:

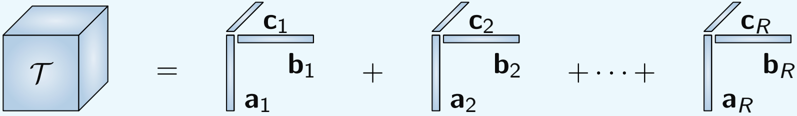
$$\mathbf{T}_{[1,2;3]} = \mathbf{E} \cdot \mathbf{F}^{\mathsf{T}} = \mathbf{E} \cdot \mathbf{M}^{-1} \cdot \mathbf{M} \cdot \mathbf{F}^{\mathsf{T}} = (\mathbf{A} \odot \mathbf{B}) \cdot \mathbf{C}^{\mathsf{T}}$$

Obtain $\hat{\mathbf{C}}^{\mathsf{T}} = \mathbf{M} \cdot \mathbf{F}^{\mathsf{T}}$ from CPD (up to permutation/scaling)

Unmix:

$$\mathbf{T}_{[1,2;3]} = (\mathbf{A} \odot \mathbf{B}) \cdot \mathbf{C}^{\mathsf{T}} \Rightarrow \mathbf{T}_{[1,2;3]} \cdot (\hat{\mathbf{C}}^{\mathsf{T}})^{\dagger} = \mathbf{A} \odot \mathbf{B}$$

$\forall r$: rank-1 approximation

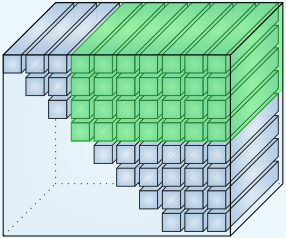


Two factor matrices subtensor have f.c.r.: variant for incomplete tensors

Select full $(\tilde{I} \times \tilde{J} \times K)$ subtensor $\quad \tilde{I} \leqslant I, \tilde{J} \leqslant J$

Obtain $\hat{\mathbf{C}}$ from CPD subtensor $\quad$ (up to perm/scaling)

Only part of data is used



Unmix:

$$\mathbf{T}_{[1,2;3]} = (\mathbf{A} \odot \mathbf{B}) \cdot \mathbf{C}^{\mathsf{T}} \Rightarrow \mathbf{T}_{[1,2;3]} \cdot (\hat{\mathbf{C}}^{\mathsf{T}})^{\dagger} = \mathbf{A} \odot \mathbf{B}$$

$\forall r$: rank-1 approximation

$$\mathbf{T}^{(inc)}_{[1,2;3]} = \mathbf{D}^{(mask)} \cdot (\mathbf{A} \odot \mathbf{B}) \cdot \mathbf{C}^{\mathsf{T}} \Rightarrow \mathbf{T}^{(inc)}_{[1,2;3]} \cdot (\hat{\mathbf{C}}^{\mathsf{T}})^{\dagger} = \mathbf{D}^{(mask)} \cdot (\mathbf{A} \odot \mathbf{B})$$

$\forall r$: rank-1 completion

Uniqueness: some intuition

Assumption: $\mathbf{C}$ has full column rank

$$\begin{aligned} \mathbf{T}_{[1,2;3]} &= (\mathbf{A} \odot \mathbf{B}) \cdot \mathbf{C}^{\intercal} \\ \mathbf{T}_{[1,2;3]} &= (\mathbf{A} \odot \mathbf{B}) \cdot \mathbf{M} \cdot \mathbf{M}^{-1} \cdot \mathbf{C}^{\intercal} \end{aligned}$$

Necessary and sufficient: only $\mathbf{M} = \mathbf{DP}$ preserves CPD structure
all other (nonsingular) $\mathbf{M}$ increase rank in columns

Rank-1 structure is ground for separation!

Compare to matrix case: $\mathbf{A} \cdot \mathbf{C}^{\intercal} = (\mathbf{A} \cdot \mathbf{M}) \cdot (\mathbf{M}^{-1} \cdot \mathbf{C}^{\intercal})$
no ground for separation

Uniqueness: one factor matrix has full column rank

Special case: tensor is long in one mode ("sample mode") (factor matrix **C**)
Khatri–Rao product second compound matrices:

$$\mathbf{U} = C_2(\mathbf{A}) \odot C_2(\mathbf{B}) \in \mathbb{C}^{\frac{I(I-1)}{2}\frac{J(J-1)}{2} \times \frac{R(R-1)}{2}}$$

$$u_{i_1 i_2 j_1 j_2, r_1 r_2} = \begin{vmatrix} a_{i_1 r_1} & a_{i_1 r_2} \\ a_{i_2 r_1} & a_{i_2 r_2} \end{vmatrix} \cdot \begin{vmatrix} b_{j_1 r_1} & b_{j_1 r_2} \\ b_{j_2 r_1} & b_{j_2 r_2} \end{vmatrix}$$

$$1 \leq i_1 < i_2 \leq I \qquad 1 \leq j_1 < j_2 \leq J \qquad 1 \leq r_1 < r_2 \leq R$$

Theorem: if **U** and **C** have full rank, then CPD is unique

[Jiang and Sidiropoulos, 2004; De Lathauwer, 2006]

Pencil-based computation: one factor matrix has f.c.r.

Assumption: $\mathbf{C}_2(\mathbf{A}) \odot \mathbf{C}_2(\mathbf{B})$ and $\mathbf{C}$ have full column rank

Rank-revealing factorization:
$$\mathbf{T}_{[1,2;3]} = \mathbf{E} \cdot \mathbf{F}^{\mathsf{T}} \qquad \text{(find R)}$$
$$\mathbf{T}_{[1,2;3]} = \mathbf{E} \cdot \mathbf{M}^{-1} \cdot \mathbf{M} \cdot \mathbf{F}^{\mathsf{T}}$$
$$\mathbf{T}_{[1,2;3]} = (\mathbf{A} \odot \mathbf{B}) \cdot \mathbf{C}^{\mathsf{T}}$$

Construct $\mathbf{P}$: for $i_1 < i_2, j_1 < j_2, r_1 \leqslant r_2,$ stack in $\mathbf{P} \in \mathbb{K}^{\frac{I(I-1)}{2}\frac{J(J-1)}{2} \times \frac{R(R+1)}{2}}$

$$p_{i_1 i_2 j_1 j_2, r_1 r_2} = e_{i_1 j_1, r_1} e_{i_2 j_2, r_2} + e_{i_1 j_1, r_2} e_{i_2 j_2, r_1} - e_{i_1 j_2, r_1} e_{i_2 j_1, r_2} - e_{i_1 j_2, r_2} e_{i_2 j_1, r_1}$$

Theorem: $\text{null}(\mathbf{P}) = \text{span}(\text{vec}(\mathbf{V}_1), \cdots, \text{vec}(\mathbf{V}_R))$

such that
$$\mathbf{V}_1 = \mathbf{W} \cdot \Lambda_1 \cdot \mathbf{W}^{\mathsf{T}} \qquad \text{with} \quad \mathbf{W} = \mathbf{M}^{-1}$$
$$\vdots$$
$$\mathbf{V}_R = \mathbf{W} \cdot \Lambda_R \cdot \mathbf{W}^{\mathsf{T}}$$

[De Lathauwer, 2006]

$$\mathcal{V} = \sum_r \mathbf{w}_r \otimes \mathbf{w}_r \otimes \mathbf{d}_r \qquad \text{all factor matrices f.c.r. (!)}$$

Computation: from **C** to **A** and **B**

Assumption: **C** has full column rank

Rank-revealing factorization:

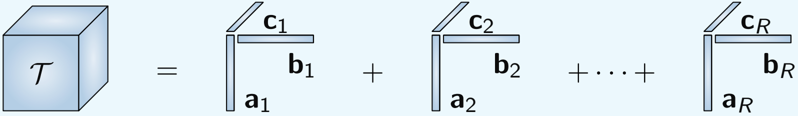
$$\mathbf{T}_{[1,2;3]} = \mathbf{E} \cdot \mathbf{F}^\top = \mathbf{E} \cdot \mathbf{M}^{-1} \cdot \mathbf{M} \cdot \mathbf{F}^\top = (\mathbf{A} \odot \mathbf{B}) \cdot \mathbf{C}^\top$$

Obtain $\quad \hat{\mathbf{C}}^\top = \mathbf{M} \cdot \mathbf{F}^\top$ from CPD $\qquad$ (up to permutation/scaling)

Unmix:

$$\mathbf{T}_{[1,2;3]} = (\mathbf{A} \odot \mathbf{B}) \cdot \mathbf{C}^\top \Rightarrow \mathbf{T}_{[1,2;3]} \cdot (\hat{\mathbf{C}}^\top)^\dagger = \mathbf{A} \odot \mathbf{B}$$

$\forall r$: rank-1 approximation



One factor matrix has f.c.r.: variant for incomplete tensors (1)

Assumption: $\mathbf{D}^{(mask,2\times2)} \cdot (\mathbf{C}_2(\mathbf{A}) \odot \mathbf{C}_2(\mathbf{B}))$ and $\mathbf{C}$ have full column rank

Rank-revealing factorization:

$$\mathbf{T}_{[1,2;3]} = \mathbf{E} \cdot \mathbf{F}^{\mathsf{T}} = \mathbf{E} \cdot \mathbf{M}^{-1} \cdot \mathbf{M} \cdot \mathbf{F}^{\mathsf{T}} = (\mathbf{A} \odot \mathbf{B}) \cdot \mathbf{C}^{\mathsf{T}}$$

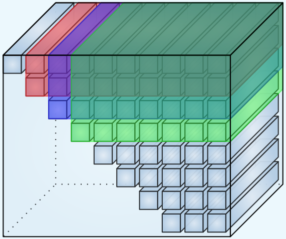
Construct $\mathbf{P}$:

for all $\quad i_1 < i_2, j_1 < j_2, \quad r_1 \leqslant r_2 \quad$ such that $\quad \mathcal{T}\left(\begin{bmatrix} i_1 \\ i_2 \end{bmatrix}, \begin{bmatrix} j_1 \\ j_2 \end{bmatrix}, :\right) \quad$ is fully observed

stack $\quad p_{i_1 i_2 j_1 j_2, r_1 r_2} = e_{i_1 j_1, r_1} e_{i_2 j_2, r_2} + e_{i_1 j_1, r_2} e_{i_2 j_2, r_1} - e_{i_1 j_2, r_1} e_{i_2 j_1, r_2} - e_{i_1 j_2, r_2} e_{i_2 j_1, r_1}$

in $\quad \mathbf{P}^{(\mathrm{mask},2\times2)} = \mathbf{D}^{(\mathrm{mask},2\times2)} \cdot \mathbf{P}$

[Sørensen and De Lathauwer, 2019]



One factor matrix has f.c.r.: variant for incomplete tensors (2)

Assumption: $\mathbf{D}^{(mask,2\times 2)} \cdot (\mathbf{C}_2(\mathbf{A}) \odot \mathbf{C}_2(\mathbf{B}))$ and $\mathbf{C}$ have full column rank

Rank-revealing factorization:

$$\mathbf{T}_{[1,2;3]} = \mathbf{E} \cdot \mathbf{F}^{\mathsf{T}} = \mathbf{E} \cdot \mathbf{M}^{-1} \cdot \mathbf{M} \cdot \mathbf{F}^{\mathsf{T}} = (\mathbf{A} \odot \mathbf{B}) \cdot \mathbf{C}^{\mathsf{T}}$$

Construct:

$$\mathbf{P}^{(\text{mask},2\times 2)}$$

Theorem:

$$\begin{aligned} \text{null}(\mathbf{P}) \; &= \; \text{span}(\text{vec}(\mathbf{V}_1), \cdots, \text{vec}(\mathbf{V}_R)) \\ &\qquad \text{such that} \quad \begin{array}{c} \mathbf{V}_1 = \mathbf{W} \cdot \Lambda_1 \cdot \mathbf{W}^{\mathsf{T}} \\ \vdots \\ \mathbf{V}_R = \mathbf{W} \cdot \Lambda_R \cdot \mathbf{W}^{\mathsf{T}} \end{array} \qquad \text{with} \quad \mathbf{W} = \mathbf{M}^{-1} \end{aligned}$$

[Sørensen and De Lathauwer, 2019]

$$\mathcal{V} = \sum_r \mathbf{w}_r \otimes \mathbf{w}_r \otimes \mathbf{d}_r \qquad \text{all factor matrices f.c.r. (!)}$$

One factor matrix has f.c.r.: variant for incomplete tensors (3)

Assumption: $\mathbf{D}^{(mask,2\times 2)} \cdot (\mathbf{C}_2(\mathbf{A}) \odot \mathbf{C}_2(\mathbf{B}))$ and $\mathbf{C}$ have full column rank

Rank-revealing factorization:

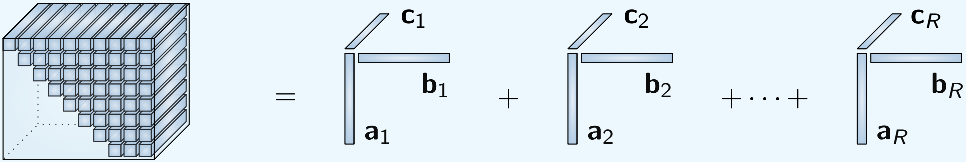
$$\mathbf{T}_{[1,2;3]} = \mathbf{E} \cdot \mathbf{F}^\mathsf{T} = \mathbf{E} \cdot \mathbf{M}^{-1} \cdot \mathbf{M} \cdot \mathbf{F}^\mathsf{T} = (\mathbf{A} \odot \mathbf{B}) \cdot \mathbf{C}^\mathsf{T}$$

Obtain $\hat{\mathbf{C}}^\mathsf{T} = \mathbf{M} \cdot \mathbf{F}^\mathsf{T}$ from auxiliary CPD (up to permutation/scaling)

Unmix:

$$\mathbf{T}^{(inc)}_{[1,2;3]} = \mathbf{D}^{(mask)} \cdot (\mathbf{A} \odot \mathbf{B}) \cdot \mathbf{C}^\mathsf{T} \Rightarrow \mathbf{T}^{(inc)}_{[1,2;3]} \cdot (\hat{\mathbf{C}}^\mathsf{T})^\dagger = \mathbf{D}^{(mask)} \cdot (\mathbf{A} \odot \mathbf{B})$$

$\forall r$: rank-1 completion



Uniqueness: none of the factor matrices has f.c.r. (1)

The k-rank of a matrix $\mathbf{A}$ is the maximal number such that any set of k columns of $\mathbf{A}$ is linearly independent.

Deterministic bound: For $\mathcal{T} \in \mathbb{K}^{I \times J \times K}$ uniqueness if

$$k(\mathbf{A}) + k(\mathbf{B}) + k(\mathbf{C}) \geq 2R + 2$$

[Kruskal, 1977; Sidiropoulos and Bro, 2000; Stegeman and Sidiropoulos, 2007; Domanov and De Lathauwer, 2013b]

Generic version:

$$\min(I, R) + \min(J, R) + \min(K, R) \geq 2R + 2$$

Computation: pencil-based

[Domanov and De Lathauwer, 2014]

Uniqueness: none of the factor matrices has f.c.r. (2)

Generic: $(I-1)(J-1) \geq R \quad K \geq R$
is necessary and sufficient
algebraic geometry

Compare to Jiang and Sidiropoulos [2004]; De Lathauwer [2006]:

$$I(I-1)J(J-1) \geq 2R(R-1) \quad \text{and} \quad K \geq R$$

$$\text{Approximately:} \quad \frac{IJ}{\sqrt{2}} \geq R \quad K \geq R$$

Compare to Kruskal [1977]:

$$\min(I,R) + \min(J,R) + \min(K,R) \geq 2R+2$$

Relaxed deterministic conditions: $\mathbf{C}$ has rank $R-1, R-2, \ldots$
$(3 \times 3), (4 \times 4), \ldots$minors

Pencil-based computation

[Domanov and De Lathauwer, 2013a,b, 2014, 2017]

Conclusion

- Fibers fully observed or fully missing
- Extensions of deterministic CPD uniqueness conditions
- Extensions of pencil-based CPD computation
- Guaranteed, exact tensor completion by GEVD under deterministic conditions (!)
- Generalization to partially observed fibers
- Generalization to MLSVD etc.

Canonical Polyadic Decomposition of Incomplete Tensors: an Algebraic Study

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Workshop Low-rank Optimization and Applications
MPI MiS Leipzig, April 1-5, 2019

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