Nonnegative Tucker Decomposition: Introduction, Identifiability and Algorithms

Giovanni Barbarino
Université de Mons, Belgium

INdAM Workshop
Low-rank Structures and Numerical Methods in Matrix and Tensor Computations

Joint work with

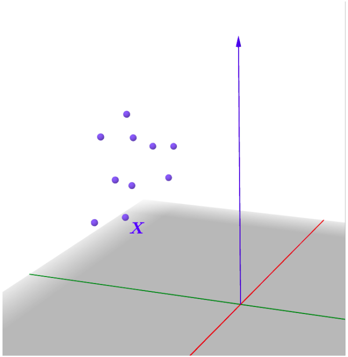
Nicolas Gillis
UMons

Subhayan Saha
UMons

NMF and Tri-NMF

Geometric interpretation of NMF

Given $X \in \mathbb{R}_+^{m \times n}$ and $r \leq \min\{m, n\}$, a NMF is $X = WH^\top$ with $W \in \mathbb{R}_+^{m \times r}$, $H \in \mathbb{R}_+^{n \times r}$



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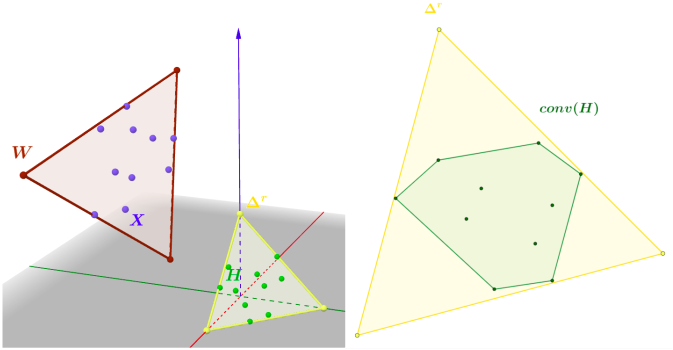
One can scale X and W such that $H^\top$ is column stochastic:

$$\underbrace{XD_X}_{\widetilde{X}} = \underbrace{WD_W}_{\widetilde{W}} \underbrace{D_W^{-1}H^\top D_X}_{\widetilde{H}^\top} \implies e^\top \widetilde{H}^\top = e^\top \widetilde{W}\widetilde{H}^\top = e^\top \widetilde{X} = e^\top \implies \textbf{conv}\,(\widetilde{X}) \subseteq \textbf{conv}\,(\widetilde{W})$$



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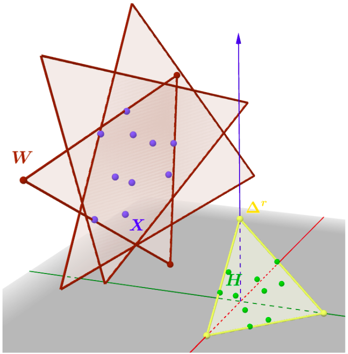

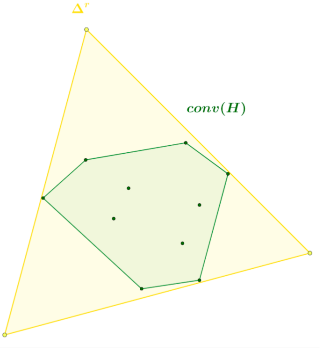

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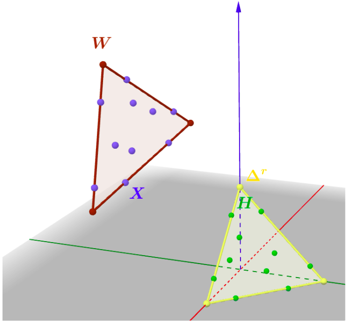

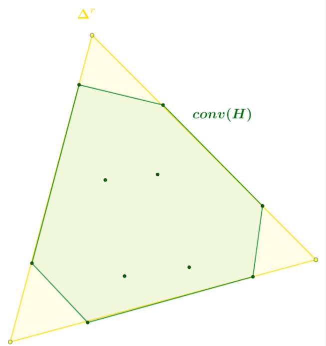

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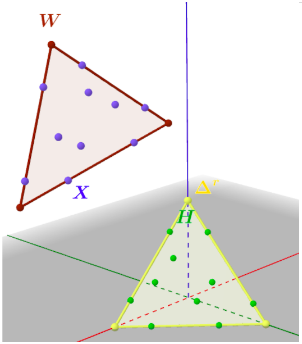
So we choose the Minimum Volume decomposition

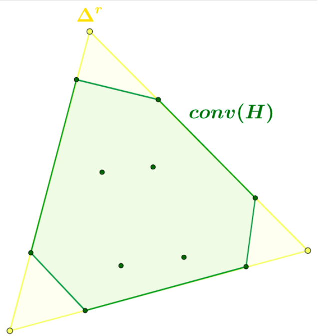
$$\min_{W,H} \ \mathrm{Vol}(W) \quad \text{s.t.}$$

$$X = WH^\top, He = e, H \geq 0$$

or $\quad \textbf{conv}(X) \subseteq \textbf{conv}(W)$

MinVol and SSC





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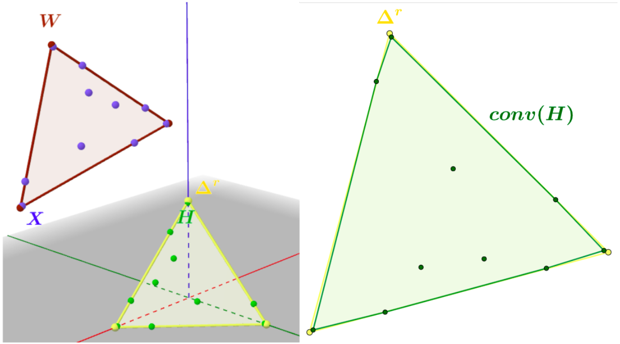
Theorem Let $X = WH^\top$ a Separable decomposition and $r = \text{rank}(X)$. Then the MinVol solution $W_\#$ is unique and coincides with W up to permutation of columns



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Separable: $W \triangleleft X \iff \mathbf{conv}\,(W) = \mathbf{conv}\,(X) \iff I \triangleleft H^\top$

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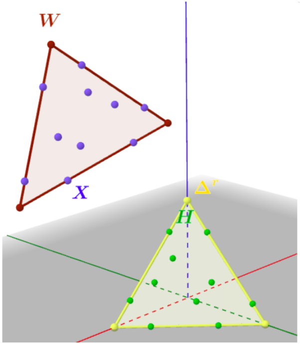
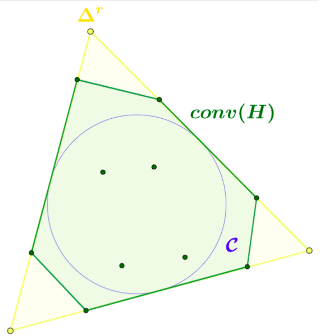
Theorem (Fu et al., 2018). Let $X = WH^\top$ a SSC decomposition and $r = \text{rank}(X)$. Then the MinVol solution $W_\#$ is unique and coincides with W up to permutation of columns





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SSC: $\quad \mathcal{C} \subseteq \mathbf{conv}\,(H) \quad + \quad [\dots]$

Nonnegative Matrix TRI-Factorization

Given $T \in \mathbb{R}^{n_1 \times n_2}$, a Tri-NMF is $T = U_1 \, G \, U_2^\top$ such that $U_i \geq 0 \in \mathbb{R}_+^{n_i \times r_i}$ and $G_+ \in \mathbb{R}^{r_1 \times r_2}$

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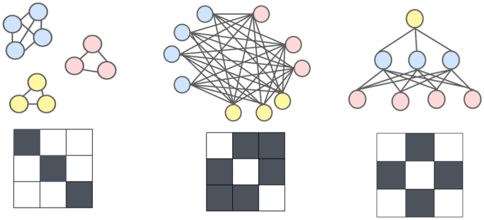

If $U_1 = U_2$ are binary with orthogonal columns, $T(i,j) = \text{Bernoulli}\Big(U_1(i,k_i)\, G(k_i,k_j)\, U_1(j,k_j)\Big)$ is the stochastic block model (SBM) widely used in community and role detection for the clustering of directed graphs

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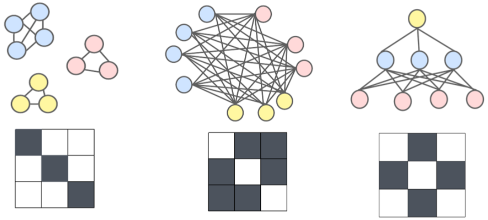

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Theorem (B., Saha, Gillis, 2025). Let $X = U_1 G U_2$ be a matrix of rank r where $U_i \in \mathbb{R}^{n_i \times r}$ satisfy the SSC. Any optimal solution, (U_1^*, G^*, U_2^*), of

$$\min_{U_i \in \mathbb{R}^{n_i \times r}, G \in \mathbb{R}^{r \times r}} |\det(G)| \;\text{ such that }\; X = U_1 G U_2^\top, U_i e = e, U_i \geq 0$$

uniquely identifies (U_1, G, U_2), meaning that $U_i^* = U_i$ and $G^* = G$ up to permutations

Nonnegative Tucker Decomposition

Tucker Decomposition (TD)

For $\mathcal{T} \in \mathbb{R}^{n_1 \times n_2 \times n_3}$, find the core $\mathcal{G} \in \mathbb{R}^{r_1 \times r_2 \times r_3}$ and factor matrices $U_i \in \mathbb{R}^{n_i \times r_i}$ s.t.

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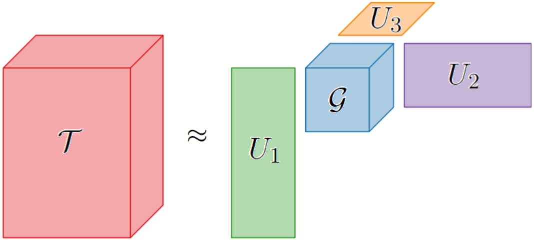

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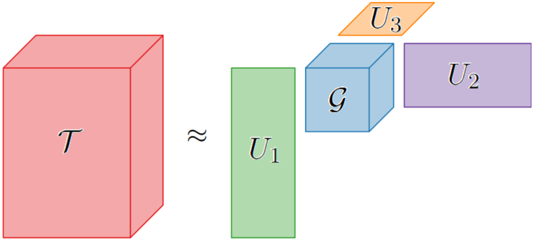

TD is a generalization of the canonical polyadic (CP) decomposition where $\mathcal{G}$ is diagonal

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  Applications: image classification, clustering, hyperspectral image denoising and compression, audio pattern extraction, image fusion, EEG signal analysis, ...

Application: community detection in multilayer graphs

Example: $59 \times 214 \times 214$ (goods $\times$ countries $\times$ countries) $\sim U_2 = U_3$

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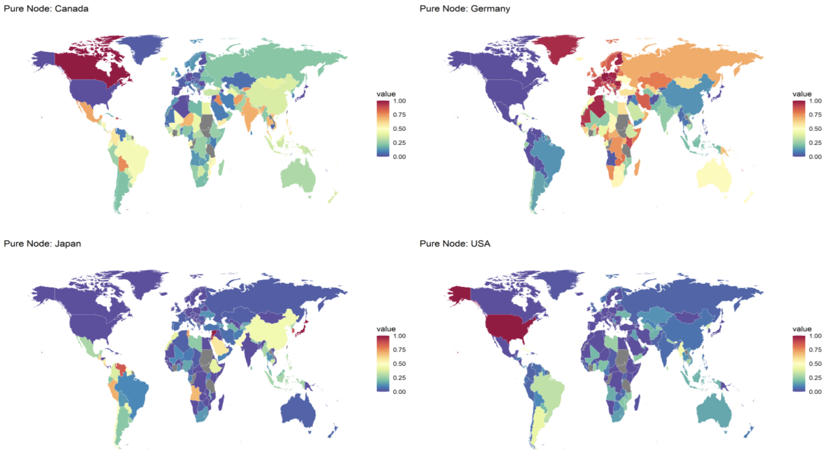
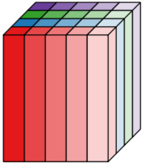


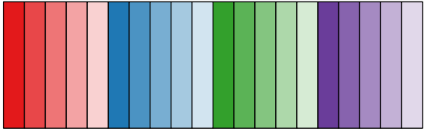
Agterberg, Zhang: Estimating higher-order mixed memberships .... J. American Statistical Association, 2024.

Identifiability of Order-3 nTD

Identifiability of order-3 nTDs: Unfoldings



Mode-1 fibers



Mode-1 unfolding : $\mathcal{T}_{(1)}^{\top}$

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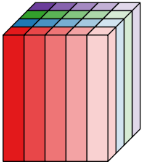

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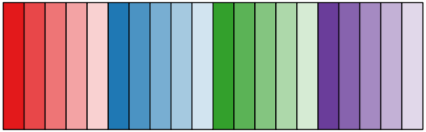

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Notation: $\mathcal{T}_{(1)} \in \mathbb{R}^{n_2 n_3 \times n_1}$ stacks fibers in mode 1 by row and

$$\mathcal{T} = (U_1, U_2, U_3).\mathcal{G} \implies \underbrace{\mathcal{T}_{(1)}}_{n_2 n_3 \times n_1} = \underbrace{(U_2 \otimes U_3)}_{n_2 n_3 \times r_2 r_3} \underbrace{\mathcal{G}_{(1)}}_{r_2 r_3 \times r_1} \underbrace{U_1^{\top}}_{r_1 \times n_1}$$

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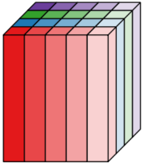

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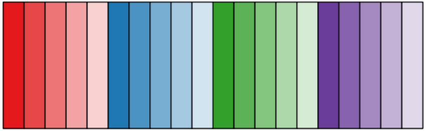

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If $X = V_1 S V_2^{\top}$ with V_i SSC
then any solution of MinVol(S)
uniquely identifies (V_1, S, V_2)

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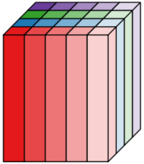

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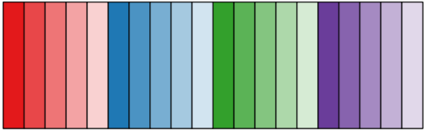

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Order-3 nTD is uniquely identifiable under the following assumptions:

1. $r_1 = r_3 r_2$, because $\mathcal{G}_{(1)} \in \mathbb{R}^{r_3 r_2 \times r_1}$
2. $(U_2 \otimes U_3)$ and U_1 satisfy the SSC
3. $\text{rank}(\mathcal{G}_{(1)}) = r_1$

If $X = V_1 S V_2{}^\top$ with V_i SSC
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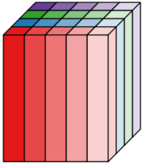
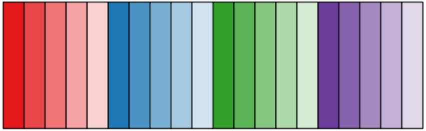
Identifiability of order-3 nTDs: Unfoldings



Mode-1 fibers



Mode-1 unfolding : $\mathcal{T}_{(1)}^\top$

Notation: $\mathcal{T}_{(1)} \in \mathbb{R}^{n_2 n_3 \times n_1}$ stacks fibers in mode 1 by row and

$$\mathcal{T} = (U_1, U_2, U_3).\mathcal{G} \implies \underbrace{\mathcal{T}_{(1)}}_{n_2 n_3 \times n_1} = \underbrace{(U_2 \otimes U_3)}_{n_2 n_3 \times r_2 r_3} \underbrace{\mathcal{G}_{(1)}}_{r_2 r_3 \times r_1} \underbrace{U_1^\top}_{r_1 \times n_1}$$

Order-3 nTD is uniquely identifiable under the following assumptions:

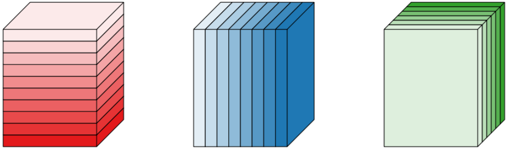
1. $r_1 = r_3 r_2$, because $\mathcal{G}_{(1)} \in \mathbb{R}^{r_3 r_2 \times r_1}$
2. $(U_2 \otimes U_3)$ and U_1 satisfy the SSC
3. $\text{rank}(\mathcal{G}_{(1)}) = r_1$

If $X = V_1 S V_2{}^\top$ with V_i SSC then any solution of MinVol(S) uniquely identifies (V_1, S, V_2)

Issues: $r_1 = r_3 r_2$, $(U_2 \otimes U_3)$ SSC not natural, order d tensor $\rightarrow \mathcal{T}_{(1)} \in \mathbb{R}^{n^{d-1} \times n}$ to factorize

Identifiability of order-3 nTDs: Slices I

Define the k-th slices of $\mathcal{T}$ along the third mode: $\mathcal{T}_k^{(3)} = \mathcal{T}(:,:,k)$



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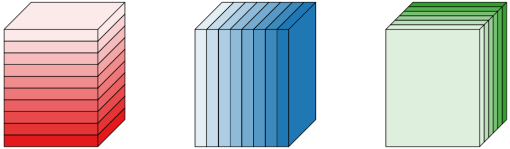

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If $\mathcal{T} = (U_1, U_2, U_3).\mathcal{G}$ then

$$\mathcal{T}_k^{(3)} = U_1 \Big(\sum_{p \in [r_3]} (U_3)_{k,p} \mathcal{G}_k^{(3)} \Big) U_2^\top$$

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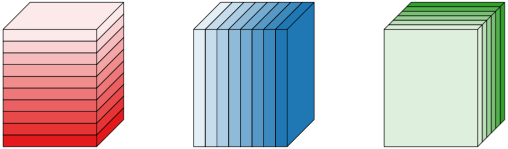

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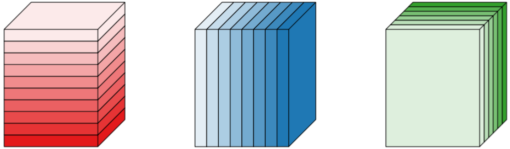

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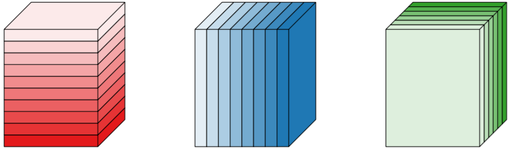

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Define the $\mathcal{J} := (k_3, k_4, \ldots, k_d)$-th slices of $\mathcal{T}$ along all modes except the first and second:

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Assumptions:

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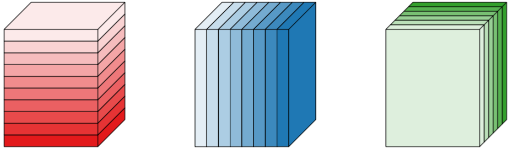

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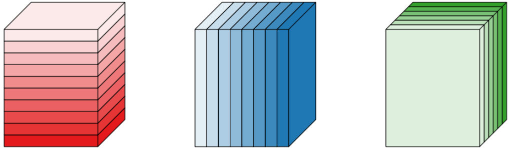

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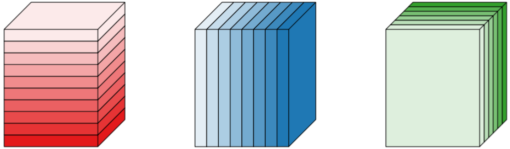

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Bad Assumptions: $(U_3 \otimes \cdots \otimes U_d)$ is SSC

Summary

Table 1: Main conditions on the U_i's, $\mathcal{G}$ and $\mathcal{T}$ to have an identifiability procedure for order-3 nTD.

	$\mathcal{G}$	U_i's	$\mathcal{T}$
Unfolding	$\text{rank}(\mathcal{G}_{(3)}) = r_3 = r_1 r_2$	$U_1 \otimes U_2$ is SSC U_3 is SSC	
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- Rank conditions can be modified to $T_\alpha^{(3)} := \sum_i \alpha_i \mathcal{T}_i^{(3)}$ with random vector α that only requires one $\mathcal{T}_i^{(3)}$ to be full rank for $\text{rank}(T_\alpha^{(3)}) = r_1$ with probability 1 without knowing i

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6. Stay tuned for the second part of this work on algorithms, with codes.

Thank you for your attention!

B., Saha, Gillis, *Identifiability of Nonnegative Tucker Decompositions - Part I: Theory*,
https://arxiv.org/abs/2505.12713