On Identifiable Polytope Characterization for Polytopic Matrix Factorization

Bariscan Bozkurt and Alper T. Erdogan, Electrical-Electronics Engineering and KUIS AI-CENTER, Koc University

IEEE ICASSP 2022

Polytopic Matrix Factorization

- **Latent Vectors:** $\mathcal{S}_g = \{\mathbf{s}_g(1), \ldots, \mathbf{s}_g(N)\} \subset \mathcal{P}$ where $\mathcal{P}$ is a polytope in $\subset \mathbb{R}^r$.
  Define $\mathbf{S}_g = \begin{bmatrix} \mathbf{s}_g(1) & \ldots & \mathbf{s}_g(N) \end{bmatrix} \in \mathbb{R}^{r \times N}$.
- **Linear Transformation:** Linearly transformed latent vectors:

$$\mathbf{y}(k) = \mathbf{H}_g \mathbf{s}_g(k), \quad k \in \{1, \ldots, N\}.$$

where $\mathbf{H}_g \in \mathbb{R}^{M \times r}$ is full column-rank.

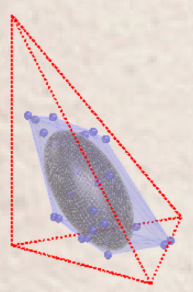
Observation matrix: $\mathbf{Y} = \mathbf{H}_g \mathbf{S}_g \in \mathbb{R}^{M \times N}$.

- **Goal:** Obtain estimates of $\mathbf{H}_g$ and $\mathbf{S}_g$ satisfying:

$$\begin{aligned} \mathbf{H} &= \mathbf{H}_g \mathbf{D}^{-1} \mathbf{\Pi}^T \\ \mathbf{S} &= \mathbf{\Pi} \mathbf{D} \mathbf{S}_g, \end{aligned}$$

where $\mathbf{\Pi}$ is a permutation matrix and $\mathbf{D}$ is a full-rank diagonal matrix.

PMF: Sufficiently Scattered Set



$\mathcal{S}_g$ is a sufficiently scattered set of $\mathcal{P}$ iff

- $\text{conv}(\mathcal{S}_g) \supset \mathcal{E}_{\mathcal{P}}$ where $\mathcal{E}_{\mathcal{P}}$ is the maximum volume inscribed ellipsoid of $\mathcal{P}$,
- $\text{bd}(\mathcal{P}) \cap \text{conv}(\mathcal{S}_g) = \text{bd}(\mathcal{P}) \cap \mathcal{E}_{\mathcal{P}}$.

Det-Max Criterion

Det-Max Criterion for Matrix Factorization

$$\begin{aligned} \text{maximize} \quad & \det(\mathbf{R_s}) \\ \text{subject to} \quad & \mathbf{R_s} = \tfrac{1}{N} \textstyle\sum_{k=1}^{N} \mathbf{S}_{:,k} \mathbf{S}_{:,k}^T \\ & \mathbf{Y} = \mathbf{H}\mathbf{S} \\ & \mathbf{S}_{:,k} \in \mathcal{D}, \ k = 1, \ldots, N. \end{aligned}$$

If $\mathcal{P}$ is an identifiable polytope, and $\mathcal{S}_g$ is a sufficiently scattered set of $\mathcal{P}$, then any global optimum $(\mathbf{H}_*, \mathbf{S}_*)$ of Det-Max Criterion satisfy

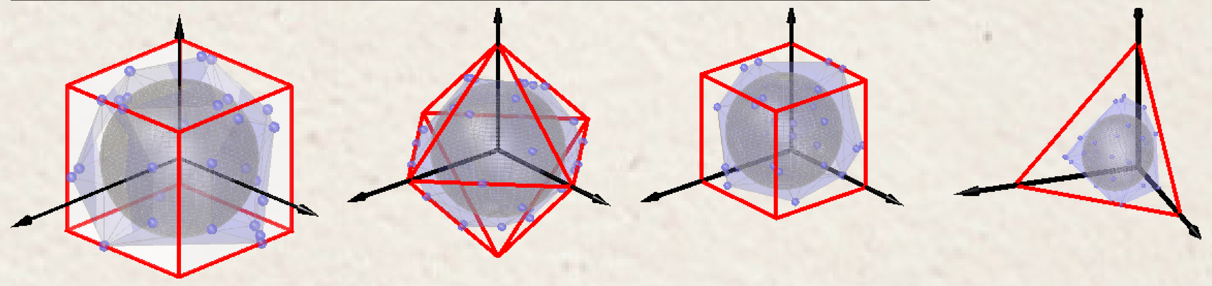
$$\begin{aligned} \mathbf{H}_* &= \mathbf{H}_h \mathbf{D}^{-1} \mathbf{\Pi}^T \\ \mathbf{S}_* &= \mathbf{\Pi} \mathbf{D} \mathbf{S}_g, \end{aligned}$$

Identifiable Polytopes

Fundamental Theorem of PMF

A polytope $\mathcal{P}$ is identifiable if its symmetry group is restricted to component permutations and sign alterations.

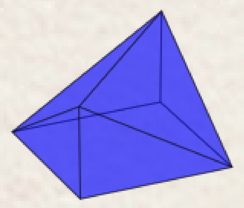
Example: Four Special Polytopes:



$\mathcal{B}_\infty$	$\mathcal{B}_1$	$\mathcal{B}_\infty \cap \Re^r_+$	$\mathcal{B}_1 \cap \Re^r_+$
Antisparse	Sparse	Nonnegative Antisparse	Nonnegative Sparse

Example: A Polytope with Mixed Features:

$$\mathcal{P}_{\text{ex}} = \left\{ \mathbf{s} \in \mathbb{R}^3 \ \middle| \ s_1, s_2 \in [-1, 1], s_3 \in [0, 1], \left\| \begin{bmatrix} s_1 \\ s_2 \end{bmatrix} \right\|_1 \leq 1, \left\| \begin{bmatrix} s_2 \\ s_3 \end{bmatrix} \right\|_1 \leq 1 \right\}$$



- s_1, s_2: signed, s_3: nonnegative
- s_1, s_2: mutually sparse
- s_2, s_3: mutually sparse

Brute Force Approach

- Let $\mathbf{V}_{\mathcal{P}} \in \mathbb{R}^{n \times m}$ be the vertex matrix of $\mathcal{P} \in \mathbb{R}^n$ containing m vertices of $\mathcal{P}$ in its columns.
- Let $\mathbf{\Pi} \in \mathbb{R}^{m \times m}$ denote a permutation matrix.
- $\mathcal{P}$ is identifiable $\iff$ the set $\{\mathbf{G} : \mathbf{G}\mathbf{V}_{\mathcal{P}} = \mathbf{V}_{\mathcal{P}}\mathbf{\Pi}, \mathbf{\Pi} \in \mathbb{R}^{m \times m}\}$ only contains signed permutation matrices.
- Brute force approach requires a search on all possible permutation matrices.
- **Factorial Complexity !**
- **We can exploit the group structure.**

Group Structure

Lemma

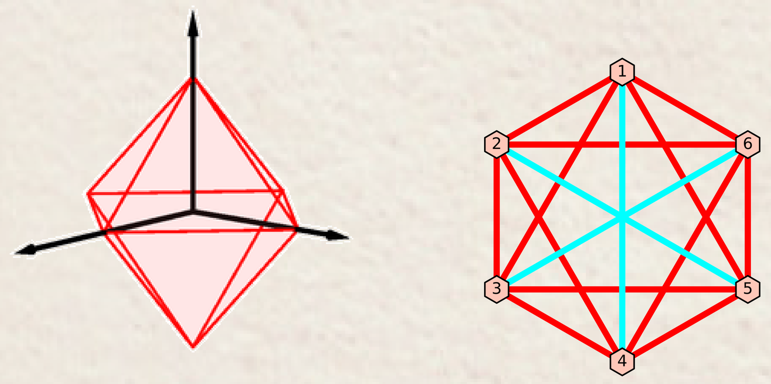
For a given polytope $\mathcal{P} \in \mathbb{R}^n$ with $\mathbf{V}_{\mathcal{P}} \in \mathbb{R}^{n \times m}$, the set $\{\mathbf{G} : \mathbf{G}\mathbf{V}_{\mathcal{P}} = \mathbf{V}_{\mathcal{P}}\mathbf{\Pi}, \mathbf{\Pi} \in \mathbb{R}^{m \times m}\}$ together with the matrix multiplication forms a group. We denote it with $\mathscr{G}(\mathcal{P})$.

Theorem

Let $Gen(\mathscr{G}(\mathcal{P})) = \{\mathbf{G}_1, \mathbf{G}_2, \ldots, \mathbf{G}_r\}$ be the generating set of $\mathscr{G}(\mathcal{P})$ for a given polytope $\mathcal{P} \in \mathbb{R}^n$. Then, $\mathcal{P}$ is identifiable if and only if each element of $Gen(\mathscr{G}(\mathcal{P}))$ is a signed permutation matrix.

Graph Representation

Find $Gen(\mathscr{G}(\mathcal{P}))$ via graph automorphism algorithms.



$\mathcal{B}_1$ $\quad$ $G_{\mathcal{B}_1}$

- Let $\mathcal{P} \in \mathbb{R}^n$ be polytope with vertex matrix $\mathbf{V}_{\mathcal{P}} \in \mathbb{R}^{n \times m}$.
- Let $\mathbf{Q} = \mathbf{V}_{\mathcal{P}}\mathbf{V}_{\mathcal{P}}^T \in \mathbb{R}^{n \times n}$, and $\mathbf{C} = \mathbf{V}_{\mathcal{P}}^T\mathbf{Q}^{-1}\mathbf{V}_{\mathcal{P}} \in \mathbb{R}^{m \times m}$.
- Construct an edge-colored complete graph $G_{\mathcal{P}}$ with m nodes where each pair of distinct nodes are connected.
- The edge color from i^{th} node to j^{th} node is given by $\mathbf{V}_{\mathcal{P}_{:,i}}^T \mathbf{Q}^{-1} \mathbf{V}_{\mathcal{P}_{:,j}}$ (entry of $\mathbf{C}_{i,j}$).
- Graph Automorphism Group: $\mathscr{G}(G_{\mathcal{P}}) = \{\mathbf{\Pi} \in \mathbb{R}^{m \times m} : \mathbf{C} = \mathbf{\Pi}^T \mathbf{C} \mathbf{\Pi}\}$
- $\mathscr{G}(G_{\mathcal{P}}) \cong \mathscr{G}(\mathcal{P})$ ($\cong$ denotes isomorphism.)

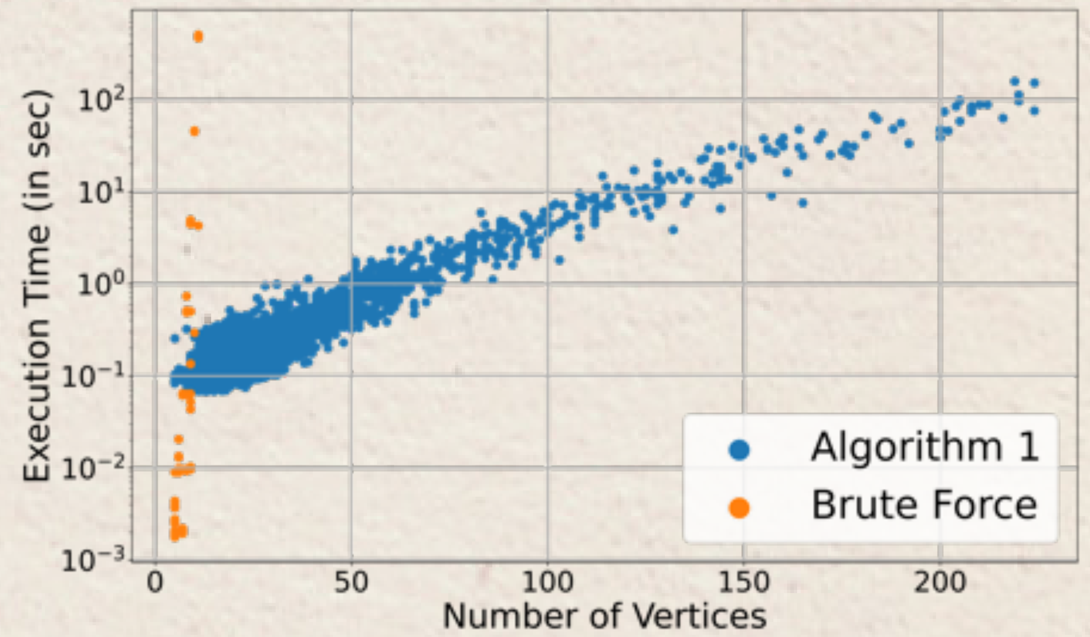
Identifiability Approach

Identifiability Characterization

- Construct $G_{\mathcal{P}}$ from a given polytope $\mathcal{P} \in \mathbb{R}^n$
- Compute $Gen(\mathscr{G}(G_{\mathcal{P}}))$ using graph automorphism algorithm.
- Find $Gen(\mathscr{G}(\mathcal{P}))$ from $Gen(\mathscr{G}(G_{\mathcal{P}}))$.
- Check if each element in $Gen(\mathscr{G}(\mathcal{P}))$ is signed permutation.

Numerical Example

- Random polytopes in $\mathbb{R}^n$, for $n \leq 10$.
- Random nonnegative $s_j \in [0, 1]$, or signed, i.e., $s_j \in [-1, 1]$ components.
- Random sparse sub-vectors, $\left\| \begin{bmatrix} s_{j_1^{(i)}} & s_{j_2^{(i)}} & \ldots & s_{j_{l_i}^{(i)}} \end{bmatrix} \right\|_1 \leq 1$



Selected References

[1] Gokcan Tatli and Alper T. Erdogan, *Polytopic matrix factorization: Determinant maximization based criterion and identifiability*, IEEE Transactions on Signal Processing, vol.69, no.16, pp. 5431-47, 2021.

[2] David Bremner, Mathieu Dutour Sikirić, Dimitrii V. Pasechnik, Thomas Rehn, and Achill Schürmann, *Computing symmetry groups of polyhedra*, LMS *Journal of Computation and Mathematics*, vol. 17, no. 1, pp.565-581, 2014.

[3] Tommi Junttila and Petteri Kaski, *Engineering an efficient canonical labeling tool for large and sparse graphs.* Proceedings of the Meeting on Algorithm Engineering & Experiments. New Orleans, Louisiana: Society for Industrial and Applied Mathematics, 2007, 135-149.