Polytopic Matrix Factorization (PMF): A New Data Decomposition Tool

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and have found that it is complete and satisfactory in all respects,
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[I dedicate this thesis to those who strive for a better world.]

ABSTRACT

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Matrix factorization methods are widely used in signal processing and machine learning applications. These methods lay the foundation of a large number of algorithms utilized in problems of those areas. As one of the main problems, we try to discover the information hidden inside input data. As a general solution strategy for this problem, input data is modeled as a product of two factors/matrices. This is known as Blind Source Separation (Blind Data Decomposition) in the signal processing literature. In this thesis, we introduce Polytopic Matrix Factorization (PMF) as a novel data decomposition approach. We model input data as unknown linear transformations of some latent vectors drawn from a polytope. The choice of polytope determines the presumed structure of latent vectors and their relationships. We first propose the identifiability criterion and identifiability conditions of PMF regarding the latent vectors. We introduce a sufficient condition for identifiability, which requires that the maximum volume inscribed ellipsoid of the polytope is contained in the convex hull of the latent vectors with a particular tightness constraint. We propose PMF identifiability results of special polytope cases corresponding to widely utilized feature attributes in applications. Then, a generalized version of PMF is presented with the characterization of eligible polytope choices and we propose to use a decision algorithm to determine these eligible polytopes. The proposed PMF tool is extended by considering a special class of linear mappings on eligible polytopes. We further extend PMF as Bounded Matrix Factorization and provide identifiability results of some bounded sets referring to polytopes. We furthermore present a PMF algorithm and interesting examples that utilize PMF as a data decomposition tool. PMF enables us to use infinitely many polytope choices and bounded sets in characterizing latent vectors. Therefore, it is possible to define different presumed structures and relations for latent vectors such as nonnegativity, sparsity and such

attributes in subvector level. In brief, we present a novel data decomposition tool that provides a high degree of flexibility in terms of presumed structures of latent vectors and offer examples illustrating this flexibility with different eligible sets and corresponding feature attributes.

ÖZETÇE

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Matrisleri çarpanlarına ayırma yöntemleri sinyal işleme ve makine öğrenmesi uygulamalarında yaygın olarak kullanılmaktadır. Bu yöntemler, bu alanlardaki problemlerde kullanılan çok sayıda algoritmanın temelini oluşturur. Biz de temel problemlerden biri olan girdi verisinin içine gömülü bilgiyi keşfetmeye çalışıyoruz. Bu problem için genel bir çözüm stratejisi olarak, girdi verisi iki faktör/matrisin çarpımı olarak modellenmiştir. Bu, sinyal işleme literatüründe Kör Kaynak Ayrımı (Kör Veri Ayrıştırma) olarak bilinir. Bu tezde, yeni bir veri ayrıştırma yaklaşımı olarak Polytopic Matrix Factorization'ı (PMF) tanıtıyoruz. Girdi verilerini, bir politoptan gelen bazı gizli vektörlerin bilinmeyen doğrusal dönüşümleri olarak modelliyoruz. Politop seçimi, gizli vektörlerin varsayılan yapısını ve bunların ilişkilerini belirliyor. İlk olarak, gizli vektörlere ilişkin olarak PMF'nin tanımlanabilirlik kriterini ve tanımlanabilirlik koşullarını sunuyoruz. Tanımlanabilirlik için, politopa sığabilecek maksimum hacimli elipsoidin, özel bir sıkışma kısıtlaması ile gizli vektörlerin dışbükey kabuğunda bulunmasını gerektiren yeterli bir koşul tanıtıyoruz. Uygulamalarda yaygın olarak kullanılan niteliklere karşılık gelen özel politop durumlarının PMF tanımlanabilirlik sonuçlarını sunuyoruz. Ardından, PMF'in uygulanabileceği politopların karakterizasyonunu ile PMF'nin genelleştirilmiş bir versiyonunu sunuyoruz ve bu politopları belirlemek için bir karar algoritması kullanmayı öneriyoruz. PMF'i, PMF'e uygun politoplar üzerinde özel bir doğrusal işlem sınıfını düşünerek genişletiyoruz. PMF'i Bounded Matrix Factorization olarak daha da genişletiyoruz ve politoplara atıfta bulunarak bazı sınırlı kümelerin tanımlanabilirlik sonuçlarını sağlıyoruz. Ayrıca bir PMF algoritması ve PMF'i veri ayrıştırma aracı olarak kullanan ilginç örnekler sunuyoruz. PMF, gizli vektörleri karakterize etmede sonsuz sayıda politop ve sınırlı seti seçenek olarak kullanmamızı sağlıyor. Bu nedenle, alt vektör düzeyinde negatif olmama, seyreklik ve benzeri nitelikler gibi gizli vektörler için farklı varsayılan yapılar ve ilişkiler tanımlamak mümkündür. Özetle, gizli vektörlerin yapısal varsayımları

açısından yüksek derecede esneklik sağlayan yeni bir veri ayrıştırma aracı sunuyoruz ve bu esnekliği PMF'e uygun farklı setler ve bu setlere karşılık gelen nitelikler ile anlatan örnekler sunuyoruz.

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ABBREVIATIONS

PMF	Polytopic Matrix Factorization
BMF	Bounded Matrix Factorization
NMF	Nonnegative Matrix Factorization
BCA	Bounded Component Analysis
ICA	Independent Component Analysis
MVIE	Maximum Volume Inscribed Ellipsoid

Chapter 1

INTRODUCTION

Matrix factorization methods are primary algorithmic tools for various signal processing and machine learning applications (see, for example, [Cichocki et al., 2009, Fu et al., 2019, Comon and Jutten, 2010, Smaragdis and Brown, 2003, Xu et al., 2003] and the references therein).

Revealing hidden information in observed data is the central problem in several applications. Matrix factorization approaches offer solutions by modeling observation vectors as linear combinations of some latent factors with unique attributes. A critical question is: *which assumptions about the generative model, especially the latent component features, enable a unique identification of the original factors from their linear combinations*, up to potentially some unresolvable permutation, sign, and scaling ambiguities? In terms of the existing literature, we can list two group of assumptions on latent factors: stochastic and deterministic (structural) assumptions. In terms of stochastic assumptions, Independent Component Analysis can be regarded as the main framework in which the observable data is modeled as the linear combinations of statistically independent variables. ICA has a variety of applications, [Comon, 1994, Hyvärinen et al., 2001]. Basic examples of ICA application areas include electroencephalograms (EEGs) [Makeig et al., 1996], functional magnetic resonance imaging (fMRI) [Calhoun et al., 2009] and calcium imaging [Mukamel et al., 2009] data analysis, audio source separation [Makino et al., 2007], and hyperspectral image decomposition [Moussaoui et al., 2008]. Under the stochastic assumptions category, we can also include approaches that exploit the time structure of random processes as an alternative or complementary to ICA (e.g., [Pham and Cardoso, 2001]).

Under the deterministic (structural) assumptions category, we can list approaches exploiting three main component attributes: nonnegativity, sparseness, and antisparseness. Nonnegative Matrix Factorization (NMF), Sparse Component Analysis (SCA) and Bounded Component Analysis (BCA) are such approaches. Polytopic Matrix Factorization (PMF) can exploit all these deterministic structures and some combinations. Therefore, our focus will be deterministic (structural) assumptions category and we will mention these approaches in the following section in conjunction with PMF. Part of this thesis addresses this fundamental problem: *which assumptions about the generative model, especially the latent component features, enable a unique identification of the original factors from their linear combinations*, in terms of deterministic (structural) assumptions. We significantly extend the existing pool of assumptions (nonnegativity, sparseness, and antisparseness) about the latent factor domains that enable unsupervised identification of the corresponding generative models. Specifically, this thesis makes following contributions,

- We propose a generalized unsupervised data decomposition framework called Polytopic Matrix Factorization (PMF) for matrix factorization approaches that assume deterministic structures for latent factors.

- We propose to use Det-Max criterion for identifiability and define a novel geometric identifiability condition based on the MVIE of the polytope.

- Existing BCA and SCA approaches ([Erdogan, 2013, Babatas and Erdogan, 2018]) use polytopes ℓ_∞-norm-ball and ℓ_1-norm-ball for antisparse and sparse components, respectively. In both approaches, the identifiability condition requires latent vectors to include vertices of those polytopes. We relax this strict identifiability condition to sufficient scattering, given in Definition (3.3.2), in existing BCA and SCA approaches ([Erdogan, 2013, Babatas and Erdogan, 2018]).

- We extend existing pool of identifiable polytopes, that enable unsupervised identification, and characterize this set of polytopes with respect to PMF framework.

- We provide determinant of scaled sample covariance matrix as another/alternative identifiability criterion for PMF framework, which will probably help to propose a information theoretical perspective in the future.

- We extend the description of identifiable set based on identifiable polytopes and provide Bounded Matrix Factorization as an extension to PMF and propose identifiability results of some bounded sets.

- We provide a Bayesian interpretation for PMF framework.

Polytopic Matrix Factorization (PMF) approach shows that if original vectors are "sufficiently scattered", a technical term with a precise definition, samples from polytopes with certain symmetry restrictions can be retrieved from their lossless linear mixtures. The richness of the infinite set of eligible polytopes enables PMF to render combinations of various feature characteristics, such as sparseness and nonnegativeness, and ranges heterogeneously to different latent factor subsets. We provide examples to illustrate the flexible description of latent vectors with such heterogeneous features in PMF framework.

Chapter 2

STRUCTURED MATRIX FACTORIZATION METHODS FOR BLIND DATA DECOMPOSITION

Matrix factorization methods lay the foundation of a large number of algorithms utilized in signal processing and machine learning problems. As one of the main problems, we try to discover the information buried in input data. In general, the solution to this problem starts with modeling input data as a product of two factors/matrices. This solution model with the problem of discovering buried data is known as Blind Data Decomposition, Blind Source Separation, in the literature.

2.1 Blind Source Separation/Data Decomposition

In previous section, we listed two groups of assumptions (stochastic and deterministic) for blind data decomposition methods. Blind data decomposition approaches with deterministic assumptions can be grouped into two with respect to the number of factor matrices that uses prior information. These are called structured matrix factorization (SMF) and semi-structured matrix factorization. Structured matrix factorization methods use a prior information or some assumption to decompose a given input data. Some examples of prior information or assumptions utilized in data decomposition can be rank, sign, sparsity and a combination these three. Similarly, semi-structured matrix factorization methods use some prior knowledge or assumption to decompose a given input data. However, only the left factor or the right factor is considered to be a subject for these assumptions. Now, we focus on blind data decomposition approaches that exploit deterministic assumptions.

2.1.1 Bounded Component Analysis

Bounded Component Analysis was proposed as a blind source separation approach in [Cruces, 2010] to replace the source independence assumption in ICA approaches with a weaker assumption called domain separability. A geometric BCA approach that utilizes from volume ratios of objects, defined with respect to output samples, was proposed in [Erdogan, 2013] based on determinant maximization. The observable data is modeled as a linear combination of bounded components. BCA approaches exploit the potential magnitude boundedness of components instead of statistical independence assumption. Such relaxation on the independence assumption enables the separation of dependent/correlated and independent components from their linear mixtures. The deterministic geometric framework in [Erdogan, 2013] demonstrates the dependent source separation capability through natural image separation and the short packet length separation capability for digital communication signals. This framework was later extended to sparse bounded sources [Babatas and Erdogan, 2018] and convolutive mixtures of bounded sources [Inan and Erdogan, 2014, Babatas and Erdogan, 2020]. These Bounded Component Analysis (BCA) frameworks assume ℓ_∞-norm-ball for the domain of sources. Their identifiability is proven only under the condition that factor components contain vertices of aforementioned polytope ℓ_∞-norm-ball. Numerical experiments show that this assumption is more stringent than necessary and can be potentially relaxed.

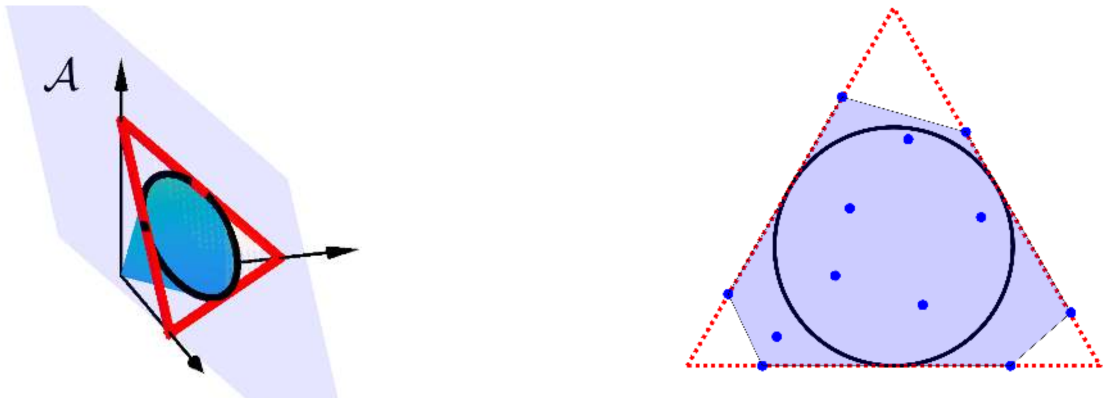
2.1.2 Sparse Component Analysis

As the name suggests, Sparse Component Analysis (SCA) exploits the sparseness assumption for component vectors. The data is modeled as a linear combination of sparse components. In Sparse Component Analysis (SCA) frameworks, [Georgiev et al., 2005, Elad, 2010, Babatas and Erdogan, 2018], sources are assumed to be contained in ℓ_1-norm-ball. Its famous application area is the dictionary learning problem [Olshausen and Field, 1997], where the columns of observation matrix are represented as a weighted combination of the minimum number of dictionary elements. This approach lays the foundation for the *sparse coding* principle, which has been utilized in both computational neuroscience [Olshausen and Field, 1997] and machine learning. Similar to BCA framework in [Erdogan, 2013], SCA framework in [Babatas and Erdogan, 2018] [Lee et al., 2007] proposes that model's identifiability is valid only under the condition that the original component samples in the generative model contain all the corresponding polytope vertices, i.e., corner points of ℓ_1-norm-ball.

2.1.3 Nonnegative Matrix Factorization

Nonnegative Matrix Factorization (NMF) is among the most popular matrix factorization approaches, where nonnegativity is assumed as a domain restriction. The observable data is modeled as a linear combination of some nonnegative components. Basic applications of NMF include document mining [Xu et al., 2003], feature extraction for natural images [Lee and Seung, 1999], source separation for hyperspectral images [Yokoya et al., 2011], community detection[Huang and Fu, 2019] and audio mixtures [Smaragdis and Brown, 2003, Ozerov and Févotte, 2009].

Earlier NMF approaches assume vertex inclusion for identifiability, which is similar to existing BCA and SCA approaches. This assumption is called "separability", "pure pixel" or "groundedness" sufficient condition on the NMF/SSMF frameworks [Donoho and Stodden, 2003, Laurberg et al., 2008], requiring that latent vectors include the vertices of the unit simplex or their scaled versions. If we assume that the latent vectors are randomly drawn from their domains, the probability of the vertex inclusion is very low. Therefore, from the practical plausibility standpoint, we desire less stringent sufficient conditions. To address this issue, weaker "sufficiently scattered conditions" were introduced for NMF. These conditions are mainly based on the enclosure of the second order cone $\mathcal{C} = \{\mathbf{x} \mid \mathbf{x}^T\mathbf{1} \geq \sqrt{r-1}\|\mathbf{x}\|_2, \mathbf{x} \in \mathbb{R}^r\}$ as a measure of spread inside the nonnegative orthant. Figure 2.1.(a) illustrates $\mathcal{C}$ for the three-dimensional case. A common approach employed in NMF algorithms is to preprocess inputs to enforce unit ℓ_1-norm constraints on the nonnegative latent vectors. As a result of this normalization, the original vectors in nonnegative orthant $\mathbb{R}^r_+$ are mapped to the unit simplex $\Delta_r = \{\mathbf{x} \mid \mathbf{1}^T\mathbf{x} = 1, \mathbf{x} \geq 0, \mathbf{x} \in \mathbb{R}^r\}$, which is the



(a) (b)

Figure 2.1: Sufficient scattering condition for NMF: (a) 3D illustration of the unit simplex Δ_r (triangle with the red boundary), the second order cone $\mathcal{C}$, and the hyperplane $\mathcal{A}$. (b) an illustration of sufficiently scattered samples (dots) and their convex hull in relation to $\mathcal{C} \cap \mathcal{A}$.

region with the triangular boundary in Figure 2.1.(a). Due to this mapping, we can focus on the $r-1$ dimensional affine subspace $\mathcal{A} = \{\mathbf{x} \mid \mathbf{1}^T\mathbf{x} = 1, \mathbf{x} \in \mathbb{R}^r\}$. Figure 2.1.(b) illustrates the restriction to $\mathcal{A}$, where the latent vectors are represented with the dots, and $\text{bd}(\mathcal{C} \cap \mathcal{A})$ is the circle.

Based on this geometric setting, Fu *et al.* [Fu et al., 2018] proposed the combination of the following conditions for sufficient scattering:

(NMF.SS.i) $\text{cone}(\mathbf{S}) \supseteq \mathcal{C}$,

(NMF.SS.ii) $\text{cone}(\mathbf{S})^d \cap \text{bd}(\mathcal{C}^d) = \{\gamma \mathbf{e}_k \mid \gamma > 0, k = 1, \ldots r\}$.

The notation $\mathcal{K}^d$ in (NMF.SS.ii) represents the dual cone of $\mathcal{K}$, as defined in Table 3.1. The first condition, (NMF.SS.i), ensures that the conic hull of the columns of $\mathbf{S}$ contains $\mathcal{C}$. Restricted to the affine subspace $\mathcal{A}$, this condition is equivalent to that in which the convex hull of the (normalized) latent vectors, the purple shaded region in Figure 2.1.(b), contains $\mathcal{C} \cap \mathcal{A}$. The second condition, (NMF.SS.ii), limits the tightness of the enclosure by effectively constraining the points of tangency between $\mathcal{C}$ and cone($\mathbf{S}$).

Part of this thesis extends the sufficient scattering approach to PMF by replacing the second order cone $\mathcal{C}$ in NMF with the Maximum Volume Inscribed Ellipsoid (MVIE) of the polytope. This new condition is much weaker than the vertex inclusion assumption used in BCA and SCA identifiability analysis for ℓ_1 and ℓ_∞-norm balls [Erdogan, 2013, Babatas and Erdogan, 2018].

Chapter 3

POLYTOPIC MATRIX FACTORIZATION (PMF)

3.1 PMF Problem

For the PMF problem, we assume the following generative data model introduced in [Tatli and Erdogan, 2021b]: the input matrix $\mathbf{Y} \in \mathbb{R}^{M \times N}$ is given by

$$\mathbf{Y} = \mathbf{H}_g \mathbf{S}_g, \tag{3.1}$$

where

- $\mathbf{H}_g \in \mathbb{R}^{M \times r}$ is the ground truth of the left-factor matrix, which is assumed to be full column rank; and
- $\mathbf{S}_g \in \mathbb{R}^{r \times N}$ is the ground truth of the right-factor matrix, where we assume $r \leq \min(M, N)$. The fundamental assumption of the PMF framework can be written as

  $$\mathbf{S}_{g_{:,j}} \in \mathcal{P}, \; j = 1, \ldots, N, \tag{3.2}$$

  where $\mathcal{P}$ is a convex polytope.

- Following two canonical forms are used to describe $\mathcal{P}$:
  - **H-Form** (*Intersections of Half-spaces*): A polytope $\mathcal{P}$ can be defined in the form

    $$\mathcal{P} = \{\mathbf{x} \mid \langle \mathbf{a}_i, \mathbf{x} \rangle \leq b_i, i = 1, ..., f\}, \tag{3.3}$$

    where f represents the number of faces and $\mathbf{a}_i$ correspond to face normals. Each inequality in 3.3 corresponds to a half-space, whose intersection forms the convex polyhedron. When this intersection is bounded, we call it convex polytope.

– **V-Form** (*Convex Hull of Vertices*): Let $\mathbf{v}_1, ..., \mathbf{v}_m$ represent the vertices, or the extreme points, of a convex polytope $\mathcal{P}$. Here, m represents the number of vertices, and then we can write

$$\mathcal{P} = \text{conv}(\begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \dots & \mathbf{v}_m \end{bmatrix}). \tag{3.4}$$

Each form of the representation of polytopes can be converted to another one. The conversion relation between these two canonical forms is referred as the *polyhedral representation conversion problem* [Bremner et al., 2009].

PMF targets to obtain a factorization of the input data $\mathbf{Y}$ in the form $\mathbf{Y} = \mathbf{HS}$ such that these factors satisfy

$$\mathbf{H} = \mathbf{H}_g \mathbf{\Pi}^T \mathbf{D}^{-1}, \tag{3.5}$$

$$\mathbf{S} = \mathbf{D}\mathbf{\Pi}\mathbf{S}_g, \tag{3.6}$$

where $\mathbf{\Pi} \in \mathbb{R}^{r \times r}$ is a permutation matrix that represents unresolvable ambiguity in obtaining the ordering of the columns (rows) of $\mathbf{H}_g$ ($\mathbf{S}_g$) and $\mathbf{D} \in \mathbb{R}^{r \times r}$ is a full rank diagonal matrix that corresponds to the scaling ambiguity.

In Section 3.4, we provide PMF identifiability results using four particular polytopes of practical interest:

i. $\mathcal{P} = \mathcal{B}_\infty$, i.e., the unit ℓ_∞-norm-ball, which we refer to as the "antisparse" PMF case hereafter;

ii. $\mathcal{P} = \mathcal{B}_1$, i.e., the unit ℓ_1-norm-ball, which we refer to as the "sparse" PMF case;

iii. $\mathcal{P} = \mathcal{B}_\infty \cap \mathbb{R}^r_+ = \{\mathbf{x} \mid \mathbf{0} \leq \mathbf{x} \leq \mathbf{1}\}$, which is referred to as the "antisparse nonnegative" PMF case; and

iv. $\mathcal{P} = \mathcal{B}_1 \cap \mathbb{R}^r_+ = \{\mathbf{x} \mid \mathbf{1}^T\mathbf{x} \leq 1, \mathbf{x} \geq 0\}$, which is referred to as the "sparse nonnegative" PMF case.

We extend these results for a wider range (infinite number) of polytopes in Section 3.5.

Table 3.1 outlines the basic notations used throughout the article.

Table 3.1

NOTATION

Notation	Meaning
$\mathbf{S}_{j,:}$ $(\mathbf{S}_{:,j})$	j^{th} row (column) of matrix $\mathbf{S}$
$\mathbf{e}_k$	Standard basis vector which is all zeros except 1 at the k^{th} index
$\langle \mathbf{x}, \mathbf{y} \rangle$	Euclidean inner product between the vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ defined as $\mathbf{y}^T\mathbf{x}$
$\mathcal{B}_p$	unit ℓ_p-norm-ball defined as $\{\mathbf{x} \mid \|\mathbf{x}\|_p \leq 1\}$
$\mathcal{S}^{*,\mathbf{d}}$	the polar of the set $\mathcal{S}$ with respect to the point $\mathbf{d}$ (See Appendix A)
$\text{conv}(\mathbf{S})$	the convex hull of the columns of $\mathbf{S}$
$\text{cone}(\mathbf{S})$	the conic hull of the columns of $\mathbf{S}$
$\mathcal{K}^d$	the dual cone of the cone $\mathcal{K}$ which is defined as $\{\mathbf{x} \mid \langle \mathbf{x}, \mathbf{y} \rangle \geq 0, \forall \mathbf{y} \in \mathcal{K}\}$
$\text{ext}(\mathcal{P})$	the set of extreme points (vertices, or corner points) of the polytope $\mathcal{P}$
$\text{bd}(\mathcal{S})$	the boundary of the set $\mathcal{S}$
$\mathbf{A}(S)$	the image of the set S under the linear transformation with matrix $\mathbf{A}$
$\mathbf{1}(\mathbf{0})$	a vector or a matrix with all ones (zeros) of the appropriate dimensions
$\mathbb{R}^r_+$	The r-dimensional nonnegative orthant
$\mathbf{A} \succ (\succeq) \mathbf{0}$	$\mathbf{A}$ is a positive (semi)definite matrix
$\alpha\mathcal{S} + \mathbf{d}$	The image of the set $\mathcal{S}$ under the transformation $f(\mathbf{x}) = \alpha\mathbf{x} + \mathbf{d}$

3.2 Identifiability Criterion

3.2.1 Det-Max Identifiability

For the PMF framework, we use the determinant maximization (Det-Max) approach as the identification criterion, which is given in [Tatli and Erdogan, 2021b] and previously utilized in different NMF [Chan et al., 2011, Fu et al., 2018, Fu et al., 2019] and BCA [Erdogan, 2013, Inan and Erdogan, 2014, Babatas and Erdogan, 2018] frameworks. Therefore, the following optimization problem is provided in [Tatli and Erdogan, 2021b] for obtaining the estimates of $\mathbf{H}_g$ and $\mathbf{S}_g$ from the input matrix $\mathbf{Y}$.

$$\underset{\mathbf{H} \in \mathbb{R}^{M \times r}, \mathbf{S} \in \mathbb{R}^{r \times N}}{\text{maximize}} \quad \det(\mathbf{S}\mathbf{S}^T) \tag{3.7a}$$

$$\text{subject to} \quad \mathbf{Y} = \mathbf{H}\mathbf{S}, \tag{3.7b}$$

$$\mathbf{S}_{:,j} \in \mathcal{P}, \quad j = 1, \ldots, N. \tag{3.7c}$$

Definition 3.2.1. *Det-Max Identifiable PMF Generative Setting*: The generative data model described by (3.1) and (3.2) is called "Det-Max identifiable PMF setting" if all of the solution pairs $(\mathbf{H}, \mathbf{S})$ of the corresponding *Det-Max problem* in (3.7) satisfy the forms

$$\mathbf{H} = \mathbf{H}_g \mathbf{\Pi}^T \mathbf{D}^{-1}, \tag{3.8}$$

$$\mathbf{S} = \mathbf{D}\mathbf{\Pi}\mathbf{S}_g, \tag{3.9}$$

where $\mathbf{\Pi} \in \mathbb{R}^{r \times r}$ is a permutation matrix that represents unresolvable ambiguity in obtaining the ordering of the columns (rows) of $\mathbf{H}_g$ ($\mathbf{S}_g$) and $\mathbf{D} \in \mathbb{R}^{r \times r}$ is a full rank diagonal matrix that corresponds to the scaling ambiguity.

3.3 PMF Identifiability Conditions with Data Models

We provide identifiability conditions for the Det-Max criterion introduced in Section 3.2.1. These criteria assume that the columns of the $\mathbf{S}_g$ are well spread inside $\mathcal{P}$ so that the solution of the optimization problem in 3.7 guarantees unique factors of the input data up to acceptable ambiguities.

3.3.1 Strongly Scattered PMF Data Model

We briefly mention Det-Max based BCA approaches in Section 2.1.1. As a keynote, earlier versions of them assumed vertex inclusion as an identifiability criterion for $\mathcal{B}_\infty$ [Erdogan, 2013] and $\mathcal{B}_1$ [Babatas and Erdogan, 2018]. This sufficient condition is similar to the "separability", "pure pixel" or "groundedness" sufficient condition of the NMF/SSMF frameworks [Donoho and Stodden, 2003, Laurberg et al., 2008], which assume that latent vectors include the vertices of the unit simplex or their scaled versions due to scaling ambiguity. Considering inclusion of polytope vertices, we introduced *Strongly Scattered PMF Data Model* in [Tatli and Erdogan, 2021a].

Definition 3.3.1. *Strongly Scattered PMF Data Model*: A PMF Data Model is called strongly scattered if the columns of $\mathbf{S}_g$ contains $\text{ext}(\mathcal{P})$.

This strong scattering assumption is hard to achieve for practical applications. Therefore, we need more useful identifiability conditions in terms of practical plausibility.

3.3.2 Sufficiently Scattered PMF Data Model

In Section, we mention sufficient scattering condition as an approach introduced for NMF in [Fu et al., 2018]. Now, we propose a similar approach for PMF by using the MVIE of the polytope instead of second order cone $\mathcal{C}$. Appendix B.1 introduces MVIE as an object and explains how we find the MVIE for a given polytope. As a result, we introduce Sufficiently Scattered PMF Data Model by using a MVIE-based approach.

Definition 3.3.2. *Sufficiently Scattered PMF Data Model and Sufficiently Scattered Factor*: A PMF Data Model is called Sufficiently Scattered if

- *(PMF.SS.i)* $\mathcal{P} \supseteq \text{conv}(\mathbf{S}_g) \supset \mathcal{E}_{\mathcal{P}}$, and,
- *(PMF.SS.ii)* $\text{conv}(\mathbf{S}_g)^{*,\mathbf{g}_{\mathcal{P}}} \cap \text{bd}(\mathcal{E}_{\mathcal{P}}^{*,\mathbf{g}_{\mathcal{P}}}) = \text{ext}(\mathcal{P}^{*,\mathbf{g}_{\mathcal{P}}})$.

where $\mathbf{g}_{\mathcal{P}}$ is the center of $\mathcal{E}_{\mathcal{P}}$. We refer such $\mathbf{S}_g$ as *Sufficiently Scattered Factor* of polytope $\mathcal{P}$.

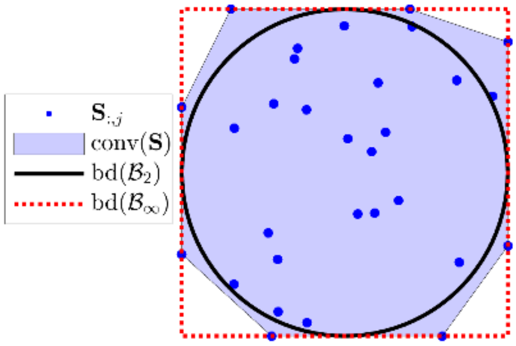


Figure 3.1: *Sufficiently scattered case* example for 2D antisparse PMF.

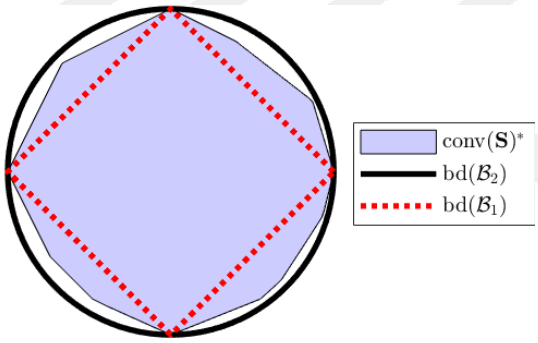


Figure 3.2: Polar sets for the example in Figure 3.1.

3.4 *Special Polytope Cases*

In this section, we provide details about special polytope cases introduced in Section 3.1. Later, in Section 3.5, we continue with the generalization of all of the identifiable polytopes. These special polytopes corresponds to sparse/antisparse and nonnegative/signed component attributes for PMF setting. Therefore, they are crucial for a wide range of existing applications. Besides this practical importance, they help us for a better understanding of PMF idea.

3.4.1 Antisparse PMF

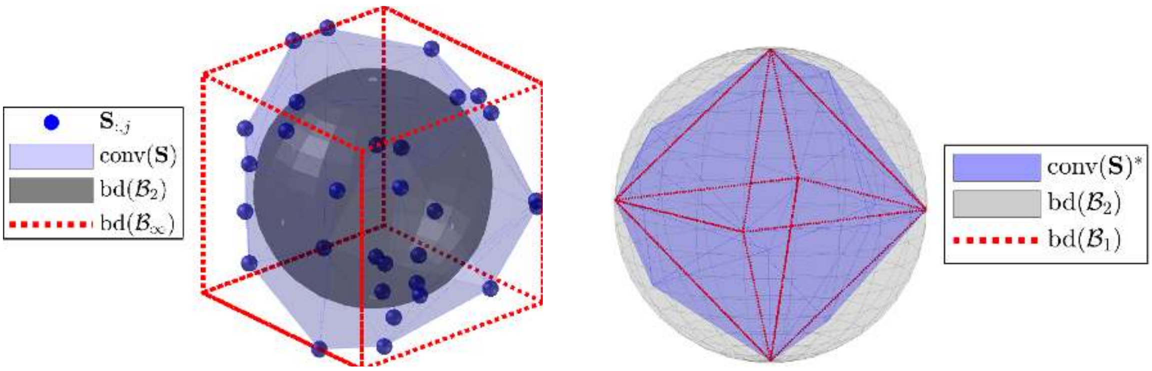
In this PMF case, columns of the $\mathbf{S}_g$ matrix are spread inside the ℓ_∞-norm-ball; i.e., $\mathcal{P} = \mathcal{B}_\infty$. Strongly Scattered and Sufficiently Scattered PMF Data Settings force columns of $\mathbf{S}_g$ to be contain or closer to corner points. Therefore, components of these columns come close to the maximum magnitude values together, which leads to name antisparse [Fuchs, 2011, Jégou et al., 2012]. Another name for the factorized version of this setting is "democratic representations" [Studer et al., 2014]. In Section 2.1.1, we mention a BCA framework proposed in [Erdogan, 2013], where $\mathcal{B}_\infty$ is used as a domain choice. Therefore, latent vectors are belong to $\mathcal{B}_\infty$. Similarly, this BCA approach uses determinant maximization as an identifiability criterion. However, an unconstrained optimization problem with a penalty terms is employed for this criterion rather than using a constraint optimization problem with $\mathcal{B}_\infty$ constraint. As another main difference, this BCA approach requires inclusion of vertices as the identifiability criterion, which is relaxed in PMF with the Sufficiently Scattered PMF Data Model. In this section, we prove that we can use Sufficiently Scattered PMF Data Model for $\mathcal{B}_\infty$ to get identifiable results. Therefore, the strong vertex inclusion condition is not further required.

In Appendix B.1.1, using Theorem 9, we showed that the MVIE for $\mathcal{B}_\infty$ is $\mathcal{B}_2$. Therefore, the corresponding MVIE parameters in (B.1) are $\mathbf{C}_{\mathcal{B}_\infty} = \mathbf{I}$ and $\mathbf{g}_{\mathcal{B}_\infty} = \mathbf{0}$.

In Section 3.3.2, Figures 3.1 and 3.2 offered illustrations for the convex hull of sufficiently scattered samples in $\mathcal{B}_\infty$, the polytope $\mathcal{B}_\infty$, its MVIE $\mathcal{E}_{\mathcal{B}_\infty}$ and their polars, in a two-dimensional setting. Figure 3.3.(a) illustrates a sufficiently scattered selection of the columns of $\mathbf{S}$ for the three-dimensional case ($r = 3$), where the vertices of $\mathcal{B}_\infty$ are not included in the samples. The corresponding three-dimensional polar domain picture is provided in Figure 3.3.(b).

The following theorem characterizes the identifiability of antisparse PMF problem for Sufficiently Scattered PMF Data Model; therefore, covers Strongly Scattered PMF Data Model.

Theorem 1. *Given the general PMF setting outlined in Section 3.1, if* $\mathbf{S}_g$ *is a sufficiently scattered factor for antisparse PMF according to Definition 3.3.2, then*



(a) (b)

Figure 3.3: Sufficiently scattered case example for 3D antisparse PMF: (a) sample domain, (b) polar domain.

all global optima $\mathbf{H}_*, \mathbf{S}_*$ *of the Det-Max problem in (3.7) for* $\mathcal{P} = \mathcal{B}_\infty$ *satisfy*

$$\mathbf{H}_* = \mathbf{H}_g \mathbf{\Pi}^T \mathbf{D}, \tag{3.10}$$

$$\mathbf{S}_* = \mathbf{D}\mathbf{\Pi}\mathbf{S}_g, \tag{3.11}$$

where $\mathbf{\Pi} \in \mathbb{R}^{r\times r}$ *is a permutation matrix and* $\mathbf{D} \in \mathbb{R}^{r\times r}$ *is an invertible diagonal matrix with* ± 1 *entries on its diagonal.*

Proof. The full column rank condition on $\mathbf{H}_g$ and the constraint $\mathbf{Y} = \mathbf{HS}$ forces any feasible point to have the same row space as $\mathbf{S}_g$. Therefore,

$$\mathbf{S} = \mathbf{A}\mathbf{S}_g, \tag{3.12}$$

for some full rank $\mathbf{A} \in \mathbb{R}^{r\times r}$ matrix. This reduces problem of finding optimal $\mathbf{S}$ to finding an optimal $\mathbf{A}$, which provides us to write $\det(\mathbf{S}\mathbf{S}^T)$, i.e., objective function in (3.7), in the following way,

$$\det(\mathbf{S}\mathbf{S}^T) = |\det(\mathbf{A})|^2 \det(\mathbf{S}_g\mathbf{S}_g^T).$$

Here, we have a constant term on the right-hand side. Therefore, the objective function (3.7) can be simplified and the optimization problem can be written as

$$\underset{\mathbf{A} \in \mathbb{R}^{r\times r}}{\text{maximize}} \quad |\det(\mathbf{A})| \tag{3.13a}$$

$$\text{subject to} \quad \|\mathbf{A}\mathbf{S}_{g:,j}\|_\infty \leq 1, \quad j = 1, \ldots, N. \tag{3.13b}$$

for the antisparse PMF case.

Then, the remaining part of the proof can be divided into three parts for a better understanding.

Step I: *This part shows that rows of any feasible* $\mathbf{A}$ *are belong to conv*$(\mathbf{S}_g)^*$*, due to the constraint in (3.13b).*

First, we can write $\mathbf{A}_{i,:}\mathbf{S}_{g:,j} \leq 1$ for all (i,j) index pairs directly from the constraint in (3.13b). This inequality, $\mathbf{A}_{i,:}\mathbf{S}_{g:,j} \leq 1$, for all (i,j) index pairs implies that $\mathbf{A}_{i,:}$ satisfies

$$\mathbf{A}_{i,:}\mathbf{s} = \mathbf{A}_{i,:}\mathbf{S}_g\boldsymbol{\lambda} \leq 1, \quad \boldsymbol{\lambda} > 0, \mathbf{1}^T\boldsymbol{\lambda} = 1,$$

for all $i \in \{1, \ldots, r\}$ and $\mathbf{s} \in \text{conv}(\mathbf{S}_g)$. This is equivalent to the fact that each row of $\mathbf{A}$ lies within the polar set of $\text{conv}(\mathbf{S}_g)$; i.e.,

$$\mathbf{A}_{i,:}^T \in \text{conv}(\mathbf{S}_g)^*, \quad \forall i \in \{1, \ldots, r\}.$$

In reference to the three-dimensional polar domain picture in Figure 3.3.(b), the rows of $\mathbf{A}$ lie in the polytopic shaded region corresponding to $\text{conv}(\mathbf{S}_g)^*$.

Step II: *This step shows that any optimal solution* $\mathbf{A}_*$ *of (3.13) is a real orthogonal matrix by using (PMF.SS.i) and Hadamard's inequality.*

The polar of sufficiently scattered condition (PMF.SS.i) can be written as

$$\text{conv}(\mathbf{S}_g)^* \subset \mathcal{B}_2, \tag{3.14}$$

which implies $\|\mathbf{A}_{i,:}\|_2 \leq 1$ for all rows of $\mathbf{A}$. Hadamard's inequality-based bound on the objective

$$|\det(\mathbf{A})| \leq \|\mathbf{A}_{1,:}^T\|_2\|\mathbf{A}_{2,:}^T\|_2 \ldots \|\mathbf{A}_{r,:}^T\|_2 \leq 1,$$

is achieved if and only if the rows of $\mathbf{A}$ are on $\text{bd}(\mathcal{B}_2)$ and they are orthogonal.

In other words, any optimal solution $\mathbf{A}_*$ is a real orthogonal matrix. Therefore, for the example case in Figure 3.3, the rows of $\mathbf{A}_*$ should lie on the boundary of the unit sphere in Figure 3.3.(b). At the same time, they should be members of $\text{conv}(\mathbf{S}_g)^*$, purple shaded region in the same figure.

Step III: *This step shows that each row of $\mathbf{A}_*$ has only one nonzero element by using the constraint (PMF.SS.ii).*

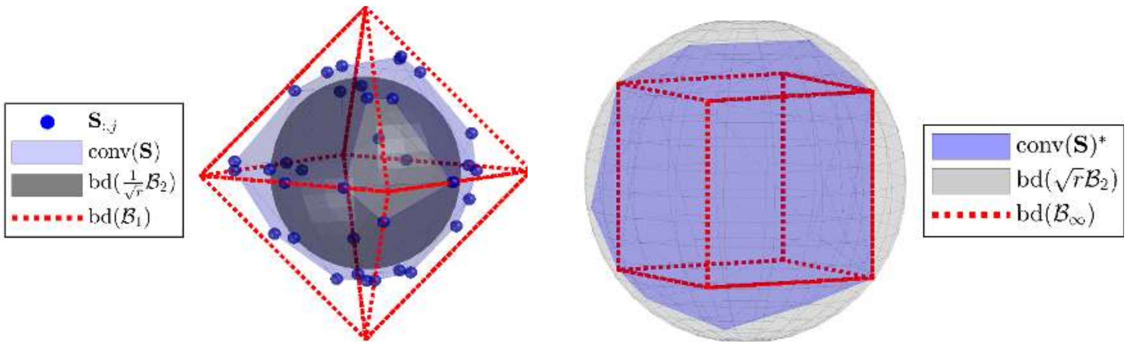
The sufficiently scattered condition (PMF.SS.ii), $\text{conv}(\mathbf{S}_g)^* \cap \text{bd}(\mathcal{B}_2) = \text{ext}(\mathcal{B}_1)$, restricts the rows of any optimal solution $\mathbf{A}_*$, which are located on the boundary of the unit sphere in Figure 3.3.(b), to the vertices of $\mathcal{B}_1$. This condition implies that, the rows of $\mathbf{A}_*$ are standard basis vectors (or their negatives). Therefore, we can write $\mathbf{A}_* = \mathbf{D\Pi}$, where $\mathbf{D} \in \mathbb{R}^{r\times r}$ is a diagonal matrix with ± 1 entries on its diagonal and $\mathbf{\Pi} \in \mathbb{R}^{r\times r}$ is a permutation matrix. Due to the equality constraint in (3.7b), $\mathbf{H}_* = \mathbf{H}_g\mathbf{A}^{-1}$; therefore, (3.10) and (3.11) follow. $\square$

3.4.2 Sparse PMF

In the sparse PMF setting, the columns of $\mathbf{S}_g$ are contained in the ℓ_1-norm-ball; i.e., $\mathcal{P} = \mathcal{B}_1$. [Donoho, 2006] and [Candès and Wakin, 2008] indicated the relation between sparsity and ℓ_1-norm constraints, where ℓ_1-norm can be considered as convex substitute of ℓ_0-norm under proper conditions. Additionally, we previously mention the sparse version of BCA approach [Babatas and Erdogan, 2018], adopted from antisparse BCA in reference [Erdogan, 2013]. As an important keynote, similar to antisparse BCA case, identifiability of sparse BCA is based on vertex inclusion. Since the sparsity is represented by ℓ_1-norm-ball here, vertices of $\mathcal{B}_1$ are required to be included in columns of $\mathbf{S}_g$ for identifiability.

In this section, we extend this result by proposing identifiability of Sufficiently Scattered PMF Data model for sparse PMF problem.

In Appendix B.1.1, using Theorem 9, we show that the MVIE of $\sqrt{r}\mathcal{B}_1$ is $\mathcal{B}_2$. Therefore, the MVIE of $\mathcal{B}_1$ is $\mathcal{E}_{\mathcal{B}_1} = \frac{1}{\sqrt{r}}\mathcal{B}_2$. The polar of an hypersphere is another hypersphere with the reciprocal radius. Therefore, $\mathcal{E}^*_{\mathcal{B}_1} = \sqrt{r}\mathcal{B}_2$. For a visual illustration of the sufficient scattering condition for $\mathcal{P} = \mathcal{B}_1$, we consider the example in Figure 3.4.(a) for $r = 3$. The sample points, represented by dots, in Figure 3.4.(a) do not contain the vertices of $\mathcal{B}_1$. Furthermore, both $\text{bd}(\mathcal{B}_1)$ and the edges of $\text{conv}(\mathbf{S})$ intersect $\text{bd}(\frac{1}{\sqrt{r}}\mathcal{B}_2)$ at identical points due to the polar domain sufficient scattering constraint (PMF.SS.ii), as illustrated in Figure 3.4.(b). The polar of $\mathcal{B}_1$ is $\mathcal{B}_\infty$, the



(a) (b)

Figure 3.4: Sufficiently scattered case example for 3D sparse PMF: (a) sample domain, (b) polar domain.

boundary of which is plotted as the red cube in Figure 3.4.(b). Its vertices and $\text{conv}(\mathbf{S})^*$ intersect the boundary of $\mathcal{E}^*_{\mathcal{P}}$ at identical points. The following theorem characterizes the identifiability of the sparse PMF problem, based on the sufficiently scattering condition in Definition 3.3.2:

Theorem 2. *Given the general PMF setting outlined in Section 3.1, if $\mathbf{S}_g$ is a sufficiently scattered factor for sparse PMF according to Definition 3.3.2, then all global optima $\mathbf{H}_*, \mathbf{S}_*$ of the Det-Max problem in (3.7) with $\mathcal{P} = \mathcal{B}_1$ satisfy*

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

where $\mathbf{\Pi} \in \mathbb{R}^{r \times r}$ is a permutation matrix and $\mathbf{D} \in \mathbb{R}^{r \times r}$ is a diagonal matrix with ± 1 entries on its diagonal.

Proof. Using the same arguments in the proof of Theorem 1, we write the optimization problem equivalent to (3.7) for the sparse PMF case as

$$\underset{\mathbf{A} \in \mathbb{R}^{r\times r}}{\text{maximize}} \quad |\det(\mathbf{A})| \tag{3.15a}$$

$$\text{subject to} \quad \|\mathbf{A}\mathbf{S}_{g\,,j}\|_1 \leq 1, \quad j = 1, \ldots, N. \tag{3.15b}$$

The proof consists of three fundamental steps:

<u>Step I:</u> *This step shows that any feasible* $\mathbf{A}^T$ *maps elements of* $\mathcal{B}_\infty$ *into* $\sqrt{r}\mathcal{B}_2$ *due to (3.15b) and (PMF.SS.i).*

We start with the identity $\mathbf{S} = \mathbf{A}\mathbf{S}_g$, as asserted in the previous proof. The second constraint of the *Det-Max problem* for the sparse case is equivalent to $\|\mathbf{A}\mathbf{S}_{g_{:,j}}\|_1 \leq 1, \ \ j = 1, \ldots, N$, which can be equivalently restated as

$$\mathbf{q}_i^T \mathbf{A}\mathbf{S}_{g_{:,j}} \leq 1, \ \ j = 1, \ldots, N, \ \forall \mathbf{q}_i \in \operatorname{ext}(\mathcal{B}_\infty).$$

Therefore, the equivalent condition for the second constraint can be written as

$$\mathbf{A}^T \mathbf{q}_i \in \operatorname{conv}(\mathbf{S}_g)^* \quad \forall \mathbf{q}_i \in \operatorname{ext}(\mathcal{B}_\infty). \tag{3.16}$$

Since $\mathbf{S}_g$ is a sufficiently scattered factor,

$$\operatorname{conv}(\mathbf{S}_g)^* \subset \sqrt{r}\mathcal{B}_2, \tag{3.17}$$

and therefore,

$$\mathbf{A}^T \mathbf{q}_i \in \sqrt{r}\mathcal{B}_2 \quad \forall \mathbf{q}_i \in \operatorname{ext}(\mathcal{B}_\infty) \tag{3.18}$$

<u>Step II:</u> *We show that any* $\mathbf{A}$ *satisfying (3.18) and maximizing* $|\det(\mathbf{A})|$ *is a real orthogonal matrix*

Based on this observation, an upper bound on the objective can be obtained through the optimization setting

$$\begin{aligned} \underset{\mathbf{A} \in \mathbb{R}^{r \times r}}{\text{maximize}} \quad & |\det(\mathbf{A})| \quad \textit{Sparse UB-I} \\ \text{subject to} \quad & \|\mathbf{A}^T \mathbf{q}_i\|_2^2 \leq r, \ \forall \mathbf{q}_i \in \operatorname{ext}(\mathcal{B}_\infty). \end{aligned}$$

This setting can also be bounded above by the setting with a more relaxed constraint

$$\begin{aligned} \underset{\mathbf{A} \in \mathbb{R}^{r \times r}}{\text{maximize}} \quad & |\det(\mathbf{A})| \quad \textit{Sparse UB-II} \\ \text{subject to} \quad & \sum_{\mathbf{q}_i \in \operatorname{ext}(\mathcal{B}_\infty)} \|\mathbf{A}^T \mathbf{q}_i\|_2^2 \leq 2^r r. \end{aligned}$$

Note that the constraint part of the above setting can be compactly rewritten as $Tr(\mathbf{A}\mathbf{A}^T\mathbf{Q}\mathbf{Q}^T) \leq 2^r r$, where $\mathbf{Q} = \begin{bmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \ldots & \mathbf{q}_{2^r} \end{bmatrix} \in \mathbb{R}^{r \times 2^r}$. Due to the symmetry of the extreme points of $\operatorname{ext}(\mathcal{B}_\infty)$, we can write $\mathbf{Q}\mathbf{Q}^T = 2^r\mathbf{I}$. As a result, the constraint expression in *sparse UB-II* is further simplified to $\|\mathbf{A}\|_F^2 \leq r$, or equivalently to,

$$\sqrt{\sum_{i=1}^{r} \sigma_i^2(\mathbf{A})} \leq \sqrt{r}. \tag{3.19}$$

For the objective of the *sparse UB-II*, we can write

$$\begin{aligned}
|\det(\mathbf{A})| &= \prod_{i=1}^{r} \sigma_i(\mathbf{A}) \\
&\leq \left(\frac{1}{r}\sum_{i=1}^{r} \sigma_i(\mathbf{A})\right)^r. && (3.20)\\
&\leq \left(\frac{1}{r}\sqrt{\sum_{i=1}^{r} \sigma_i^2(\mathbf{A})\sqrt{r}}\right)^r && (3.21)\\
&\leq 1, && (3.22)
\end{aligned}$$

where (3.20) is due to the arithmetic-geometric mean inequality, (3.21) is due to the Cauchy-Schwarz inequality, and (3.22) is due to (3.19). The equality holds if and only if $\sigma_1(\mathbf{A}) = \sigma_2(\mathbf{A}) = \ldots\ldots = \sigma_r(\mathbf{A}) = 1$, which is equivalent to the condition that $\mathbf{A}$ is real orthogonal.

Step III: *We use the sufficient scattering condition (PMF.SS.ii) together with the orthogonality of optimal $\mathbf{A}_*$ to show that any optimal point of (3.15) has the desired form, i.e., the product of a permutation and a diagonal matrix.*

If a real orthogonal matrix $\mathbf{A}$ exists that satisfies (3.16) and $\mathbf{A}^T\mathbf{q}_i \in \mathrm{bd}(\sqrt{r}\mathcal{B}_2)$, then matrix $\mathbf{A}$ corresponds to an optimal solution since $|\det(\mathbf{A})|$ achieves its upper bound of 1. Since $\mathbf{S}_g$ is a sufficiently scattered factor, $\mathrm{conv}(\mathbf{S}_g)^* \cap \mathrm{bd}(\sqrt{r}\mathcal{B}_2) = \mathrm{ext}(\mathcal{B}_\infty)$; the equivalent condition for the global optimality of $\mathbf{A}$ is

$$\mathbf{A}_*^T\mathbf{q}_i \in \mathrm{ext}(\mathcal{B}_\infty) \ \ \forall \mathbf{q}_i \in \mathrm{ext}(\mathcal{B}_\infty), \ \ \text{and } \mathbf{A}_*^T\mathbf{A}_* = \mathbf{I}.$$

In other words, $\mathbf{A}_*$ is a global optimum if and only if it is real orthogonal and maps $\mathrm{ext}(\mathcal{B}_\infty)$ to itself. The orthogonality of $\mathbf{A}_*$ implies $\|\mathbf{A}_{*i,:}\|_2 = 1$. Furthermore, since $\mathrm{sign}(\mathbf{A}_{*i,:}^T) \in \mathrm{ext}(\mathcal{B}_\infty)$, then

$$\mathbf{A}_{*i,:}\mathrm{sign}(\mathbf{A}_{*i,:}^T) = \|\mathbf{A}_{*i,:}^T\|_1 = 1,$$

where the last equality is because $\mathbf{A}_*\text{sign}(\mathbf{A}_{*i,:}^T) = \mathbf{q}_j$ for some $\mathbf{q}_j \in \text{ext}(\mathcal{B}_\infty)$, and therefore, its i^{th} row is equal to 1 (as $\|A_{*i,:}^T\|_1$ is nonnegative). As a result, $\mathbf{A}_{*i,:}$ can only have one nonzero entry, which has a magnitude of 1. Since the rows of $\mathbf{A}_*$ are orthogonal, the global optima characterization is given by $\mathbf{A}_* = \mathbf{D}\mathbf{\Pi}$, where $\mathbf{D}$ and $\mathbf{\Pi}$ are as stated in the theorem. □

3.4.3 Antisparse Nonnegative PMF

This case corresponds to following polytope choice

$$\begin{aligned}\mathcal{P} = \mathcal{B}_{\infty,+} &= \{\mathbf{x} \mid \mathbf{0} \leq \mathbf{x} \leq \mathbf{1}, \mathbf{x} \in \mathbb{R}_+^r\}, \\ &= \mathcal{B}_\infty \cap \mathbb{R}_+^r = 0.5\mathcal{B}_\infty + 0.5\mathbf{1}.\end{aligned}$$

As seen from the given definition, this polytope is shifted and scaled version of $\mathcal{B}_\infty$. Therefore, we apply the same shift and scaling to find MVIE of $\mathcal{B}_{\infty,+}$.

Antisparse nonnegative PMF is the special case of antisparse BCA introduced in [Erdogan, 2013]. However, [Erdogan, 2013] requires vertex inclusion for identifiability. In the following theorem, we propose identifiability of Sufficiently Scattered PMF Data Model, which requires a weaker condition than vertex inclusion.

Theorem 3. *Given the general PMF setting outlined in Section 3.1, if $\mathbf{S}_g$ is a sufficiently scattered factor for antisparse nonnegative PMF according to Definition 3.3.2, then all global optima $\mathbf{H}_*, \mathbf{S}_*$ of the Det-Max problem in (3.7) with $\mathcal{P} = B_{\infty,+}$ satisfy*

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

where $\mathbf{\Pi} \in \mathbb{R}^{r\times r}$ is a permutation matrix.

Proof. Following the same treatment in the proof of Theorem 1, we can write the equivalent form of the optimization in (3.7) for nonnegative antisparse PMF as

$$\underset{\mathbf{A} \in \mathbb{R}^{r\times r}}{\text{maximize}} \quad |\det(\mathbf{A})| \tag{3.23a}$$

$$\text{subject to} \quad 0 \leq \mathbf{A}_{i,:}\mathbf{S}_{g_{:,j}} \leq 1, \quad i = 1, \dots, r, \tag{3.23b}$$

$$j = 1, \ldots, N.$$

The proof consists of three major steps.

Step I: *We use (3.23b) and (PMF.SS.i) to show that the columns(rows) of any feasible* $\mathbf{A}$ *of (3.23) lie in* $\mathcal{B}_2$.

Due to (PMF.SS.i), which is $\mathcal{E}_{\mathcal{B}_{\infty,+}} \subset \text{conv}(\mathbf{S}_g)$, for all $\mathbf{s} \in \mathcal{E}_{\mathcal{B}_{\infty,+}}$ the constraint (3.23b) holds. Therefore, for any $i \in \{1, \ldots, r\}$, we have

$$0 \leq 0.5\mathbf{A}_{i,:}\mathbf{u} + 0.5\mathbf{A}_{i,:}\mathbf{1} \leq 1, \quad \forall \mathbf{u} \in \mathcal{B}_2, \tag{3.24}$$

where we used $\mathcal{E}_{\mathcal{B}_{\infty,+}} = \{0.5\mathbf{u} + 0.5\mathbf{1}, \|\mathbf{u}\|_2 \leq 1\}$. If we substitute $\mathbf{u} = \frac{(\mathbf{A}_{i,:})^T}{\|\mathbf{A}_{i,:}\|_2}$ and $\mathbf{u} = -\frac{(\mathbf{A}_{i,:})^T}{\|\mathbf{A}_{i,:}\|_2}$ in (3.24), we obtain

$$0 \leq 0.5\|\mathbf{A}_{i,:}\|_2 + 0.5\mathbf{A}_{i,:}\mathbf{1} \leq 1, \text{ and,} \tag{3.25}$$

$$0 \leq -0.5\|\mathbf{A}_{i,:}\|_2 + 0.5\mathbf{A}_{i,:}\mathbf{1} \leq 1, \tag{3.26}$$

respectively, for all $i = 1, \ldots, r$. The summation of (3.25) and the sign reversed (3.26) lead to $\|\mathbf{A}_{i,:}\|_2 \leq 1$ for all rows of $\mathbf{A}$. In other words, the rows(columns) of any feasible $\mathbf{A}$ should be in $\mathcal{B}_2$.

Step II: *We now show any optimal solution* $\mathbf{A}_*$ *of (3.23) should be a real orthogonal matrix.*

Using Hadamard's inequality and $\|\mathbf{A}_{i,:}\|_2 \leq 1$ from the previous step, we can place an upper bound on the objective function in (3.23a) as

$$|\det(\mathbf{A})| \leq \|\mathbf{A}_{1,:}\|_2\|\mathbf{A}_{2,:}\|_2 \ldots \|\mathbf{A}_{r,:}\|_2 \leq 1. \tag{3.27}$$

This bound is achieved if and only if the rows form an orthonormal set. Therefore, any optimal solution $\mathbf{A}_*$ of (3.23) is a real orthogonal matrix.

Step III: *We use (PMF.SS.ii) to show that all global optima of (3.23) are permutation matrices.*

If we substitute a real orthogonal $\mathbf{A}_*$ in (3.26), we obtain $\mathbf{A}_{*i,:}\mathbf{1} \geq 1$. Combining this inequality with (3.23b), we can write

$$2\mathbf{A}_{*i,:}\mathbf{S}_{g_{:,j}} \leq 2 \leq 1 + \mathbf{A}_{*i,:}\mathbf{1}. \tag{3.28}$$

Reorganizing the left and right terms of this expression, we obtain

$$2\mathbf{A}_{*i,:}(\mathbf{S}_{g_{:,j}} - 0.5\mathbf{1}) \leq 1 \tag{3.29}$$

for all the columns of $\mathbf{S}_g$. Based on this inequality, we conclude that $2\mathbf{A}_{*i,:}$ lies in $\text{conv}(\mathbf{S}_g)^{*,0.5\mathbf{1}}$ for all the rows of $\mathbf{A}_*$. Furthermore, since $\mathbf{A}_*$ is also real orthogonal,

$$2\mathbf{A}_{*i,:} \in \text{conv}(\mathbf{S}_g)^{*,0.5\mathbf{1}} \cap \text{bd}(2\mathcal{B}_2). \tag{3.30}$$

Due to the sufficiently scattered constraint (PMF.SS.ii), which is $\text{conv}(\mathbf{S}_g)^{*,0.5\mathbf{1}} \cap \text{bd}(2\mathcal{B}_2) = \text{ext}(2\mathcal{B}_1)$, $\mathbf{A}_{*i,:} \in \text{ext}(\mathcal{B}_1)$. Furthermore, due to the condition $\mathbf{A}_{*i,:}\mathbf{1} \geq 1$, $\mathbf{A}_*$ is a global optimum if and only if its rows are positive standard basis vectors that are orthogonal to each other, i.e., $\mathbf{A}_*$ is a permutation matrix. □

3.4.4 Sparse Nonnegative PMF

As defined in Section 3.1.(iv), the polytope for sparse nonnegative factors is given by

$$\mathcal{P} = \mathcal{B}_{1,+} = \{\mathbf{x} \mid \mathbf{x} \geq \mathbf{0}, \mathbf{1}^T\mathbf{x} \leq 1\} = \mathcal{B}_1 \cap \mathbb{R}^r_+. \tag{3.31}$$

We are not aware of any nonnegative matrix factorization results that make explicit use of the polytope $\mathcal{B}_{1,+}$, and provide the corresponding identifiability conditions. In this section, we provide identifiability results for this polytope, again based on the sufficient scattering assumption in Definition 3.3.2. For this purpose, we derive the MVIE $\mathcal{E}_{\mathcal{B}_{1,+}}$ in Appendix B.1.2. The MVIE derivation in this case is relatively more involved compared to other special cases (Section 3.1.(i)-(iii)). This is due to the fact the MVIE in this case is not spherical, and therefore, Theorem 9 is not applicable. The inscribed ellipsoid parameters obtained in Appendix B.1.2 are

$$\begin{aligned} \mathbf{C}_{\mathcal{B}_{1,+}} &= \frac{1}{\sqrt{r}}\left(\frac{1}{\sqrt{r+1}}\mathbf{I} - \frac{\sqrt{r+1}-1}{r^2+r}\mathbf{1}\mathbf{1}^{\mathbf{T}}\right), \\ \mathbf{g}_{\mathcal{B}_{1,+}} &= \frac{1}{r+1}\mathbf{1}. \end{aligned} \tag{3.32}$$

To obtain the polar of the polytope $\mathcal{P}$, we first use the canonical form for the polytope shifted by $-\mathbf{g}_{\mathcal{B}_{1,+}}$ in the form

$$\mathcal{P} - \mathbf{g}_{\mathcal{B}_{1,+}} = \{\mathbf{x} \mid \mathbf{1}^T(\mathbf{x} + \frac{1}{r+1}\mathbf{1}) \leq 1, -\mathbf{e}_i^T(\mathbf{x} + \frac{1}{r+1}\mathbf{1}) \leq 0, i \in \{1, \dots, r\}\}.$$

After some algebraic manipulations, we can convert it into standard form (A.2) in Appendix A:

$$\mathcal{P} - \mathbf{g}_{\mathcal{B}_{1,+}} = \{\mathbf{x} \mid (r+1)\mathbf{1}^T\mathbf{x} \leq 1, -(r+1)\mathbf{e}_i^T\mathbf{x} \leq 1, i \in \{1, \ldots, r\}\}.$$

Therefore, based on the procedure in Appendix A, the polar of $\mathcal{B}_{1,+}$ can be written as

$$\mathcal{B}_{1,+}^{*,\frac{1}{r+1}\mathbf{1}} = \operatorname{conv}(-(r+1)\mathbf{e}_1, \ldots, -(r+1)\mathbf{e}_r, (r+1)\mathbf{1}), \tag{3.33}$$

which is a polytope with $(r+1)$ vertices (Note that $\mathcal{B}_{1,+}$ has $(r+1)$ faces).

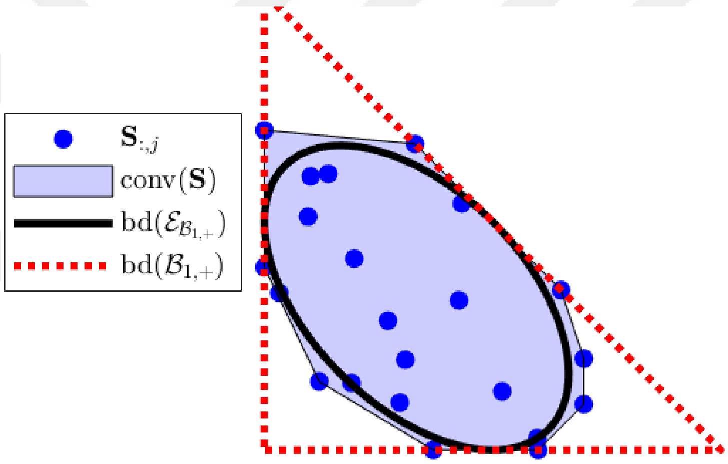


Figure 3.5: 2D Sufficiently scattered case example.

Figure 3.5 illustrates $\mathcal{B}_{1,+}$, its MVIE and an example set of sufficiently scattered samples for $r = 2$. These samples clearly do not contain the vertices of $\mathcal{B}_{1,+}$. The convex hull of the samples contains the nonspherical MVIE and is tangent to its boundary at the points where the polytope is tangent.

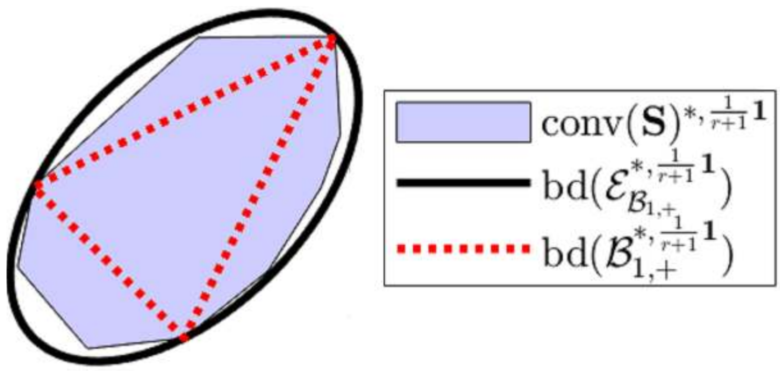


Figure 3.6: Polar sets for the example in Figure 3.5.

The picture corresponding to the polars of the sets in Figure 3.5 is provided in Figure 3.6. The polar of the polytope $\mathcal{B}_{1,+}$ is a triangular region, the boundary of which is shown with dashed-red lines. We note that as expected from (PMF.SS.ii), $\text{conv}(\mathbf{S})^{*,\frac{1}{r+1}\mathbf{1}}$ intersects the boundary of $\mathcal{E}_{\mathcal{B}_{1,+}}^{*,\frac{1}{r+1}\mathbf{1}}$ only at the vertices of $\mathcal{B}_{1,+}^{*,\frac{1}{r+1}\mathbf{1}}$. Figure 3.7 illustrates a sufficiently scattered distribution of columns of $\mathbf{S}$ for the three-dimensional case.

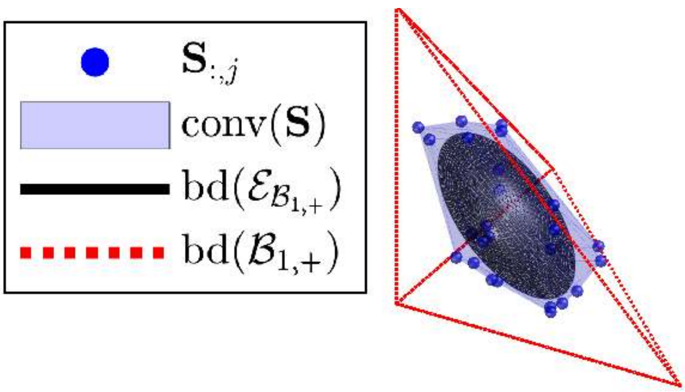


Figure 3.7: 3D Sufficiently scattered case example.

We characterize the identifiability condition for the nonnegative sparse PMF problem through the following theorem.

Theorem 4. *Given the general PMF setting outlined in Section 3.1, if* $\mathbf{S}_g$ *is a sufficiently scattered factor for sparse nonnegative PMF according to Definition 3.3.2,* *then all global optima* $\mathbf{H}_*, \mathbf{S}_*$ *of the Det-Max problem in (3.7) for* $\mathcal{P} = \mathcal{B}_{1,+}$ *satisfy*

$$\mathbf{H}_* = \mathbf{H}_g \mathbf{\Pi}^T, \tag{3.34}$$

$$\mathbf{S}_* = \mathbf{\Pi} \mathbf{S}_g, \tag{3.35}$$

where $\mathbf{\Pi} \in \mathbb{R}^{r\times r}$ *is a permutation matrix.*

Proof. Following the same arguments in the proof of Theorem 1, we start with the equivalent determinant maximization formulation for the nonnegative sparse PMF:

$$\underset{\mathbf{A}\in\mathbb{R}^{r\times r}}{\text{maximize}} \quad |\det(\mathbf{A})| \tag{3.36a}$$

$$\text{subject to} \quad 0 \leq \mathbf{A}_{i,:}\mathbf{S}_{g_{:,j}} \leq 1, \quad i = 1,\ldots,r, \quad j = 1,\ldots,N, \tag{3.36b}$$

$$\mathbf{1}^T\mathbf{A}\mathbf{S}_{g_{:,j}} \leq 1 \quad j = 1,\ldots,N. \tag{3.36c}$$

The proof consists of four steps.

Step I: *We use the polytopic constraints (3.36b) and (3.36c), and the sufficient scattering condition (PMF.SS.i) to show that optimal* $\mathbf{A}_*$ *is a real orthogonal matrix with* $\mathbf{1}^T\mathbf{A}_*\mathbf{1} = r$ *and* $\|\mathbf{A}_{*i,:}\|_2 = \mathbf{A}_{*i,:}\mathbf{1} = 1$ *for all* $i = 1,\ldots,r$*.*

Based on the sufficient scattering condition (PMF.SS.i), which is $\text{conv}(\mathbf{S}_g) \supset \mathcal{E}_{\mathcal{B}_{1,+}}$ (as illustrated in Figures 3.5 and 3.7), any member of the MVIE should satisfy the constraints (3.36b) and (3.36c). Therefore, we have

$$0 \leq \mathbf{A}_{i,:}\mathbf{C}_{\mathcal{B}_{1,+}}\mathbf{u} + \frac{1}{r+1}\mathbf{A}_{i,:}\mathbf{1} \leq 1, \quad \forall \mathbf{u} \in \mathcal{B}_2, \tag{3.37}$$

$$\mathbf{1}^T\mathbf{A}\mathbf{C}_{\mathcal{B}_{1,+}}\mathbf{u} + \frac{1}{r+1}\mathbf{1}^T\mathbf{A}\mathbf{1} \leq 1, \quad \forall \mathbf{u} \in \mathcal{B}_2, \tag{3.38}$$

Specifically, if we substitute $\mathbf{u} = -\frac{(\mathbf{A}_{i,:}\mathbf{C}_{\mathcal{B}_{1,+}})^T}{\|\mathbf{C}_{\mathbf{A}_{i,:}\mathcal{B}_{1,+}}\|_2}$ in (3.37), we obtain

$$\|\mathbf{A}_{i,:}\mathbf{C}_{\mathcal{B}_{1,+}}\|_2 \leq \frac{1}{r+1}\mathbf{A}_{i,:}\mathbf{1}, \tag{3.39}$$

which further implies

$$\mathbf{A}_{i,:}\mathbf{C}^2_{\mathcal{B}_{1,+}}(\mathbf{A}_{i,:})^T \leq \left(\frac{1}{r+1}\mathbf{A}_{i,:}\mathbf{1}\right)^2, \tag{3.40}$$

for all $i = 1, \ldots, r$. Inserting (B.18) for $\mathbf{C}^2_{\mathcal{B}_{1,+}}$ (derived in Appendix B.1.2) in (3.40), we obtain

$$\frac{1}{r(r+1)}\left(\|\mathbf{A}_{i,:}\|_2^2 - \frac{(\mathbf{A}_{i,:}\mathbf{1})^2}{r+1}\right) \leq \frac{(\mathbf{A}_{i,:}\mathbf{1})^2}{(r+1)^2}.$$

Simplifying this expression, we have

$$\|\mathbf{A}_{i,:}\|_2^2 \leq (\mathbf{A}_{i,:}\mathbf{1})^2, \tag{3.41}$$

for all $i = 1, \ldots, r$. If we substitute $\mathbf{u} = \mathbf{0}$ in (3.37), we obtain $\mathbf{A}_{i,:}\mathbf{1} \geq 0$. Therefore, we can rewrite (3.41) as $\|\mathbf{A}_{i,:}\|_2 \leq \mathbf{A}_{i,:}\mathbf{1}$. Furthermore, if we substitute $\mathbf{u} = \frac{1}{\sqrt{r}}\mathbf{1}$ in (3.38), we have

$$\frac{1}{\sqrt{r}}\mathbf{1}^T\mathbf{A}\mathbf{C}_{\mathcal{B}_{1,+}}\mathbf{1} + \frac{1}{r+1}\mathbf{1}^T\mathbf{A}\mathbf{1} \leq 1. \tag{3.42}$$

Inserting (3.32) for $\mathbf{C}_{\mathcal{B}_{1,+}}$ in (3.42), and after applying some simplifications, we obtain

$$\mathbf{1}^T\mathbf{A}\mathbf{1} \leq r. \tag{3.43}$$

Replacing the constraints of (3.36) with (3.41) and (3.43), we obtain the following optimization problem, the solution of which provides an upper bound for (3.36):

$$\underset{\mathbf{A} \in \mathbb{R}^{r \times r}}{\text{maximize}} \quad |\det(\mathbf{A})| \tag{3.44a}$$

$$\text{subject to} \quad \mathbf{A}_{i,:}\mathbf{1} \geq \|\mathbf{A}_{i,:}\|_2, \quad i = 1, \ldots, r, \tag{3.44b}$$

$$\mathbf{1}^T\mathbf{A}\mathbf{1} \leq r. \tag{3.44c}$$

The optimal value of the objective function (3.44a) is bounded from above by

$$\begin{aligned}
|\det(\mathbf{A})| &\leq \|\mathbf{A}^T_{1,:}\|_2\|\mathbf{A}^T_{2,:}\|_2 \ldots \|\mathbf{A}^T_{r,:}\|_2, && (3.45)\\
&\leq (\mathbf{A}_{1,:}\mathbf{1})(\mathbf{A}_{2,:}\mathbf{1}) \ldots (\mathbf{A}_{r,:}\mathbf{1}), && (3.46)\\
&\leq (\frac{1}{r}\mathbf{1}^T\mathbf{A}\mathbf{1})^r, && (3.47)\\
&\leq 1, && (3.48)
\end{aligned}$$

where the expression in (3.45) is Hadamard's inequality, (3.47) is due to the arithmetic-geometric mean inequality, and (3.48) is due to (3.44c). Therefore, for any optimal solution $\mathbf{A}_*$ of (3.36), we have

$$|\det(\mathbf{A}_*)| \leq 1. \tag{3.49}$$

The equality in (3.49) is achieved if and only if $\mathbf{A}_*$ is a real orthogonal matrix with

$$\mathbf{1}^T\mathbf{A}_*\mathbf{1} = r, \text{ and } \|\mathbf{A}_{*i,:}\|_2 = \mathbf{A}_{*i,:}\mathbf{1} = 1, i = 1, \ldots, r. \tag{3.50}$$

Furthermore, since the identity matrix, $\mathbf{I}$, is clearly a feasible point for (3.36), its determinant corresponds to a lower bound. Therefore, for any optimal solution $\mathbf{A}_*$ of (3.36), we obtain

$$|\det(\mathbf{A}_*)| \geq 1. \tag{3.51}$$

Combining the lower bound in (3.51) and the upper bound in (3.49) and with the equality conditions in (3.45)–(3.48), we conclude that $\mathbf{A}_*$ is an optimal solution for the problem in (3.36) only if $\mathbf{A}_*$ is a real orthogonal matrix satisfying (3.50).

Step II: *We show that the scaled rows of the global optima of (3.36) are in $conv(\mathbf{S}_g)^{*,\frac{1}{r+1}\mathbf{1}}$.*

A global optimal point $\mathbf{A}_*$ satisfies (3.36b), therefore, we can write $\mathbf{A}_{*i,:}\mathbf{S}_{g:,j} \geq 0$ for all possible (i, j) pairs. Multiplying this expression by $-(r + 1)$, we obtain

$$-(r + 1)\mathbf{A}_{*i,:}\mathbf{S}_{g:,j} \leq 0.$$

From the previous step, we also have $\mathbf{A}_{*i,:}\mathbf{1} = 1$. Combining these expressions, we can write

$$-(r + 1)\mathbf{A}_{*i,:}\left(\mathbf{S}_{g:,j} - \frac{1}{r+1}\mathbf{1}\right) \;\leq\; 1,$$

which implies

$$-(r + 1)(\mathbf{A}_{*i,:})^T \in \text{conv}(\mathbf{S}_g)^{*,\frac{1}{r+1}\mathbf{1}} \text{ for all } i \in \{1, \ldots, r\}.$$

We will show in the fourth step that these scaled rows of $\mathbf{A}_*$ are also the vertices of $\mathcal{B}_{1,+}^{*,\frac{1}{r+1}\mathbf{1}}$.

Furthermore, scaling (3.36c) with $(r + 1)$, we can write

$$((r + 1)\mathbf{A}_*^T\mathbf{1})^T\mathbf{S}_{g:,j} \leq r + 1 \text{ for all } j \in \{1, \ldots, N\}.$$

Replacing r on the right with $\mathbf{1}^T\mathbf{A}_*\mathbf{1}$ (based on (3.50)), we have

$$((r + 1)\mathbf{A}_*^T\mathbf{1})^T\mathbf{S}_{g:,j} \leq \mathbf{1}^T\mathbf{A}_*\mathbf{1} + 1. \tag{3.52}$$

Reorganizing (3.52), leads to

$$((r+1)\mathbf{A}_*^T\mathbf{1})^T\left(\mathbf{S}_{g_{:,j}}-\frac{1}{r+1}\mathbf{1}\right)\leq 1,$$

from which we conclude $(r+1)\mathbf{A}_*{}^T\mathbf{1}\in\text{conv}(\mathbf{S}_g)^{*,\frac{1}{r+1}\mathbf{1}}$.

<u>Step III:</u> *We show that the* $-(r+1)$ *scaled rows of the global optima* $\mathbf{A}_*$ *of (3.36) are on the boundary of the polar ellipsoid* $\mathcal{E}_{\mathcal{P}}^{*,\frac{1}{r+1}\mathbf{1}}$.

From Appendix A, the polar of the ellipsoid in (B.1) is given by

$$\mathcal{E}_{\mathcal{P}}^{*,\mathbf{g}_P}=\{\mathbf{C}_P^{-1}\mathbf{u}\mid\|\mathbf{u}\|_2\leq 1,\mathbf{u}\in\mathbb{R}^r\},$$

the boundary of which can be written as

$$\text{bd}(\mathcal{E}_{\mathcal{P}}^{*,\mathbf{g}_P})=\{\mathbf{x}\mid\|\mathbf{x}^T\mathbf{C}_P\|_2=1\}. \tag{3.53}$$

To check whether $-(r+1)(\mathbf{A}_{*i,:})^T$ is on the boundary of the polar of the MVIE, we evaluate the norm expression in (3.53):

$$\begin{aligned}\|(r+1)\mathbf{A}_{*i,:}\mathbf{C}_{\mathcal{B}_{1,+}}\|_2^2 &= (r+1)^2\mathbf{A}_{*i,:}\mathbf{C}_{\mathcal{B}_{1,+}}^2\mathbf{A}_{*i,:}^T,\\ &= \tfrac{r+1}{r}\left(\|\mathbf{A}_{*i,:}\|_2^2-\tfrac{(\mathbf{A}_{*i,:}\mathbf{1})^2}{r+1}\right), &(3.54)\\ &= 1. &(3.55)\end{aligned}$$

We used (B.18) to obtain (3.54), and (3.50) to simplify (3.54) into (3.55). As a result,

$$-(r+1)(\mathbf{A}_{*i,:})^T\in\text{bd}(\mathcal{E}_{\mathcal{P}}^{*,\mathbf{g}_P}).$$

Therefore, the rows of the global optimum $\mathbf{A}_*$ lie in the boundary of the polar domain ellipsoid illustrated in Figure 3.6.

Similarly, we can show $(r+1)\mathbf{A}_*{}^T\mathbf{1}\in\text{bd}(\mathcal{E}_{\mathcal{P}}^{*,\mathbf{g}_P})$ through

$$\begin{aligned}\|(r+1)\mathbf{1}^T\mathbf{A}_*\mathbf{C}_{\mathcal{B}_{1,+}}\|_2^2 &= (r+1)^2\mathbf{1}^T\mathbf{A}_*\mathbf{C}_{\mathcal{B}_{1,+}}^2\mathbf{A}_*{}^T\mathbf{1},\\ &= \frac{r+1}{r}\left(\mathbf{1}^T\mathbf{A}_*\mathbf{A}_*{}^T\mathbf{1}-\frac{(\mathbf{1}^T\mathbf{A}_*\mathbf{1})^2}{r+1}\right), &(3.56)\\ &= 1. &(3.57)\end{aligned}$$

We again used (B.18) to obtain (3.56), and (3.50) to simplify (3.56) into (3.57).

Step IV: *We combine the results of the previous steps and (PMF.SS.ii) to show that all global optima for (3.36) are permutation matrices.*

Combining the results of the second and third steps of the proof, we deduce that

$$-(r+1)(\mathbf{A}_{*i,:})^T \in \text{conv}(\mathbf{S}_g)^{*,\frac{1}{r+1}\mathbf{1}} \cap \text{bd}(\mathcal{E}_{\mathcal{P}}^{*,\frac{1}{r+1}\mathbf{1}}) \text{ for all } i \in \{1,\dots,r\}$$

and

$$(r+1){\mathbf{A}_*}^T\mathbf{1} \in \text{conv}(\mathbf{S}_g)^{*,\frac{1}{r+1}\mathbf{1}} \cap \text{bd}(\mathcal{E}_{\mathcal{P}}^{*,\frac{1}{r+1}\mathbf{1}}).$$

The sufficient scattering condition (PMF.SS.ii) dictates that

$$\text{conv}(\mathbf{S}_g)^{*,\frac{1}{r+1}\mathbf{1}} \cap \text{bd}(\mathcal{E}_{\mathcal{B}_{1,+}}^{*,\frac{1}{r+1}\mathbf{1}}) = \text{ext}(\mathcal{B}_{1,+}^{*,\frac{1}{r+1}\mathbf{1}}).$$

Due to the canonical description in (3.33),

$$\text{ext}(\mathcal{B}_{1,+}^{*,\frac{1}{r+1}\mathbf{1}}) = \{-(r+1)\mathbf{e}_1, ..., -(r+1)\mathbf{e}_r, (r+1)\mathbf{1}\}. \tag{3.58}$$

This condition is visible in Figure 3.6 as a triangle intersecting the boundaries of the ellipsoid and $\text{conv}(\mathbf{S}_g)^{*,\frac{1}{r+1}\mathbf{1}}$ at its $(r+1)$ vertices only. Therefore, we conclude that the set $\{(r+1)\mathbf{A}_*^T\mathbf{1}, (r+1)(\mathbf{A}_{*i,:})^T, i \in \{1,\dots,r\}\}$ are all vertices of $\mathcal{B}_{1,+}^{*,\frac{1}{r+1}\mathbf{1}}$ given by (3.58). This equivalence together with (3.50) lead to the conclusion that the rows of $\mathbf{A}_*$ are the standard basis vectors; therefore, $\mathbf{A}_*$ is a permutation matrix. □

3.5 Generalized PMF

This section provides the characterization of identifiable polytopes with respect to *Det-Max Criterion*. We first provide a definition and continue with polytopes that are identifiable for strongly scattered PMF data models.

Definition 3.5.1. *Permutation-and/or-Sign-Only Invariant Set*: Given a set E, we refer to it as Permutation-and/or-Sign-Only Invariant set, if and only if $\mathbf{A}(E) = E$ holds for only some $\mathbf{A} = \mathbf{D}\mathbf{\Pi}$, where $\mathbf{\Pi}$ is a permutation matrix and $\mathbf{D}$ is a full rank diagonal matrix with diagonal entries in $\{-1, 1\}$.

Theorem 5. *Characterization of Polytopes that are Det-Max Identifiable with respect to the Strongly Scattered PMF Data Model : All strongly scattered PMF data* *models corresponding to a non-degenerate polytope $\mathcal{P}$ are identifiable if and only if $ext(\mathcal{P})$ is a Permutation-and/or-Sign-Only Invariant set.*

Proof. "If" part: using the same arguments in the proof of Theorem 1, we write the optimization problem equivalent to (3.66) for the generalized PMF as

$$\underset{\mathbf{A}\in\mathbb{R}^{r\times r}}{\text{maximize}} \quad |\det(\mathbf{A})| \tag{3.59a}$$

$$\text{subject to} \quad \mathbf{A}\mathbf{S}_{g:,j} \in \mathcal{P}, \quad j = 1,\ldots,N. \tag{3.59b}$$

For this optimization problem, it is obvious that the identity matrix, $\mathbf{I}$, is a feasible solution. Therefore, the value of the objective function at $\mathbf{A} = \mathbf{I}$ forms the following lower bound

$$|\det(\mathbf{A}_*)| \geq 1. \tag{3.60}$$

for any optimal solution $\mathbf{A}_*$.

By definition of the strongly scattered data models, convex hull of source elements is equal to polytope $\mathcal{P}$, which can be written as

$$\text{conv}(\mathbf{S}_g)) = \mathcal{P}. \tag{3.61}$$

Therefore,

$$\mathbf{A}(\text{conv}(\mathbf{S}_g)) = \mathbf{A}(\mathcal{P}).$$

The constrain in (3.73b) and convexity of $\mathcal{P}$ implies that

$$\mathbf{A}(\text{conv}(\mathbf{S}_g)) \subseteq \mathcal{P}. \tag{3.62}$$

Then, considering 3.61 and 3.62, we can show that

$$\mathbf{A}(\mathcal{P}) \subseteq \mathcal{P},$$

which implies the following upper bound,

$$|\det(\mathbf{A})| \leq 1. \tag{3.63}$$

Now, (3.51) and (3.63) imply $|\det(\mathbf{A}_*)| = 1$ and $\mathbf{A}_*(\mathcal{P}) = \mathcal{P}$ for optimal $\mathbf{A}_*$. This is equivalent to write

$$\mathbf{A}_*(\text{ext}(\mathcal{P})) = \text{ext}(\mathcal{P}). \tag{3.64}$$

since $\mathcal{P}$ is a convex polytope. Therefore, if $\text{ext}(\mathcal{P})$ is *Permutation-and/or-Sign-Only Invariant*, then the PMF Data Model is Det-Max identifiable.

"Only if" part: Let $\mathbf{V}_{\mathcal{P}} \in \Re^{r\times K}$ represent a matrix containing all K vertices of $\mathcal{P}$ in its columns. Then $\mathbf{S}_g = \mathbf{V}_{\mathcal{P}}\mathbf{L}_g$ for some $\mathbf{L}_g \in \Re^{K\times K}$ is a matrix with convex combination weights in its columns. If there exists an $\mathbf{A}_*$ matrix for which $\mathbf{A}_*(\text{ext}(\mathcal{P})) = \text{ext}(\mathcal{P})$ holds then $\mathbf{A}_*\mathbf{V}_{\mathcal{P}} = \mathbf{V}_{\mathcal{P}}\mathbf{\Gamma}$ for some permutation matrix $\mathbf{\Gamma}$. The corresponding $\mathbf{S} = \mathbf{A}_*\mathbf{S}_g = \mathbf{A}_*\mathbf{V}_{\mathcal{P}}\mathbf{L}_g = \mathbf{V}_{\mathcal{P}}\mathbf{\Gamma}\mathbf{L}_g = \mathbf{V}_{\mathcal{P}}\mathbf{L}'_g$ where $\mathbf{L}'_g = \mathbf{\Gamma}\mathbf{L}_g$ is another matrix with convex combination weights in its columns, obtained from $\mathbf{L}_g$ by shuffling in its rows. Therefore, the corresponding $\mathbf{S}$ is feasible. Full rank condition on $\mathbf{V}_{\mathcal{P}}$ from non-degeneracy of $\mathcal{P}$ and $\mathbf{A}_*\mathbf{V}_{\mathcal{P}} = \mathbf{V}_{\mathcal{P}}\mathbf{\Gamma}$ imply $|\det(\mathbf{A}_*)| = 1$. Therefore, all matrices satisfying (3.64) are optimal Det-Max solutions for strongly scattered PMF Data Models. Therefore, if there exists an $\mathbf{A}_*$ that satisfies (3.64) but not equal to the product of a diagonal sign and a permutation matrix, then all strongly scattered PMF Data Models corresponding to $\mathcal{P}$ will be unidentifiable. $\square$

The next theorem shows that the use of the weaker scattering notion leads to the same condition of polytope eligibility for PMF Data Model identifiability:

Theorem 6. *Characterization of Polytopes that are Det-Max Identifiable with respect to the Sufficiently Scattered PMF Data Model : All sufficiently scattered PMF data models corresponding to a non-degenerate polytope $\mathcal{P}$ are identifiable if and only if ext($\mathcal{P}$) is a Permutation-and/or-Sign-Only Invariant set.*

Proof. We will first show the "if" part: Let $(\mathcal{P}, \mathbf{S}_g, \mathbf{H}_g)$ be any sufficiently scattered PMF model for $\mathcal{P}$. Let $\mathbf{A}_*$ be any optimal solution of the corresponding Det-Max problem. We will show that $\mathbf{A}_*(\text{ext}(\mathcal{P})) = \text{ext}(\mathcal{P})$. We start by noting that the constraint part of Det-Max problem imposes

$$\text{conv}(\mathbf{A}_*\mathbf{S}_g) \subseteq \mathcal{P}, \tag{3.65}$$

and from the feasibility of the identity matrix $\mathbf{A} = \mathbf{I}$, the optimal solution satisfies

$$|\det(\mathbf{A}_*)| \geq \det(\mathbf{I}) = 1.$$

Then, due to the sufficient scattering of $\mathbf{S}_g$, the constraints in Definition 3.3.2 hold. The first constraint along with (3.65) imply that

$$\mathbf{A}_*(\mathcal{E}_\mathcal{P}) \subset \mathcal{P},$$

i.e., an ellipsoid in $\mathcal{P}$ with

$$\mathrm{vol}(\mathbf{A}_*(\mathcal{E}_\mathcal{P})) = |\det(\mathbf{A}_*)|\mathrm{vol}(\mathcal{E}_P) \geq \mathrm{vol}(\mathcal{E}_\mathcal{P}),$$

using the lower bound $|\det(\mathbf{A}_*)| \geq 1$. Due to the uniqueness of MVIE for $\mathcal{P}$ we deduce that $|\det(\mathbf{A}_*)| = 1$ and

$$\mathbf{A}_*(\mathcal{E}_\mathcal{P}) = \mathcal{E}_\mathcal{P}. \tag{3.66}$$

In other words, sufficient scattering condition places an upper bound on $|\det(\mathbf{A}_*)|$ and restricts optimal $\mathbf{A}_*$ to map $\mathcal{E}_\mathcal{P}$ to itself. Consequently, according to Lemma 2 and Lemma 3, (3.66) corresponds to

$$\mathbf{A}_*^{-T}(\mathcal{E}_\mathcal{P}^{*,\mathbf{g}_\mathcal{P}}) = \mathcal{E}_\mathcal{P}^{*,\mathbf{g}_\mathcal{P}} \tag{3.67}$$

where $\mathcal{E}_\mathcal{P}^{*,\mathbf{g}_\mathcal{P}}$ is also an ellipsoid. Therefore, (3.67) implies

$$\mathbf{A}_*^{-T}(\mathrm{bd}(\mathcal{E}_\mathcal{P}^{*,\mathbf{g}_\mathcal{P}})) = \mathrm{bd}(\mathcal{E}_\mathcal{P}^{*,\mathbf{g}_\mathcal{P}}). \tag{3.68}$$

By the reversing property of polar sets given in Appendix A, (3.65) corresponds to

$$\mathcal{P}^{*,\mathbf{g}_\mathcal{P}} \subseteq \mathbf{A}_*^{-T}(\mathrm{conv}(\mathbf{S}_g)^{*,\mathbf{g}_\mathcal{P}}),$$

which implies

$$\mathbf{A}_*^{-T}(\mathrm{conv}(\mathbf{S}_g)^{*,\mathbf{g}_\mathcal{P}}) \supset \mathrm{ext}(\mathcal{P}^{*,\mathbf{g}_\mathcal{P}}). \tag{3.69}$$

From the second constraint of sufficient scattering, we obtain $\mathrm{conv}(\mathbf{S}_g)^{*,\mathbf{g}_\mathcal{P}} \supset \mathrm{ext}(\mathcal{P}^{*,\mathbf{g}_\mathcal{P}})$, $\mathrm{bd}(\mathcal{E}_\mathcal{P}^{*,\mathbf{g}_\mathcal{P}}) \supset \mathrm{ext}(\mathcal{P}^{*,\mathbf{g}_\mathcal{P}})$ and

$$\mathbf{A}^{-T}(\mathrm{conv}(\mathbf{S}_g)^{*,\mathbf{g}_\mathcal{P}}) \cap \mathrm{bd}(\mathcal{E}_\mathcal{P}^{*,\mathbf{g}_\mathcal{P}}) = \mathbf{A}^{-T}(\mathrm{ext}(\mathcal{P}^{*,\mathbf{g}_\mathcal{P}})), \tag{3.70}$$

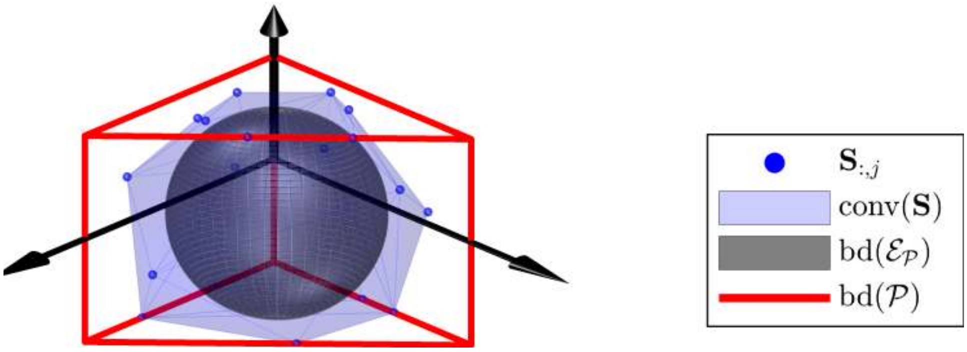


Figure 3.8: An example polytope corresponding to one signed and two nonnegative-mutually sparse sources.

where we also inserted (3.68). In addition, (3.69) implies

$$\mathbf{A}^{-T}(\text{conv}(\mathbf{S}_g)^{*,\mathbf{g}_\mathcal{P}}) \cap \text{bd}(\mathcal{E}_\mathcal{P}^{*,\mathbf{g}_\mathcal{P}}) \supseteq \text{ext}(\mathcal{P}^{*,\mathbf{g}_\mathcal{P}}). \tag{3.71}$$

Combining (3.70) and (3.71), we obtain

$$\mathbf{A}_*^{-T}(\text{ext}(\mathcal{P}^{*,\mathbf{g}_\mathcal{P}})) \supseteq \text{ext}(\mathcal{P}^{*,\mathbf{g}_\mathcal{P}}).$$

Since the sets on both sides have the same cardinality, it boils down to the equality

$$\mathbf{A}_*^{-T}(\text{ext}(\mathcal{P}^{*,\mathbf{g}_\mathcal{P}})) = \text{ext}(\mathcal{P}^{*,\mathbf{g}_\mathcal{P}}),$$

which corresponds to $\mathbf{A}_*^{-T}(\mathcal{P}^{*,\mathbf{g}_\mathcal{P}}) = \mathcal{P}^{*,\mathbf{g}_\mathcal{P}}$. This is equivalent to $\mathbf{A}_*(\mathcal{P}) = \mathcal{P}$, which corresponds to (3.64) by the convexity of $\mathcal{P}$. Therefore, the condition that $\text{ext}(\mathcal{P})$ is a *Permutation-and/or-Sign-Only Invariant Set* leads to the restriction that $\mathbf{A}_* = \mathbf{D\Pi}$, with diagonal sign matrix $\mathbf{D}$ and the permutation matrix $\mathbf{\Pi}$, hence guaranteeing identifiability.

For the "only if" part: follows the same arguments as the "only if" part of Theorem 5. □

We provide an example for the better understanding of Theorem 6.

3.5.1 Example

As asserted by Theorem 6, polytopes are only constrained to obey the restricted symmetry condition, i.e. only permutation and/or sign only invariance. This result offers a rich set of possibilities for selecting polytopes enabling high flexibility about shaping conditions on the desired factors.

In order to illustrate this point and provide the corresponding geometrical picture, we consider an example with three components where $s_3 \in [-1, 1]$ is signed and $s_1, s_2 \in [0, 1]$ are non-negative. Furthermore, we require $\| \begin{bmatrix} s_1 & s_2 \end{bmatrix} \|_1 \leq 1$, i.e., a sparsity enforcing condition on this subvector. The corresponding polytope, its MVIE and some sufficiently scattered sample points (with their convex hull) are shown on the left of Figure 3.8. Such sample points can be obtained from their lossless linear mixtures as the solution of the Det-Max optimization framework, through, for example, the algorithm proposed in Section 3.8.

3.6 Sample Covariance Matrix as Identifiability Criterion

Polytopic Matrix Factoriation (PMF) employs determinant maximization (Det-Max) approach as the identifiability criterion. The objective function of the Det-Max Problem in (3.7a) corresponds to the determinant of the scaled sample correlation matrix $\mathbf{R_s} = \frac{1}{N}\mathbf{S}\mathbf{S}^T = \frac{1}{N}\sum_{j=1}^{N} \mathbf{S}_{:,j}\mathbf{S}_{:,j}^T$. When the mean of samples is zero, the objective function amounts to generalized variance, which is denoted as the product of the eigenvalues of the covariance matrix [Sengupta, 2004].

We propose to use generalized variance as an alternative identifiability criterion to the determinant of the scaled sample correlation matrix for any value of sample mean including nonzero ones. For this purpose, we need to show the equivalency of scaled sample correlation and generalized variance as objective functions under the constrains given in (3.7b) and (3.7c). Therefore, we first write the equivalent form of the problem in (3.7). As we have shown in the proof of Theorem 1, the full column rank condition on $\mathbf{H}_g$ and the constraint $\mathbf{Y} = \mathbf{H}\mathbf{S}$ in (3.7b) implies that any feasible point $\mathbf{S}$ has the same row space as $\mathbf{S}_g$, which further implies

$$\mathbf{S} = \mathbf{A}\mathbf{S}_g, \tag{3.72}$$

for some full rank $\mathbf{A} \in \mathbb{R}^{r \times r}$ matrix. Therefore, the objective function in (3.7a) can be written as

$$\det(\mathbf{S}\mathbf{S}^T) = |\det(\mathbf{A})|^2 \det(\mathbf{S}_g\mathbf{S}_g^T).$$

Since the second term on the right-hand side is constant, we can write the equivalent problem of (3.7) as

$$\begin{aligned} \underset{\mathbf{A} \in \mathbb{R}^{r\times r}}{\text{maximize}} \quad & |\det(\mathbf{A})| && (3.73a) \\ \text{subject to} \quad & \mathbf{A}\mathbf{S}_{g:,j} \in \mathcal{P}, \quad j = 1, \ldots, N. && (3.73b) \end{aligned}$$

Formulating the sample mean as $\frac{1}{N}\mathbf{S}\mathbf{1}$, generalized variance (GV) can be written in the following way,

$$\begin{aligned} \text{GV} &= \det((\mathbf{S} - \frac{1}{N}\mathbf{S}\mathbf{1}\mathbf{1}^T)(\mathbf{S} - \frac{1}{N}\mathbf{S}\mathbf{1}\mathbf{1}^T)^T) && (3.74) \\ &= \det(\mathbf{S}\mathbf{S}^T - \frac{1}{N}\mathbf{S}\mathbf{1}\mathbf{1}^T\mathbf{S}^T). && (3.75) \end{aligned}$$

Exploiting generalized variance as the objective function of PMF optimization problem given in (3.7), we can write the following optimization problem,

$$\begin{aligned} \underset{\mathbf{H} \in \mathbb{R}^{M\times r}, \mathbf{S} \in \mathbb{R}^{r\times N}}{\text{maximize}} \quad & \det(\mathbf{S}\mathbf{S}^T - \frac{1}{N}\mathbf{S}\mathbf{1}\mathbf{1}^T\mathbf{S}^T) && (3.76a) \\ \text{subject to} \quad & \mathbf{Y} = \mathbf{H}\mathbf{S}, && (3.76b) \\ & \mathbf{S}_{:,j} \in \mathcal{P}, \quad j = 1, \ldots, N. && (3.76c) \end{aligned}$$

Then, using the parametrization in (3.72), the objective function in (3.76a), i.e., generalized variance expression in (3.75), can be written as

$$\begin{aligned} \text{GV} &= \det(\mathbf{A}\mathbf{S}_g\mathbf{S}_g^T\mathbf{A}^T - \frac{1}{N}\mathbf{A}\mathbf{S}_g\mathbf{1}\mathbf{1}^T\mathbf{S}_g^T\mathbf{A}^T) && (3.77) \\ &= \det(\mathbf{A}(\mathbf{S}_g\mathbf{S}_g^T - \frac{1}{N}\mathbf{S}_g\mathbf{1}\mathbf{1}^T\mathbf{S}_g^T)\mathbf{A}^T) && (3.78) \\ &= |\det(\mathbf{A})|^2 \det(\mathbf{S}_g\mathbf{S}_g^T - \frac{1}{N}\mathbf{S}_g\mathbf{1}\mathbf{1}^T\mathbf{S}_g^T). && (3.79) \end{aligned}$$

Since the second term on the right-hand side is constant, the optimization problem in (3.76) boils down to the optimization problem in (3.73). In the end, we prove that optimization problems in (3.76) and (3.7) are equivalent, since both boil down to the optimization problem in (3.73).

3.7 Characterization of Identifiable Polytopes

For the characterization of identifiable polytopes with respect to sufficiently scattered condition, Theorem 6 is proposed in [Tatli and Erdogan, 2021a]. According to this theorem, Theorem 2 in [Tatli and Erdogan, 2021a], for a given polytope $\mathcal{P}$, any sufficiently scattered data model is called "Det-Max identifiable" if and only if $\mathcal{P}$ satisfies a particular symmetry condition, which is called *Permutation-and/or-Sign-Only Invariance* in [Tatli and Erdogan, 2021a] and given in Section 3.5.

3.8 Algorithm

To illustrate use of PMF framework, we adopt the iterative algorithm in [Fu et al., 2016] which is originally proposed for the SSMF framework.

We start by introducing the Determinant Minimization (Det-Min problem), equivalent to the Det-Max problem in (3.7) under the equality constraint in (3.7b) [Fu et al., 2019]:

$$\underset{\mathbf{H}\in\mathbb{R}^{M\times r},\mathbf{S}\in\mathbb{R}^{r\times N}}{\text{minimize}} \quad \det(\mathbf{H}^T\mathbf{H}) \tag{3.80a}$$

$$\text{subject to} \quad \mathbf{Y} = \mathbf{HS}, \tag{3.80b}$$

$$\mathbf{S}_{:,j} \in \mathcal{P}, \quad j = 1, \ldots, N. \tag{3.80c}$$

Similar to [Fu et al., 2016], we employ the Lagrangian optimization,

$$\underset{\mathbf{H},\mathbf{S}}{\text{minimize}} \quad \|\mathbf{Y} - \mathbf{HS}\|_F^2 + \lambda \log\det(\mathbf{H}^T\mathbf{H} + \tau\mathbf{I}) \tag{3.81a}$$

$$\text{subject to} \quad \mathbf{S}_{:,j} \in \mathcal{P}, \quad j = 1, \ldots, N. \tag{3.81b}$$

corresponding to (3.80), where $\tau > 0$ is a hyperparameter to ensure that the objective function is bounded from below.

Algorithm 1 Det-Min algorithm for PMF

Input: $\mathbf{Y}$; r; Initial $\mathbf{H}, \mathbf{S}$; τ.

$t = 0$;

$\mathbf{X}^{(t)} = \mathbf{S}$,$\mathbf{F}^{(t)} = \mathbf{I}$,$\mathbf{H}^{(t)} = \mathbf{H}$,$\mathbf{S}^{(t)} = \mathbf{S}$, $q^{(t)} = 1$;

repeat

select $L^{(t)}$;

$\mathbf{S}_{:,l}^{(t+1)} \leftarrow P_{\mathcal{P}}\left(\mathbf{X}_{:,l}^{(t)} - (\mathbf{H}^{(t)})^T(\mathbf{Y}_{:,l} - \mathbf{H}^{(t)}\mathbf{X}_{:,l}^{(t)})\right)$ for $l = 1, \ldots, N$;

$q^{(t+1)} \leftarrow \frac{1+\sqrt{1+(q^{(t)})^2}}{2}$;

$\mathbf{X}_{:,l}^{(t+1)} \leftarrow \mathbf{S}_{:,l}^{(t+1)} + \frac{q^{(t)}-1}{q^{(t+1)}}(\mathbf{S}_{:,l}^{(t+1)} - \mathbf{S}_{:,l}^{(t)})$ for $l = 1, \ldots, N$;

$\mathbf{H}^{(t+1)} \leftarrow \mathbf{Y}(\mathbf{S}^{(t+1)})^T(\mathbf{S}^{(t+1)}(\mathbf{S}^{(t+1)})^T + \lambda\mathbf{F}^{(t)})$;

$t \leftarrow t + 1$;

$\mathbf{F}^{(t)} \leftarrow ((\mathbf{H}^{(t)})^T\mathbf{H}^{(t)} + \tau\mathbf{I})^{-1}$.

until some stopping criterion is reached.

Output: $\mathbf{H}^{(t)}$;$\mathbf{S}^{(t)}$.

The corresponding steps are provided in Algorithm 1, which is the algorithm in [Fu et al., 2016], except that the projection onto the unit simplex is replaced with the projection to polytope, $P_{\mathcal{P}}(\cdot)$. The following are examples of this projection operator:

- *Antisparse Case:* $\mathbf{X} = P_{\mathcal{B}_\infty}(\bar{\mathbf{X}})$ defines an elementwise projection operator to $\mathcal{B}_\infty$, which can be written as

$$X_{ij} = \begin{cases} \bar{X}_{ij} & \text{if } |\bar{X}_{ij}| < 1, \\ \text{sign}(\bar{X}_{ij}) & \text{otherwise.} \end{cases}$$

- *Sparse Case*: For $P_{\mathcal{B}_1}(\cdot)$, the projection onto the ℓ_1-norm-ball has no closed-form solution; however, efficient iterative algorithms, such as [Duchi et al., 2008], exist.

- *Antisparse Nonnegative Case:* The projection operator is a simple modification of $P_{\mathcal{B}_\infty}(\cdot)$, where elementwise projections are performed over $[0, 1]$ instead of $[-1, 1]$.

- *Sparse Nonnegative Case:* We can simplify the projection operator $\mathcal{B}_1$ to obtain the projection onto $\mathcal{B}_{1,+}$ (see [Duchi et al., 2008]).

3.9 Numerical Experiments

3.9.1 Special Polytopes

This section provides experiments for special polytopes covered in Section 3.4. Our standard sample generation process includes a conversion step between polytope representations. As the dimension of samples increases, this step becomes highly complex. Therefore, we propose an alternative way of sample generation for high dimensions. Additionally, we propose an alternative method for sample generation in high dimensions, which is similar to the method used in [Lin et al., 2015, Fu et al., 2016]. According to this alternative method, we first choose random samples inside the enlarged version of the MVIE and then, we project these points to the polytope. This 2 step procedure can be explained in the following way:

S1 Generate N samples from the inflated version of the MVIE of the polytope: we first generate N random i.i.d. Gaussian vector samples $\mathbf{w}_i \sim \mathcal{N}(\mathbf{0}, \frac{\rho^2}{r}\mathbf{I}), i = 1, \dots N$, in $\mathbb{R}^r$, the norms of which concentrate around the mean $E(\|\mathbf{w}_i\|_2) = \rho$. We call ρ "inflation constant" and choose $\rho > 1$. Then, we saturate vectors with norm greater than ρ by defining $\mathbf{u}_i = \rho\mathbf{w}_i/\|\mathbf{w}_i\|_2$ if $\|\mathbf{w}_i\|_2 > \rho$ and $\mathbf{u}_i = \mathbf{w}_i$ otherwise. The resulting $\mathbf{u}_i$ vectors are random samples in the hypersphere $\rho\mathcal{B}_2$, i.e., expanded unit hypersphere. Finally, we map the samples $\mathbf{u}_i$ into the inflated version of $\mathcal{E}_\mathcal{P}$ using $\mathbf{z}_i = \mathbf{C}_\mathcal{P}\mathbf{u}_i + \mathbf{g}_\mathcal{P}$. Therefore, the resulting samples lie in $\rho(\mathcal{E}_\mathcal{P} - \mathbf{g}_\mathcal{P}) + \mathbf{g}_\mathcal{P}$, the ρ-inflated version of the MVIE.

S2. Project the samples $\mathbf{z}_i$ onto the polytope: i.e., $\mathbf{S}_{g:,i} = P_\mathcal{P}(\mathbf{z}_i), i = 1, \dots, N$.

Figure 3.12.(a) illustrates the proposed sample generation for $\mathcal{P} = \mathcal{B}_\infty$ and $r = 2$. The inflation constant is selected as $\rho = 0.85\sqrt{r}$. Note that the choice $\rho = 1$ corresponds to the MVIE, and $\rho = \sqrt{r}$ corresponds to the minimum volume enclosing sphere of $\mathcal{B}_\infty$. Therefore, when $\rho < \sqrt{r}$, the vertices of $\mathcal{B}_\infty$ are not covered by the inflated MVIE.

For the experiments with polytopes in Section 3.4, we took $r = 10$ and $M = 20$. At each realization, we independently generated $\mathbf{H}_g$ as a 20×10 i.i.d. Gaussian matrix with zero mean and unity variance. We used different empirical λ parameter choices for different polytope and sample size selections to improve the SIR performance. We conducted this experiment for 300 realizations. Figure 3.12.(b) shows the SIR obtained as a function of ρ for $\mathcal{P} = \mathcal{B}_\infty$ and $N = 500$. In Figure 3.9, for the choice $\rho = 0.85\sqrt{r}$, we show the SIR as a function of the sample size N for all four polytopes in Section 3.4. Both Figure 3.12 and 3.9 confirm that the sufficiently scattered set generation probability increases with the increasing values of ρ and N as expected.

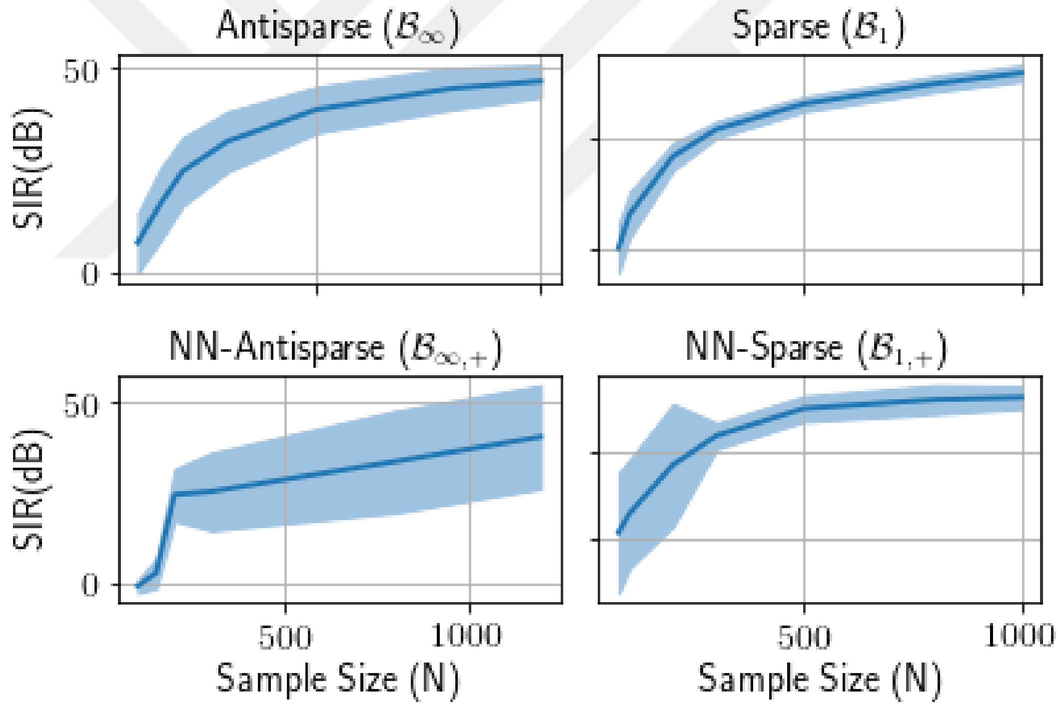


Figure 3.9: SIR (mean-solid line with std. envelope) as a function of sample size N for the polytopes in Section 3.4.

3.9.2 Polytope with Local Features

To illustrate the feature shaping flexibility provided by the PMF framework, we consider the following example polytope:

$$\mathcal{P}_{\text{ex}} = \left\{ \mathbf{x} \in \mathbb{R}^3 \;\middle|\; \begin{array}{l} x_1, x_2 \in [-1,1], x_3 \in [0,1], \\ \left\| \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \right\|_1 \leq 1, \left\| \begin{bmatrix} x_2 \\ x_3 \end{bmatrix} \right\|_1 \leq 1 \end{array} \right\},$$

which corresponds to the assignment of the following local attributes:

- x_3 is nonnegative and x_1, x_2 are signed; and
- $\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ and $\begin{bmatrix} x_2 \\ x_3 \end{bmatrix}$ are sparse subvectors.

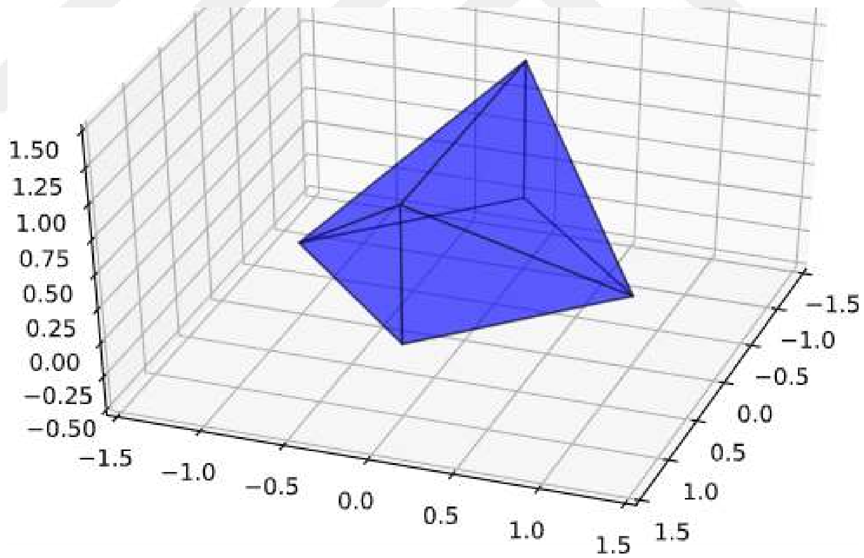


Figure 3.10: Polytope $\mathcal{P}_{\text{ex}}$.

The polytope $\mathcal{P}_{\text{ex}}$, shown in Figure 3.10, has 6 vertices placed in the columns of the following matrix:

$$\mathbf{V}_{\mathcal{P}_{\text{ex}}} = \begin{bmatrix} 1 & -1 & 0 & 0 & 1 & -1 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix}.$$

Checking all of the possible permutations of the columns of this matrix reveals that the vertex set satisfies the desired symmetry restriction; therefore, $\mathcal{P}_{\text{ex}}$ is identifiable. To illustrate both the identifiability of $\mathcal{P}_{\text{ex}}$ and the convergence behavior of the algorithm for sufficiently scattered samples, we conducted the following experiment. With each run of the experiment, we generate a set of sufficiently scattered samples from $\mathcal{P}_{\text{ex}}$ using the procedure described below.

S1. Generate the polar domain set $\text{conv}(\mathbf{S})^{*,\mathbf{g}_{\mathcal{P}_{\text{ex}}}}$ in **V-Form** (3.4): For this purpose we generate L samples from $\text{conv}(\mathbf{S})^{*,\mathbf{g}_{\mathcal{P}_{\text{ex}}}}$, the columns of $\mathbf{K} \in \mathbb{R}^{r\times L}$, and define $\text{conv}(\mathbf{S})^{*,\mathbf{g}_{\mathcal{P}_{\text{ex}}}} = \text{conv}(\mathbf{K})$:

i. According to the condition (PMF.SS.ii) in Definition 3.3.2, the elements of $\text{ext}(\mathcal{P}^{*,\mathbf{g}_{\mathcal{P}_{\text{ex}}}})$ should be the vertices of $\text{conv}(\mathbf{S})^{*,\mathbf{g}_{\mathcal{P}_{\text{ex}}}}$. Therefore, we first include elements of $\text{ext}(\mathcal{P}_{\text{ex}}^{*,\mathbf{g}_{\mathcal{P}_{\text{ex}}}})$ in $\mathbf{K}$, by setting:

$$\mathbf{K}_{:,1:7} = \begin{bmatrix} 1 & 1 & -1 & -1 & 0 & 0 & 0 \\ 1 & -1 & 1 & -1 & 1.6 & -1.6 & 0 \\ 0 & 0 & 0 & 0 & 1.6 & 1.6 & -8/3 \end{bmatrix}.$$

Note that $\text{conv}(\mathbf{K}_{,1:7}) = \mathcal{P}_{\text{ex}}{}^{*,\mathbf{g}_{\mathcal{P}_{\text{ex}}}}$. If we set $L = 7$, and therefore, skip the next step (S1.ii), our procedure would generate the vertices of $\mathcal{P}_{\text{ex}}$, which is a sufficiently scattered set.

ii. According to (PMF.SS.ii), the remaining vertices of $\mathcal{P}^{*,\mathbf{g}_{\mathcal{P}_{\text{ex}}}}$ should be in the interior of $\mathcal{E}^*_{\mathcal{P}_{\text{ex}}}$. Therefore, we generate $L-7$ random points in the interior of $\mathcal{E}^*_{\mathcal{P}_{\text{ex}}}$. For this purpose, we generate $L-7$ i.i.d. r-dimensional random samples in $0.9\mathcal{B}_2$. Then we multiply these vectors with $\mathbf{C}_P^{-1}$ to obtain the remaining columns of $\mathbf{K}$.

iii. We find **V-Form** for $\text{conv}(\mathbf{S})^{*,\mathbf{g}_{\mathcal{P}_{\text{ex}}}}$ by applying a numerical convex hull algorithm (such as ConvexHull function of Python's Scipy library [Virtanen et al., 2020]) to the columns of $\mathbf{K}$. The output of this step is the matrix $\mathbf{V} \in \mathbb{R}^{r\times L'}$ containing the vertices of $\mathcal{P}^{*,\mathbf{g}_{\mathcal{P}_{\text{ex}}}}$.

S2. Convert the representation of $\text{conv}(\mathbf{S})^{*,\mathbf{g}_{\mathcal{P}_{\text{ex}}}}$ from **V-Form** to **H-Form**: We convert the representation of $\text{conv}(\mathbf{S})^{*,\mathbf{g}_{\mathcal{P}_{\text{ex}}}}$ from **V-Form** in (3.4) to **H-Form** in (3.3). For this purpose, we use the PYPOMAN (a PYthon module for POlyhedral MANipulations) software package (`duality.compute_polytope_halfspaces` function.) [Caron, 2020]. The output of this stage are the hyperplane parameters $(\mathbf{a}_i, b_i), i = 1, \ldots, f$, for the **H-Form**.

S3. Find the vertices of $\text{conv}(\mathbf{S}_g)$: We first perform the normalization on the hyperplane parameters to obtain $(\mathbf{a}_i/b_i, 1), i = 1, \ldots, f$. Note that according to the polar conversion described in Appendix A, obtaining **V-Form** for $\mathcal{P}_{\text{ex}}$ in (A.3) from the **H-Form** for $\text{conv}(\mathbf{S})^{*,\mathbf{g}_{\mathcal{P}_{\text{ex}}}}$ in (A.2), the vectors $\{\mathbf{a}_i/b_i + \mathbf{g}_{\mathcal{P}_{\text{ex}}}, i = 1, \ldots, f\}$ are the vertices of $\text{conv}(\mathbf{S}_g)$, where $\mathbf{g}_{\mathcal{P}_{\text{ex}}} = [0, 0, 0.375]$. Therefore, we can set

$$\mathbf{S}_{g:,1:f} = \begin{bmatrix} \frac{\mathbf{a}_1}{b_1} + \mathbf{g}_{\mathcal{P}_{\text{ex}}} & \frac{\mathbf{a}_2}{b_2} + \mathbf{g}_{\mathcal{P}_{\text{ex}}} & \ldots & \frac{\mathbf{a}_f}{b_f} + \mathbf{g}_{\mathcal{P}_{\text{ex}}} \end{bmatrix}.$$

Note that f, the number of vertices of conv $(\mathbf{S}_g)$ (or faces of its polar), is a random quantity.

In the experiments, we chose $L = 30$. The $\mathbf{H}_g$ matrix is generated as a 4×3 i.i.d. Gaussian matrix (with zero mean and unity variance). We added zero mean i.i.d. Gaussian noise to the input matrix $\mathbf{Y} = \mathbf{H}_g\mathbf{S}_g$. The projection operation $P_{\mathcal{P}_{\text{ex}}}$ onto $\mathcal{P}_{\text{ex}}$ is implemented through 5 alternating iterations of the following.

- the projection onto the rectangle corresponding to the range constraints, implemented by elementwise clipping operations;
- the projection onto the ℓ_1-norm-ball for $\begin{bmatrix} x_1 & x_2 \end{bmatrix}^T$;
- the projection onto the ℓ_1-norm-ball for $\begin{bmatrix} x_2 & x_3 \end{bmatrix}^T$.

For the algorithm hyperparameters, we selected $\tau = 10^{-8}$, $L^{(t)} = 5\|(\mathbf{H}^{(t)})^T\mathbf{H}^{(t)}\|_2$ and $\lambda = 0.01$.

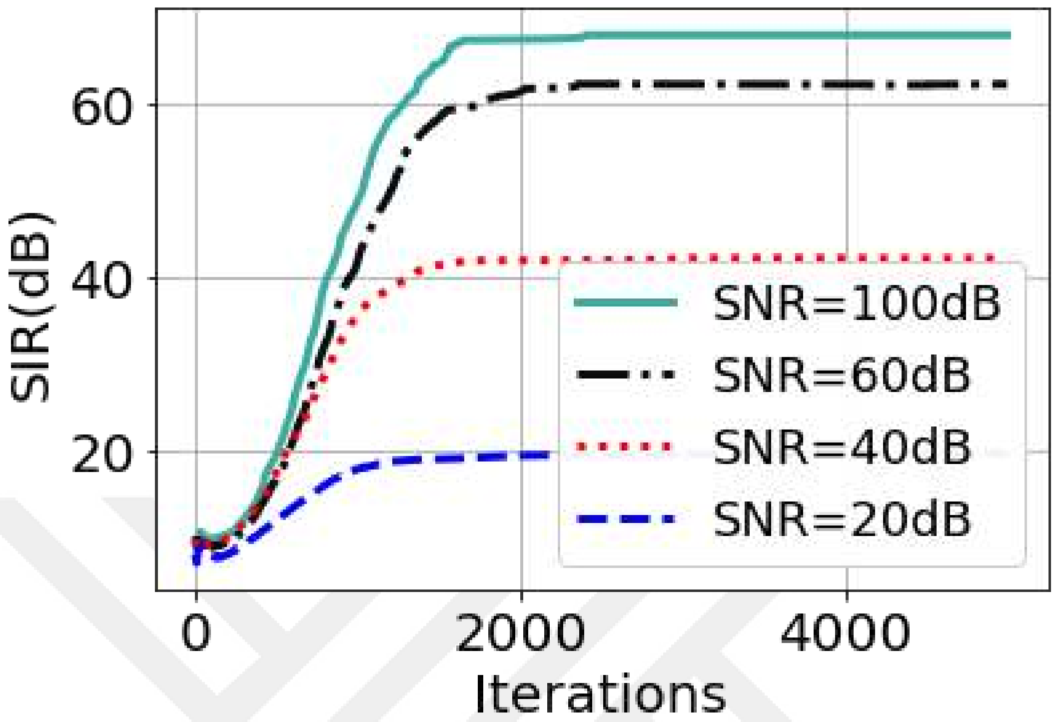
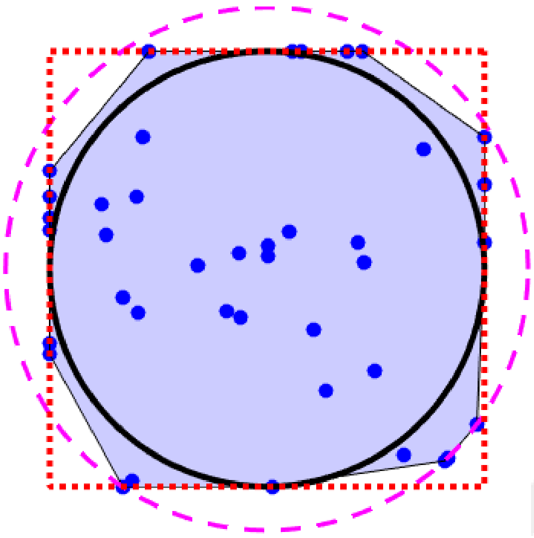


Figure 3.11: Average SIR convergence curves for $\mathcal{P}_{\text{ex}}$.

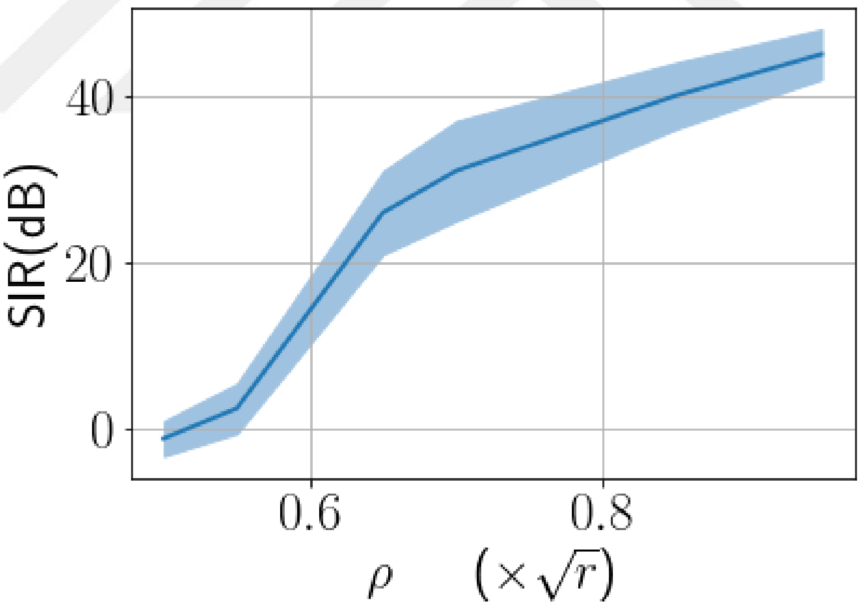
The convergence of the algorithm in terms of the signal-to-interference ratio (SIR), averaged over 100 realizations, as a function of the iterations is shown in Figure 3.11 for different signal-to-noise-ratio (SNR) levels. These experiments confirm the identifiability under the sufficiently scattered condition.

3.9.3 Sparse Dictionary Learning for Natural Image Patches

As the second example, we applied sparse PMF to 12×12 image patches obtained from Olshausen's prewhitened natural images (available at http://www.rctn.org/bruno/sparsenet/). These patches are vectorized (into 144×1 vectors) and placed in the columns of the $\mathbf{Y}$ matrix. The columns of the $\mathbf{H} \in \mathbb{R}^{144\times 144}$ matrix obtained from the sparse PMF algorithm (with $\lambda = 1$, $\tau = 10^{-6}$ and $L^{(t)} = 4\|(\mathbf{H}^{(t)})^T\mathbf{H}^{(t)}\|_2$) to 12×12 images (rescaled to the $0-1$ range) are shown in Figure 3.13. It is interesting to note that, although we used a different normative approach (based on determinant maximization) than [Olshausen and Field, 1997], we obtained similar Gabor-like edge features for the natural image patches.



(a)



(b)

Figure 3.12: (a) Sample generation example for Section 3.9.1: $\mathcal{P} = \mathcal{B}_\infty$ $(r = 2)$, the dashed circle represents the boundary of the inflated MVIE for $\rho = 0.85\sqrt{r}$. (b) SIR (mean-solid line with std. envelope) as a function of ρ for $\mathcal{B}_\infty$, $r = 10$ and $N = 500$.

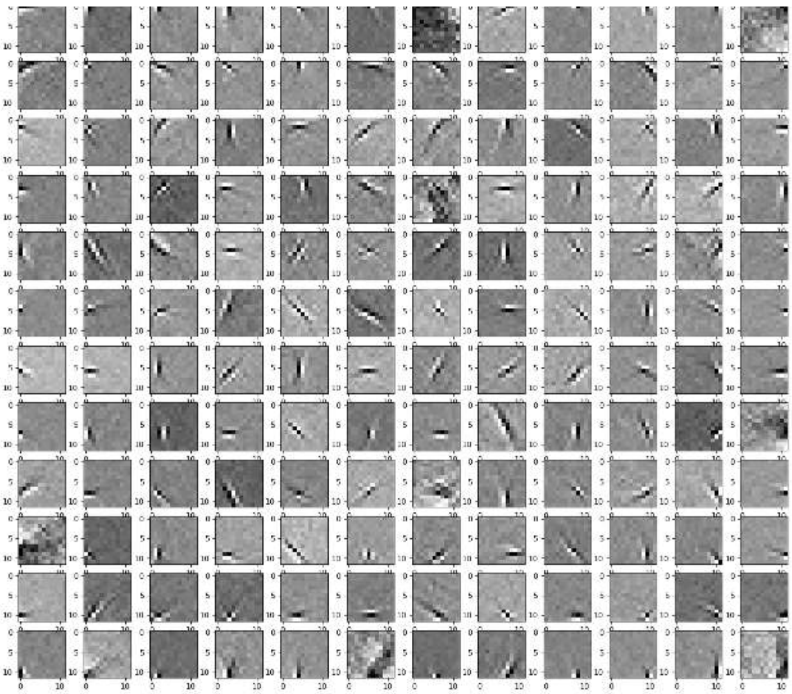


Figure 3.13: Dictionary obtained by sparse PMF for prewhitened natural image patches.

Chapter 4

EXTENDING POLYTOPIC MATRIX FACTORIZATION

4.1 Identifiability Under Diagonal Linear Mappings

Theorem 7. *Preservation of Identifiability Under a Diagonal Linear Mapping: Let $\mathcal{P} \in \mathbb{R}^n$ be a Det-Max Identifiable polytope with respect to the Det-Max Criterion and $\mathcal{P}_f$ is its image under the linear mapping $f(\mathbf{x}) = \mathbf{A}\mathbf{x}$, where $\mathbf{A} = \mathbf{P}\mathbf{\Lambda} \in \mathbb{R}^{n\times n}$ is the product of the permutation matrix $\mathbf{P}$ and the full rank diagonal matrix $\mathbf{\Lambda}$, then $\mathcal{P}_f$ is identifiable with respect to the Det-Max criterion.*

Proof. Consider the generative data setting

$$\mathbf{Y} = \mathbf{H}_{f,g}\mathbf{S}_{f,g} \tag{4.1}$$

where the $\mathbf{H}_{f,g} \in \Re^{M\times r}$ is full rank and the columns of $\mathbf{S}_{f,g} \in \Re^{r\times N}$ are in $\mathcal{P}_f$. We further assume that $\mathbf{S}_{f,g}$ is sufficiently scattered in $\mathcal{P}_f$. The data matrix $\mathbf{S}_{f,g}$ can be written as

$$\mathbf{S}_{f,g} = \mathbf{A}\mathbf{S}_g \tag{4.2}$$

where the columns of $\mathbf{S}_g$ are in $\mathcal{P}$. Plugging in (4.2) in (4.1), we obtain

$$\mathbf{Y} = \mathbf{H}_g\mathbf{S}_g \tag{4.3}$$

where $\mathbf{H}_g = \mathbf{H}_{f,g}\mathbf{A}$. Let $\mathcal{E}_{\mathcal{P}_f}(\mathbf{C}_{\mathcal{P}_f}, \mathbf{g}_{\mathcal{P}_f})$ denote the MVIE of $\mathcal{P}_f$. Its inverse image $\mathcal{E}_{\mathcal{P}}(\mathbf{C}_{\mathcal{P}}, \mathbf{g}_{\mathcal{P}})$, where $\mathbf{C}_{\mathcal{P}} = \mathbf{A}^{-1}\mathbf{C}_{\mathcal{P}_f}$ and $\mathbf{g}_{\mathcal{P}} = \mathbf{A}^{-1}\mathbf{g}_{\mathcal{P}_f}$ is the MVIE for $\mathcal{P}$, as f is a bijective mapping. Furthermore, due to the same property, the fact that $\mathbf{S}_{f,g}$ is sufficiently scattered in $\mathcal{P}_f$ implies $\mathbf{S}_g$ is sufficiently scattered in $\mathcal{P}$.

The *Det-Max Problem* for $\mathcal{P}_f$ can be written as

$$\begin{aligned}
&\underset{\mathbf{H}_f\in\mathbb{R}^{M\times r},\mathbf{S}_f\in\mathbb{R}^{r\times N}}{\text{maximize}} && \det(\mathbf{S}_f\mathbf{S}_f^T) \\
&\text{subject to} && \mathbf{Y}=\mathbf{H}_f\mathbf{S}_f, \\
& && \mathbf{S}_{f:,j}\in\mathcal{P}_f,\ j=1,\ldots,N.
\end{aligned}$$

Using the identity, $\mathbf{S}_f = \mathbf{A}\mathbf{S}$ where the columns of $\mathbf{S}$ are in $\mathcal{P}$, we can rewrite this optimization problem as

$$\begin{aligned}
&\underset{\mathbf{H}\in\mathbb{R}^{M\times r},\mathbf{S}\in\mathbb{R}^{r\times N}}{\text{maximize}} && \det(\mathbf{S}\mathbf{S}^T)(\det(\mathbf{A}))^2 \\
&\text{subject to} && \mathbf{Y}=\mathbf{H}\mathbf{S}, \\
& && \mathbf{S}_{:,j}\in\mathcal{P},\ j=1,\ldots,N.
\end{aligned}$$

Since $\mathcal{P}$ is identifiable and $\mathbf{S}_g$ is sufficiently scattered in $\mathcal{P}$, a global optimum point of the above optimization satisfies

$$\mathbf{S}_* = \mathbf{\Pi}_*\mathbf{D}_*\mathbf{S}_g \tag{4.4}$$

for some permutation matrix $\mathbf{\Pi}_*$ and the diagonal matrix $\mathbf{D}_*$. Since $\mathbf{S}_{f*} = \mathbf{A}\mathbf{S}_*$, we have

$$\begin{aligned}
\mathbf{S}_{f*} &= \mathbf{A}\mathbf{\Pi}_*\mathbf{D}_*\mathbf{A}^{-1}\mathbf{S}_{f,g} && (4.5)\\
&= \mathbf{P}\mathbf{\Lambda}\mathbf{\Pi}_*\mathbf{D}_*\mathbf{\Lambda}^{-1}\mathbf{P}^T\mathbf{S}_{f,g} && (4.6)\\
&= \mathbf{P}\mathbf{\Pi}_*\widehat{\mathbf{\Lambda}}\mathbf{D}_*\mathbf{\Lambda}^{-1}\mathbf{P}^T\mathbf{S}_{f,g} && (4.7)\\
&= \mathbf{P}\mathbf{\Pi}_*\mathbf{P}^T\mathbf{D}_{f*}\mathbf{S}_{f,g} && (4.8)\\
&= \mathbf{\Pi}_{f*}\mathbf{D}_{f*}\mathbf{S}_{f,g}, && (4.9)
\end{aligned}$$

where $\mathbf{\Pi}_{f*} = \mathbf{P}\mathbf{\Pi}_*\mathbf{P}^T$ is a permutation matrix, $\widehat{\mathbf{\Lambda}} = \mathbf{\Pi}_*^T\mathbf{\Lambda}\mathbf{\Pi}_*$ and $\mathbf{D}_{f*} = \mathbf{P}\widehat{\mathbf{\Lambda}}\mathbf{D}_*\mathbf{\Lambda}^{-1}\mathbf{P}^T$ are diagonal matrices. As a result, $\mathcal{P}_f$ is identifiable with respect to the *Det-Max Criterion.* □

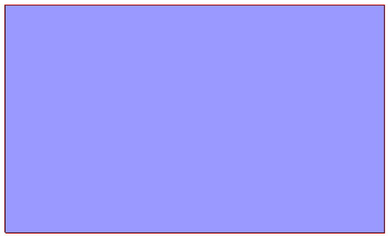


Figure 4.1: An example of identifiable 2D polytope transformed from $\mathcal{B}_\infty$.

4.2 Bounded Matrix Factorization

In this section, we propose an alternative sufficient scattering definition to further extend PMF identifiability. Up to that point, MVIE inclusion is always required for being identifiable with respect to the *Det-Max Criterion*. Now, we provide a further extension that does not require direct inclusion of MVIE. Then, we call this new extension Bounded Matrix Factorization.

Lemma 1. *Alternative Sufficient Scattering Definition for Polytopes Guaranteeing Identifiability for Sufficiently Scattered PMF Data Models*: For such identifiable polytopes, second criterion in Definition 3.3.2 manifests as the structure in which $\mathrm{bd}(\mathrm{conv}(\mathbf{S}))$ intersects with $\mathcal{E}_\mathcal{P}$ only at the $\mathrm{bd}(\mathcal{P})$ intersections of $\mathcal{E}_\mathcal{P}$. Therefore, we can say that, given a polytope $\mathcal{P}$ which guarantees identifiability for Sufficiently Scattered PMF Data Models , $\mathbf{S} \in \Re^{r \times N}$ is called sufficiently scattered in $\mathcal{P}$ if

- $\mathcal{P} \supset \mathrm{conv}(\mathbf{S}) \supset \mathcal{E}_\mathcal{P}$, and,
- $\mathrm{bd}(\mathrm{conv}(\mathbf{S})) \cap \mathcal{E}_\mathcal{P} = \mathrm{bd}(\mathcal{P}) \cap \mathcal{E}_\mathcal{P}$.

Proof. Without loss of generality, assume that $\mathcal{E}_\mathcal{P}$ is origin centered. Then, using the **V-Form** representation in Section 3.1, polytope $P \in \Re^r$ can be represented as

$$P = \{\mathbf{x} \mid \langle \mathbf{a}_i, \mathbf{x} \rangle \leq b_i, i = 1, ..., r\} \tag{4.10}$$

where $b_i > 0$. Using appropriate scaling, we can consider b_i=1, $\forall i = 1, ..., r$. Then, the polar of P can be represented as convex hull of a_i's.

$$P^* = conv(a_1, ..., a_r),$$

where $a_1, ..., a_r$ correspond to extreme points of P^* by the convexity of P^*. To be more precise, each hyperplane in (4.10) corresponds to an extreme point in the polar set.

Now, using the second criterion in Definition 3.3.2, we can deduce following

$$\text{ext}(\mathcal{P}^{*,\mathbf{g}_{\mathcal{P}}}) \quad \subset \quad \text{ext}(\mathcal{E}_{\mathcal{P}}^{*,\mathbf{g}_{\mathcal{P}}}) \tag{4.11}$$

$$\text{ext}(\mathcal{P}^{*,\mathbf{g}_{\mathcal{P}}}) \quad \subseteq \quad \text{ext}(\text{conv}(\mathbf{S}_g)^{*,\mathbf{g}_{\mathcal{P}}}). \tag{4.12}$$

which, in turn, yield that the hyperplane representation of conv$(\mathbf{S}_g)$ contains $\mathbf{a}_i$'s for $i = 1, ..., r$ similar to the representation in (4.10), where each hyperplane intersects with $\mathcal{E}_{\mathcal{P}}$. Due to the second constraint in Definition 3.3.2, (PMF.SS.ii), hyperplane representation of conv$(\mathbf{S}_g)$ includes only those hyperplanes among the ones intersect with $\mathcal{E}_{\mathcal{P}}$. Therefore, sufficiently scattered condition for polytopes guaranteeing identifiability for Sufficiently Scattered PMF Data Models can be written in the given alternative way. □

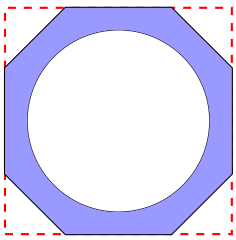


Figure 4.2: An interesting example that satisfies the alternative definition of sufficient scattering, referring to $\mathcal{B}_\infty$, in Lemma 1.

In the light of this alternative definition, we propose the following theorem for Det-Max identifiability of bounded subsets of Det-Max Identifiable polytopes.

Theorem 8. *Identifiable Bounded Subset : Let $\mathcal{P} \in \mathbb{R}^n$ be an identifiable polytope with respect to the Det-Max criterion and $\mathcal{P}_S$ is its subset. If $\mathcal{P}_S$ satisfies*

- $Co(\mathcal{P}_S) \supset \mathcal{E}_{\mathcal{P}}$,

- $bd(Co(\mathcal{P}_S)) \cap \mathcal{E}_{\mathcal{P}} = bd(\mathcal{P}) \cap \mathcal{E}_{\mathcal{P}}$,

then it is also identifiable with respect to the Det-Max Criterion.

Proof. If $\mathbf{S}_g$ is a sufficiently scattered set in $\mathcal{P}_S$ with respect to alternative definition of sufficient scattering, then

- $\mathrm{conv}(\mathbf{S}_g) \supset \mathcal{E}_{\mathcal{P}}$,

- $\mathrm{bd}(\mathrm{conv}(\mathbf{S}_g)) \cap \mathcal{E}_{\mathcal{P}} = \mathrm{bd}(\mathrm{Co}(\mathcal{P}_S)) \cap \mathcal{E}_{\mathcal{P}} = \mathrm{bd}(\mathcal{P}) \cap \mathcal{E}_{\mathcal{P}}$.

Therefore, $\mathbf{S}_g$ is also sufficiently scattered in $\mathcal{P}$. Since $\mathbf{S}_g$ is the determinant maximizing solution with the larger constraint set $\mathcal{P}$, it is also the feasible and the determinant maximizing solution with the constraint set $\mathcal{P}_S$. As a result $\mathbf{S}_g$ is identifiable, which implies the identifiability of the set $\mathcal{P}_S$.

$\square$

For a sufficiently scattered $\mathbf{S}$ of a given identifiable polytope $\mathcal{P}$, $\mathrm{conv}(\mathbf{S})$ is a subpolytope of $\mathcal{P}$ which clearly satisfies the required conditions in Theorem 8, which leads to the following corollary:

Corollary .1. *Identifiability of Sufficiently Scattered Subsets: Let $\mathcal{P} \in \mathbb{R}^n$ be an identifiable polytope with respect to the Det-Max Criterion, then for any sufficiently scattered factor $\mathbf{S}$ of $\mathcal{P}$, conv($\mathbf{S}$) is an identifiable bounded subset of $\mathcal{P}$.*

Chapter 5

BAYESIAN INTERPRETATION

5.1 Bayesian Interpretation with Inverse-Wishart Distribution

For the Bayesian interpretation of PMF problem, we assume the following data model with additional stochastic assumptions: the input matrix $\mathbf{Y} \in \mathbb{R}^{M\times N}$ is given by

$$\mathbf{Y} = \mathbf{H}_g\mathbf{S}_g + \mathbf{V}, \tag{5.1}$$

where

- $\mathbf{H}_g \in \mathbb{R}^{M\times r}$ is the ground truth of the left-factor matrix, which is assumed to be full column rank; and
- $\mathbf{S}_g \in \mathbb{R}^{r\times N}$ is the ground truth of the right-factor matrix, where we assume $r \leq \min(M, N)$ and

$$\mathbf{S}_{g_{:,j}} \in \mathcal{P},\ j = 1, \ldots, N, \tag{5.2}$$

  where $\mathcal{P}$ is a convex polytope; and
- $\mathbf{V} \in \mathbb{R}^{M\times N}$ is the noise matrix.

<u>Stochastic Assumptions</u>

- Let row partition of $\mathbf{H}_g$ given by $\begin{bmatrix} \mathbf{h}_1^T \\ \mathbf{h}_2^T \\ \ldots \\ \mathbf{h}_M^T \end{bmatrix}$, where $\mathbf{h}_i \in \mathbb{R}^N$ for $i = 1, \ldots, M$. We assume that $\mathbf{h}_i$'s are i.i.d. random variables with $\mathbf{h}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{\Sigma}_\mathbf{h}),\ i = 1, \ldots M$, in $\mathbb{R}^N$ and $\mathbf{\Sigma}_\mathbf{h} \sim \mathcal{IW}(\mathbf{\Psi}, \mathbf{v})$, where $\mathbf{\Psi} \in \mathbb{R}^{N\times N}$ and $\mathbf{v} \in \mathbb{R}$ are given parameters.

- $\mathbf{S}_{g_{:,j}}$'s are i.i.d. random variables and uniformly distributed inside $\mathcal{P}$, for $j = 1, \ldots, N$.

- $\mathbf{V}_{:,j}$'s are i.i.d. random variables with $\mathbf{V}_{:,j} \sim \mathcal{N}(\mathbf{0}, \sigma_{\mathbf{v}})$, for $j = 1, \ldots N$.

Then, the Maximum a Posteriori (MAP) estimation of $(\mathbf{H}, \mathbf{S}, \mathbf{\Sigma_h})$ can be written as

$$\underset{\mathbf{H},\mathbf{S},\mathbf{\Sigma_h}}{\text{maximize}} \quad \log f(\mathbf{H}, \mathbf{S}|\mathbf{Y}; \mathbf{\Sigma_h}),$$

which can be rearranged in the following form:

$$\underset{\mathbf{H},\mathbf{S},\mathbf{\Sigma_h}}{\text{maximize}} \quad \log f(\mathbf{Y}|\mathbf{H}, \mathbf{S}) + \log f(\mathbf{S}) + \log f(\mathbf{H}|\mathbf{\Sigma_h}) + \log f(\mathbf{\Sigma_h}).$$

In this objective function, the first term can be written as

$$\log f(\mathbf{Y}|\mathbf{H}, \mathbf{S}) = -\frac{1}{2\sigma_{\mathbf{v}}^2}||\mathbf{Y} - \mathbf{HS}||_F^2 + c_1,$$

where c_1 is a constant number. The second term $\log f(\mathbf{S})$ enforces $\mathbf{S}_{g_{:,j}}$'s to be contained in $\mathcal{P}$, since $\mathbf{S}_{g_{:,j}}$'s are uniformly distributed in $\mathcal{P}$. Therefore, this term corresponds to following constraint

$$\mathbf{S}_{g_{:,j}} \in \mathcal{P}, \ j = 1, \ldots, N. \tag{5.3}$$

The logarithm of conditional normal distribution $\log f(\mathbf{H}|\mathbf{\Sigma_h})$ is written as

$$\begin{aligned}
\log f(\mathbf{H}|\mathbf{\Sigma_h}) &= -\frac{M}{2}\log\det(\mathbf{\Sigma_h}) - \frac{1}{2}\sum_{1}^{M}\mathbf{h}_i^T\mathbf{\Sigma_h}^{-1}\mathbf{h}_i + c_2, &(5.4)\\
&= -\frac{M}{2}\log\det(\mathbf{\Sigma_h}) - \frac{1}{2}\mathrm{Tr}(\mathbf{\Sigma_h}^{-1}\sum_{1}^{M}\mathbf{h}_i\mathbf{h}_i^T), &(5.5)\\
&= -\frac{M}{2}\log\det(\mathbf{\Sigma_h}) - \frac{1}{2}\mathrm{Tr}(\mathbf{\Sigma_h}^{-1}\mathbf{H}^T\mathbf{H}) &(5.6)
\end{aligned}$$

where c_2 is a constant. The Inverse-Wishart distribution of $\log f(\mathbf{\Sigma_h})$ can be written as

$$\frac{\mathbf{v}}{2}\log\det(\mathbf{\Psi}) - \frac{N + \mathbf{v} + 1}{2}\log\det(\mathbf{\Sigma_h}) - \log(2^{v\frac{N}{2}})\Gamma_N(\frac{v}{2}) - \frac{1}{2}\mathrm{Tr}(\mathbf{\Psi}\mathbf{\Sigma_h}^{-1}) \tag{5.7}$$

Then, we differentiate $\log f(\mathbf{H}|\mathbf{\Sigma_h})$ and $\log f(\mathbf{\Sigma_h})$ with respect to $\mathbf{\Sigma_h}^{-1}$ to find the maximizer. Therefore, we can write following equations,

$$\frac{M}{2}\mathbf{\Sigma_h} - \frac{1}{2}\mathbf{H}^T\mathbf{H} = \mathbf{0}, \tag{5.8}$$

$$\frac{N + \mathbf{v} + 1}{2}\mathbf{\Sigma_h} - \frac{1}{2}\mathbf{\Psi}^T = \mathbf{0}. \tag{5.9}$$

From (5.8) and (5.9),

$$(N + \mathbf{v} + M + 1)\mathbf{\Sigma_h} = \mathbf{H}^T\mathbf{H} + \mathbf{\Psi}^T.$$

If we insert this to the summation of $\log f(\mathbf{H}|\mathbf{\Sigma_h})$ and $\log f(\mathbf{\Sigma_h})$, this summation is simplified as

$$-c_3 \log\det(\mathbf{H}^T\mathbf{H} + \mathbf{\Psi}), \tag{5.10}$$

where c_3 is a constant. In the end, the optimization problem is transformed into a form, that is solvable by our PMF algorithm,

$$\underset{\mathbf{H},\mathbf{S}}{\text{minimize}} \quad \frac{1}{2\sigma_{\mathbf{v}}^2}||\mathbf{Y} - \mathbf{HS}||_F^2 + c_3 \log\det(\mathbf{H}^T\mathbf{H} + \mathbf{\Psi})) \tag{5.11a}$$

$$\text{subject to} \quad \mathbf{S}_{:,j} \in \mathcal{P}, \quad j = 1, \ldots, N. \tag{5.11b}$$

Chapter 6

CONCLUSION

6.1 Conclusions

We introduced PMF as a novel structured matrix factorization approach. This new approach can be considered as a generalized version of existing approaches in terms of structural assumptions, since it can exploit sparseness, nonnegativeness and antisparseness for latent factor discovery. We also proposed a geometric approach for identifiability analysis, which provided practically plausible conditions for the applicability of the PMF framework. Therefore, we relaxed identifiability conditions of existing BCA and SCA approaches, that require inclusion of all vertices of the polytope.

We provided identifiability results of infinite number of polytopes by generalizing the idea of PMF. Having infinite choices of identifiable polytopes positions PMF as a general framework with a diverse set of feature representation selections.Therefore, we can consider some heterogeneous frameworks such as some part of the latent vectors are assumed sparse and remaining part can be assumed nonnegative. Such heterogeneous frameworks would be beneficial in various machine learning problems, which we consider as a future work.

The extension of PMF as Bounded Matrix Factorization broadened identifiable set description. Therefore, we proposed identifiability results of some bounded sets. This could also make possible use of PMF in some integer matrix factorization problems, which is a future direction for us.

We can foresee more and various future extensions including underdetermined data models, fully structured matrix factorization, noise/outlier analysis and efficient algorithms for PMF framework.

BIBLIOGRAPHY

[Babatas and Erdogan, 2018] Babatas, E. and Erdogan, A. T. (2018). An algorithmic framework for sparse bounded component analysis. *IEEE Transactions on Signal Processing*, 66(19):5194–5205.

[Babatas and Erdogan, 2020] Babatas, E. and Erdogan, A. T. (2020). Time and frequency based sparse bounded component analysis algorithms for convolutive mixtures. *Signal Processing*, page 107590.

[Ball, 1992] Ball, K. (1992). Ellipsoids of maximal volume in convex bodies. *Geometriae Dedicata*, 41(2):241–250.

[Boyd and Vandenberghe, 2004] Boyd, S. and Vandenberghe, L. (2004). *Convex Optimization*. Cambridge University Press.

[Bremner et al., 2009] Bremner, D., Sikiric, M. D., and Schürmann, A. (2009). Polyhedral representation conversion up to symmetries. In *CRM proceedings*, volume 48, pages 45–72.

[Brondsted, 2012] Brondsted, A. (2012). *An Introduction to Convex Polytopes*, volume 90. Springer Science & Business Media.

[Calhoun et al., 2009] Calhoun, V. D., Liu, J., and Adalı, T. (2009). A review of group ica for fmri data and ica for joint inference of imaging, genetic, and erp data. *Neuroimage*, 45(1):S163–S172.

[Candès and Wakin, 2008] Candès, E. J. and Wakin, M. B. (2008). An introduction to compressive sampling. *IEEE Signal Processing Magazine*, 25(2):21–30.

[Caron, 2020] Caron, S. (2020). Python module for polyhedral manipulations – PYPOMAN. version 1.0. Available: `https://scaron.info/doc/pypoman/`.

[Chan et al., 2011] Chan, T.-H., Ma, W.-K., Ambikapathi, A., and Chi, C.-Y. (2011). A simplex volume maximization framework for hyperspectral endmember extraction. *IEEE Transactions on Geoscience and Remote Sensing*, 49(11):4177–4193.

[Cichocki et al., 2009] Cichocki, A., Zdunek, R., Phan, A. H., and Amari, S. (2009). *Nonnegative Matrix and Tensor Factorizations: Applications to Exploratory Multi-way Data Analysis and Blind Source Separation*. John Wiley & Sons.

[Comon, 1994] Comon, P. (1994). Independent component analysis, a new concept? *Signal processing*, 36(3):287–314.

[Comon and Jutten, 2010] Comon, P. and Jutten, C. (2010). *Handbook of Blind Source Separation: Independent Component Analysis and Applications*. Academic press.

[Cruces, 2010] Cruces, S. (2010). Bounded component analysis of linear mixtures: A criterion of minimum convex perimeter. *IEEE Transactions on Signal Processing*, 58(4):2141–2154.

[Donoho and Stodden, 2003] Donoho, D. and Stodden, V. (2003). When does non-negative matrix factorization give a correct decomposition into parts? *Advances in Neural Information Processing Systems*, 16:1141–1148.

[Donoho, 2006] Donoho, D. L. (2006). For most large underdetermined systems of equations, the minimal ℓ_1-norm near-solution approximates the sparsest near-solution. *Communications on Pure and Applied Mathematics*, 59(7):907–934.

[Duchi et al., 2008] Duchi, J., Shalev-Shwartz, S., Singer, Y., and Chandra, T. (2008). Efficient projections onto the ℓ_1-ball for learning in high dimensions. In *Proceedings of the 25th International Conference on Machine learning*, pages 272–279.

[Elad, 2010] Elad, M. (2010). *Sparse and Redundant Representations: From Theory to Applications in Signal and Image Processing.* Springer Science & Business Media.

[Erdogan, 2013] Erdogan, A. T. (2013). A class of bounded component analysis algorithms for the separation of both independent and dependent sources. *IEEE Transactions on Signal Processing*, 61(22):5730–5743.

[Fu et al., 2018] Fu, X., Huang, K., and Sidiropoulos, N. D. (2018). On identifiability of nonnegative matrix factorization. *IEEE Signal Processing Letters*, 25(3):328–332.

[Fu et al., 2019] Fu, X., Huang, K., Sidiropoulos, N. D., and Ma, W.-K. (2019). Nonnegative matrix factorization for signal and data analytics: Identifiability, algorithms, and applications. *IEEE Signal Process. Mag.*, 36(2):59–80.

[Fu et al., 2016] Fu, X., Huang, K., Yang, B., Ma, W.-K., and Sidiropoulos, N. D. (2016). Robust volume minimization-based matrix factorization for remote sensing and document clustering. *IEEE Transactions on Signal Processing*, 64(23):6254–6268.

[Fuchs, 2011] Fuchs, J.-J. (2011). Spread representations. In *2011 Conference Record of the Forty Fifth Asilomar Conference on Signals, Systems and Computers (ASILOMAR)*, pages 814–817. IEEE.

[Georgiev et al., 2005] Georgiev, P., Theis, F., and Cichocki, A. (2005). Sparse component analysis and blind source separation of underdetermined mixtures. *IEEE Transactions on Neural Networks*, 16(4):992–996.

[Huang and Fu, 2019] Huang, K. and Fu, X. (2019). Detecting overlapping and correlated communities without pure nodes: Identifiability and algorithm. In *International Conference on Machine Learning*, pages 2859–2868.

[Hyvärinen et al., 2001] Hyvärinen, A., Karhunen, J., and Oja, E. (2001). Independent component analysis, adaptive and learning systems for signal processing, communications, and control. *John Wiley & Sons, Inc*, 1:11–14.

[Inan and Erdogan, 2014] Inan, H. A. and Erdogan, A. T. (2014). A convolutive bounded component analysis framework for potentially nonstationary independent and/or dependent sources. *IEEE Transactions on Signal Processing*, 63(1):18–30.

[Jégou et al., 2012] Jégou, H., Furon, T., and Fuchs, J.-J. (2012). Anti-sparse coding for approximate nearest neighbor search. In *2012 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)*, pages 2029–2032. IEEE.

[Laurberg et al., 2008] Laurberg, H., Christensen, M. G., Plumbley, M. D., Hansen, L. K., and Jensen, S. H. (2008). Theorems on positive data: On the uniqueness of NMF. *Computational Intelligence and Neuroscience*, 2008.

[Lee and Seung, 1999] Lee, D. D. and Seung, H. S. (1999). Learning the parts of objects by non-negative matrix factorization. *Nature*, 401(6755):788–791.

[Lee et al., 2007] Lee, H., Battle, A., Raina, R., and Ng, A. Y. (2007). Efficient sparse coding algorithms. In *Advances in Neural Information Processing Systems*, pages 801–808.

[Lin et al., 2015] Lin, C.-H., Ma, W.-K., Li, W.-C., Chi, C.-Y., and Ambikapathi, A. (2015). Identifiability of the simplex volume minimization criterion for blind hyperspectral unmixing: The no-pure-pixel case. *IEEE Transactions on Geoscience and Remote Sensing*, 53(10):5530–5546.

[Makeig et al., 1996] Makeig, S., Bell, A. J., Jung, T.-P., and Sejnowski, T. J. (1996). Independent component analysis of electroencephalographic data. In *Advances in neural information processing systems*, pages 145–151.

[Makino et al., 2007] Makino, S., Lee, T.-W., and Sawada, H. (2007). *Blind speech separation*, volume 615. Springer.

[Moussaoui et al., 2008] Moussaoui, S., Hauksdottir, H., Schmidt, F., Jutten, C., Chanussot, J., Brie, D., Douté, S., and Benediktsson, J. A. (2008). On the decomposition of mars hyperspectral data by ica and bayesian positive source separation. *Neurocomputing*, 71(10-12):2194–2208.

[Mukamel et al., 2009] Mukamel, E. A., Nimmerjahn, A., and Schnitzer, M. J. (2009). Automated analysis of cellular signals from large-scale calcium imaging data. *Neuron*, 63(6):747–760.

[Olshausen and Field, 1997] Olshausen, B. A. and Field, D. J. (1997). Sparse coding with an overcomplete basis set: A strategy employed by v1? *Vision Research*, 37(23):3311–3325.

[Ozerov and Févotte, 2009] Ozerov, A. and Févotte, C. (2009). Multichannel nonnegative matrix factorization in convolutive mixtures for audio source separation. *IEEE Transactions on Audio, Speech, and Language Processing*, 18(3):550–563.

[Pham and Cardoso, 2001] Pham, D.-T. and Cardoso, J.-F. (2001). Blind separation of instantaneous mixtures of nonstationary sources. *IEEE Transactions on signal processing*, 49(9):1837–1848.

[Sengupta, 2004] Sengupta, A. (2004). Generalized variance. In Kotz, S., Read, C. B., Balakrishnan, N., and Vidakovic, B., editors, *Encyclopedia of Statistical Sciences*. Wiley Online Library.

[Smaragdis and Brown, 2003] Smaragdis, P. and Brown, J. C. (2003). Non-negative matrix factorization for polyphonic music transcription. In *2003 IEEE Workshop on Applications of Signal Processing to Audio and Acoustics (IEEE Cat. No. 03TH8684)*, pages 177–180. IEEE.

[Studer et al., 2014] Studer, C., Goldstein, T., Yin, W., and Baraniuk, R. G. (2014). Democratic representations. *arXiv preprint arXiv:1401.3420*.

[Tatli and Erdogan, 2021a] Tatli, G. and Erdogan, A. T. (2021a). Generalized polytopic matrix factorization. In *ICASSP 2021-2021 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)*, pages 3235–3239. IEEE.

[Tatli and Erdogan, 2021b] Tatli, G. and Erdogan, A. T. (2021b). Polytopic matrix factorization: Determinant maximization based criterion and identifiability. *Submitted to IEEE Transactions on Signal Processing*.

[Virtanen et al., 2020] Virtanen, P., Gommers, R., and Oliphant, T. E. *et al.*. (2020). SciPy 1.0: Fundamental Algorithms for Scientific Computing in Python. *Nature Methods*, 17:261–272.

[Xu et al., 2003] Xu, W., Liu, X., and Gong, Y. (2003). Document clustering based on non-negative matrix factorization. In *Proceedings of the 26th annual international ACM SIGIR conference on Research and development in informaion retrieval*, pages 267–273.

[Yokoya et al., 2011] Yokoya, N., Yairi, T., and Iwasaki, A. (2011). Coupled nonnegative matrix factorization unmixing for hyperspectral and multispectral data fusion. *IEEE Transactions on Geoscience and Remote Sensing*, 50(2):528–537.

Appendix A

CONVEX ANALYSIS PRELIMINARY

A.1 Polar of a Set

The polar of a set $C \subset \mathbb{R}^r$ with respect to the point $\mathbf{d} \in \mathbb{R}^r$ is defined as

$$C^{*,\mathbf{d}} = \{\mathbf{x} \in \mathbb{R}^r | \langle \mathbf{x}, \mathbf{y} - \mathbf{d} \rangle \leq 1 \ \forall \mathbf{y} \in C\}. \tag{A.1}$$

When $\mathbf{d} = \mathbf{0}$, we simplify the notation as C^*. Based on this notation, we can write $C^{*,\mathbf{d}} = (C - \mathbf{d})^*$. A polytope containing the origin as an interior point can be written as

$$\mathcal{P} = \{\mathbf{x} \ | \langle \mathbf{a}_i, \mathbf{x} \rangle \leq 1, i = 1, ..., f\}, \tag{A.2}$$

the polar of which is given by (Theorem 9.1 in [Brondsted, 2012])

$$\mathcal{P}^* = \text{conv}(\begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \dots & \mathbf{a}_f \end{bmatrix}). \tag{A.3}$$

Therefore, the face normals $\mathbf{a}_i$ of the polytope $\mathcal{P}$ are the vertices of its polar $\mathcal{P}^*$. Note that if $\mathbf{d}$ is an interior point of $\mathcal{P}$, to calculate $\mathcal{P}^{*,\mathbf{d}}$, one can write $\mathcal{P} - \mathbf{d}$ in the form (A.2) and use $\mathcal{P}^{*,\mathbf{d}} = (\mathcal{P} - \mathbf{d})^*$ and (A.3). For an ellipsoid $\mathcal{E}_P \subset \mathbb{R}^r$ defined by

$$\mathcal{E}_\mathcal{P} = \{\mathbf{C}_\mathcal{P}\mathbf{u} + \mathbf{g}_\mathcal{P} \mid \|\mathbf{u}\|_2 \leq 1, \mathbf{u} \in \mathbb{R}^r\}, \tag{A.4}$$

where $\mathbf{C} \in \mathbb{R}^{r \times r}$ and $\mathbf{g} \in \mathbf{R}^r$, its polar with respect to its center $\mathbf{g}_p$ can be written as

$$\mathcal{E}_\mathcal{P}^{*,\mathbf{g}_P} \quad = \quad \{\mathbf{x} \mid \langle \mathbf{x}, \mathbf{C}_P\mathbf{u} \rangle \leq 1, \forall \|\mathbf{u}\|_2 \leq 1, \mathbf{u} \in \mathbb{R}^r\},$$

which can be simplified to

$$\mathcal{E}_\mathcal{P}^{*,\mathbf{g}_P} = \{\mathbf{C}_P^{-1}\mathbf{u} \mid \|\mathbf{u}\|_2 \leq 1, \mathbf{u} \in \mathbb{R}^r\}. \tag{A.5}$$

A particular property of polar operation that we use in the article is the reversal of the set inclusion: if $A \subset B$ holds then we have $B^{*,\mathbf{d}} \subset A^{*,\mathbf{d}}$.

Lemma 2. *On Linear Transformations of Ellipsoids*: Given a full rank square transformation matrix $\mathbf{A}$ with real entries and an ellipsoid $\mathcal{E}$. $\mathbf{A}(\mathcal{E}) = \mathcal{E}$ implies $\mathbf{A}(\mathrm{bd}(\mathcal{E})) = \mathrm{bd}(\mathcal{E})$, and $\mathbf{A}(\mathcal{E}) = \mathcal{E}$ implies $\mathbf{Ag} = \mathbf{g}$, where $\mathbf{g}$ is the center of ellipsoid $\mathcal{E}$.

Lemma 3. *Polar of the Transformed Set*: Polar of a set S with respect to the point $\mathbf{d}$ is defined as

$$S^{*,\mathbf{d}} = \{\mathbf{x} \in \Re^n | \langle \mathbf{x}, \mathbf{y} - \mathbf{d} \rangle \leq 1 \ \forall \mathbf{y} \in S\}$$

from (A.1). In the light of this definition, we can characterize the polar of the transformed set $\mathbf{A}(S)$ in the following way,

$$(\mathbf{A}(S))^{*,\mathbf{d}} \quad = \quad \{\mathbf{x} \in \Re^n | \langle \mathbf{x}, \mathbf{Ay} - \mathbf{d} \rangle \leq 1 \ \forall \mathbf{y} \in S\}$$

which corresponds to the set $\mathbf{A}^{-T}(S^{*,\mathbf{d}})$, when $\mathbf{Ad} = \mathbf{d}$.

Appendix B

MAXIMUM VOLUME INSCRIBED ELLIPSOID

B.1 MVIE

The MVIE of a polytope $\mathcal{P}$ can be represented with (see Section 8.4.2, Page 400 of [Boyd and Vandenberghe, 2004])

$$\mathcal{E}_{\mathcal{P}} = \{\mathbf{C}_{\mathcal{P}}\mathbf{u} + \mathbf{g}_{\mathcal{P}} \mid \|\mathbf{u}\|_2 \leq 1\}, \tag{B.1}$$

where, for a polytope defined by (3.3), the pair ($\mathbf{C}_{\mathcal{P}} \in \mathbb{R}^{r\times r}, \mathbf{g}_{\mathcal{P}} \in \mathbb{R}^r$) is obtained as the optimal solution of the optimization problem:

$$\underset{\mathbf{C}\in\mathbb{R}^{r\times r},\mathbf{g}\in\mathbb{R}^r}{\text{minimize}} \quad -\log\det\mathbf{C} \tag{B.2a}$$

$$\text{subject to} \quad \|\mathbf{C}\mathbf{a}_i\|_2 + \mathbf{a}_i^T\mathbf{g} \leq b_i, \quad i = 1, \ldots, f, \tag{B.2b}$$

$$\mathbf{C} \succeq \mathbf{0}. \tag{B.2c}$$

B.1.1 Spherical MVIEs

The following theorem by Fritz John [Ball, 1992] is useful for identifying spherical MVIEs:

Theorem 9. *$\mathcal{B}_2$ is the ellipsoid of maximal volume contained in the convex body $C \subset \mathbb{R}^r$ if and only if $\mathcal{B}_2 \subset C$ and, for some $m \geq r$, there are unit 2-norm vectors $\{\mathbf{u}_1, \ldots, \mathbf{u}_m\} \subset \mathbb{R}^r$ on the boundary of C, and positive numbers $\{c_i, i = 1, \ldots, m\}$ for which $\sum_{i=1}^m c_i\mathbf{u}_i = 0$ and $\sum_{i=1}^m c_i\mathbf{u}_i\mathbf{u}_i^T = \mathbf{I}_r$.*

Based on Theorem 9, we can show that the special polytope $\mathcal{B}_\infty$ (Section 3.1.i.) has $\mathcal{B}_2$ as its MVIE, with the choices of $\mathbf{u}_i = \mathbf{e}_i, i = 1, \ldots, r$ and $\mathbf{u}_i = -\mathbf{e}_{i-r}, i = r+1, \ldots 2r$, $c_i = 1, i = 1, \ldots, r$. Similarly, the MVIE of $\sqrt{r}\mathcal{B}_1$ is also $\mathcal{B}_2$, which can be justified by Theorem 9, through the choice of $\mathbf{u}_i = \frac{1}{\sqrt{r}}\mathbf{q}_i, i = 1, \ldots, 2^r$, where vectors $\mathbf{q}_i$ are all possible distinct sign vectors with ±1 entries.

B.1.2 MVIE for $\mathcal{B}_{1,+}$

We can obtain the MVIE parameters $(\mathbf{C}_P, \mathbf{g}_P)$ of the polytope $\mathcal{B}_{1,+}$, as the optimal solution of the following optimization problem:

$$\underset{\mathbf{C} \in \mathbb{R}^{r\times r}, \mathbf{g} \in \mathbb{R}^r}{\text{minimize}} \quad -\log\det\mathbf{C} \tag{B.3a}$$

$$\text{subject to} \quad \|\mathbf{C}\mathbf{e}_i\|_2 - \mathbf{e}_i^T\mathbf{g} \leq 0, \quad i = 1, \ldots, r, \tag{B.3b}$$

$$\|\mathbf{C}\mathbf{1}\|_2 + \mathbf{1}^T\mathbf{g} \leq 1, \tag{B.3c}$$

$$\mathbf{C} \succeq \mathbf{0}, \tag{B.3d}$$

which is obtained by applying the description of $\mathcal{B}_{1,+}$ in (3.31) to the generic MVIE optimization problem in (B.2). To find the solution of (B.3), we utilize the following Karush-Kuhn-Tucker (KKT) optimality conditions [Boyd and Vandenberghe, 2004] for the solution pair $(\mathbf{C}_P, \mathbf{g}_P)$:

$$-\mathbf{C}_P^{-1} + \sum_{i=1}^{r} \lambda_i \frac{\mathbf{C}_P\mathbf{e}_i\mathbf{e}_i^T}{\|\mathbf{C}_P\mathbf{e}_i\|_2} + \lambda_{r+1}\frac{\mathbf{C}_P\mathbf{1}\mathbf{1}^T}{\|\mathbf{C}_P\mathbf{1}\|_2} - \mathbf{W} = \mathbf{0}, \tag{B.4}$$

$$\lambda_i(\|\mathbf{C}_P\mathbf{e}_i\|_2 - \mathbf{e}_i^T\mathbf{g}_P) = 0, \text{ for all } i = 1, \ldots, r, \tag{B.5}$$

$$\lambda_{r+1}(\|\mathbf{C}_P\mathbf{1}\|_2 + \mathbf{1}^T\mathbf{g}_P - 1) = 0, \tag{B.6}$$

$$-\sum_{i=1}^{r} \lambda_i\mathbf{e}_i + \lambda_{r+1}\mathbf{1} = \mathbf{0}, \tag{B.7}$$

$$Tr(\mathbf{W}\mathbf{C}_P) = \mathbf{0}, \tag{B.8}$$

where (B.4) and (B.7) represent stationarity conditions of $\mathbf{C}_P$ and $\mathbf{g}_P$, respectively. The remaining KKT equations – (B.5), (B.6) and (B.8) – are known as complementary slackness conditions, which involve optimal dual variables $\lambda_1, \lambda_2, ..., \lambda_{r+1} \in \mathbb{R}_+$ and $\mathbf{W} \succeq \mathbf{0}$ corresponding to the inequality constraints in (B.3b), (B.3c) and (B.3d), respectively. Based on the optimization in (B.3) and the corresponding optimality conditions in (B.4)-(B.8), we can deduce the following:

- $\mathbf{C}_P$ is nonsingular, i.e., $\mathbf{C}_P \succ \mathbf{0}$, otherwise the objective function $-\log\det\mathbf{C}_P$ becomes infinite under the primal feasibility condition $\mathbf{C} \succeq \mathbf{0}$ in (B.3d). Therefore, the nonsingularity of $\mathbf{C}$ implies $\mathbf{W} = \mathbf{0}$ due the KKT condition given in (B.8).

- The condition in (B.7) is equivalent to $\lambda_1 = \lambda_2 = ... = \lambda_{r+1} = \lambda$, further implying that either all or none of the corresponding primal feasibility conditions are binding, i.e., the inequalities corresponding to these dual variables, (B.3b) and (B.3c), are equalities at the optimal point. If we assume none of them are binding, the KKT conditions (B.6) and (B.7) imply that $\lambda_1 = \lambda_2 = ... = \lambda_{r+1} = 0$, which further implies $\mathbf{W} \neq \mathbf{0}$ due to (B.4). This outcome contradicts our earlier finding that $\mathbf{W} = \mathbf{0}$. Therefore, we conclude that

$$\lambda_1 = \lambda_2 = ... = \lambda_{r+1} > 0, \tag{B.9}$$

and all corresponding inequalities are binding, i.e., $\|\mathbf{C}_P\mathbf{e}_i\|_2 - \mathbf{e}_i^T\mathbf{g}_P = 0$ for $i = 1, \ldots, r$ and $\|\mathbf{C}_P\mathbf{1}\|_2 + \mathbf{1}^T\mathbf{g}_P = 1$ hold.

- Using (B.9) and $\mathbf{W} = \mathbf{0}$, the expression in (B.4) can be rewritten as

$$-\mathbf{C}_P^{-1} + \lambda \left(\sum_{i=1}^{r} \frac{\mathbf{C}_P\mathbf{e}_i\mathbf{e}_i^T}{\|\mathbf{C}_P\mathbf{e}_i\|_2} + \frac{\mathbf{C}_P\mathbf{1}\mathbf{1}^T}{\|\mathbf{C}_P\mathbf{1}\|_2} \right) = \mathbf{0}. \tag{B.10}$$

If we multiply both sides of (B.10) by $\mathbf{C}_P^{-1}$, and rearrange the terms, we obtain

$$\mathbf{C}_P^{-2} = \lambda \left(\sum_{i=1}^{r} \frac{\mathbf{e}_i\mathbf{e}_i^T}{\|\mathbf{C}_P\mathbf{e}_i\|_2} + \frac{\mathbf{1}\mathbf{1}^T}{\|\mathbf{C}_P\mathbf{1}\|_2} \right). \tag{B.11}$$

Using the binding constraints $\|\mathbf{C}_P\mathbf{e}_i\|_2 = \mathbf{e}_i^T\mathbf{g}_P$ and $\|\mathbf{C}_P\mathbf{1}\|_2 = 1 - \mathbf{1}^T\mathbf{g}_P$, (B.11) can be rewritten as

$$\mathbf{C}_P^{-2} = \lambda \left(\mathbf{G}^{-1} + \frac{\mathbf{1}\mathbf{1}^T}{1 - \mathbf{1}^T\mathbf{g}_P} \right), \tag{B.12}$$

where $\mathbf{G} \in \mathbb{R}^{r\times r}$ is a diagonal matrix, the i^{th} diagonal entry of which is equal to $\mathbf{e}_i^T\mathbf{g}$ for all i=1, ..., r. Applying the matrix inversion lemma to the right hand side of (B.12), we have

$$\mathbf{C}_P^2 = \lambda^{-1} \left(\mathbf{G} - \mathbf{g}_P\mathbf{g}_P^T \right). \tag{B.13}$$

Multiplying (B.13) by the ones-vector from both the left and right yields

$$\mathbf{1}^T\mathbf{C}_P^2\mathbf{1} = \lambda^{-1}\mathbf{1}^T\mathbf{g}_P \left(1 - \mathbf{1}^T\mathbf{g}_P \right). \tag{B.14}$$

The binding constraint $\|\mathbf{C}_P\mathbf{1}\|_2 = 1 - \mathbf{1}^T\mathbf{g}_P$ can be used to obtain an alternative expression

$$\mathbf{1}^T\mathbf{C}_P^2\mathbf{1} = (1 - \mathbf{1}^T\mathbf{g}_P)^2. \tag{B.15}$$

Equating the right hand sides of (B.14) and (B.15), we have

$$\lambda = \frac{\mathbf{1}^T\mathbf{g}_P}{1 - \mathbf{1}^T\mathbf{g}_P} = \frac{1}{1 - \mathbf{1}^T\mathbf{g}_P} - 1. \tag{B.16}$$

- Squaring both sides of the binding constraint $\|\mathbf{C}_P\mathbf{e}_i\|_2 = \mathbf{e}_i^T\mathbf{g}$, we obtain $\mathbf{e}_i^T\mathbf{C}_P^2\mathbf{e}_i = (\mathbf{e}_i^T\mathbf{g}_P)^2 = g_{P,i}^2$, where $g_{P,i}$ stands for $\mathbf{e}_i^T\mathbf{g}_P$. Inserting the expression for $\mathbf{C}_P^2$ in (B.13), we obtain

$$\lambda^{-1}(g_{P,i} - g_{P,i}^2) = g_{P,i}^2,$$

which leads to

$$\lambda = \frac{1 - g_{P,i}}{g_{P,i}} = \frac{1}{g_{P,i}} - 1, \quad \forall i \in \{1, \ldots, r\}. \tag{B.17}$$

Combining (B.16) and (B.17), we can write

$$1 - \mathbf{1}^T\mathbf{g} = g_{P,i}, \quad \forall i \in \{1, \ldots, r\}.$$

From this expression and (B.17), we obtain $\mathbf{g}_P = \frac{1}{r+1}\mathbf{1}$ and $\lambda = r$. Inserting these values into (B.13) yields

$$\mathbf{C}_P^2 = \frac{1}{r}\left(\frac{1}{r+1}\mathbf{I} - \frac{1}{(r+1)^2}\mathbf{1}\mathbf{1}^T\right), \tag{B.18}$$

the square root of which is given by

$$\mathbf{C}_P = \frac{1}{\sqrt{r}}\left(\frac{1}{\sqrt{r+1}}\mathbf{I} - \frac{\sqrt{r+1} - 1}{r(r+1)}\mathbf{1}\mathbf{1}^T\right).$$