

IDENTIFIABILITY OF SECOND-ORDER MULTIDIMENSIONAL ICA

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ABSTRACT

In this paper, we consider the identifiability of second-order blind separation of multidimensional components. By maximizing the likelihood for piecewise-stationary Gaussian data, we obtain that the maximum likelihood (ML) solution is equivalent to joint block diagonalization (JBD) of the sample covariance matrices of the observations. Small-error analysis of the solution indicates that the identifiability of the model depends on the positive-definiteness of a matrix, which is a function of the latent source covariance matrices. By analysing this matrix, we derive necessary and sufficient conditions for the model to be identifiable. These are also the sufficient and necessary conditions for JBD of any set of real positive-definite symmetric matrices to be unique.

Index Terms— Joint block diagonalization, identifiability, uniqueness, multidimensional ICA

1. INTRODUCTION

In this paper, we discuss the identifiability of second-order multidimensional ICA (MICA). We show that the identifiability analysis provides necessary and sufficient conditions for the existence of a unique solution to joint block diagonalization (JBD) of a set of real, positive-definite symmetric matrices.

The relationship between blind separation and JBD has been established recently in various works [1, 2, 3]. For the one-dimensional case, second-order blind separation of stationary sources has been shown [4] to be solvable by joint diagonalization (JD) of several covariance matrices, as long as the covariances of the different sources, at different time lags, are not proportional. Gutch et al. [5] have recently presented analogous conditions for the multidimensional case. In [5], the discussion is based on whitened second-order wide-sense stationary sources and the proofs of the theorems in [5, Sec. 1.3] are omitted. On the other hand, De Lathauwer [6] has proved that existence and uniqueness of JBD, up to trivial indeterminacies and for $Q > 2$ matrices, are guaranteed with probability one when the entries of the source covariance matrices are drawn from a continuous probability density function.

In this paper, we take a route different than that of [5]. Our analysis is based on multidimensional ICA of piecewise-stationary sources. We show in Sec. 2 that the maximum-likelihood solution, for Gaussian data and non-orthogonal mixing matrix (that is, avoiding any whitening constraints) can be obtained by minimizing a contrast function, which is a JBD criterion. Small-error analysis of this contrast function leads to the observation that identifiability of the model relies on the invertibility of a matrix \mathcal{H} which connects the relative gradient with the perturbations due to finite data. In [7, 8], a closed-form expression for the error covariance was derived, based on the assumption that \mathcal{H} was invertible. In [9], a quasi-Newton algorithm which minimizes the contrast function was proposed. The quasi-Newton step at each iteration is based on calculating the inverse of \mathcal{H} . However, the conditions on the data for \mathcal{H} to be invertible have not yet been discussed. In Sec. 3 the invertibility of matrix \mathcal{H} is studied, and the problem is simplified to determining when a matrix, which is a function of the source covariance matrices, is positive-definite. The derivation is concluded with a theorem, which states sufficient and necessary conditions for the identifiability of the model, in terms of the latent unnormalized, non-whitened, source covariance matrices. A short discussion of our results follows, in Sec. 4.

2. PROBLEM FORMULATION

The data model which motivates our analysis is as follows. Consider T observations of an $m \times 1$ vector $\mathbf{x}(t)$, modeled as a sum of $n \leq m$ components $\mathbf{x}(t) = \sum_{i=1}^n \mathbf{x}_i(t)$. It is assumed that the i th component $\mathbf{x}_i(t)$ (an $m \times 1$ vector) has an underlying structure of $\mathbf{x}_i(t) = \mathbf{A}_i \mathbf{s}_i(t)$, where \mathbf{A}_i , the i th column block of the $m \times m$ matrix \mathbf{A} , has dimension $m \times m_i$. Vector $\mathbf{s}_i(t)$ has dimension $m_i \times 1$ and $\sum_{i=1}^n m_i = m$, such that $\mathbf{A} = [\mathbf{A}_1, \dots, \mathbf{A}_n]$, $\mathbf{s}(t) = [\mathbf{s}_1^\dagger(t), \dots, \mathbf{s}_n^\dagger(t)]^\dagger$, and

$$\mathbf{x}(t) = \mathbf{A} \mathbf{s}(t) \quad 1 \leq t \leq T. \quad (1)$$

Let us consider a piecewise stationary model as follows. The observation interval $[1, T]$ is partitioned into Q domains \mathcal{D}_q , $q = 1, \dots, Q$, where domain q contains n_q samples, so that $\sum_{q=1}^Q n_q = T$. We assume that $\mathbf{s}(t)$ is independent of $\mathbf{s}(t')$

if $t \neq t'$ and that, for any $t \in \mathcal{D}_q$, $\mathbf{s}(t)$ has zero mean and covariance matrix $\mathbf{R}_S^{(q)}$. The linear model (1) implies that $\mathbf{R}_X^{(q)} = \mathbf{A}\mathbf{R}_S^{(q)}\mathbf{A}^\dagger$, where $\mathbf{R}_X^{(q)}$ is the covariance matrix of $\mathbf{x}(t)$ for $t \in \mathcal{D}_q$. The model of dependent sources corresponds to the block-diagonal structure

$$\mathbf{R}_S^{(q)} \triangleq \begin{bmatrix} \mathbf{R}_{S,11}^{(q)} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \ddots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{R}_{S,nn}^{(q)} \end{bmatrix}, \quad (2)$$

where $\mathbf{R}_{S,ii}^{(q)}$ is the $m_i \times m_i$ covariance matrix of $\mathbf{s}_i(t)$ for $t \in \mathcal{D}_q$. The set $\{\mathbf{R}_S^{(q)}\}_{q=1}^Q$ is such that it cannot be further jointly block diagonalized into smaller blocks. Hence, $\{\mathbf{R}_S^{(q)}\}_{q=1}^Q$ is *JBD-irreducible*. This notion of irreducibility is analogous to that proposed by [3, 10]. A formal definition of the finest JBD-irreducible structure can be found in [11, Theorem 1].

It is shown in [7, 8] that separation, up to the unavoidable scale and permutation indeterminacies, can be obtained by minimizing the contrast function

$$C(\mathbf{A}) \triangleq \langle D(\mathbf{A}^{-1}\overline{\mathbf{R}}_X\mathbf{A}^{-\dagger}, \text{bdiag}_m\{\mathbf{A}^{-1}\overline{\mathbf{R}}_X\mathbf{A}^{-\dagger}\}) \rangle, \quad (3)$$

where $D(\cdot, \cdot)$ denotes the Kullback-Leibler [12] divergence between any two $m \times m$ positive-definite matrices. $\langle \cdot \rangle$ denotes a weighted average of any sequence indexed by q with weights n_q , $\langle \mathbf{M} \rangle = \frac{1}{T} \sum_{q=1}^Q n_q \mathbf{M}^{(q)}$. $\overline{\mathbf{R}}_X^{(q)} \triangleq \frac{1}{n_q} \sum_{t \in \mathcal{D}_q} \mathbf{x}(t)\mathbf{x}^\dagger(t)$ denotes the empirical counterpart and natural estimate of $\mathbf{R}_X^{(q)}$, and $\text{bdiag}_m\{\mathbf{M}\}$ returns the block-diagonal matrix with block pattern $\mathbf{m} \triangleq [m_1, \dots, m_n]^\dagger$ which has the same diagonal blocks as \mathbf{M} and has zeros in the off-diagonal blocks. Therefore, $\min_{\mathbf{A}} C(\mathbf{A})$ can be understood as *joint block diagonalization* (JBD) of the set of covariance matrices $\{\mathbf{R}_X^{(q)}\}_{q=1}^Q$ by matrix \mathbf{A}^{-1} . We denote the minimizer of (3) as $\hat{\mathbf{A}}$. If $\mathbf{s}(t)$ is normally distributed, then the solution of (3) yields the ML estimate of \mathbf{A} [7, 8].

The first step in studying the performance of component separation using (3) is defining suitable error terms. The estimation error in the i th component can be written as [7, 8]

$$\hat{\mathbf{x}}_i(t) - \mathbf{x}_i(t) = - \sum_{j \neq i}^n \mathcal{E}_{ji} \mathbf{x}_i(t) + \sum_{j \neq i}^n \mathcal{E}_{ij} \mathbf{x}_j(t), \quad (4)$$

where the $m \times m$ matrices \mathcal{E}_{ij} , \mathcal{E}_{ji} represent the pairwise error terms between component i and j . The component estimates are obtained from $\hat{\mathbf{x}}_i(t) = \hat{\mathbf{P}}_i \mathbf{x}(t)$, where \mathbf{P}_i are the $m \times m$ oblique projection matrices onto $\text{Span}(\mathbf{A}_i)$ along $\text{Span}(\mathbf{A}_j)$ for all $j \neq i$, and $\hat{\mathbf{P}}_i$ are their estimates, with \mathbf{A}_i replaced with $\hat{\mathbf{A}}_i$, etc. Similarly, we define $\mathbf{\Pi}_i = \mathbf{A}_i \mathbf{A}_i^\sharp$, the orthogonal projection onto $\text{Span}(\mathbf{A}_i)$, where \mathbf{A}_i^\sharp denotes the Moore-Penrose pseudo-inverse (22) of \mathbf{A}_i . Then,

$\mathcal{E}_{ij} = (\hat{\mathbf{P}}_i - \mathbf{P}_i)\mathbf{\Pi}_j$ [7, 8]. The added value of working with projections instead of the mixing matrix is that the projection matrices do not suffer from the scale ambiguity and thus also \mathcal{E}_{ij} are well-defined, in this sense. It can be shown [7, 8] that in the small-errors regime, these errors can be expressed as a function of the $m \times m$ model cross-covariance matrices $\mathbf{R}_{X_i X_j}^{(q)}$ and their finite-sample counterparts $\overline{\mathbf{R}}_{X_i X_j}^{(q)} \triangleq \frac{1}{n_q} \sum_{t \in \mathcal{D}_q} \mathbf{x}_i(t)\mathbf{x}_j^\dagger(t)$, as follows:

$$\begin{bmatrix} \mathbf{g}_{ij} \\ \mathbf{g}_{ji} \end{bmatrix} = -\mathcal{H} \cdot \begin{bmatrix} \text{vec}\{\mathcal{E}_{ij}\} \\ \text{vec}\{\mathcal{E}_{ji}\} \end{bmatrix} + \text{higher-order terms}, \quad (5)$$

where $\mathbf{g}_{ij} = \langle \text{vec}\{\mathbf{R}_{X_i X_i}^\sharp \overline{\mathbf{R}}_{X_i X_j}\} \rangle$ is the vectorized (i, j) th block of the relative gradient of $C(\mathbf{A})$ [7, 8];

$$\mathcal{H} = \begin{bmatrix} \mathbf{H}_{ij} & \mathcal{T}_{m,m} \\ \mathcal{T}_{m,m} & \mathbf{H}_{ji} \end{bmatrix} \quad (6)$$

is a symmetric matrix with

$$\mathbf{H}_{ij} = \langle \mathbf{R}_{X_j X_j} \otimes \mathbf{R}_{X_i X_i}^\sharp \rangle, \quad (7)$$

and $\mathcal{T}_{m,m}$ is the commutation matrix [13], see Appendix A. The $\text{vec}\{\cdot\}$ operator stacks the columns of a $p \times q$ matrix into a $pq \times 1$ vector. \otimes denotes the Kronecker product [14]. As can be seen from (5), for the parameter estimates to be consistent, that is, for the covariance of the errors \mathcal{E}_{ij} to decrease as the cross-correlation between components $\overline{\mathbf{R}}_{X_i X_j}^{(q)}$ approaches zero, matrix \mathcal{H} must be full-rank. This observation can be rephrased as the requirement for the identifiability of the parametric model. Since the solution of (5) is related to JBD (3), the invertibility of \mathcal{H} is also related to the existence of a unique solution to the JBD. A counter-example is given in Sec. 4.

3. INVERTIBILITY OF \mathcal{H}

As a first stage in the analysis of \mathcal{H} , we state that the inverse of \mathcal{H} , when exists, is given by

$$\mathcal{H}^{-1} = \mathcal{H}_{\Pi}^\sharp + \mathcal{H} - \mathcal{H}_{\Pi}, \quad (8)$$

where

$$\mathcal{H}_{\Pi} = \begin{bmatrix} \mathbf{H}_{ij} & \mathcal{T}_{m,m}^{\Pi_{ij}} \\ \mathcal{T}_{m,m}^{\Pi_{ji}} & \mathbf{H}_{ji} \end{bmatrix}, \quad (9)$$

and

$$\mathcal{T}_{m,m}^{\Pi_{ij}} \triangleq (\mathbf{\Pi}_j \otimes \mathbf{\Pi}_i) \mathcal{T}_{m,m} (\mathbf{\Pi}_i \otimes \mathbf{\Pi}_j). \quad (10)$$

It is important at this point to mention that in [7, 8] it is shown that $\text{Cov}\left(\begin{bmatrix} \mathbf{g}_{ij} \\ \mathbf{g}_{ji} \end{bmatrix}\right) = \frac{1}{T} \mathcal{H}_{\Pi}$ and asymptotically, that is, $T \rightarrow \infty$ with $\frac{n_q}{T}$ fixed $\forall q$, $\text{Cov}\left(\begin{bmatrix} \text{vec}\{\mathcal{E}_{ij}\} \\ \text{vec}\{\mathcal{E}_{ji}\} \end{bmatrix}\right) = \frac{1}{T} \mathcal{H}_{\Pi}^\sharp$. That is, if a solution to (5) exists, then \mathcal{H}_{Π} and \mathcal{H}_{Π}^\sharp are covariance matrices of rank $2m_i m_j$. This rank is due to the fact

that \mathbf{g}_{ij} and \mathbf{E}_{ij} each reflect a correlation between an m_i -dimensional element and an m_j -dimensional one. Therefore, the problem of finding the condition for the invertibility of \mathcal{H} can be rephrased as finding the condition for \mathcal{H}_Π and \mathcal{H}_Π^\sharp to be positive-semidefinite symmetric with rank $2m_i m_j$.

In order to further simplify our task, we now break down \mathcal{H}_Π and \mathcal{H}_Π^\sharp into more basic components. With some algebra, \mathcal{H}_Π can be rewritten as

$$\mathcal{H}_\Pi = \mathcal{I} \mathcal{A} \mathcal{R} \mathcal{A}^\dagger \mathcal{I}, \quad (11)$$

where $\mathcal{I} = \begin{bmatrix} \mathbf{I}_{m^2 \times m^2} & \mathbf{0}_{m^2 \times m^2} \\ \mathbf{0}_{m^2 \times m^2} & \mathcal{T}_{m,m} \end{bmatrix}$ is always invertible, $\mathcal{A} = \begin{bmatrix} \mathbf{A}_j \otimes \mathbf{A}_i^\dagger & \mathbf{0}_{m^2 \times m_i m_j} \\ \mathbf{0}_{m^2 \times m_i m_j} & \mathbf{A}_j^\dagger \otimes \mathbf{A}_i \end{bmatrix}$ is rank-deficient $\forall n > 1$, and

$$\mathcal{R} = \begin{bmatrix} \langle \mathbf{R}_{S,jj} \otimes \mathbf{R}_{S,ii}^{-1} \rangle & \mathbf{I}_{m_i m_j \times m_i m_j} \\ \mathbf{I}_{m_i m_j \times m_i m_j} & \langle \mathbf{R}_{S,jj}^{-1} \otimes \mathbf{R}_{S,ii} \rangle \end{bmatrix}$$

is a $2m_i m_j \times 2m_i m_j$ symmetric matrix. If \mathcal{R} is invertible, that is, \mathcal{R} has rank- $2m_i m_j$, then

$$\mathcal{H}_\Pi^\sharp = \mathcal{I} \mathcal{A}^\dagger \mathcal{R}^{-1} \mathcal{A} \mathcal{I}^\dagger. \quad (12)$$

Notation (12) can be verified by checking the four properties of the pseudoinverse (22). We have thus reduced the conditions on \mathcal{H}_Π or \mathcal{H}_Π^\sharp to the requirement that \mathcal{R} be positive-definite and symmetric. The conditions for \mathcal{R} to be strictly positive-definite and symmetric are given by the following theorem, whose proof is given in Appendix B.

Theorem 1. Given $\{\mathbf{R}_{S,ii}^{(q)}\}_{q=1}^Q$ and $\{\mathbf{R}_{S,jj}^{(q)}\}_{q=1}^Q$, $Q > 2$, two JBD-irreducible sequences of positive-definite symmetric matrices, then $\begin{bmatrix} \langle \mathbf{R}_{S,jj} \otimes \mathbf{R}_{S,ii}^{-1} \rangle & \mathbf{I} \\ \mathbf{I} & \langle \mathbf{R}_{S,jj}^{-1} \otimes \mathbf{R}_{S,ii} \rangle \end{bmatrix}$ is positive-definite if

1. $m_i \neq m_j$, or
2. $m_i = m_j$ and there does not exist an $m_i \times m_i$ invertible matrix \mathbf{M} such that $\forall q$,

$$\mathbf{R}_{S,jj}^{(q)} = \mathbf{M} \mathbf{R}_{S,ii}^{(q)} \mathbf{M}^\dagger. \quad (13)$$

Note that Theorem 1 is applicable for any normalization of $\mathbf{R}_{S,jj}^{(q)}$, regardless of the arbitrary block-diagonal scale ambiguity between \mathbf{A} and $\mathbf{s}(t)$. We have thus obtained all the necessary and sufficient conditions for \mathcal{R} to be positive-definite and symmetric, and thus also for \mathcal{H}_Π^\sharp and \mathcal{H}^{-1} to have the required rank.

It remains now to prove (8). The proof is based on showing that the term which we denote “ \mathcal{H}^{-1} ” indeed obeys $\mathcal{H}^{-1} \mathcal{H} = \mathbf{I} = \mathcal{H} \mathcal{H}^{-1}$. Given (8),

$$\begin{aligned} \mathcal{H}^{-1} \mathcal{H} &= (\mathcal{H}_\Pi^\sharp + \mathcal{J})(\mathcal{H}_\Pi + \mathcal{J}) \\ &= \mathcal{H}_\Pi^\sharp \mathcal{H}_\Pi + \mathcal{H}_\Pi^\sharp \mathcal{J} + \mathcal{J} \mathcal{H}_\Pi + \mathcal{J} \mathcal{J} \end{aligned} \quad (14)$$

$$\begin{aligned} \mathcal{H} \mathcal{H}^{-1} &= (\mathcal{H}_\Pi + \mathcal{J})(\mathcal{H}_\Pi^\sharp + \mathcal{J}) \\ &= \mathcal{H}_\Pi \mathcal{H}_\Pi^\sharp + \mathcal{J} \mathcal{H}_\Pi^\sharp + \mathcal{H}_\Pi \mathcal{J} + \mathcal{J} \mathcal{J}, \end{aligned} \quad (15)$$

where $\mathcal{J} \triangleq \mathcal{H} - \mathcal{H}_\Pi$. From (6), (9) and (10),

$$\mathcal{J} = \begin{bmatrix} \mathbf{0}_{m^2 \times m^2} & \mathcal{T}_{m,m} (\mathbf{I} - \mathbf{\Pi}_i \otimes \mathbf{\Pi}_j) \\ \mathcal{T}_{m,m} (\mathbf{I} - \mathbf{\Pi}_j \otimes \mathbf{\Pi}_i) & \mathbf{0}_{m^2 \times m^2} \end{bmatrix}.$$

For the fourth term in (14) and (15),

$$\mathcal{J} \mathcal{J} = \begin{bmatrix} \mathbf{I} - \mathbf{\Pi}_j \otimes \mathbf{\Pi}_i & \mathbf{0}_{m^2 \times m^2} \\ \mathbf{0}_{m^2 \times m^2} & \mathbf{I} - \mathbf{\Pi}_i \otimes \mathbf{\Pi}_j \end{bmatrix} \quad (16)$$

due to (20). For the first term on the RHS of (14) and (15), one can use the explicit forms (11) and (12) to obtain

$$\mathcal{H}_\Pi^\sharp \mathcal{H}_\Pi = \begin{bmatrix} \mathbf{\Pi}_j \otimes \mathbf{\Pi}_i & \mathbf{0}_{m^2 \times m^2} \\ \mathbf{0}_{m^2 \times m^2} & \mathbf{\Pi}_i \otimes \mathbf{\Pi}_j \end{bmatrix}, \quad (17)$$

and $\mathcal{H}_\Pi^\sharp \mathcal{H}_\Pi = \mathcal{H}_\Pi \mathcal{H}_\Pi^\sharp$ due to the symmetry of \mathcal{H}_Π . For the second and third terms on the RHS of (14) and (15), combining (11) or (12) with the symmetry of \mathcal{J} yields

$$\mathcal{J} \mathcal{H}_\Pi = \mathcal{H}_\Pi \mathcal{J} = \mathcal{J} \mathcal{H}_\Pi^\sharp = \mathcal{H}_\Pi^\sharp \mathcal{J} = \mathbf{0}_{2m^2 \times 2m^2}. \quad (18)$$

Substituting (17), (18) and (16) in (14) and (15) yields $\mathcal{H} \mathcal{H}^{-1} = \mathbf{I} = \mathcal{H}^{-1} \mathcal{H}$. This confirms the desired identity (8) and thus the invertibility of \mathcal{H} . Note that the derivation of (17) and (18) has relied on the fact that the decomposition (12) exists; that is, on the assumption that \mathcal{R} is invertible. Hence, the invertibility of \mathcal{H} follows from Theorem 1.

4. DISCUSSION

In the above, we have obtained necessary and sufficient conditions for the identifiability of the MICA model of Sec. 2. Our analysis was based on the observation that the consistency of errors between the model parameters and their corresponding estimates (i.e., solutions of (3)) depends on the invertibility of the 2-by-2 symmetric block matrix¹ \mathcal{H} . Strictly speaking, since these conditions are based on small-error analysis, they imply *local* identifiability.

As a counter example, let us consider the case that Theorem 1 does not hold. Namely, that $\mathbf{R}_{S,jj}^{(q)} = \mathbf{M} \mathbf{R}_{S,ii}^{(q)} \mathbf{M}^\dagger \forall q$. Given two statistically independent components of the same dimension, such that $i = 1, j = 2$, let us define two new vectors $\mathbf{y}_1(t) = \frac{1}{\sqrt{2}}(\mathbf{s}_1(t) - \mathbf{M}^{-1} \mathbf{s}_2(t))$ and $\mathbf{y}_2(t) = \frac{1}{\sqrt{2}}(\mathbf{s}_1(t) + \mathbf{M}^{-1} \mathbf{s}_2(t))$, and $\mathbf{y}(t) = [\mathbf{y}_1(t); \mathbf{y}_2(t)]$. Then, $\mathbf{R}_Y^{(q)} = \begin{bmatrix} \mathbf{R}_{S,11}^{(q)} & \mathbf{0} \\ \mathbf{0} & \mathbf{R}_{S,11}^{(q)} \end{bmatrix} \forall q$. In other words, one can obtain exact JBD of the set of covariance matrices of these components without actually statistically separating them. In this case, the errors terms \mathbf{E}_{ij} and their covariances may be arbitrarily large, regardless of how close $\overline{\mathbf{R}}_{X_i X_j}^{(q)}$ are to their (zero) mean.

¹The analogous matrix in [7, Eq. (22)] is equal to (9) up to right- and left-multiplication by the invertible matrix $\begin{bmatrix} \mathbf{0}_{m^2 \times m^2} & \mathbf{I}_{m^2 \times m^2} \\ \mathcal{T}_{m,m} & \mathbf{0}_{m^2 \times m^2} \end{bmatrix}$. The current notation is compatible with [8].

The derived Theorem 1 is similar to that given in [5] and to the claim in [15, Sec. 2.2], without the whitening and orthonormality constraints.

Theorem 1 is analogous to the notion of ‘‘simplicity’’, as proposed by [5]. As argued in [5], all the statistically independent sources for which (13) holds with equality should be gathered into one ‘simple’ factor, and the decomposition of s into such ‘simple’ factors is unique, up to an arbitrary invertible mixture within each such factor. However, unlike [5], we obtain Theorem 1 as a by-product of our performance analysis, and without any orthogonality prerequisite on the mixing or de-mixing matrix. We also provide a full proof of the Theorem.

It should be noted that Theorem 1 reduces, in the one-dimensional case, to the condition that the covariance matrices of the different sources, as a function of the domain index, should not be proportional [4].

A. KRONECKER PRODUCT, VEC AND PSEUDOINVERSE PROPERTIES

For ease of reference, we list some useful algebraic properties. These properties can be found in [13] and [14]. The $mn \times mn$ commutation matrix $\mathcal{T}_{m,n}$ [13] is such that

$$\text{vec}\{M^\dagger\} = \mathcal{T}_{m,n} \text{vec}\{M\} \quad (19)$$

for any $m \times n$ matrix M . The commutation matrix is isometric and satisfies $\mathcal{T}_{n,m} \mathcal{T}_{m,n} = I$. Hence, $\mathcal{T}_{n,m} = \mathcal{T}_{m,n}^{-1}$. One also has $\mathcal{T}_{n,m} = \mathcal{T}_{m,n}^\dagger$. For any two matrices $M_{m \times n}$ and $N_{p \times q}$,

$$N \otimes M = \mathcal{T}_{p,m} (M \otimes N) \mathcal{T}_{n,q} \quad (20)$$

and

$$\mathcal{T}_{m,p} (N \otimes M) = (M \otimes N) \mathcal{T}_{n,q}. \quad (21)$$

Definition A.1. The Moore-Penrose pseudoinverse of a matrix M is the matrix M^\sharp that obeys

$$MM^\sharp M = M, \quad MM^\sharp = (MM^\sharp)^\dagger \quad (22a)$$

$$M^\sharp MM^\sharp = M^\sharp, \quad M^\sharp M = (M^\sharp M)^\dagger. \quad (22b)$$

B. INVERTIBILITY OF \mathcal{H}_Ξ

Let $\Xi_i^{(q)}$ and $\Xi_j^{(q)}$, $q = 1, \dots, Q$ denote invertible symmetric matrices of dimensions $m_i \times m_i$ and $m_j \times m_j$, respectively, and

$$\mathcal{H}_\Xi = \begin{bmatrix} \langle \Xi_j \otimes \Xi_i^{-1} \rangle & I \\ I & \langle \Xi_j^{-1} \otimes \Xi_i \rangle \end{bmatrix}. \quad (23)$$

We look for sufficient and necessary conditions on the sequences $\{\Xi_i^{(q)}\}_{q=1}^Q$ and $\{\Xi_j^{(q)}\}_{q=1}^Q$ for the strict positivity: $\mathcal{H}_\Xi > 0$.

\mathcal{H}_Ξ is positive-definite if and only if $x^\dagger \mathcal{H}_\Xi x = 0$ for all non-zero vectors x with real entries. Since $n_q > 0$, the condition $x^\dagger \mathcal{H}_\Xi x = 0$ is equivalent to $x^\dagger \mathcal{H}_\Xi^{(q)} x = 0 \forall q$, where each

$$\mathcal{H}_\Xi^{(q)} \triangleq \begin{bmatrix} \Xi_j^{(q)} \otimes \Xi_i^{-1(q)} & I \\ I & \Xi_j^{-1(q)} \otimes \Xi_i^{(q)} \end{bmatrix}$$

is *always* singular. Without loss of generality, we can look for x in the form

$$x = \begin{bmatrix} \text{vec}\{M\} \\ -\text{vec}\{N\} \end{bmatrix},$$

where M and N are $m_i \times m_j$ matrices. With the factorization

$$\mathcal{H}_\Xi^{(q)} = \begin{bmatrix} \Xi_j^{\frac{1}{2}(q)} \otimes \Xi_i^{-\frac{1}{2}(q)} \\ \Xi_j^{-\frac{1}{2}(q)} \otimes \Xi_i^{\frac{1}{2}(q)} \end{bmatrix} \begin{bmatrix} \text{vec}\{M\} \\ -\text{vec}\{N\} \end{bmatrix}^\dagger$$

we have

$$x^\dagger \mathcal{H}_\Xi^{(q)} x = \left\| \begin{bmatrix} \Xi_j^{\frac{1}{2}(q)} \otimes \Xi_i^{-\frac{1}{2}(q)} \\ \Xi_j^{-\frac{1}{2}(q)} \otimes \Xi_i^{\frac{1}{2}(q)} \end{bmatrix}^\dagger \begin{bmatrix} \text{vec}\{M\} \\ -\text{vec}\{N\} \end{bmatrix} \right\|^2$$

and therefore, the condition for positive-definiteness becomes

$$\begin{bmatrix} \Xi_j^{\frac{1}{2}(q)} \otimes \Xi_i^{-\frac{1}{2}(q)} & \Xi_j^{-\frac{1}{2}(q)} \otimes \Xi_i^{\frac{1}{2}(q)} \end{bmatrix} \begin{bmatrix} \text{vec}\{M\} \\ -\text{vec}\{N\} \end{bmatrix} = 0 \quad \forall q.$$

Using $\text{vec}\{MXN\} = (N^\dagger \otimes M) \text{vec}\{X\}$ [14] for any matrices M, N, X of compatible dimensions, the latter can be rewritten as

$$\Xi_i^{-\frac{1}{2}(q)} M \Xi_j^{\frac{1}{2}(q)} = \Xi_i^{\frac{1}{2}(q)} N \Xi_j^{-\frac{1}{2}(q)} \quad \forall q, \quad (24)$$

which is equivalent to

$$M \Xi_j^{(q)} = \Xi_i^{(q)} N \quad \forall q. \quad (25)$$

(25) can be simplified into $M' T_j^{(q)} = T_i^{(q)} M' \forall q$, where

$$T_i^{(q)} = \langle \Xi_i \rangle^{-\frac{1}{2}} \Xi_i^{(q)} \langle \Xi_i \rangle^{-\frac{1}{2}}, \quad (26)$$

and $M' = \langle \Xi_i \rangle^{-\frac{1}{2}} M \langle \Xi_j \rangle^{\frac{1}{2}}$ (analogously for index j) so that $\langle T_i \rangle = I$.

We now introduce a Lemma. This lemma and its proof can be found in Murota et al. [11, Lemma A.4].

Lemma 1. Let $\{R^{(q)}\}_{q=1}^Q$ and $\{P^{(q)}\}_{q=1}^Q$ be two sequences of $Q > 2$ positive-definite symmetric matrices of size $p \times p$ and $r \times r$, respectively. Assume that both sequences are JBD-irreducible. Then, the equation

$$MR^{(q)} = P^{(q)}M \quad \forall q \quad (27)$$

for a $p \times r$ matrix M has a non-zero solution only if $r = p$ and that solution must be proportional (i.e., up to a scalar factor) to a $p \times p$ orthonormal matrix.

By identifying $\mathbf{P}^{(q)}$ with $\mathbf{T}_i^{(q)}$ and $\mathbf{R}^{(q)}$ with $\mathbf{T}_j^{(q)}$, and applying Lemma 1, it turns out that for $m_i \neq m_j$, \mathcal{H}_{Ξ} is always positive-definite and symmetric. For $m_i = m_j$, \mathcal{H}_{Ξ} is not positive-definite if and only if there exists an orthonormal matrix \mathbf{O} such that

$$\mathbf{O}\mathbf{T}_j^{(q)} = \mathbf{T}_i^{(q)}\mathbf{O} \quad \forall q. \quad (28)$$

Eq. (28) defines an orthogonal equivalence relation between $\mathbf{T}_i^{(q)}$ and $\mathbf{T}_j^{(q)}$. By rewriting (28) explicitly we obtain

$$\mathbf{O}\langle\Xi_j\rangle^{-\frac{1}{2}}\Xi_j^{(q)}\langle\Xi_j\rangle^{-\frac{1}{2}} = \langle\Xi_i\rangle^{-\frac{1}{2}}\Xi_i^{(q)}\langle\Xi_i\rangle^{-\frac{1}{2}}\mathbf{O} \quad \forall q,$$

where $\langle\Xi_j\rangle^{-\frac{1}{2}}\Xi_j^{(q)}\langle\Xi_j\rangle^{-\frac{1}{2}}$ is the whitened version of $\Xi_j^{(q)}$, and similarly for $\Xi_i^{(q)}$. By changing sides, the latter equation can be rewritten as

$$\Xi_j^{(q)} = \langle\Xi_j\rangle^{\frac{1}{2}}\mathbf{O}^\dagger\langle\Xi_i\rangle^{-\frac{1}{2}}\Xi_i^{(q)}\langle\Xi_i\rangle^{-\frac{1}{2}}\mathbf{O}\langle\Xi_j\rangle^{\frac{1}{2}} \quad \forall q.$$

This is equivalent to normalizing $\Xi_i^{(q)}$ by $\langle\Xi_j\rangle^{\frac{1}{2}}\mathbf{O}^\dagger\langle\Xi_i\rangle^{-\frac{1}{2}}$. However, since $\langle\Xi_j\rangle$ and $\langle\Xi_i\rangle$ are in fact arbitrary symmetric positive-definite matrices, then $\langle\Xi_j\rangle^{\frac{1}{2}}\mathbf{O}^\dagger\langle\Xi_i\rangle^{-\frac{1}{2}}$ can be any invertible matrix. We summarize the results of this section in Theorem 1, which also replaces $\Xi_i^{(q)}$ and $\Xi_j^{(q)}$ with $\mathbf{R}_{S,ii}^{(q)}$ and $\mathbf{R}_{S,jj}^{(q)}$, respectively.

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