BLOCK JACOBI-TYPE METHODS FOR NON-ORTHOGONAL JOINT DIAGONALISATION

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ABSTRACT

In this paper, we study the problem of non-orthogonal joint diagonalisation of a set of real symmetric matrices via simultaneous conjugation. A family of block Jacobi-type methods are proposed to optimise two popular cost functions for the non-orthogonal joint diagonalisation, namely, the off-norm function and the log-likelihood function. By exploiting the appropriate underlying manifold, namely the so-called oblique manifold, rigorous analysis shows that, under the exact non-orthogonal joint diagonalisation setting, the proposed methods converge locally quadratically fast to a joint diagonaliser. Finally, performance of our methods is investigated by numerical experiments for both exact and approximate non-orthogonal joint diagonalisation.

Index Terms— Independent component analysis (ICA), non-orthogonal joint diagonalisation (NoJD), oblique manifold, block Jacobi-type method, local quadratic convergence.

1. INTRODUCTION

In recent years, joint diagonalisation of a set of matrices has attracted considerable attention in the areas of statistical signal processing and multivariate statistics. It has become a prominent tool for the problem of linear independent component analysis (ICA). In general, after a whitening process of the source signals, usually via principal component analysis (PCA), a linear ICA problem is expected to be solved by a joint diagonalisation of a set of matrices, which are derived from certain statistics of the whitened sources, with an orthogonality constraint on the diagonalising matrix [5]. Unfortunately, it has been shown in [4] that linear ICA performed by an orthogonal joint diagonalisation (OJD) might have a serious limitation of degraded performance, especially when additive noise is present. Furthermore, some diagonality criterion, namely the weighted least square (WLS) based criterion, might result in poor performance of joint diagonalisation, since this criterion is practically distorted by the whitening process [12].

To avoid the aforementioned limits of OJD, a natural relaxation of OJD, namely the non-orthogonal joint diagonalisation (NoJD), has been recently proposed and studied with increasing attention. Generally speaking, a criterion or measure of diagonality of a set of matrices can be constructed mainly in three different forms, specifically, off-norm formulation [7], log-likelihood formulation [8], and subspace fitting formulation [10]. Note that log-likelihood based criteria only apply to a set of positive definite matrices. Nowadays, various numerical algorithms for optimising these diagonality criteria have been developed in the community. To list a few, they include Newton-type methods [7], Gauss-Newton methods [10], Jacobi-type methods [8, 11], and so on. In this work, we focus on developing Jacobi-type NoJD methods.

Different to the more algebraic approaches taken in [8, 11], we treat Jacobi-type method as an optimisation approach on a smooth manifold. It is known that, by the construction of the so-called Exact NoJD and certain diagonality criteria, the oblique manifold is an appropriate setting for these scenarios [1, 3]. Recent work in [6] proposes a block Jacobi-type method on a smooth manifold, which has been applied successfully to the problem of independent subspace analysis (ISA) in [9]. The task of this paper is to develop block Jacobi-type NoJD methods from a geometric optimisation perspective, which optimise two particular NoJD cost functions, specifically the off-norm function and the log-likelihood function.

The paper is organised as follows. Section 2 provides a brief introduction to the NoJD problem and some basic concepts of the oblique manifold required in our derivation. In Section 3, we analyse the critical point set of two NoJD cost functions under the Exact NoJD setting. By exploiting the block diagonal structure of the Hessians at the joint diagonaliser, a family of block Jacobi-type NoJD methods is proposed. Meanwhile, local convergence properties of these methods are presented as well. Finally, in Section 4, performance of the proposed algorithms is investigated by numerical experiments for both the Exact NoJD and Approximate NoJD settings.

2. MATHEMATICAL PRELIMINARIES

Given a set of $m \times m$ real symmetric matrices $\{C_i\}_{i=1}^n$, constructed by

$$C_i = A_i A_i^\top, \quad i = 1, \ldots, n,$$  (1)

where $\Lambda_i = \text{diag}(\lambda_{i1}, \ldots, \lambda_{im}) \in \mathbb{R}^{m \times m}$ with $\lambda_{ij} \neq 0$ for $j = 1, \ldots, m$ and $A_i \in \mathbb{R}^{m \times m}$ non-singular. The problem of estimating the matrix $A_i$ given only the set $\{C_i\}_{i=1}^n$ is equivalent to finding a non-singular matrix $X \in \mathbb{R}^{m \times m}$ such that the set of matrices $\{Y_i\}_{i=1}^n$, computed by

$$Y_i = X^\top C_i X, \quad i = 1, \ldots, n,$$  (2)

are simultaneously diagonalised. We refer to this problem as the Exact NoJD problem. In a generic situation, a joint diagonaliser $X$ can only be determined up to column-wise permutation and scaling, i.e., if $X$ is a diagonaliser, so is any $XDP$ where $D$ is an $m \times m$ invertible diagonal matrix and $P$ an $m \times m$ permutation matrix. For any $j = 1, \ldots, m$, let us denote $\bar{X}_j = (\bar{x}_{ij})_{i=1}^m \in \mathbb{R}^m$. According to theorem 2.3 in [3], the Exact NoJD problem (2) has a unique joint diagonaliser, which refers to that column-wise permutation and scaling are the only indeterminacies in identifying the diagonaliser, if and only if any pair $(\bar{x}_j, \bar{x}_k)$ for $j \neq k$ are linearly independent.

To deal with the scaling ambiguity, the oblique manifold is shown to be an appropriate setting for Exact NoJD [3]. Note that

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in [1], \( \mathcal{OB}(m) \) is differently defined. We, however, think that for our application, the rank condition is indispensable. Let denote the \( m \times m \) oblique manifold by
\[
\mathcal{OB}(m) := \{ X \in \mathbb{R}^{m \times m} | \text{ddiag}(X^T X) = I_m, \text{rk} X = m \},
\]
where \( \text{ddiag}(Z) \) forms a diagonal matrix, whose diagonal entries are just those of \( Z \), and \( I_m \) is the \( m \times m \) identity matrix. Thus, we define the off-norm function [7], a NoJD cost function, as follows
\[
f_1 : \mathcal{OB}(m) \rightarrow \mathbb{R}, \quad X \mapsto \frac{1}{2} \sum_{i=1}^m \| \text{off}(X^T C_i X) \|^2_F, \tag{4}
\]
where \( \| Z \|_F \) is the Frobenius norm.

In the specific application of linear ICA, however, due to the presence of additive noise or estimation errors, exact joint diagonalisation is hardly possible to achieve. Thus in general, the task is eventually to find a matrix \( X \in \mathbb{R}^{m \times m} \) such that the matrices \( \{ Y_i \}_{i=1}^n \) under the construction (2) are jointly as diagonal as possible. We refer to this problem as the Approximate NoJD problem. It is important to notice that the off-norm function (4) is not column-wise scale invariant with respect to the matrix \( X \), except if \( X \) is an exact joint diagonaliser. So to overcome this limit, a log-likelihood based cost function is proposed, see [8],
\[
f_2 : \mathcal{OB}(m) \rightarrow \mathbb{R}, \quad X \mapsto \log \det \text{ddiag}(X^T C_i X) - \log \det (X^T C_i X). \tag{5}
\]
Although this function is in fact column-wise scale invariant, it unfortunately applies only to the scenario where the set of matrices to be jointly diagonalised are positive definite.

More recently, to avoid these drawbacks with the functions (4) and (5), a new subspace fitting based cost function is developed in [2]. Following our analysis in the next section, however, we can show that this cost function does not share the features, which we will derive for both the off-norm function and the log-likelihood function. In other words, the block Jacobi-type NoJD method developed in this work cannot be applied to it. Therefore, discussion and analysis on the subspace fitting function as in [2] are omitted.

Before we continue, let us review some basic concepts of \( \mathcal{OB}(m) \). It is known that \( \mathcal{OB}(m) \) is an \( m(m-1) \) dimensional smooth manifold. The tangent space of \( \mathcal{OB}(m) \) at \( X \in \mathcal{OB}(m) \) is defined by
\[
T_X \mathcal{OB}(m) = \{ H \in \mathbb{R}^{m \times m} | \text{ddiag}(X^T H) = 0 \}. \tag{6}
\]
Let denote the set of all \( m \times m \) matrices with all diagonal entries equal to zero by
\[
\text{off}(m) = \{ Z \in \mathbb{R}^{m \times m} | z_{ii} = 0, \text{ for } i = 1, \ldots, m \}. \tag{7}
\]

**Lemma 1** For every point \( X \in \mathcal{OB}(m) \), the following map \( \mu_X : \text{off}(m) \rightarrow \mathcal{OB}(m) \),
\[
Z \mapsto X(I_m + Z) \text{ddiag} \left( \frac{1}{|x_{11}^1 + \cdots + x_{m1}^m|}, \ldots, \frac{1}{|x_{1m}^1 + \cdots + x_{mm}^m|} \right), \tag{8}
\]
where \( Z = \{ z_1, \ldots, z_m \} \in \text{off}(m) \) and \( e_i \) is the \( i \)-th standard basis vector of \( \mathbb{R}^m \), is a smooth parameterisation around \( X \) with the following properties. For a given \( X = [x_1, \ldots, x_m] \in \mathcal{OB}(m) \) and \( \Theta = [\theta_1, \ldots, \theta_m] \in \text{off}(m) \),
\begin{itemize}
  \item[(i)] \( \mu_X(0) = X \), and
  \item[(ii)] \( H : = D \mu_X(0) (\Theta) \in T_X \mathcal{OB}(m) \), where
\end{itemize}
\[
H = [\Pi(x_1)X \theta_1, \ldots, \Pi(x_m)X \theta_m]. \tag{9}
\]
Here \( \Pi(x_i) := I_m - x_i x_i^T \) is the orthogonal projection operator onto the complement of \( \text{span}(x_i) \).

### 3. DERIVATION OF BLOCK JACOBI-TYPE METHODS FOR EXACT NOJD

All analysis and derivation in this section are undertaken under the Exact NoJD setting. In Section 3.1, we first provide critical point analysis of the functions (4) and (5). The Hessians of both functions at a joint diagonaliser are shown to be positive definite and have the nice structure of being block diagonal. This leads to a family of block Jacobi-type NoJD methods in Section 3.2.

#### 3.1. Analysis of Cost Functions for Exact NoJD

##### 3.1.1. The Off-norm Function

Taking the first derivative of \( f_1 \), evaluated at \( X \in \mathcal{OB}(m) \) in tangent direction \( H \in T_X \mathcal{OB}(m) \), we get
\[
D f_1(X) H = \sum_{i=1}^n \text{tr} \left( \text{off}(X^T C_i X) X^T C_i H \right). \tag{10}
\]
Let \( X^* \in \mathcal{OB}(m) \) be a joint diagonaliser, obviously
\[
D f_1(X^*) H = 0, \tag{11}
\]
i.e., any diagonaliser of the Exact NoJD problem (2) is a critical point of \( f_1 \). We now calculate the Hessian of \( f_1 \) at such an \( X^* \), i.e., the symmetric bilinear form \( H_{f_1}(X^*) : T_X \mathcal{OB}(m) \times T_X \mathcal{OB}(m) \rightarrow \mathbb{R} \). Using Lemma 1, we get
\[
H_{f_1}(X^*)(H, H) = \frac{1}{m} \text{tr} (f_1 \circ \mu_X \circ (\Theta))|_{\Theta = 0}
= \sum_{i=1}^n \text{tr} \left( \left( \text{off}(X^T C_i H) + \text{off}(H^T C_i X^*) \right) X^T C_i H \right). \tag{12}
\]
By the construction of Exact NoJD (1), we know \( X^* = A^{-T} \Delta \in \mathcal{OB}(m) \) a joint diagonaliser. Here \( \Delta = \text{diag} \{ \delta_1, \ldots, \delta_m \} \in \mathbb{R}^{m \times m} \) normalises each column of \( A^{-T} \). It is then equivalent to \( A = (X^*)^{-T} \Delta \). Thus, we can compute
\[
X^T C_i H = X^T C_i X^* = \Delta \Lambda_i \Delta (X^*)^{-1} H = \Delta \Lambda_i (X^*)^{-1} H. \tag{13}
\]
Let us denote \( D_i = \text{diag} \{ d_{i1}, \ldots, d_{im} \} = \Delta \Lambda_i \Delta_i, \text{ i.e. } d_{ij} = \delta_{ij}^2 \lambda_{ij} \). By recalling Eq (9), a direct computation gives
\[
H_{f_1}(X^*)(H, H) = \sum_{1 \leq j \leq k \leq m} (d_{ij} \delta_{jk} + d_{ik} \delta_{kj})^2
= \sum_{1 \leq j \leq k \leq m} \left[ \frac{\theta_{jk}}{\theta_{kj}} \right] \left[ \frac{\theta_{jk}}{\theta_{kj}} \right]^T = \frac{\theta_{jk}}{\theta_{kj}}. \tag{14}
\]
Clearly, the Hessian of \( f_1 \) at a joint diagonaliser \( X^* \) is at least positive semi-definite, and diagonal, in terms of \( 2 \times 2 \) blocks, with respect to the standard basis of the parameter space \( \mathbb{R}^{m \times (m-1)} \). Then, the definiteness of the Hessian depends on the determinant of \( B_1^{jk} \)'s, which is computed by
\[
det(B_1^{jk}) = \left( \sum_{i=1}^n d_{ij}^2 \right) \left( \sum_{i=1}^n d_{ik}^2 \right) - \left( \sum_{i=1}^n d_{ij} d_{ik} \right)^2.
= \delta_{ij}^2 (\sum_{i=1}^n \lambda_{ij}^2) \left( \sum_{i=1}^n \lambda_{ik}^2 \right) - \left( \sum_{i=1}^n \lambda_{ij} \lambda_{ik} \right)^2. \tag{15}
\]
By the Cauchy-Schwarz inequality, it can be shown that \( \det(B_{jk}^{ik}) \) is certainly non-negative, and equal to zero if and only if \( \lambdalj = (\lambdaij)_{i=1}^n \) in \( \mathbb{R}^2 \) and \( \lambdaj^k \) are linearly dependent. Thus, by recalling the uniqueness condition of solutions of Exact NoJD, i.e. theorem 2.3 in [3], we conclude

**Lemma 2** Let the Exact NoJD problem (2) have a unique joint diagonaliser. Then the Hessian of the off-norm function (4) at the joint diagonaliser is positive definite.

### 3.1.2. The Log-likelihood Function

Now we briefly apply a similar analysis to the log-likelihood function \( f_2 \) (5). Note that, we now assume that the set of matrices \( \{C_i\}_{i=1}^n \) are all positive definite, i.e. \( \lambdaij > 0 \) for all \( i = 1, \ldots , n \) and \( j = 1, \ldots , m \).

The first derivative of \( f_2 \) is computed by

\[
Df_2(X) = \nabla \left( \text{log} \prod_{i=1}^n \text{det}(X_i^T X_i) \right).
\]

It can be shown that a joint diagonaliser \( X^* \in \mathbb{O}(m) \) of the Exact NoJD (2) is a critical point of \( f_2 \), i.e., \( Df_2(X^*) = 0 \). Similarly, the Hessian of \( f_2 \) at \( X^* \), i.e. the symmetric bilinear form \( Hf_2(X^*) \), is given by

\[
Hf_2(X^*) = \frac{d^2 f_2}{d\mu_{X^*}} \bigg|_{\mu_{X^*}}.
\]

Using that \( d_{ijk} = \lambda_{jk} i^2 \), we compute

\[
\det(B_{jk}^{ik}) = \left( \sum_{i=1}^n d_{ijk} \right)^2 - n^2 = \left( \sum_{i=1}^n \lambda_{ijk} \right)^2 - n^2. \tag{19}
\]

By Chebyshev’s sum inequality, the determinant \( \det(B_{jk}^{ik}) \) is non-negative, and equal to zero if and only if \( \lambda_{lij} \) and \( \lambda_{lj^k} \) are linearly dependent. Thus we conclude

**Lemma 3** Let the set of matrices \( \{C_i\}_{i=1}^n \), constructed by (1) be all positive definite, and the Exact NoJD problem (2) have a unique joint diagonaliser. Then the Hessian of the log-likelihood function (5) at the joint diagonaliser is positive definite.

It is important to notice that, the Hessian of the log-likelihood function \( f_2 \) at a joint diagonaliser shares the same block diagonal structure as the Hessian of the off-norm function \( f_1 \).

### 3.2. Block Jacobi-type Exact NoJD Algorithm

In this subsection, we develop a family of block Jacobi-type methods, which optimise the functions \( f_1 \) and \( f_2 \), by using the block diagonal structure of the Hessians at a joint diagonaliser shared by both functions.

A block Jacobi-type method consists of an iterative application of so-called grouped variable sweep operations. Let \( \Theta_{jk} = \{(\theta_{jk})_{i=1}^n \in \text{off}(m) \) be a zero matrix except for the \( jk \)-th entry, and denote \( \bar{\Theta} = \{(\theta_{jk})_{i=1}^n \in \mathbb{R}^2 \). For any point \( X \in \mathbb{O}(m) \), we construct a family of maps \( \nu_{jk}^{(X)} \)

\[
\nu_{jk}^{(X)} : \mathbb{R}^2 \rightarrow \mathbb{O}(m), \quad \bar{\Theta} \mapsto \mu_X (\Theta_{jk}). \tag{20}
\]

Then, a block Jacobi-type method for optimising the functions \( f_1 \) and \( f_2 \) is described as

**Algorithm 1** Block Jacobi-type NoJD Method

1. **Step 1:** Given an initial guess \( X_0 \in \mathbb{O}(m) \) and set \( s = 0 \).
2. **Step 2:** Set \( s = s + 1 \) and let \( X_s = X_{s-1} \).
   - **For** \( 1 \leq j < k \leq m \), update
     
     \[
     X_s \leftarrow \nu_{jk}^{(X_s)} (\bar{\Theta}),
     \]
     
     where
     
     \[
     \Theta = \{ \arg \min_{\bar{\Theta} \in \mathbb{R}^2} f_1(\Theta) \} \oplus f_2(\Theta).
     \]
     
   - **otherwise**, go to Step 2.

**Theorem 1** Let the Exact NoJD problem (2) have a unique joint diagonaliser. Then the block Jacobi-type method, Algorithm 1, converges locally quadratically fast to the joint diagonaliser.

Let us look at Algorithm 1 a bit closer. Within a sweep (Step 2) with \( X_s = [x_{s1}^T, \ldots , x_{sn}^T] \in \mathbb{O}(m) \), the \( (j,k) \)-th iteration solves essentially a NoJD problem of the set of 2 \( \times \) 2 symmetric matrices \( \{B_{jk}^{ij}\}_{i=1}^n \), constructed by

\[
B_{jk}^{ij} = \begin{bmatrix}
\theta_{jk}^{(i)} & b_{jk}^{(i)} \\
b_{jk}^{(i)} & b_{jk}^{(i)}
\end{bmatrix} \in \mathbb{R}^2,
\]

where \( b_{jk}^{(i)} = x_{ij}^{(s)} C_i x_{jk}^{(s)} \).

It has been shown in [11] that, under the Exact NoJD setting, a joint diagonaliser of such a subproblem (21) can be obtained in closed-form. In other words, the so-called DNJD algorithm in [11] is a special case of Algorithm 1. Therefore, the local convergence property of the DNJD follows directly from Theorem 1. Nevertheless, in general, the \( (j,k) \)-th iteration minimises the following functions, either

\[
f_1 \circ \nu_{jk}^{(X)} : \mathbb{R}^2 \rightarrow \mathbb{R}, \quad \bar{\Theta} \mapsto \sum_{i=1}^n \frac{(b_{jk}^{(i)} + b_{jk}^{(i)} \theta_{jk} + b_{jk}^{(i)} \theta_{jk} + b_{jk}^{(i)} \theta_{jk})^2}{\|x_{ij} + \theta_{jk} x_{jk}\|}, \tag{22}
\]

or

\[
f_2 \circ \nu_{jk}^{(X)} : \mathbb{R}^2 \rightarrow \mathbb{R}, \quad \bar{\Theta} \mapsto \sum_{i=1}^n \log(b_{jk}^{(i)} + 2b_{jk}^{(i)} \theta_{jk} + b_{jk}^{(i)} \theta_{jk}^2) + \log(b_{jk}^{(i)} \theta_{jk}^2 + 2\theta_{jk}^{(i)} \theta_{jk} + b_{jk}^{(i)} - \log(1 - \theta_{jk} \theta_{jk}^2)) \tag{23}
\]
4. NUMERICAL EXPERIMENTS

It is well known that performance of block Jacobi-type methods significantly depends on the techniques to solve the subproblems, e.g. in our case, minimising either (22) or (23). In this section, we will demonstrate local convergence properties of two concrete Jacobi-type NoJD methods under both the Exact and Approximate NoJD settings.

For the off-norm function based methods, i.e. minimising the function (22), although the DNJD algorithm in [11], which occupies a closed-form update derived under the Exact NoJD setting, has demonstrated its effectiveness even for Approximate NoJD by numerical evidence. There is however no theory to guarantee its convergence. In our experiment, we utilise a Gauss-Newton method to minimise (22). In the following, we refer to the resulting Jacobi-type method as Gauss-Newton-Jacobi NoJD method.

For the log-likelihood function based methods, it seems almost impossible to derive a closed-form solution for minimising (23), even under the Exact NoJD setting. Nevertheless, an efficient algorithm, developed in a Jacobi-style by Pham [8], minimises the upper bound of (23) instead, whose minimum point can be found in closed-form, and appears to coincide with the minimum point of (23) under the Exact NoJD setting. In our experiment, we adapt Pham’s algorithm on the oblique manifold.

The task of our experiment is to jointly diagonalise a set of symmetric matrices \( \{ C_i \}_{i=1}^n \), constructed by

\[
C_i = A \Lambda_i A^\top + \epsilon E_i, \quad i = 1, \ldots, n,
\]

where \( A \in \mathbb{R}^{m \times m} \) is a randomly picked matrix in \( OB(m) \), diagonal entries of \( \Lambda_i \) are drawn from a uniform distribution on the interval \((0, 11)\), \( E_i \in \mathbb{R}^{m \times m} \) is the symmetric part of an \( m \times m \) matrix, whose entries are generated from a uniform distribution on the unit interval \((-0.5, 0.5)\), representing additive noise, and \( \epsilon \in \mathbb{R} \) is the noise level. We set \( m = n = 20 \), and run six tests, for both the Gauss-Newton-Jacobi algorithm and Pham’s algorithm, in accordance with increasing noise, by using \( \epsilon = t \times 10^{-s} \) where \( t = 0, \ldots, 5 \).

The convergence of algorithms is measured by the distance of the accumulation point \( X^* \in OB(m) \) to the current iterate \( X_k \in OB(m) \), i.e., \( \| X_k - X^* \|_F \). According to Fig. 1 and 2, it is clear that both algorithms converge locally quadratically fast to a joint diagonaliser under the Exact NoJD setting, i.e., \( \epsilon = 0 \). Although Pham’s algorithm was claimed in [8] to converge locally quadratically fast to a joint diagonaliser under the Approximate NoJD setting, such a property indeed holds no longer for both algorithms with the presence of noise. They appear to converge only linearly fast.

5. REFERENCES


