Intrinsic Newton's Method on Oblique Manifolds for Overdetermined Blind Source Separation

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Abstract— **This paper studies the problem of Overdetermined Blind Source Separation (OdBSS), a challenging problem in signal processing. It aims to recover desired sources from outnumbered observations without knowing either the source distributions or the mixing process. It is well-known that performance of standard BSS algorithms, which usually utilize a whitening step as a pre-process to reduce the dimensionality of observations, might be seriously limited due to its blind trust on the data covariance matrix. In this paper, we develop efficient OdBSS algorithms without dimensionality reduction. In particular, our algorithms solve a problem of simultaneous diagonalization of a set of symmetric matrices. By exploiting the appropriate underlying manifold, namely the so-called oblique manifold, intrinsic Newton's method is developed to optimize two popular cost functions for the simultaneous diagonalization of symmetric matrices, i.e., the off-norm function and the log-likelihood function. Performance of the proposed algorithms is investigated by several numerical experiments.**

I. INTRODUCTION

Linear Blind Source Separation (BSS) addresses the problem of recovering linearly mixed sources from only several observed mixtures without knowing either the source distributions or the mixing process. A popular assumption of the sources being *mutually statistically independent* leads to the concept of linear Independent Component Analysis (ICA), which has become a prominant statistical method for solving the linear BSS problem. A common linear BSS model, usually refered to as the *determined linear BSS model*, assumes that the number of sources is equal to the number of observations. In this work, we are interested in the problem of extracting a fewer number of signals from a number of observations, i.e. the problem of overdetermined linear ICA. Its applications can be found in image analysis and biomedical data analysis.

A widely-used linear ICA procedure consists of two steps [1]: (i) the observations are firstly whitened, usually by Principal Component Analysis (PCA), and (ii) a number of desired signals are extracted from the whitened observations according to mutual statistical independence. Step (i) reduces complexity of step (ii) and meanwhile copes with uniqueness of source extraction [2]. Such a procedure results in the so-called whitened linear ICA problem. It is well-known [3] that, in real applications, i.e. problems with only a finite number of samples, performance of linear ICA methods with whitening is limited due to statistical inefficiency. Recent work in [4] shows that the so-called *oblique manifold* is the suitable setting for doing non-whitened linear ICA.

A popular category of ICA algorithms involve a joint diagonalization of a set of matrices, which are derived from certain statistics of the observations [2], [5]. Recently, several efficient simultaneous diagonalization based ICA algorithms have been developed in [6], [7], for the determined linear ICA problem, i.e. extracting all sources. Unfortunately, these works do not handle the current overdetermined situation. Moreover, we are aware of gradient descent algorithms on the non-compact Stiefel manifold for non-whitened overdetermined linear ICA without considering convergence properties of the proposed algorithms [8], [9]. In this work, we develop an intrinsic Newton's method for solving the OdBSS problem on an appropriate oblique manifold.

This paper is organized as follows. In Section II, we briefly introduce the overdetermined blind source separation problem. Section III presents some basic results about the oblique manifold, which are needed in our later analysis and development. Critical point analysis of two studied cost functions is provided in Section IV, followed by a quick formulation of intrinsic Newton's method on the oblique manifold. Finally in Section V, performance of the proposed algorithms is investigated by several numerical experiments.

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II. OVERDETERMINED BSS PROBLEM

Mixing model of an instantaneous OdBSS problem is given as

$$w(t) = As(t) + n(t), \tag{1}$$

where $s(t) \in \mathbb{R}^n$ denotes the time series of n statistically independent signals, $A \in \mathbb{R}^{m\times n}$ with $m > n$ is the mixing matrix of full rank, $w(t) \in \mathbb{R}^m$ denotes m observed linear mixtures, and $n(t) \in \mathbb{R}^m$ are certain noises. We denote by $s_i(t) \in \mathbb{R}$ and $w_i(t) \in \mathbb{R}$ the i-th components of $s(t)$ and $w(t)$, respectively. By the construction of linear ICA, the source signals $s(t)$ are assumed to be *mutually statistically independent* and, without loss of generality, to have *zero mean* and *unit variance*, i.e.,

$$\mathbb{E}[s(t)] = 0, \quad \text{and} \quad \mathbb{E}[s(t)s(t)^\top] = I_n, \tag{2}$$

where $I_n \in \mathbb{R}^{n\times n}$ is the identity matrix. The task of OdBSS is to extract k source signals with $k \leq n$, by finding a demixing matrix $X \in \mathbb{R}^{m\times k}$ based only on the observations $w(t)$ via the demixing model

$$y(t) = X^\top w(t), \tag{3}$$

where $y(t) \in \mathbb{R}^k$ denotes k extracted source signals.

It is well-known that under certain conditions, the OdBSS problem can be solved effectively by only using second-order statistics. The first scenario studied in this work assumes that sources $s(t)$ are nonstationary, namely, covariance of $s(t)$, and thus consequently, $w(t)$ as well, is time-varying. A simple approach to separate nonstationary sources [10] is to simultaneously diagonalize a set of covariance matrices of $w(t)$ at different time periods, which are symmetric positive semi-definite. A more general approach of using second-order statistics is to simultaneous diagonalize a set of time-lagged covariance matrices, constructed as follows,

$$R(\tau) := \mathbb{E}\left[w(t)w(t+\tau)^\top\right] \tag{4}$$

where $\tau > 0$ is a time lag. Note that $R(\tau)$ is symmetric indefinite in general. In this paper, we are interested in solving the following problem. Given a set of matrices $\{C_i\}_{i=1}^N \subset \mathbb{R}^{m\times m}$, constructed as second-order statistics of the observations $w(t)$, the task is to find a matrix $X \in \mathbb{R}^{m\times k}$ being of full rank, such that

$$X^\top C_i X, \qquad \text{for all } i = 1, \ldots, N, \tag{5}$$

are simultaneously diagonalized, or approximately simultaneously diagonalized subject to certain diagonality measure.

It is well-known [2], [11] that, if an $X^* \in \mathbb{R}^{m\times k}$ extracts k desired sources, the demixing matrix X^* can only be identified up to arbitrary column-wise scaling and permutation of columns, i.e., any X^*DP, where D is a $k\times k$ invertible diagonal matrix and P a $k\times k$ permutation matrix, extracts the same k sources. It is known that the ambiguity due to column-wise scaling can be eliminated by a pre-whitening process. For a non-whitened approach, one needs an appropriate setting to handle the column-wise scaling, namely the oblique manifold [12]. Now let us denote the $m\times k$ oblique manifold by

$$\mathcal{O}(m,k) := \left\{X \in \mathbb{R}^{m\times k} \,|\, \operatorname{ddiag}(X^\top X) = I_k, \operatorname{rk} X = k\right\}, \tag{6}$$

where rk is the rank, and $\operatorname{ddiag}(Z)$ forms a diagonal matrix, whose diagonal entries are just those of Z.

Straightforwardly, two popular cost functions of measuring diagonality of matrices, namely, the off-norm function [13] and the log-likelihood based cost function [10], are adapted to the present overdetermined scenario as follows

$$\begin{aligned} f_1 \colon \mathcal{O}(m,k) &\to \mathbb{R}, \\ X &\mapsto \frac{1}{4}\sum_{i=1}^n \left\| \operatorname{off}(X^\top C_i X)\right\|_{\mathrm{F}}^2, \end{aligned} \tag{7}$$

where $\operatorname{off}(Z) = Z - \operatorname{ddiag}(Z)$ is a matrix by setting the diagonal entries of Z to zero and $\|\cdot\|_{\mathrm{F}}$ is the Frobenius norm, and

$$\begin{aligned} f_2 \colon \mathcal{O}(m,k) &\to \mathbb{R}, \\ X &\mapsto \frac{1}{2}\sum_{i=1}^n \log \frac{\det \operatorname{ddiag}\left(X^\top C_i X\right)}{\det\left(X^\top C_i X\right)}. \end{aligned} \tag{8}$$

It is important to notice that the off-norm function (7) is *column-wise scale invariant* with respect to the matrix X, only if the OdBSS problem is noiseless. Performance of both functions in terms of separation quality is out of scope of this paper.

III. Structure of Oblique Manifold

In order to formulate an intrinsic Newton's method on the oblique manifold $\mathcal{O}(m,k)$, we introduce the Riemannian gradient and the Riemannian Hessian on $\mathcal{O}(m,k)$. We endow $\mathcal{O}(m,k)$ with the Riemannian metric inherited from $\mathbb{R}^{n\times k}$ by the inner product

$$g \colon \mathbb{R}^{n\times k} \times \mathbb{R}^{n\times k} \to \mathbb{R}, \quad g(A,B) := \operatorname{tr}(A^\top B). \tag{9}$$

It will be useful for understanding the upcoming formulas, if we recall the fact that $\mathcal{O}(m,k)$ is an open and dense Riemannian submanifold of the well understood k-times product of the $(m-1)$-sphere with the usual Euclidean metric

$$\overline{\mathcal{O}(m,k)} = \underbrace{S^{m-1} \times \cdots \times S^{m-1}}_{k-\text{times}} =: (S^{m-1})^k. \tag{10}$$

Here, $\overline{\mathcal{O}}(m,k)$ denotes the closure of $\mathcal{O}(m,k)$. It follows, that

$$\dim \mathcal{O}(m,k) = k \dim S^{m-1} = k(m-1) \tag{11}$$

and, the tangent spaces and the geodesics for $\mathcal{O}(m,k)$ and $(S^{m-1})^k$ coincide. In other words, a geodesic on $\mathcal{O}(m,k)$ is exactly the connected component of a geodesic on $(S^{m-1})^k$ restricted to $\mathcal{O}(m,k)$. Concretely, the tangent space at some $X \in \mathcal{O}(m,k)$ is given by

$$T_X\mathcal{O}(m,k) = \{\Xi \in \mathbb{R}^{m\times k} \mid \operatorname{ddiag}(X^\top \Xi) = 0\}, \tag{12}$$

and the normal space by

$$N_X\mathcal{O}(m,k) = \{X\Gamma \mid \Gamma \in \mathbb{R}^{k\times k} \text{ is diagonal}\}. \tag{13}$$

Lemma 1: The orthogonal projection onto the tangent space $T_X\mathcal{O}(m,k)$ at $X \in \mathcal{O}(m,k)$ is given by

$$\begin{aligned} \operatorname{pr} \colon \mathbb{R}^{m\times k} &\to T_X\mathcal{O}(m,k), \\ \operatorname{pr}(A) &:= A - X\operatorname{ddiag}(X^\top A). \end{aligned} \tag{14}$$

Proof: We first show that for $\operatorname{pr}(A) \in T_X\mathcal{O}(m,k)$,

$$\begin{aligned} &\operatorname{ddiag}(X^\top \operatorname{pr}(A)) \\ =\ &\operatorname{ddiag}(X^\top(A - X\operatorname{ddiag}(X^\top A)) \\ =\ &\operatorname{ddiag}(X^\top A) - \operatorname{ddiag}(X^\top X(\operatorname{ddiag} X^\top A)) \\ =\ &\operatorname{ddiag}(X^\top A) - \operatorname{ddiag}(X^\top X)(\operatorname{ddiag} X^\top A) \\ =\ &0, \end{aligned} \tag{15}$$

because $\operatorname{ddiag}(X^\top X) = I_k$. For orthogonality of the projection, let $\Xi \in T_X\mathcal{O}(m,k)$, i.e. $\operatorname{ddiag}(\Xi^\top X) = 0$. We compute

$$\begin{aligned} \operatorname{tr}(\Xi^\top \operatorname{pr}(A)) &= \operatorname{tr}(\Xi^\top A) - \operatorname{tr}(\Xi^\top X\operatorname{ddiag}(X^\top A)) \\ &= \operatorname{tr}(\Xi^\top A), \end{aligned} \tag{16}$$

following the fact that $\operatorname{ddiag}(\Xi^\top X) = 0$ implies $\operatorname{ddiag}(\Xi^\top X\Gamma) = 0$ for any diagonal matrix Γ, thus, $\operatorname{tr}(\Xi^\top X\operatorname{ddiag}(X^\top A)) = 0$. The result follows. ■

Now, let us recall the great circle μ_x of S^{m-1} at $x \in S^{m-1}$ for a given tangent direction $\xi \in T_x S^{m-1}$, defined as follows

$$\mu_{x,\xi}\colon \mathbb{R} \to S^{m-1},$$
$$\mu_{x,\xi}(t) := \begin{cases} x, & \|\xi\| = 0; \\ x \cos t\|\xi\| + \xi \frac{\sin t\|\xi\|}{\|\xi\|}, & \text{otherwise.} \end{cases} \quad (17)$$

Clearly, $\mu_{x,\xi}(0) = x$ and $\dot{\mu}_{x,\xi}(0) = \xi$. Geodesics of $\mathcal{O}(m,k)$ are given as follows.

Lemma 2: Geodesics $\gamma_{X,\Xi}\colon \mathbb{R} \to \mathcal{O}(m,k)$ through $X = [x_1, \ldots, x_k] \in \mathcal{O}(m,k)$ in direction $\Xi = [\xi_1, \ldots, \xi_k] \in T_X\mathcal{O}(m,k)$ on $(S^{m-1})^k$ and hence, by restriction, on $\mathcal{O}(m,k)$ are given by

$$\gamma_{X,\Xi}(t) = [\mu_{x_1,\xi_1}(t), \ldots, \mu_{x_k,\xi_k}(t)]. \quad (18)$$

Proof: Since $x_i^\top x_i = 1$ and $\xi_i^\top x_i = 0$ for $i = 1, \ldots k$, we have $\dot{\gamma}_{X,\Xi}(0) = \Xi$. Moreover, it can be shown that $\ddot{\gamma}_{X,\Xi}(0)$ lies in the normal space of X since

$$\ddot{\gamma}_{X,\Xi}(0) = X \operatorname{diag}(-\|\xi_1\|^2, \ldots, -\|\xi_k\|^2), \quad (19)$$

hence the result follows. ■

IV. INTRINSIC NEWTON'S METHOD

In this section, we firstly provide a critical point analysis of the two cost functions defined in (7) and (8), followed by development of an intrinsic Newton's method for optimizing both functions.

We compute the first derivative of f_1 as defined in (7) at $X \in \mathcal{O}(m,k)$ in direction $\Xi \in T_X\mathcal{O}(m,k)$ as

$$\mathrm{D}\, f_1(X)\Xi = \operatorname{tr}\left(\Xi^\top C_i X \operatorname{off}(X^\top C_i X)\right). \quad (20)$$

Let $X^* \in \mathcal{O}(m,k)$ be an exact joint diagonalizer, obviously

$$\mathrm{D}\, f_1(X^*)\Xi = 0, \quad (21)$$

i.e., any exact diagonalizer of the simultaneous diagonalization problem (5) is a critical point of f_1. By taking the second derivative of f_1 at $X \in \mathcal{O}(m,k)$ in direction $\Xi \in T_X\mathcal{O}(m,k)$, it gives

$$\begin{aligned} \mathrm{D}^2 f_1(X)(\Xi,\Xi) &= \tfrac{\mathrm{d}^2}{\mathrm{d}\,t^2}(f_1 \circ \gamma_{X,\Xi})(t)\Big|_{t=0} \\ &= \sum_{i=1}^{N} \operatorname{tr}\left(\Xi^\top C_i \Xi \operatorname{off}\big(X^\top C_i X\big)\right) \\ &\quad - \operatorname{tr}\left(\operatorname{ddiag}(\Xi^\top \Xi) X^\top C_i X \operatorname{off}\big(X^\top C_i X\big)\right) \\ &\quad + \operatorname{tr}\left(\Xi^\top C_i X \left(\operatorname{off}\big(X^\top C_i \Xi\big) + \operatorname{off}\big(\Xi^\top C_i X\big)\right)\right). \end{aligned} \quad (22)$$

where $\gamma_{X,\Xi}$ is the geodesic on $\mathcal{O}(m,k)$ as defined in (18). It is easy to see that the first two terms on the right-hand side in (22) evaluated at a joint diagonalizer $X^* \in \mathcal{O}(m,k)$ are equal to zero. Let $\Xi = [\xi_1, \ldots, \xi_k] \in T_{X^*}\mathcal{O}(m,k)$. Then we evaluate the third term at X^* as

$$\begin{aligned} &\operatorname{tr}\left(\Xi^\top C_i X^* \left(\operatorname{off}\big(X^{*\top} C_i \Xi + \Xi^\top C_i X^*\big)\right)\right) \\ &= \sum_{p,q=1}^{k} \sum_{i=1}^{N} \xi_p^\top C_i x_q^* x_q^{*\top} C_i \xi_p + \xi_p^\top C_i x_q^* x_p^{*\top} C_i \xi_q. \end{aligned} \quad (23)$$

A direct computation shows that the second summation on the right-hand side of (23) is equal to zero as well. By the construction of OdBSS, i.e. the second-order statistics C_i's are not of full rank, we conclude the following result.

Lemma 3: Any exact joint diagonalizer $X^* \in \mathcal{O}(m,k)$ of the noiseless OdBSS problem as defined in (5) is a critical point of the off-norm function f_1, defined in (7). The Hessian of f_1 at X^* is *positive semidefinite*.

Remark 1: Obviously, the semidefiniteness of the Hessian of f_1 at desired critical point will cause troubles for Newton's method to converge. Nevertheless, noiseless OdBSS problem can be efficiently solved by a pre-whitened BSS approach. When noises are present, in general, it is reasonable to assume that the Hessian of f_1 at X^* is positive definite.

In what follows, we quickly derive a critical point analysis of the log-likelihood based cost function f_2, defined in (8), in the same manner as for f_1. The first derivative of f_2 at $X \in \mathcal{O}(m,k)$ in direction $\Xi \in T_X\mathcal{O}(m,k)$ is computed by

$$\begin{aligned} \mathrm{D} f_2(X)\Xi = \sum_{i=1}^{N} \operatorname{tr}\Bigg(\Xi^\top C_i X \Big(\big(\operatorname{ddiag}(X^\top C_i X)\big)^{-1} \\ - (X^\top C_i X)^{-1}\Big)\Bigg). \end{aligned} \quad (24)$$

It can be easily shown that an exact joint diagonalizer $X^* \in \mathcal{O}(m,k)$ is a critical point of f_2. A tedious computation leads to the the second derivative of f_2 at $X \in \mathcal{O}(m,k)$ in direction $\Xi \in T_X\mathcal{O}(m,k)$ as follows

$$\begin{aligned} &\mathrm{D}^2 f_2(X)(\Xi,\Xi) = \tfrac{\mathrm{d}^2}{\mathrm{d}\,t^2}(f_2 \circ \gamma_{X,\Xi})(t)\Big|_{t=0} \\ &= \sum_{i=1}^{N} \operatorname{tr}\Bigg(\Big(\big(\operatorname{ddiag}(X^\top C_i X)\big)^{-1} - \big(X^\top C_i X\big)^{-1}\Big) \cdot \\ &\quad \cdot \Big(\Xi^\top C_i \Xi - \operatorname{ddiag}(\Xi^\top \Xi) X^\top C_i X\Big)\Bigg) \\ &\quad + \operatorname{tr}\Bigg(\Xi^\top C_i X \Big(\big(X^\top C_i X\big)^{-1} \big(\Xi^\top C_i X + X^\top C_i \Xi\big) \cdot \\ &\quad \cdot \big(X^\top C_i X\big)^{-1} - \big(\operatorname{ddiag}(X^\top C_i X)\big)^{-1} \cdot \\ &\quad \cdot \operatorname{ddiag}\big(\Xi^\top C_i X + X^\top C_i \Xi\big)\big(\operatorname{ddiag}\big(X^\top C_i X\big)\big)^{-1}\Big)\Bigg). \end{aligned} \quad (25)$$

The first term on the right-hand side from above can be shown to be equal to zero at $X^* \in \mathcal{O}(m,k)$. Let us denote

$$\begin{aligned} \Lambda &:= \operatorname{diag}(\lambda_1, \ldots, \lambda_k) \\ &= \big(X^{*\top} C_i X^*\big)^{-1} = \big(\operatorname{ddiag}(X^{*\top} C_i X^*)\big)^{-1}, \end{aligned} \quad (26)$$

with $\lambda_j > 0$ for all $j = 1, \ldots, k$. Then the second term in (25) evaluated at X^* is computed as

$$\begin{aligned} &\operatorname{tr}\left(\Xi^\top C_i X^* \Lambda \operatorname{off}\big(X^{*\top} C_i \Xi + \Xi^\top C_i X^*\big) \Lambda\right) \\ &= \sum_{p,q=1}^{k} \sum_{i=1}^{N} \lambda_p \lambda_q \xi_p^\top C_i x_q^* x_q^{*\top} C_i \xi_p \\ &\quad + \sum_{p,q=1}^{k} \sum_{i=1}^{N} \lambda_p \lambda_q \xi_p^\top C_i x_q^* x_p^{*\top} C_i \xi_q. \end{aligned} \quad (27)$$

By the same argument, the second summation on the right-hand side of (27) is equal to zero. Following the fact that $\lambda_j > 0$, we conclude a similar result as Lemma 3 as follows

Lemma 4: Any exact joint diagonalizer $X^* \in \mathcal{O}(m,k)$ of the noiseless OdBSS problem as defined in (5) is a critical point of the off-norm function f_2, defined in (8). The Hessian of f_2 at X^* is *positive semidefinite*.

In the rest of the section, we quickly develop an intrinsic Newton's method for minimizing...

V. NUMERICAL EXPERIMENTS

The task of our experiment is to jointly diagonalize a set of symmetric matrices $\{\widetilde{C}_i\}_{i=1}^N$, constructed by

$$\widetilde{C}_i = A\Lambda_i A^\top + \varepsilon E_i, \qquad i = 1, \ldots, N, \tag{28}$$

where $A \in \mathbb{R}^{m\times m}$ is a randomly picked matrix in $\mathcal{O}(m,k)$, diagonal entries of Λ_i are drawn from a uniform distribution on the interval $(9, 11)$, $E_i \in \mathbb{R}^{m\times m}$ 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 $\varepsilon \in \mathbb{R}$ is the noise level. We set $m = 5$, $n = 20$, and run six tests, for both the Gauss-Newton-Jacobi algorithm and Pham's algorithm, in accordance with increasing noise, by using $\varepsilon = t \times 10^{-2}$ where $t = 0, \ldots, 5$.

The convergence of algorithms is measured by the distance of the accumulation point $X^* \in \mathcal{O}(m,k)$ to the current iterate $X_k \in \mathcal{O}(m,k)$, i.e., by $\|X_k - X^*\|_{\mathrm{F}}$. According to Fig. **??** and **??**, it is clear that both algorithms converge locally quadratically fast to a joint diagonalizer under the Exact NoJD setting, i.e., $\varepsilon = 0$. Although Pham's algorithm was claimed in [10] to converge locally quadratically fast to a joint diagonalizer 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.

VI. ACKNOWLEDGMENTS

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