A STABLE AND EFFICIENT ALGORITHM FOR DIFFICULT NON-ORTHOGONAL JOINT DIAGONALIZATION PROBLEMS

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ABSTRACT

This article deals with the Non-Orthogonal Joint Diagonalization of few matrices of large size: a difficult problem that is not solved by existing methods. The proposed algorithm combines, on the one hand, the efficiency provided by the Givens and hyperbolic rotations parametrization of the mixing matrix and, on the other hand, the stability guaranteed by the minimization of the complete off-diagonal norm. The stability and the quadratic convergence of the algorithm are illustrated by numerical simulations in situations where other techniques are slow or even non-convergent. The improvement is reached at the price of a moderate increase of the computational complexity.

1. INTRODUCTION

Many Blind Source Separation (BSS) methods are based on a step of Joint Diagonalization (JD) of a set of symmetric matrices. This set contains for instance fourth-order cumulants matrices like in JADE [1, 2] or time delayed covariance matrices like in SOBI [4] according to the expected properties of the mixed sources like for instance: mutual independence and non-Gaussianity, decorrelation and spectral difference, or decorrelation and a difference of the variance temporal profiles.

The Joint Diagonalization problem consists of computing the N-by-N non-singular mixing matrix A given a set of K symmetric N-by-N matrices $\mathcal{M} \triangleq \{M_1, M_2, \ldots, M_K\}$ sharing the same structure

$$M_k = A D_k A^T \tag{1}$$

where D_k are diagonal matrices and $1 \leq k \leq K$. An equivalent objective is to compute the inverse of the mixing matrix, denoted $B \triangleq A^{-1}$, called the separation matrix because $B M_k B^T = D_k$. In practical applications, the M_k are estimated, the model (1) is only approximately true then the JD can only be approximately achieved.

The JD is said to be orthogonal (OJD) when the mixing matrix A to be estimated is required to be orthogonal. This orthogonality constraint normalizes and simplifies the JD problem but is generally based on a second-order pre-whitening step that is always approximate and this unavoidable pre-whitening error cannot be corrected a posteriori by the OJD step, which limits the estimation accuracy of the mixing matrix. Consequently many authors proposed Non-Orthogonal Joint Diagonalization (NOJD) algorithms to avoid this bias. NOJD algorithms are designed for dealing with sets of positive definite matrices [5], sets containing at least one positive matrix [6, 7, 9, 13] and also general sets of matrices [8, 10, 15]. In this paper, the last problem is adressed i.e. no assumption of definite positiveness of any matrix of $\mathcal{M}$ is needed.

This paper aims at building fast BSS methods (small K) for high dimensional applications (large N) which are very difficult contexts of Non-Orthogonal Joint Diagonalization. As a matter of fact the difficulty of the NOJD depends firstly on the diversity of the diagonal matrices D_k which is related to the unicity of the mixing matrix, and secondly on the conditionning of the mixing matrix which can make the solution very sensitive to noise. The influence of the D_k can be measured by a positive index lower than 1 called the modulus of uniqueness (see [12]). The closer to 1 is this modulus of uniqueness the more difficult is the NOJD problem. Here we will consider small sets of matrices of large size with modulus of uniqueness larger than 0.95, i.e. $K = 10$ matrices of size 100-by-100, and up to 0.99999995, i.e. $K = 2$ matrices of size 100-by-100.

It is generally believed that the Generalized EigenValue Decomposition (GEVD) of 2 matrices provides a joint diagonalizer, but this is not true in general. The sufficient condition given in [18] p. 461 for instance is not always verified. The proposed algorithm is therefore one of the few available solutions of this difficult problem.

In the following section, we introduce the notations and describe shortly the already published J-Di algorithm [14, 15]. The proposed modification of the J-Di algorithm, called J-Di+, is derived in the third section and its performance compared with the existing J-Di and FFDiag [8] algorithms in Section IV.

2. THE J-DI ALGORITHM

2.1. An Optimization on the Linear Special Group

The NOJD of a set $\mathcal{M}$ of symmetric N-by-N matrices $M_1, M_2, \ldots, M_K$ can be achieved by successive multiplications of Givens and hyperbolic rotations [1] in a Jacobi-like framework [18]. Both rotations have a determinant equal to 1 therefore this algorithm called J-Di performs an optimization in the linear special group (matrices of determinant equal

[1] This parametrization has also been proposed for solving the joint eigenvalue decomposition problem [16, 17].

to 1). By comparison, the JADE (and SOBI) optimization is achieved in the orthogonal special group (orthogonal matrices of determinant equal to 1), which is a sub-group of the linear special group. In this sense, J-Di is an Non-Orthogonal extension of the Jacobi-like OJD algorithm [1, 2] used in JADE (and SOBI).

Every matrix M_k of $\mathcal{M}$ is diagonalized by repeating the following iteration for every $1 \leq i, j \leq N$ and $1 \leq k \leq K$

$$M_k' \triangleq H(\phi, i, j)^T G(\theta, i, j)^T M_k \, G(\theta, i, j) H(\phi, i, j) \quad (2)$$

and

$$A' \triangleq AG(\theta, i, j) H(\phi, i, j)^{-1} = AG(\theta, i, j) H(-\phi, i, j) \quad (3)$$

where M_k' (resp. A') denotes the updated M_k (resp. A) matrix, $G(\theta, i, j)$ denotes the classical N-by-N Givens rotation of angle θ and indices i, j

$$G(\theta, i, j) \triangleq \begin{pmatrix} I_{i-1} & \vdots & 0 & \vdots & 0 \\ \cdots & \cos\theta & \cdots & -\sin\theta & \cdots \\ 0 & \vdots & I_{j-i-1} & \vdots & 0 \\ \cdots & \sin\theta & \cdots & \cos\theta & \cdots \\ 0 & \vdots & 0 & \vdots & I_{N-j} \end{pmatrix} \quad (4)$$

and $H(\phi, i, j)$ is the corresponding hyperbolic rotation

$$H(\phi, i, j) \triangleq \begin{pmatrix} I_{i-1} & \vdots & 0 & \vdots & 0 \\ \cdots & \cosh\phi & \cdots & \sinh\phi & \cdots \\ 0 & \vdots & I_{j-i-1} & \vdots & 0 \\ \cdots & \sinh\phi & \cdots & \cosh\phi & \cdots \\ 0 & \vdots & 0 & \vdots & I_{N-j} \end{pmatrix} \quad (5)$$

The $N(N-1)/2$ iterations over all the (i, j) for $1 \leq i < j \leq N$ are called a sweep. Several sweeps are generally necessary to reach the convergence.

2.2. Computation of the optimal angles for given i, j

The last problem to solve is now to compute the optimal angles θ and ϕ to diagonalize simultaneously all the M_k. The J-Di algorithm computes the angles that minimize only the sum of the squared i, j entries of the M_k, denoted $M_k[i, j]$, for all the k between 1 and K, i.e.

$$J(\theta, \phi, i, j) \triangleq \sum_{k=1}^{k=K} (M_k'[i, j])^2 \quad (6)$$

One must note that this minimization of $J(\theta, \phi, i, j)$ is not equivalent to the minimization of a global criterion like the norm of all the off-diagonal M_k entries because the hyperbolic rotations $H(\phi, i, j)$ are not orthogonal matrices. Nevertheless, such a partial minimization of the off-diagonal norm generally yields a very efficient diagonalization of $\mathcal{M}$ as it is illustrated in [15].

The main interest of the Givens/hyperbolic parametrization is that the trigonometric and hyperbolic function that appears at the power 4 (quartic) in $J(\theta, \phi, i, j)$ can be transformed into an easy to optimize quadratic form involving the double angles 2θ and 2ϕ. As a matter of fact, after some manipulations on Eq. 2, one can see that

$$\begin{pmatrix} M_1'[i, j] \\ \vdots \\ M_k'[i, j] \\ \vdots \\ M_K'[i, j] \end{pmatrix} = Cv(\theta, \phi) \quad (7)$$

with

$$v(\theta, \phi) \triangleq \begin{pmatrix} \sinh(2\phi) \\ -\sin(2\theta)\cosh(2\phi) \\ \cos(2\theta)\cosh(2\phi) \end{pmatrix} \quad (8)$$

and

$$C \triangleq \begin{pmatrix} \frac{M_1[i,i]+M_1[j,j]}{2} & \frac{M_1[i,i]-M_1[j,j]}{2} & M_1[i,j] \\ \vdots & \vdots & \vdots \\ \frac{M_k[i,i]+M_k[j,j]}{2} & \frac{M_k[i,i]-M_k[j,j]}{2} & M_k[i,j] \\ \vdots & \vdots & \vdots \\ \frac{M_K[i,i]+M_K[j,j]}{2} & \frac{M_K[i,i]-M_K[j,j]}{2} & M_K[i,j] \end{pmatrix} \quad (9)$$

Finally the J-Di criterion $J(\theta, \phi, i, j)$ is equal to quadratic term

$$J(\theta, \phi, i, j) \triangleq v(\theta, \phi)^T C^T C v(\theta, \phi) \quad (10)$$

where $v(\theta, \phi)$ verifies the following quadratic constraint

$$v(\theta, \phi)^T \mathrm{diag}(-1, 1, 1) v(\theta, \phi) = 1 \quad (11)$$

The global minimum is reached when $v(\theta, \phi)$ is the generalized eigenvector of $(C^T C, \mathrm{diag}(-1, 1, 1))$ of minimal positive eigenvalue (see [15] for more details).

This technique compares favorably with other NOJD methods in many contexts. But we observed lack of convergence in several very difficult NOJD situations; mainly when $\mathcal{M}$ contains few large matrices, like $K = 3$ to 4 matrices of size $N = 50$ or 100 for instance. The goal of the following section is to propose a modification of the J-Di criterion to deal with these hard NOJD contexts not covered by existing methods.

3. MINIMIZATION OF THE COMPLETE OFF-DIAGONAL NORM

A natural solution to guarantee the convergence, at least to a local minimum, of our NOJD algorithm is to minimize the complete off-diagonal norm of the matrices of $\mathcal{M}$. We propose to modify the J-Di criterion $J(\theta, \phi, i, j)$ in Eq. 6 to minimize exactly the off-diagonal norm at each (i, j) iteration of the Jacobi scheme. It means in particular that we will have to take into account not only the $M_k'[i, j]$ entries but also all the other entries of the i-th and j-th rows and columns of the M_k matrices. As a matter of fact, the Givens and hyperbolic rotations in Eq. 2 only modify the two i, j rows and the two i, j columns of the M_k matrices.

Consequently, the modified criterion to be minimized is

$$\begin{aligned} L(\theta,\phi,i,j) &\triangleq \sum_{k=1}^{k=K} (M'_k[i,j])^2 \\ &+ \sum_{k=1}^{k=K} \sum_{\substack{n=1 \\ n\neq i,j}}^{n=N} (M'_k[n,i])^2 \\ &+ \sum_{k=1}^{k=K} \sum_{\substack{n=1 \\ n\neq i,j}}^{n=N} (M'_k[n,j])^2 \end{aligned} \quad (12)$$

3.1. Minimization of the new criterion

Let's first define the vectors u_k and v_k (resp. u'_k and v'_k) equal to the i-th and j-th columns of M_k (resp. M'_k) excluding the $[i,i]$, $[j,i]$, $[i,j]$ and $[j,j]$ entries, i.e.

$$u_k \triangleq \begin{pmatrix} M_k[1,i] \\ \vdots \\ M_k[i-1,i] \\ M_k[i+1,i] \\ \vdots \\ M_k[j-1,i] \\ M_k[j+1,i] \\ \vdots \\ M_k[N,i] \end{pmatrix}, v_k \triangleq \begin{pmatrix} M_k[1,j] \\ \vdots \\ M_k[i-1,j] \\ M_k[i+1,j] \\ \vdots \\ M_k[j-1,j] \\ M_k[j+1,j] \\ \vdots \\ M_k[N,j] \end{pmatrix} \quad (13)$$

Then one can show that the update in Eq. 2 is equivalent to

$$\begin{pmatrix} \frac{{u'_1}^T u'_1 + {v'_1}^T v'_1}{2} \\ \vdots \\ \frac{{u'_k}^T u'_k + {v'_k}^T v'_k}{2} \\ \vdots \\ \frac{{u'_K}^T u'_K + {v'_K}^T v'_K}{2} \end{pmatrix} = Fw(\theta,\phi) \quad (14)$$

with

$$w(\theta,\phi) \triangleq \begin{pmatrix} \cosh(2\phi) \\ -\sin(2\theta)\sinh(2\phi) \\ \cos(2\theta)\sinh(2\phi) \end{pmatrix} \quad (15)$$

and

$$F \triangleq \begin{pmatrix} \frac{u_1^T u_1 + v_1^T v_1}{2} & \frac{u_1^T u_1 - v_1^T v_1}{2} & u_1^T v_1 \\ \vdots & \vdots & \vdots \\ \frac{u_k^T u_k + v_k^T v_k}{2} & \frac{u_k^T u_k - v_k^T v_k}{2} & u_k^T v_k \\ \vdots & \vdots & \vdots \\ \frac{u_K^T u_K + v_K^T v_K}{2} & \frac{u_K^T u_K - v_K^T v_K}{2} & u_K^T v_K \end{pmatrix} \quad (16)$$

Once again the power 2 of the trigonometric and hyperbolic functions can be reduced to 1 by considering the double angles 2θ and 2ϕ.

Finally, the new criterion is the sum of the J-Di criterion $J(\theta,\phi,i,j)$ that is quadratic in $v(\theta,\phi)$ plus a new term that is linear in $w(\theta,\phi)$

$$L(\theta,\phi,i,j) \triangleq v(\theta,\phi)^T C^T C v(\theta,\phi) + f^T w(\theta,\phi) \quad (17)$$

where

$$f^T \triangleq 2 \sum_{k=1}^{k=K} F(k,:) \quad (18)$$

which have to be minimized under the constraint

$$\begin{bmatrix} v(\theta,\phi)^T \\ w(\theta,\phi)^T \end{bmatrix} \mathrm{diag}(-1,1,1) \, [v(\theta,\phi) \; w(\theta,\phi)] = \mathrm{diag}(1,-1) \quad (19)$$

We already know how to minimize the J-Di quadratic term, it is also easy to minimize the new linear term alone but we haven't found an analytic expression of θ and ϕ that minimizes $L(\theta,\phi,i,j)$ in spite of the obvious relationship between $v(\theta,\phi)$ and $w(\theta,\phi)$. We propose to optimize $L(\theta,\phi,i,j)$ using several Newton iterations initialized at the J-Di minimum. More specifically, a fixed number of Newton iterations is used in the following simulations. An analytical expression possibly exists and would be more elegant but not necessarily more efficient in terms of speed of convergence or computational load which is what matters. As a matter of fact, the dominant computational cost is the update in Eq. 2, not the computation of θ and ϕ.

This new algorithm which minimizes $L(\theta,\phi,i,j)$ defined in Eq. 17 is called J-Di+.

3.2. Complexity

The costs of the J-Di [15] and FFDiag [8] sweeps are approximately $2KN^3$ flops mainly due to the update of $\mathcal{M}$ in Eq. 2. The cost of the improved algorithm is higher because the computation of the F matrix defined in Eq. 16 requires $3K(N-2) \times N(N-1)/2 \approx 3/2KN^3$ flops which is lower but comparable to the $\mathcal{M}$ update. In summary the complexity of the J-Di+ algorithm is less than 2 times higher than the J-Di or FFDiag complexity but we will see in the next section that this higher cost yields much better performance.

4. PERFORMANCE ANALYSIS BY NUMERICAL SIMULATIONS

The performance of the original J-Di, FFDiag and the improved J-Di+ algorithm are compared with sets of exactly diagonalizable matrices using the off-diagonal norm as index of performance. This index is plotted as a function of the number of sweeps for 30 independent trials. The mixing matrix A and the diagonal matrices D_k entries are independent and normally distributed. The figures show the performance with numbers K of matrices decreasing from situations where the three algorithms converge (here we choose $K = 10$ because larger K were investigated in [15]) until the lowest possible value for NOJD, i.e. $K = 2$, where only the new algorithm J-Di+ converges.

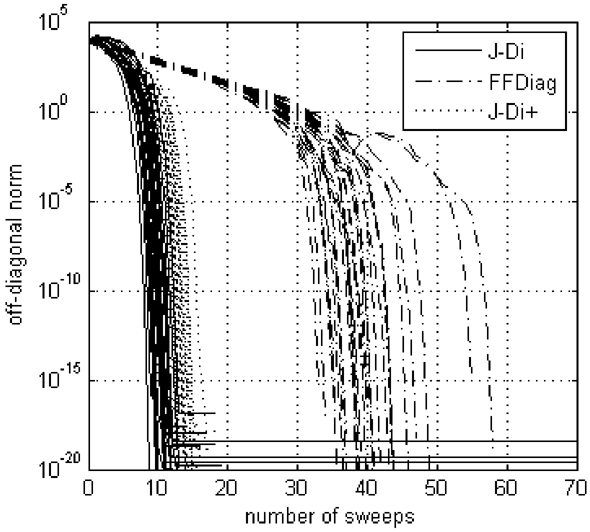

Fig. 1. Convergence of the off-diagonal norm for 30 sets of $K = 10$ matrices of size 100×100, MoU ≈ 0.95

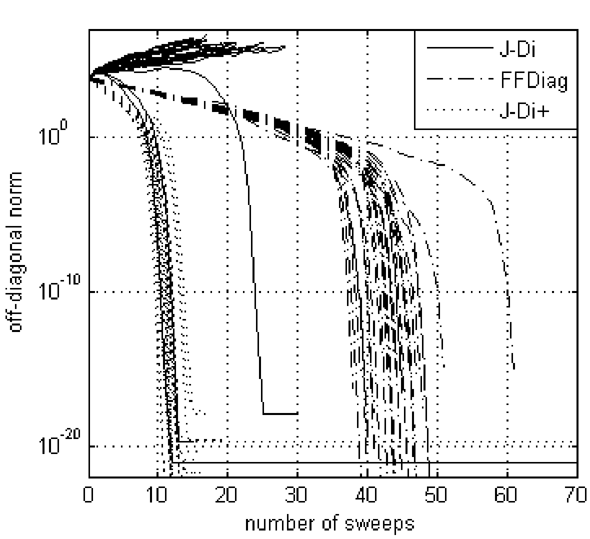

Fig. 2. Convergence of the off-diagonal norm for 30 sets of $K = 7$ matrices of size 100×100, MoU ≈ 0.98

The matrix size is $N = 100$ and the number of matrices K decreases from $K = 10$ in Fig. 1, to $K = 7$ in Fig. 2, $K = 5$ in Fig. 3, $K = 3$ in Fig. 4 and finally $K = 2$ in Fig. 5. The Modulus of Uniqueness (MoU) which measures the difficulty of the NOJD increases when K decreases; its average value is roughly equal to 0.95 for $K = 10$, 0.98 for $K = 7$, 0.995 for $K = 5$, 0.9999 for $K = 3$ and 0.99999995 for $K = 2$.

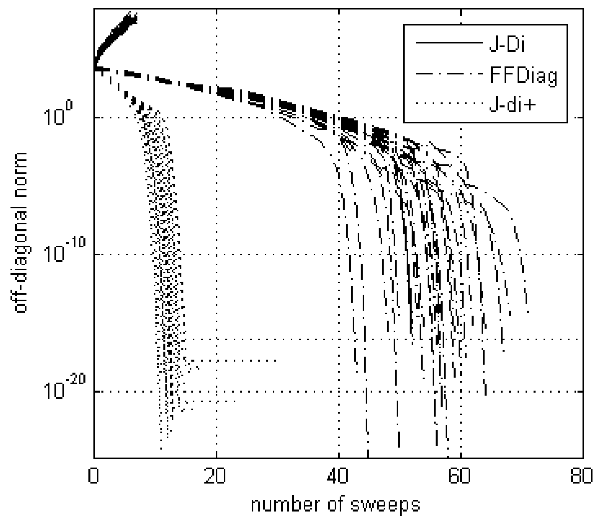

Fig. 3. Convergence of the off-diagonal norm for 30 sets of $K = 5$ matrices of size 100×100, MoU ≈ 0.995

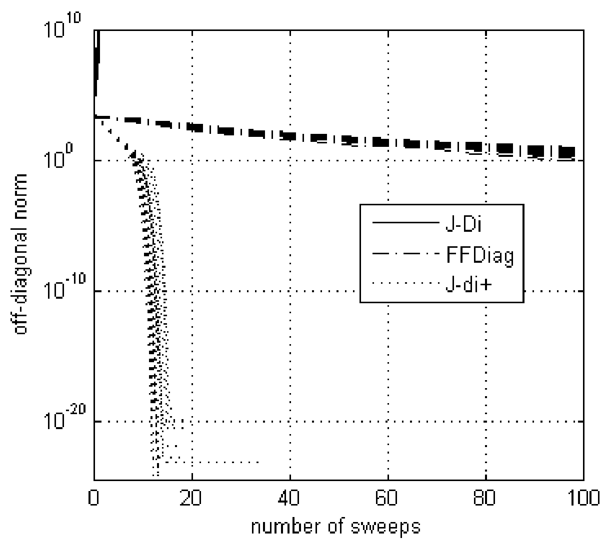

Fig. 4. Convergence of the off-diagonal norm for 30 sets of $K = 3$ matrices of size 100×100, MoU ≈ 0.9999

J-Di converges like J-Di+ for $K = 10$, diverges in few sweeps when $K = 7, 5$ or 3 and immediately if $K = 2$ (the curves corresponding to J-Di are not visible in Fig. 5). FF-Diag converges slowly (about 50 sweeps) until $K \leq 5$ and diverges for lower values of K. J-Di+ converges in every case i.e. $K = 10, 7, 5, 3$ and 2 in less than 15 to 20 sweeps (25 when $K = 2$).

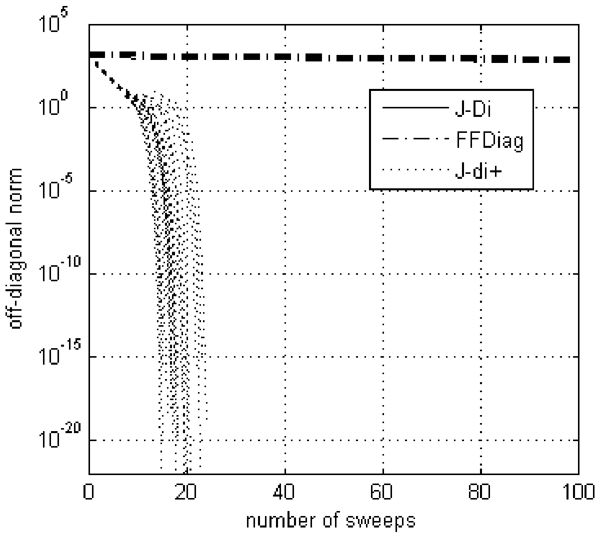

Fig. 5. Convergence of the off-diagonal norm for 30 sets of $K = 2$ matrices of size 100×100, MoU ≈ 0.99999995

5. CONCLUSION

A new Non-Orthogonal Joint Diagonalization algorithm is proposed that extends the range of application of the Non-Orthogonal Joint Diagonalization and is of interest for building fast BSS methods for very high dimension applications. The Jacobi-like iterations structure combining Givens and hyperbolic rotations of the J-Di algorithm [14, 15] is preserved but the optimal Givens and hyperbolic angles computation is modified to minimize all the off-diagonal entries of the matrix set to be jointly diagonalized. The resulting algorithm is able to deal with very difficult Joint Diagonalization problems like few (i.e. down to 2) matrices of large size, which was not possible with existing methods. This improvement is illustrated by numerical simulations. This extension of the Joint Diagonalization application domain is obtained at the price of an increase of the computational complexity lower than a factor two. But this complexity increase can be compensated by a reduction of the size of the matrix set. These results should be generalized by means of more extensive numerical simulations and, if possible, a theoretical analysis of the convergence speed.

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