WHAT CAN MAKE JOINT DIAGONALIZATION DIFFICULT?

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ABSTRACT

We show that the issues of uniqueness and noise sensitivity in the problem of matrix joint diagonalization are closely related. We address other factors important in noise sensitivity. We distinguish between orthogonal and non-orthogonal joint diagonalization and argue that the latter can be more difficult than the former. Our analysis is based on the perturbation analysis of the stationary points of certain flows for joint diagonalization. Numerical experiments support the derived results.

Index Terms— Joint Diagonalization, Sensitivity Analysis, Tensor Decomposition, Blind Signal Processing, Independent Component Analysis

1. INTRODUCTION

Matrix Joint Diagonalization (also known as Simultaneous Matrix Diagonalization) has found applications in many blind signal processing algorithms (for example [1, 2, 3, 4]), as well as in tensor decomposition methods as in [5]. In these problems, based on a model, we believe that for a set of symmetric $n \times n$ matrices $\{C_i\}_{i=1}^N$ we have:

$$C_i = A\Lambda_i A^T, \ \ 1 \leq i \leq N \tag{1}$$

where A is a non-singular $n \times n$ matrix and Λ_i is a diagonal matrix. Here A^T is the transpose of matrix A. Also denote $[\Lambda_i]_{jj}$ by λ_{ij}. The goal is to find the matrix A by observing just the set $\{C_i\}_{i=1}^N$. Note that without knowing Λ_i's we can not distinguish between A and $AD\Pi$ for any permutation Π and non-singular diagonal D (the scaling factor). In order to find A one might think of the problem of finding a non-singular matrix B such that BC_iB^T's all are diagonal and hence find A (up to scale and permutation) as B^{-1}. We call this problem the Exact Joint Diagonalization (EJD) problem. Obviously, if B is an exact joint diagonalizer, then ΠDB, is also another one. So any solution to the EJD problem can be unique only up to a permutation and a scaling factor. If the scale and permutation are the only ambiguities in the solution we say that the EJD problem has a unique solution. If the EJD problem has a unique solution then the problem of finding A and EJD are equivalent.

In practice, due to noise or estimation errors or because our underlying model is not accurate we only can have:

$$C_i \approx A\Lambda_i A^T, \ \ 1 \leq i \leq N \tag{2}$$

Again, in this case, one might think of the problem of finding a non-singular matrix B such that all BC_iB^T's are "as diagonal as possible" and hope that B^{-1} is close to A (up to the expected ambiguities). We call this problem the Joint Diagonalization (JD) problem. If the set $\{C_i\}_{i=1}^N$ is such that the solution that we find for the JD problem is very far from A^{-1} even for small values of noise or error in our model then we can say that JD for that set is a difficult problem.

In this paper we consider the factors that can make the JD problem difficult. In Section 2 we introduce a cost function for Orthogonal Joint Diagonalization (OJD) and show how it can also be used for Non-Orthogonal Joint Diagonalization (NOJD). In Section 3 we elaborate on the uniqueness properties of the EJD problem in both orthogonal and non-orthogonal cases. In Section 4 we present the actual sensitivity results and in Section 5 we provide some numerical experiments in support of the derived results.

2. ORTHOGONAL AND NON-ORTHOGONAL JD

If we assume that B is an orthogonal matrix then we call the JD problem as Orthogonal Joint Diagonalization (OJD) and if we assume that B is not orthogonal we call the problem as Non-Orthogonal Joint Diagonalization (NOJD). As one might expect these two problems have very different properties. The OJD problem together with a simple and efficient algorithm for it was introduced first in [1]. This algorithm which is a part of the JADE algorithm minimizes the cost function:

$$J_1(B) = \sum_{i=1}^{n} \left\| BC_iB^T - \mathrm{diag}(BC_iB^T) \right\|_F^2 \tag{3}$$

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where B is orthogonal, $\mathrm{diag}(X)$ is the diagonal part of the matrix X and $\|.\|_F$ is the Frobenius norm. It can be shown that the stationary points of $J_1(B)$ satisfy [6]:

$$\sum_{i=1}^{N}[BC_iB^T, \mathrm{diag}(BC_iB^T)] = 0 \tag{4}$$

where $[X, Y] = XY - YX$ is the matrix Lie bracket. Note that the OJD problem is permutation invariant but not scale invariant, i.e. if B is an orthogonal joint diagonalizer then DB can not be an orthogonal joint diagonalizer unless D has all diagonal elements of $+1$ or -1. Another observation is that given C_1, if its eigen values are distinct we can find its eigen matrix and that would be an approximation for A. But we hope that by inclusion of more matrices in the OJD process we can improve this approximation. On the other hand, it is not difficult to see that the minimum number of matrices to give enough equations to solve for a unique non-orthogonal joint diagonalizer is $N = 2$. So the NOJD problem generically is a two-matrix problem. For a given set of matrices $\{C_i\}_{i=1}^N$ NOJD gives a better approximation for the unknown non-orthogonal matrix A than OJD by introducing more degrees of freedom in the search. Exactly for the same reason NOJD can be harder as we show later.

Defining a cost function for NOJD has been a challenge. One idea is to extend J_1 from the group of orthogonal matrices $\mathrm{O}(n)$ to the group of non-singular matrices $\mathrm{GL}(n)$ and try to reduce J_1 (say by gradient method) along directions orthogonal to the directions that correspond to reduction by scaling by diagonal matrices. Note that the directions that correspond to reduction by scaling are those directions along which the non-orthogonal joint diagonalizer is invariant. Some algorithms that use this idea are introduced in [7, 6, 4]. It is possible to make this approach rigorous via the language of Lie groups and Riemannian geometry. For brevity and shortage of space we avoid further details and refer the reader to [6]. Briefly, the overall scheme is that after equipping $\mathrm{GL}(n)$ with a Natural Riemannian metric one can define $\nabla J_1(B)$ the gradient of J_1. Then we restrict $-\nabla J_1$ to the directions mentioned above and obtain a non-holonomic flow for NOJD based on J_1. Based on the stationary points of this flow, we can define B the non-orthogonal joint diagonalizer of $\{C_i\}_{i=1}^N$ via the equation:

$$\sum_{i=1}^{N}\left((BC_iB^T)^\circ BC_iB^T\right)^\circ = 0 \tag{5}$$

where $X^\circ = X - \mathrm{diag}(X)$, provided such a B exists. We mention that there are other possible formulations for the NOJD problem, as in [3] for example.

3. UNIQUENESS FOR EJD AND MODULUS OF UNIQUENESS

It is not difficult to show that [8]:

Theorem 1 *Let C_i's satisfy (1) with A orthogonal. The necessary and sufficient condition to have a unique orthogonal joint diagonalizer is that for every pair of indices $1 \le k < l \le n$ we have some $1 \le i \le N$ such that $\lambda_{ik} \ne \lambda_{il}$.*

In order to have a similar result for non-orthogonal EJD, it is convenient to define:

Defenition 1 *For the set of diagonal matrices $\{\Lambda_i\}_{i=1}^N$ let:*

$$\rho_{kl} = \frac{\sum_{i=1}^{N}\lambda_{ik}\lambda_{il}}{(\sum_{i=1}^{N}\lambda_{il}^2)^{\frac{1}{2}}(\sum_{i=1}^{N}\lambda_{ik}^2)^{\frac{1}{2}}}, \quad 1 \le k \ne l \le n \tag{6}$$

with the convention that $\rho_{kl} = 1$ if $\lambda_{ik} = 0$ for some k and all i. Let ρ be equal to one of the ρ_{kl}'s that have the maximum absolute value among all. The Modulus of Uniqueness(MU) for this set is defined as $|\rho|$.

Obviously $|\rho| \le 1$. For $N = 1$, $|\rho| = 1$ and the exact joint diagonalizer is not unique. MU captures the uniqueness in an exact sense:

Theorem 2 *Let C_i's satisfy (1). The necessary and sufficient condition to have a unique non-orthogonal joint diagonalizer is that $|\rho| < 1$.*

This means that in order to have unique solution the matrix Λ whose rows are diagonals of Λ_i's should have no co-linear columns. This result has been known in the literature of tensor decomposition, see for example [9] for references and more general results. A proof is also given in [10].

We should mention again the dramatic difference between uniqueness properties of OJD and NOJD. For a given $\{\Lambda_i\}_{i=1}^N$ with $\beta \ne 0$ and $|\rho| < 1$ in order to make $\beta = 0$ we can change the first diagonal elements of Λ_i's and set $\lambda_{i1} = \lambda_{i2}$ for all $1 \le i \le N$. Whereas in order to make $|\rho| = 1$, we can have $\lambda_{i1} = K\lambda_{i2}$ for all $1 \le i \le N$ and any number K. As a result it is much easier to degrade the uniqueness in the NOJD problem than in the OJD problem.

4. SENSITIVITY RESULTS

In order to understand the sensitivity of the JD problem we add noise to the model (1) as:

$$C_i(t) = A\Lambda_iA^T + tN_i, \ \ t \in [-\delta, \delta], \delta > 0 \tag{7}$$

where $\{N_i\}_{i=1}^N$ are symmetric error or noise matrices and t shows the noise contribution. With $t = 0$ the set $\{C_i(0)\}_{i=1}^N$ has an exact joint diagonalizer which is A^{-1}. As t varies and provided that δ is small enough, $B(t)$ the joint diagonalizer which satisfies (4) (in the orthogonal case) or (5) (in the non-orthogonal case) can be written as:

$$B(t) = (I + t\Delta)A^{-1} + o(t), \ \ t \in [-\delta, \delta] \tag{8}$$

where I is the $n \times n$ identity matrix, $\Delta \in \mathbb{R}^{n\times n}$ with $\mathrm{diag}(\Delta) = 0$ and $\frac{\|o(t)\|}{t} \to 0$ as $t \to 0$. Again we emphasize that the above equality should be understood up to scale and permutation. For the OJD problem (where $B(t)$ is orthogonal), Δ is a skew-symmetric matrix. $\|\Delta\|$ measures the sensitivity of the joint diagonalization problem to noise. The larger the $\|\Delta\|$, the more sensitive the problem is. Note that if the corresponding EJD (i.e. when $t = 0$) does not have a unique solution we expect the sensitivity to be infinity and that is what we will show. Our main tool will be to apply perturbation analysis to find Δ.

4.1. Sensitivity of the OJD Problem

Based on what preceded one can have (see [8] also):

Theorem 3 *Let $C_i = A\Lambda_i A^T + tN_i, 1 \le i \le N$ ($t \in [-\delta, \delta]$), where $A \in O(n)$, Λ_i's are diagonal and N_i's are symmetric matrices. For small enough δ we have that $B(t)$ the minimizer of $J_1(B)$ on $O(n)$ (i.e. the orthogonal joint diagonalizer of C_i's) satisfies: $B(t) = (I + t\Delta)A^T + o(t)$ where Δ is a skew-symmetric matrix whose (k,l) entry is:*

$$\Delta_{kl} = \frac{\mathcal{S}_{kl}}{\sum_{i=1}^{N}(\lambda_{ik} - \lambda_{il})^2} \tag{9}$$

and

$$\mathcal{S} = -\sum_{i=1}^{N}[(A^T N_i A)^\circ, \Lambda_i] \tag{10}$$

with $[X, Y] = XY - YX$ being the matrix Lie bracket.

The $\mathcal{S}$ in (10) manifests the effect of noise in Δ. Note that since A is orthogonal we will not have noise amplification in $\mathcal{S}$, which is in contrast to the case of NOJD, as we shall see. Also one can show that if $\min_{k\neq l}\sum_{i=1}^{N}(\lambda_{ik} - \lambda_{il})^2 = \beta$ then:

$$\|\Delta\|_F \le \frac{1}{\beta}\|\mathcal{S}\|_F \tag{11}$$

4.2. Sensitivity of the NOJD Problem

For sensitivity analysis of the NOJD problem we provide the following result. Its derivation is straightforward which for lack of space we omit. The full derivations are given in [10].

Theorem 4 *Let $C_i = A\Lambda_i A^T + tN_i, 1 \le i \le N$ ($t \in [-\delta, \delta]$). Let us define $B(t)$ the non-orthogonal joint diagonalizer for $\{C_i\}_{i=1}^N$ as (5). Then for small enough δ the joint diagonalizer can be written as: $B(t) = (I + t\Delta)A^{-1} + o(t)$ where Δ (with diag$(\Delta) = 0$) satisfies*

$$M_{kl}\begin{bmatrix}\Delta_{kl}\\ \Delta_{lk}\end{bmatrix} = \begin{bmatrix}\mathcal{T}_{kl}\\ \mathcal{T}_{lk}\end{bmatrix},\ 1 \le k < l \le n \tag{12}$$

with

$$\mathcal{T} = -\sum_{i=1}^{N}(A^{-1}N_i(A^{-1})^T)^\circ\Lambda_i \tag{13}$$

and

$$M_{kl} = \gamma_{kl}\begin{bmatrix}\frac{1}{\eta_{kl}} & \rho_{kl}\\ \rho_{kl} & \eta_{kl}\end{bmatrix} \quad 1 \le k \neq l \le N \tag{14}$$

and

$$\gamma_{kl} = (\sum_{i=1}^{N}\lambda_{ik}^2)^{\frac{1}{2}}(\sum_{i=1}^{N}\lambda_{il}^2)^{\frac{1}{2}},\ \ \eta_{kl} = \frac{(\sum_{i=1}^{N}\lambda_{ik}^2)^{\frac{1}{2}}}{(\sum_{i=1}^{N}\lambda_{il}^2)^{\frac{1}{2}}} \tag{15}$$

.

Here also $\mathcal{T}$ manifests the noise contribution in the sensitivity. In contrast to the OJD case, if A is bad-conditioned, norm of A^{-1} can be large and hence $\|\mathcal{T}\|$ can be large and we can have noise amplification. Also one can show that

$$\|\Delta\|_F < \frac{\alpha}{(1-\rho^2)}\|\mathcal{T}\|_F \tag{16}$$

where $\alpha = \max_{k\neq l}\frac{\eta_{kl}+\frac{1}{\eta_{kl}}}{\gamma_{kl}}$ and $|\rho|$ is the modulus of uniqueness for the set $\{\Lambda_i\}_{i=1}^N$ as defined before. From (16) or from (12) together with (14) it is evident that if $|\rho| \approx 1$ then $\|\Delta\|$ can be large and we can not expect an accurate solution.

4.3. Effect of the Number of Matrices

A very interesting question related to the JD problem is about the effect of the number of matrices on accuracy of the solution. As mentioned before generically $N = 1$ matrix for OJD and $N = 2$ matrices for NOJD are enough to give an answer. However, to combat noise, we may want to include more matrices. Inclusion of more matrices can have two effects: one on how $\mathcal{T}$ for NOJD (or $\mathcal{S}$ for OJD) changes and the other one on how α and especially ρ for NOJD (or β for OJD) may change. This, of course, depends on how N_i's and Λ_i's are statistically distributed. For example, consider the case of NOJD and assume that the elements of N_i's as well as the elements of Λ_i's are i.i.d with zero mean and all matrices are independent from each other. Also assume that each diagonal element of Λ_i has variance σ^2. Then, by the strong law of large numbers, we have that $\|\frac{\mathcal{T}}{N}\| \to 0$, $\rho \to 0$, $N\alpha \to 2/\sigma^2 < \infty$ as $N \to \infty$ with probability one. Hence, $\|\Delta\| \to 0$ as $N \to \infty$ with probability one. However, if N_i's and Λ_i's were of positive-definite mean then we could not reach at this conclusion. This case could be relevant when we are jointly diagonalizaing a set of correlation matrices, for example. On the other hand for small values of N such as $N = 2, 3$ or 4, and especially when n is large, $|\rho|$ can be fairly large. Moreover the cancelation or averaging that we expect to happen for large N in $\mathcal{T}$ is not likely to happen for small N.

5. NUMERICAL EXPERIMENTS

Here we perform some experiments to test our theoretical results. We generate our matrices as in (7). We draw the ele-

Table 1. (Top): Sensitivity of Index(BA) with respect to noise level t as N and hence ρ changes for NOJD. (Bottom): Sensitivity of Index(BA) with respect to noise level t as N changes for OJD.

Index(BA)	$t = 0$	$t = 10^{-4}$
$N = 2, \rho = 0.999$	.06	1.19
$N = 10, \rho = 0.946$	2×10^{-13}	.17

Index(BA)	$t = 0$	$t = 10^{-4}$
$N = 2$	6×10^{-14}	.036
$N = 10$	2×10^{-14}	0.011

ments of N_i's from standard normal distribution and the diagonal elements of Λ_i's from uniform distribution between 0 and 1. We choose $n = 10$ and vary N and t. We use $N = 2, 10$ and $t = 0, 10^{-4}$. Also we test with A orthogonal and a non-orthogonal A with condition number of 25 and $\|A\|_F = \sqrt{10}$. The reason for choosing this value for $\|A\|_F$ is that this is the norm of an orthogonal 10×10 matrix and this makes comparisons more sensible. As it was evident from our calculations the sensitivity depends on the norms of the matrices involved. So we try to be fair and not change the norms in different experiments. This means that we use the same A and set of Λ_i's and noise matrices for different experiments. For OJD (i.e. orthogonal A) we use the algorithm introduced in [1] and for NOJD (i.e. non-orthogonal A) we use the algorithm QRJ2D introduced in [7]. The output of each run is a matrix B that should be close to A (up to scale and permutation factors) and we use this index to measure the closeness:

$$\text{Index}(P) = \sum_{i=1}^{n}\left(\sum_{j=1}^{n} \frac{|p_{ij}|}{\max_k |p_{ik}|} - 1\right) + \sum_{j=1}^{n}\left(\sum_{i=1}^{n} \frac{|p_{ij}|}{\max_k |p_{kj}|} - 1\right) \tag{17}$$

with $P = BA$. Index$(BA) \geq 0$ and equality happens only when B is a column permuted and scaled version of A^{-1}. Table (1) shows the resulted Index(BA) for different tests. We should mention that the actual Index value depends on the specific algorithm used, but this table should give a sense of a trend that in general introducing more matrices improves the accuracy of JD. Also note that for NOJD with $N = 2$, $\rho = .999$ which makes the problem very sensitive as shown in the table. Again we remind that how ρ behaves in terms of N in general depends on the statistical distribution of the elements of Λ_i's. Also note that Index(BA) is lower for OJD than NOJD which corroborates the expectation that NOJD is more difficult than OJD.

6. CONCLUSIONS

We considered the sensitivity of the OJD and NOJD problems to noise. Our main result is that uniqueness of the underlying EJD problem and the condition number of the joint diagonalizer affect the level of the difficulty of the JD problem. The NOJD problem can be very sensitive when the matrices are large and the number of them is small. Inclusion of more matrices in the NOJD process can improve the accuracy of the solution via improving the modulus of uniqueness and averaging out the noise. Also we gave some intuition and experimental evidence that why NOJD is more difficult than OJD.

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