MATRIX FACTORIZATION FOR BILINEAR BLIND SOURCE SEPARATION: METHODS, SEPARABILITY AND CONDITIONING

Yannick Deville

Université de Toulouse, UPS-CNRS-OMP
IRAP (Institut de Recherche en Astrophysique et Planétologie)
14 Av. Edouard Belin, F-31400 Toulouse, France

ABSTRACT

This paper deals with a general class of blind source separation methods for bilinear mixtures, using a structure based on matrix factorization, which models the direct, i.e. mixing, function, thus not requiring the analytical form of the inverse model. This approach also initially does not set restrictions on e.g. statistical independence, nonnegativity or sparsity, but on linear independence of sources and some source products. The separation principle used for adapting the parameters of the above structure consists in fitting the observations with the above direct model. We prove (for two sources at this stage) that this principle ensures separability, i.e. unique decomposition. Associated criteria and algorithms are also described. Performance is illustrated with preprocessed hyperspectral remote sensing data. This also allows us to highlight potential conditioning issues of some practical bilinear matrix factorization (BMF) methods and to suggest how to extend them.

Index Terms— bilinear matrix factorization, direct modeling, exact fit, separability (uniqueness of decomposition)

1. INTRODUCTION

Blind source separation (BSS) methods aim at restoring a set of unknown source signals from a set of observed signals which are mixtures of these source signals [2], [3]. In most investigations, the above mixtures consist of linear combinations of source signals. More recently, various works focused on nonlinear mixing operators [2]. This especially concerns linear-quadratic (LQ), including bilinear, memoryless operators, which appear in various application fields, such as remote sensing [5], [6] and processing of scanned images involving the show-through effect [4]. This non-linearity of the mixing model is traditionally considered as an issue, coming in addition to the usual difficulties already faced when dealing with *linear* BSS. However, we hereafter introduce an original position from this point of view, by showing that mixture nonlinearity can be *exploited* in order to introduce new BSS approaches that are not applicable to linear mixtures.

This work was partly supported by the French ANR project "HYEP ANR 14-CE22-0016-01", as from Jan. 2015.

More precisely, a complete BSS investigation consists in defining five items: the considered mixing model, separating structure, separation principle (e.g. ICA), separation criterion (e.g. minimization of a given cost function) and separation algorithm. Many investigations in the literature include original contributions only for the above last item, i.e. for separation algorithms. On the contrary, considering bilinear mixtures defined in Section 2, our contributions hereafter cover a broader scope. We first define Bilinear BSS methods based on Matrix Factorization (MF), i.e. BMF methods, in Section 3. We then analyze their theoretical separability properties and discuss their practical conditioning in Section 4. Numerical simulations with realistic data are then used in Section 5, not only to illustrate the performance of a specific BMF method proposed above but mainly to highlight conditioning properties of the considered general class of BMF methods. Conclusions are eventually drawn from this investigation in Section 6.

2. BILINEAR MIXING MODEL

Considering real-valued signals which depend on a discrete variable n, the scalar form of the bilinear (memoryless, or instantaneous) mixing model reads

$$x_i(n) = \sum_{j=1}^{M} a_{ij} s_j(n) + \sum_{j=1}^{M-1} \sum_{k=j+1}^{M} b_{ijk} s_j(n) s_k(n) \quad \forall\, i \in \{1, \ldots, P\} \qquad (1)$$

where $x_i(n)$ are the values of the P observed mixed signals for the sample index n and $s_j(n)$ are the values of the M unknown source signals which yield these observations, whereas a_{ij} and b_{ijk} are respectively the linear and quadratic mixing coefficients (with unknown values in the blind case) which define the considered source-to-observation transform.

A first matrix form of that model (1) reads

$$x(n) = As(n) + Bp(n) \qquad (2)$$

where the source and observation vectors are

$$s(n) = [s_1(n), \ldots, s_M(n)]^T \qquad (3)$$

$$x(n) = [x_1(n), \ldots, x_P(n)]^T, \qquad (4)$$

978-0-9928626-3-3/15/$31.00 ©2015 IEEE

where ^{T} stands for transpose and matrix A consists of the mixing coefficients a_{ij}. The column vector $p(n)$ is composed of all source products $s_j(n)s_k(n)$ of (1), i.e. with $1 \leq j < k \leq M$, arranged in a fixed, arbitrarily selected, order (see e.g. [6] for the natural order). The matrix B is composed of all entries b_{ijk} arranged so that i is the row index of B and the columns of B are indexed by (j,k) and arranged in the same order as the source products $s_j(n)s_k(n)$ in $p(n)$.

An even more compact form of this model may be derived by stacking row-wise the vectors $s(n)$ and $p(n)$ of sources and source products in an extended vector

$$\tilde{s}(n) = \begin{bmatrix} s(n) \\ p(n) \end{bmatrix} \tag{5}$$

whereas the corresponding matrices A and B are stacked column-wise in an extended matrix

$$\tilde{A} = [A \;\; B]\,. \tag{6}$$

The bilinear mixing model (2) then yields

$$x(n) = \tilde{A}\tilde{s}(n). \tag{7}$$

A third matrix-form model may eventually be derived by stacking column-wise all available signal samples, which correspond to n ranging from 1 to N, in the matrices

$$\tilde{S} = [\tilde{s}(1), \ldots, \tilde{s}(N)] \tag{8}$$

$$X = [x(1), \ldots, x(N)]. \tag{9}$$

The single-sample model (7) thus yields its overall matrix version

$$X = \tilde{A}\tilde{S}. \tag{10}$$

3. BLIND SEPARATION METHODS BASED ON BMF

3.1. Methods using a source-constrained structure

Generally speaking, a separating system aims at providing estimates of source signals, by using adequately tuned parameters. Within this framework, a standard approach uses systems which receive the observations as their inputs and which combine them according to a model which implements a class of functions equal to the *inverse* of the class of functions corresponding to the mixing model. The parameter values of such a system define one single function within this class and should be selected so as to match those of the single function corresponding to the considered mixture. The outputs of this separating system thus yield estimates of the source signals.

Within the above overall framework, we here propose to use a different approach, by building a system which aims at modeling the *direct*, i.e. mixing, function. Since the latter function is defined by (10), the variables involved in our separating structure consist of two matrices, C and D, which respectively aim at estimating $\tilde{A}$ and $\tilde{S}$ (possibly up to some indeterminacies). The rows of $\tilde{S}$ and thus D may be seen as vectors used to decompose the row vectors of X, whereas $\tilde{A}$ and thus C contain the coefficients of this decomposition. Moreover, matrix $\tilde{S}$ is guaranteed to be constrained: as shown by (5) and (8), only its top M rows are free, i.e. they contain the source values, whereas all subsequent rows are element-wise products of the above rows. Therefore, we set the same constraint on the adaptive variable D of our separating structure. This means that the top M rows of D are master, i.e. freely tuned, variables. These M row vectors are respectively denoted as d_1 to d_M. On the contrary, all subsequent rows of D are slave variables, which are updated together with the above top M rows, so as to contain element-wise products $d_j \odot d_k$ of those top M rows. These $d_j \odot d_k$ products are only stored for $1 \leq j < k \leq M$ and arranged in a fixed, arbitrarily selected, order (see e.g. [6] for the natural order).

We already proposed to use the LQ version of the above mixing model (10) and separating structure in previous investigations, e.g. [6]. However, we stress that our previous approach was restricted to nonnegative sources and mixing coefficients. On the contrary, the approach proposed in this paper initially does not set any such restriction (nor does it require the "sum-to-one" constraint used for some parameters in [6] and in some partly similar methods for linear mixtures).

We then propose the following methods for adapting matrices C and D of the above separating structure. The separation principle consists in updating these variables associated with the direct model so that their product CD fits the observation matrix X, in order to ideally achieve $CD = X$. This class of methods and their separation principle are therefore called Bilinear Matrix Factorization, or BMF, hereafter. The relevance of this separation principle specifically for bilinear mixtures is justified in Section 4. Several criteria for adapting C and D may then be derived from this separation principle. The most natural one consists in minimizing the cost function

$$J_1 = ||X - CD||_F \tag{11}$$

(or its square), where $||.||_F$ stands for Frobenius norm. A modified version of this BMF approach may be derived as follows.

3.2. Methods using a doubly-constrained structure

In the above version of our methods, both C and the top M rows of D are master, i.e. independently updated, variables. However, since this adaptation aims at minimizing $J_1 = ||X - CD||_F$, a different adaptation scheme may be used. In this scheme, only the top M rows of D are considered as master variables. In each occurence of the loop for updating D, the slave variable C is set to its optimum value, i.e. to its value which minimizes $||X - CD||_F$ with respect to C for the considered value of D. This optimum is nothing but the least squares (LS) solution, i.e. (assuming D has full

row rank) [7]

$$C_{opt} = XD^T(DD^T)^{-1}. \quad (12)$$

Setting $C = C_{opt}$ in (11), the cost function to be optimized (only with respect to the top M rows of D) becomes

$$J_2 = ||X(I - D^T(DD^T)^{-1}D)||_F \quad (13)$$

(or its square). Using $C = C_{opt}$ is attractive, first because the number of master variables adapted when using C_{opt} and therefore J_2 is much lower than when using J_1, so that the searched space has a much lower dimension, which may decrease computational time and improve convergence properties. Moreover, C and J_2 are thus defined by a closed-form expression, which allows one to derive the gradient of J_2 with respect to the master part of D. This gradient may then be used in gradient-based optimization algorithms.

The last step of the development of BMF methods consists in defining the considered separation algorithm(s). Various algorithms may be derived for minimizing the above cost functions J_1 or preferrably J_2. As suggested above, this e.g. includes standard gradient descent and extended gradient-based minimization methods, that we will report elsewhere. Derivative-free optimization algorithms may also be used. In particular, the algorithm used hereafter to minimize J_2 is the Nelder-Mead (NM) method, as implemented in the fminsearch() Matlab function. The resulting version of our BMF methods is therefore called BMF-LS-NM. Before presenting associated test results, we analyze the theoretical properties of BMF in general and we discuss its conditioning.

4. SEPARABILITY AND CONDITIONING

We here consider the overall BMF class of BSS methods, i.e. not restricting ourselves to any resulting separation criterion or algorithm. The separation principle thus consists in selecting the observation-modeling variables C and D so that their product CD fits the observation matrix X. The above-defined structure of $\tilde{S}$ and D is then of major importance: it is the reason why one may hope this separating structure for bilinear mixtures not to suffer from unacceptably high indeterminacies. This may first be intuitively explained as follows. For an arbitrary value of the top M rows of D, the matrix product CD yields row vectors which are combinations of the M vectors d_1 to d_M and of their element-wise products $d_j \odot d_k$ with $1 \leq j < k \leq M$. Let us e.g. consider the undesired case when each vector d_j is not collinear to one of the actual source vectors which compose the top M rows of $\tilde{S}$, but is a linear combination of the latter vectors. Then, one may hope that the following property is met: the vector products $d_j \odot d_k$ have a "complex form" and are thus outside the subspace spanned by the actual source vectors and their element-wise products, i.e. outside the subspace spanned by the rows of X. Then, the product CD cannot exactly fit the observation matrix X, wathever the value of C. Therefore, conversely, the exact fit $CD = X$ may be hoped to be achieved only when D extracts the source signals, up to scaling and permutation.

We are going to give a proof for the above property but, before this, we stress that this property is a new phenomenon, i.e. only obtained thanks to the nonlinear nature of the considered mixture. On the contrary, if the mixing model is linear and D is therefore restricted to its linear part, i.e. top M rows, when each of these rows is an arbitrary linear combination of the actual source vectors, the rows of CD are linear combinations of the actual source vectors, as the rows of X. If the rows of D span the same subspace as X, the coefficients in C can then always be selected so that $CD = X$ exactly. This linear version of the MF separation principle therefore does not allow one to retrieve the sources: D may thus yield any linear *mixture* of these sources. If trying to use the (linear) MF principle for the linear mixing model, the data must therefore be further constrained. Such a constraint consists in requesting all entries of C, D and X to be nonnegative, thus leading to Nonnegative Matrix Factorization (NMF) [1], although this nonnegativity constraint has been shown not to be sufficient for ensuring the uniqueness of the linear NMF decomposition.

We now prove the above-mentioned property for bilinear mixtures, for $M = 2$ sources at this stage. The three rows of D are then d_1, d_2 and $d_1 \odot d_2$. Similarly, $\tilde{S}$ consists of the three row vectors s_1, s_2 and $s_1 \odot s_2$, which are here assumed to be linearly independent, so that they span a three-dimensional subspace. All row vectors of X belong to this subspace, and we here assume that they actually span this subspace (this only requires X to contain at least three, linearly independent, row vectors). If the exact fit condition $CD = X$ is met, the subspace spanned by $\{d_1, d_2, d_1 \odot d_2\}$ is equal to the subspace spanned by $\{s_1, s_2, s_1 \odot s_2\}$, and therefore i) the vectors d_1, d_2 and $d_1 \odot d_2$ are non-zero, linearly independent, and ii) each of them is a linear combination of the vectors s_1, s_2 and $s_1 \odot s_2$. Property ii) above yields three conditions. The first two of them read

$$d_1 = e_{11}s_1 + e_{12}s_2 + e_{13}s_1 \odot s_2 \quad (14)$$

$$d_2 = e_{21}s_1 + e_{22}s_2 + e_{23}s_1 \odot s_2 \quad (15)$$

and they therefore entail

$$\begin{aligned} d_1 \odot d_2 = {} & e_{11}e_{21}s_1 \odot s_1 + (e_{11}e_{22} + e_{12}e_{21})s_1 \odot s_2 \\ & + e_{12}e_{22}s_2 \odot s_2 \\ & + (e_{11}e_{23} + e_{13}e_{21})s_1 \odot s_1 \odot s_2 \\ & + (e_{12}e_{23} + e_{13}e_{22})s_1 \odot s_2 \odot s_2 \\ & + e_{13}e_{23}s_1 \odot s_1 \odot s_2 \odot s_2. \end{aligned} \quad (16)$$

Moreover, if the eight vectors in the set $\{s_1, s_2, s_1 \odot s_1, s_1 \odot s_2, s_2 \odot s_2, s_1 \odot s_1 \odot s_2, s_1 \odot s_2 \odot s_2, s_1 \odot s_1 \odot s_2 \odot s_2\}$ are linearly independent, the third condition contained in Property ii) above entails that all coefficients in (16) except the

one corresponding to $s_1 \odot s_2$ are null, i.e.

$$\begin{aligned} e_{11}e_{21} &= 0 && (17)\\ e_{12}e_{22} &= 0 && (18)\\ e_{11}e_{23} + e_{13}e_{21} &= 0 && (19)\\ e_{12}e_{23} + e_{13}e_{22} &= 0 && (20)\\ e_{13}e_{23} &= 0. && (21) \end{aligned}$$

Eq. (17) has two solutions. The first one is

$$e_{11} = 0. \quad (22)$$

Eq. (18)-(21) then become

$$\begin{aligned} e_{12}e_{22} &= 0 && (23)\\ e_{13}e_{21} &= 0 && (24)\\ e_{12}e_{23} + e_{13}e_{22} &= 0 && (25)\\ e_{13}e_{23} &= 0. && (26) \end{aligned}$$

Let us assume that $e_{13} \neq 0$. Then, (24)-(26) and (15) are easily shown to yield $d_2 = 0$, which is not true, as stated above. Therefore

$$e_{13} = 0. \quad (27)$$

Eq. (23)-(26) then become

$$\begin{aligned} e_{12}e_{22} &= 0 && (28)\\ e_{12}e_{23} &= 0. && (29) \end{aligned}$$

Moreover, $e_{12} = 0$ is not possible because, together with (22), (27) and (14), it would yield $d_1 = 0$. Since $e_{12} \neq 0$, (28), (29) and (15) yield

$$d_2 = e_{21}s_1. \quad (30)$$

Besides, (22), (27) and (15) yield

$$d_1 = e_{12}s_2. \quad (31)$$

Conversely, any couple of vectors defined by (30)-(31) with arbitrary non-zero coefficients e_{ij} is indeed a solution to the problem, i.e. it allows CD to exactly fit X, because the sets $\{d_1, d_2, d_1 \odot d_2\}$ and $\{s_1, s_2, s_1 \odot s_2\}$ then span the same subspace.

It may be shown in the same way that the second solution of (17), i.e. $e_{21} = 0$, leads to the solution $d_1 = e_{11}s_1$ and $d_2 = e_{22}s_2$. As an overall result, under the above assumptions, the condition set by the BMF separation principle, i.e. $CD = X$, is met if and only if the considered separating structure restores the sources up to scale factors and permutation. In other words, this BMF separation principle then ensures separability (i.e. uniqueness of the BMF decomposition up to the above indeterminacies). Unlike in the linear case, this separability is obtained without setting such constraints as nonnegativity of the data.

The above result only concerns the considered *theoretical* separation principle and the associated *exact* equality $CD = X$. When then moving to *practical* BMF methods e.g. involving the criteria based on (11) or preferrably (13), and associated algorithms, one should in addition take into account the numerical conditioning of the considered cost functions. In other words, the above analysis showed that, if CD is made exactly equal to X, then D exactly restores the source vectors (up to acceptable indeterminacies), but the following question is still open: if CD is only made to get close to X, with a given accuracy (as when using practical BMF algorithms), then with which accuracy does D restore the source vectors ? One way to get insight into this topic consists in analyzing the convergence points of BMF algorithms, as will now be illustrated.

5. TEST RESULTS

As an example, we here apply the above approach to synthetic but realistic bilinear mixtures, corresponding to the remote sensing application described in [5], [6]. The considered two source vectors s_1 and s_2 are reflectance spectra, derived from the USGS hyperspectral database: each source sample is here obtained as the average of 200 adjacent samples of an original USGS spectrum. The source vectors are thus reduced to 10 samples, which allows us to investigate how the proposed approach behaves in the difficult case when limited information is available about the sources. Similarly, only 10 mixtures of these sources are used (this models 10 pixels of an observed image). Based on the physical mixing model derived in [5], the linear mixing coefficients a_{ij} are randomly, uniformly, drawn over $[0, 1]$ and then rescaled so as to sum to one in each observed vector, whereas the second-order coefficients b_{ijk} are uniformly drawn over $[0, 0.2]$. 100 Monte-Carlo tests are performed with the above data, using the above-defined BMF-LS-NM algorithm. Its master variables d_1 and d_2 are initialized with values respectively equal to s_1 and s_2 plus random noise, with uniform distribution over $[-0.05, 0.05]$.

Performance is analyzed by first computing two error parameters involving the above initial value of D and the associated value C_{opt} of C, defined by (12). First, the normalized root-mean-square error for sources is defined as

$$E_{src} = \frac{\sqrt{\min\limits_{i \neq j \in \{1,2\}} (F_{ij})}}{\sqrt{||s_1||^2 + ||s_2||^2}} \quad (32)$$

where F_{ij} is equal to:

$$\min_{\epsilon_1 = \pm 1} \left(||s_1 + \epsilon_1 \frac{||s_1||}{||d_i||} d_i||^2 \right) + \min_{\epsilon_2 = \pm 1} \left(||s_2 + \epsilon_2 \frac{||s_2||}{||d_j||} d_j||^2 \right).$$

Then, the normalized reconstruction error is defined as

$$E_{recons} = \frac{||X - C_{opt}D||_F}{||X||_F}. \quad (33)$$

The corresponding scatter plot in the (E_{src}, E_{recons}) plane, for all 100 Monte-Carlo tests, is shown in Fig. 1.

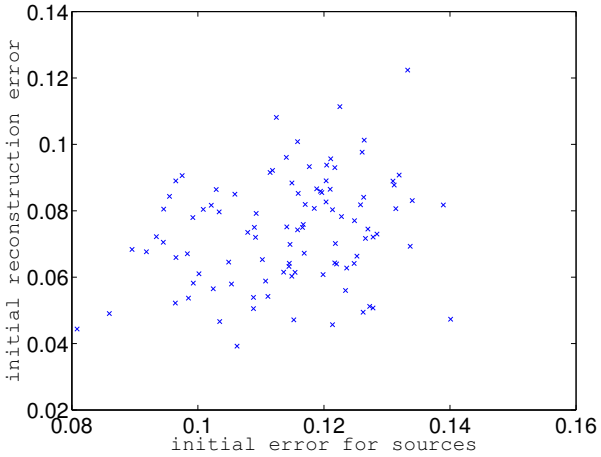

Fig. 1. Scatter plot in (E_{src}, E_{recons}) plane, before running BMF-LS-NM.

The values of the above two performance parameters are then considered for the value of D obtained after BMF-LS-NM converged, and for the associated value C_{opt} of C. The corresponding scatter plot is shown in Fig. 2.

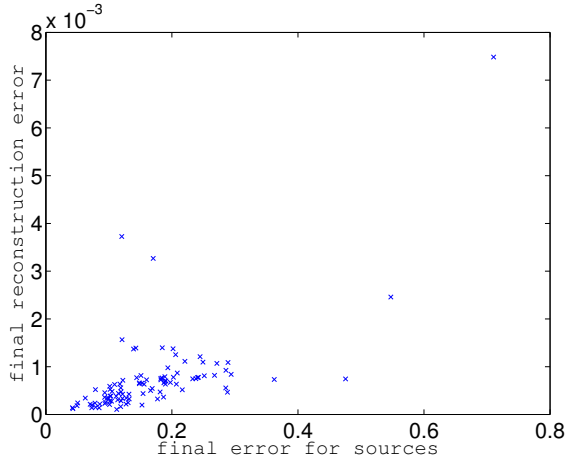

Fig. 2. Scatter plot in (E_{src}, E_{recons}) plane, after running BMF-LS-NM.

Comparing the above two plots first proves that BMF-LS-NM always succeeds in strongly decreasing the cost function J_2, as expected. Moreover, this shows that, despite this good fit of CD with respect to X obtained after convergence of BMF-LS-NM, the source estimates obtained in the top rows of D may then still be significantly different from the actual (rescaled and permuted) source vectors, thus leading to non-negligible values of E_{src} [1]. This conditioning issue is discussed hereafter.

[1] The bottom part of Fig. 2 shows that this problem cannot be avoided by selecting the runs of BMF-LS-NM yielding the lowest reconstruction error.

6. CONCLUSION

The general BMF class of BSS methods addressed in this paper is attractive because 1) it initially does not require the statistical independence, nonnegativity or sparsity of the source signals but only linear independence of sources and some element-wise source products (see the constraint defined after (16)), 2) it does not require knowing the analytical form of the inverse of the mixing model but only of the direct, i.e. mixing, model, 3) its separation principle was shown (for 2 sources at this stage) to ensure theoretical separability (i.e. uniqueness of decomposition up to the above indeterminacies). However, despite that separability, some corresponding practical cost functions and algorithms may lead to numerical conditioning issues, as illustrated above for our BMF-LS-NM method. This suggests us to further investigate the cost functions and algorithms that may be developed for the general class of BMF methods and/or to add constraints to these cost functions. These constraints for practical conditioning should be contrasted with those required for theoretical separability when addressing linear mixtures. For bilinear mixtures too, a natural constraint is nonnegativity, that we started to investigate in [6]. We will report about other constraints in future papers also dealing with BMF methods.

REFERENCES

[1] A. Cichocki, R. Zdunek, A. H. Phan, S.-I. Amari, "Nonnegative matrix and tensor factorizations. Applications to exploratory multi-way data analysis and blind source separation", Wiley, Chichester, UK, 2009.

[2] P. Comon and C. Jutten Eds, "Handbook of blind source separation. Independent component analysis and applications", Academic Press, Oxford, UK, 2010.

[3] Y. Deville, "Traitement du signal : signaux temporels et spatiotemporels - ... séparation aveugle de sources", Ellipses Editions Marketing, Paris, France, 2011.

[4] L. T. Duarte, C. Jutten, S. Moussaoui, "Bayesian source separation of linear and linear-quadratic mixtures using truncated priors", Journal of Signal Processing Systems, vol. 65, issue 3, pp. 311-323, Dec. 2011.

[5] I. Meganem, P. Déliot, X. Briottet, Y. Deville, S. Hosseini, "Linear-quadratic mixing model for reflectances in urban environments", IEEE Trans. on Geos. and Remote Sensing, vol. 52, no. 1, pp. 544-558, Jan. 2014.

[6] I. Meganem, Y. Deville, S. Hosseini, P. Déliot, X. Briottet, "Linear-quadratic blind source separation using NMF to unmix urban hyperspectral images", IEEE Transactions on Signal Processing, vol. 62, no. 7, pp. 1822-1833, April 1, 2014.

[7] A. Smilde, R. Bro, P. Geladi, "Multi-way analysis with applications in the chemical sciences", Wiley, Chichester, England, 2004.