NON-NEGATIVE SOURCE SEPARATION: RANGE OF ADMISSIBLE SOLUTIONS AND CONDITIONS FOR THE UNIQUENESS OF THE SOLUTION

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ABSTRACT

A main issue in source separation is to deal with the indeterminacies. Well known are the ordering and scale ambiguities, but other types of indeterminacies may also occur. In this paper we address these indeterminacies in the case of non-negative sources and non-negative mixing coefficients. On the one hand, we fully develop the case of two sources. On the other hand, in the general case we formulate necessary conditions for the uniqueness of the solution (up to ordering and scale ambiguities).

1. INTRODUCTION

The source separation model assumes that m observed signals of n samples $\{x_{ik}, k = 1..., n\}_{i=1}^{m}$ are a linear combination of p non-observable source signals $\{s_{jk}\}_{j=1}^{p}$. Using matrix notations, the whole mixing model is expressed as

$$\boldsymbol{X} = \boldsymbol{A}\,\boldsymbol{S}, \tag{1}$$

where $\boldsymbol{X}$ is the $(m \times n)$ data matrix, $\boldsymbol{A}$ is a $(m \times p)$ matrix of mixing coefficients, $\boldsymbol{S}$ is a $(p \times n)$ matrix of source signals. In non-negative source separation, the main constraints are $\forall\, i, j,\;\; a_{ij} \geq 0$ and $\forall\, j, k,\; s_{jk} \geq 0$, which will be denoted

$$\boldsymbol{A} \geq 0 \;\text{ and }\; \boldsymbol{S} \geq 0. \tag{2}$$

This separation problem is then formulated as follows: from the data $\boldsymbol{X}$, jointly find matrices $\boldsymbol{A}$ and $\boldsymbol{S}$ that fulfill the mixture model (1) and satisfy the constraints (2).

Some algorithms have been proposed to achieve the joint estimation of $\boldsymbol{A}$ and $\boldsymbol{S}$ [1–4]. However, before trying to effectively estimate the source signals and the mixing coefficients, it is necessary to answer some questions related to the model indeterminacies and solution uniqueness. When the solution is not unique, it is also useful to determine the range of admissible solutions. Up to our knowledge, this question has received only a few attention [5–7].

Section 2 of this paper states the problem and reformulates the scale and ordering indeterminacies in the case of non-negative source separation and section 3 addresses the case of two sources. We explicitly give the range of the admissible solutions, from which we deduce the necessary and sufficient conditions for the solution uniqueness. The results are illustrated through a simplified example in the field of spectrometry. The case of more than two sources is considered in section 4, for which necessary conditions for uniqueness are given.

2. PROBLEM STATEMENT

Throughout the paper, we assume the existence of a non-negative factorization of the data matrix $\boldsymbol{X}$. The conditions for the existence of such a factorization are discussed in [8]. Let us introduce a non-singular $(p \times p)$ matrix $\boldsymbol{T}$. From any pair $(\boldsymbol{A}, \boldsymbol{S})$, a new pair $(\tilde{\boldsymbol{A}}, \tilde{\boldsymbol{S}})$ can be defined by

$$\tilde{\boldsymbol{A}} = \boldsymbol{A}\boldsymbol{T}^{-1}, \tag{3}$$

$$\tilde{\boldsymbol{S}} = \boldsymbol{T}\boldsymbol{S}, \tag{4}$$

with no modification in the data matrix, i.e. $\boldsymbol{X} = \tilde{\boldsymbol{A}}\,\tilde{\boldsymbol{S}}$. In the unconstrained case, this transformation shows the existence of an infinite number of possible exact factorizations of the matrix $\boldsymbol{X}$. However, in the case of non-negative source separation, a possible linear transformation should lead to transformed matrices $\tilde{\boldsymbol{A}}$ and $\tilde{\boldsymbol{S}}$ satisfying

$$\tilde{\boldsymbol{A}} \geq 0 \;\text{ and }\; \tilde{\boldsymbol{S}} \geq 0. \tag{5}$$

In that respect, the remaining questions are: (i) what are the conditions on the true non-negative source signals and non-negative mixing coefficients ensuring the uniqueness of the decomposition (1) respecting the contraints (2)? (ii) If the decomposition is not unique, what is the range of admissible solutions? (iii) Among all the admissible solutions, can we define a preferable one?

In this paper only the points (i) and (ii) are addressed. However, before going further, let us reformulate the scale and ordering indeterminacies in the case of non-negative source separation.

2.1. Scale Indeterminacy

Consider the transformation defined by $\boldsymbol{T} = \mathrm{Diag}(\lambda_1, ..., \lambda_p)$ with $\lambda_i > 0$, so that $\boldsymbol{T}^{-1} = \mathrm{Diag}(1/\lambda_1, ..., 1/\lambda_p)$. The application of $\boldsymbol{T}$ and $\boldsymbol{T}^{-1}$ to $\boldsymbol{S}$ and $\boldsymbol{A}$ according to (4) and (3) corresponds to scale dilatations. Straightforwardly, we have $\tilde{\boldsymbol{A}}$, $\tilde{\boldsymbol{S}} \geq 0$ if $\boldsymbol{A}$, $\boldsymbol{S} \geq 0$. To handle this indeterminacy it is usual to impose additional constraints on the source signals (in general unit variance). Here, for convenience and without loss of generality, we assume each source signal to have coefficients summing to a unity.

2.2. Ordering Indeterminacy

The associated transformation $\boldsymbol{T}$ corresponds to a permutation of the i-th row with the j-th row of the matrix $\boldsymbol{S}$. Matrix $\boldsymbol{T}^{-1}$ then corresponds to a permutation of the i-th column with the j-th column of the matrix $\boldsymbol{A}$. Such permutation matrices having only 0 or 1 components, it is obvious that $\boldsymbol{A}$, $\boldsymbol{S} \geq 0$ implies $\tilde{\boldsymbol{A}}$, $\tilde{\boldsymbol{S}} \geq 0$. The ordering indeterminacy means that we cannot know in advance which index will be assigned to a particular source.

2.3. Definitions

Definition 1 *A pair $(\boldsymbol{A}, \boldsymbol{S})$ is said an admissible solution if both $\boldsymbol{A}$ and $\boldsymbol{S}$ satisfy (2) and jointly provide an exact factorization of $\boldsymbol{X}$ according to (1).*

Definition 2 *For a given data matrix $\boldsymbol{X}$, the solution of (1) under constraints (2) is said unique if the only sources of ambiguities are the scale and ordering indeterminacies.*

3. CASE OF TWO SOURCES

3.1. Preliminaries

In the case of two sources, the matrices $\boldsymbol{A}$ and $\boldsymbol{S}$ can be represented by

$$\boldsymbol{A} = [\boldsymbol{a}_1 \ \boldsymbol{a}_2] \ \text{ and } \ \boldsymbol{S} = [\boldsymbol{s}_1 \ \boldsymbol{s}_2]^T, \tag{6}$$

where $\{\boldsymbol{a}_j\}_{j=1}^2$ are vectors of dimension $(m, 1)$ and $\{\boldsymbol{s}_j\}_{j=1}^2$ are vectors of dimension $(n, 1)$. To analyze the model indeterminacies, let us introduce the following matrix

$$\boldsymbol{T}(\alpha, \beta) = \begin{bmatrix} 1-\alpha & \alpha \\ \beta & 1-\beta \end{bmatrix}, \tag{7}$$

in which case the inverse matrix reads

$$\boldsymbol{T}^{-1}(\alpha, \beta) = \frac{1}{1-\alpha-\beta} \begin{bmatrix} 1-\beta & -\alpha \\ -\beta & 1-\alpha \end{bmatrix}. \tag{8}$$

In order to get rid of the ordering indeterminacy, the parameters α and β can be constrained to satisfy $\alpha + \beta < 1$. Moreover, such a constraint ensures that $\boldsymbol{T}$ is invertible.

Remark 1 *Note that handling the scale ambiguity by assuming the sum of each source coefficients to be equal to unity, i.e.* $\sum_{k=1}^n \tilde{s}_{jk} = \sum_{k=1}^n s_{ik} = 1, \ \forall i, j,$ *yields*

$$\sum_{k=1}^n \tilde{s}_{jk} = \sum_{k=1}^n \sum_{i=1}^p t_{ji}\, s_{ik} = \sum_{i=1}^p \left(t_{ji} \sum_{k=1}^n s_{ik} \right), \tag{9}$$

that is $\sum_{i=1}^p t_{ji} = 1, \quad \forall j = 1, ..., p.$

3.2. Range of Admissible Solutions

Using the parametric transformation defined in (7), the non-negativity constraint of the two transformed source signals reads

$$\forall k, \quad \tilde{s}_{1k} = (1-\alpha)s_{1k} + \alpha s_{2k} \geq 0, \tag{10}$$

$$\forall k, \quad \tilde{s}_{2k} = (1-\beta)s_{2k} + \beta s_{1k} \geq 0. \tag{11}$$

The non-negativity of the transformed mixing coefficients corresponds to

$$\forall \ell, \quad \tilde{a}_{\ell 1} = \frac{(1-\beta)a_{\ell 1} - \beta a_{\ell 2}}{1-\alpha-\beta} \geq 0; \tag{12}$$

$$\forall \ell, \quad \tilde{a}_{\ell 2} = \frac{(1-\alpha)a_{\ell 2} - \alpha a_{\ell 1}}{1-\alpha-\beta} \geq 0. \tag{13}$$

The resolution of all these inequalities with $\alpha + \beta < 1$ allows to get lower and upper bounds for the admissible values of α and β. In this respect, it will be useful to introduce the two following index sets $\mathbb{K}_1 = \{k; s_{2k} > s_{1k}\}$ and $\mathbb{K}_2 = \{k; s_{1k} > s_{2k}\}$.

It can be checked that the inequalities (10) and (11) provide a lower bounds for α and β as

$$\alpha \geq \alpha_{\min} = -\min_{k \in \mathbb{K}_1} \left\{ \frac{s_{1k}}{s_{2k} - s_{1k}} \right\}, \tag{14}$$

and

$$\beta \geq \beta_{\min} = -\min_{k \in \mathbb{K}_2} \left\{ \frac{s_{2k}}{s_{1k} - s_{2k}} \right\}. \tag{15}$$

Similarly, it is easy to show that (12) and (13) are equivalent to

$$\beta \leq \beta_{\max} = \min_{\ell} \left\{ \frac{a_{\ell 1}}{a_{\ell 1} + a_{\ell 2}} \right\}, \tag{16}$$

and

$$\alpha \leq \alpha_{\max} = \min_{\ell} \left\{ \frac{a_{\ell 2}}{a_{\ell 1} + a_{\ell 2}} \right\}. \tag{17}$$

Finally, the set of all admissible solutions corresponds to

$$\tilde{\boldsymbol{S}} = \boldsymbol{T}(\alpha, \beta)\, \boldsymbol{S}, \ \text{ and } \tilde{\boldsymbol{A}} = \boldsymbol{A}\, \boldsymbol{T}^{-1}(\alpha, \beta), \tag{18}$$

for $\alpha \in [\alpha_{\min}, \alpha_{\max}]$ and $\beta \in [\beta_{\min}, \beta_{\max}]$.

3.3. Uniqueness Conditions

Proposition 1 *The decomposition of $\boldsymbol{X}$ according to*

$$\boldsymbol{X} = \boldsymbol{A}\,\boldsymbol{S},\ \textit{with}\ \boldsymbol{A}, \boldsymbol{S} \geq 0, \tag{19}$$

is unique if an only if $\exists\ (k_1, k_2, \ell_1, \ell_2)$, with $k_1 \neq k_2$ and $\ell_1 \neq \ell_2$, such that

$$\begin{cases} s_{1k_1} = 0,\ \textit{and}\ s_{2k_1} \neq 0, \\ s_{2k_2} = 0,\ \textit{and}\ s_{1k_2} \neq 0, \\ a_{\ell_1 1} = 0,\ \textit{and}\ a_{\ell_1 2} \neq 0, \\ a_{\ell_2 2} = 0,\ \textit{and}\ a_{\ell_2 1} \neq 0. \end{cases} \tag{20}$$

Proof 1 *The proof results directly from section 3.2. According to the bounds defined by (14)–(17), the range of admissible values of α and β is reduced to $\alpha = 0$ and $\beta = 0$ if and only if conditions (20) are satisfied.*

3.4. Numerical Example

Let us illustrate the range of admissible solutions of non-negative source separation with the help of an example. The mixture data are obtained by constructing two non-negative signals (p=2, n=500) and mixing coefficient profiles (m=10) similar to what we get during the analysis of multicomponent substances in analytical chemistry using spectroscopic techniques. The source signals and the mixing coefficient profiles are shown in figure (1).

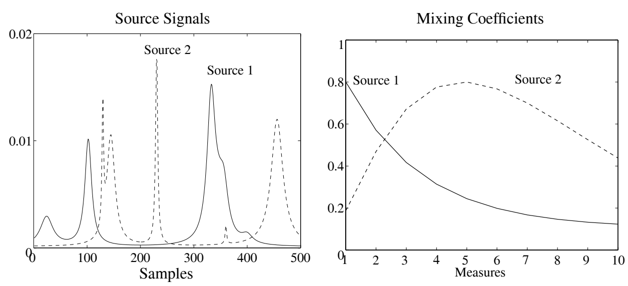

Fig. 1: Source signals and mixing coefficient profiles

The conditions for the uniqueness of the solution are not satisfied by the source signals and the mixing coefficients. Using the results of the previous section, it is easy to determine the bounds of the parameters of the possible transformation matrices

$$-0.0163 \leq \alpha \leq 0.1898, \tag{21}$$
$$-0.0198 \leq \beta \leq 0.1924. \tag{22}$$

The admissible solutions in terms of source signals and mixing coefficients are deduced according to (18) and are shown in figure 2.

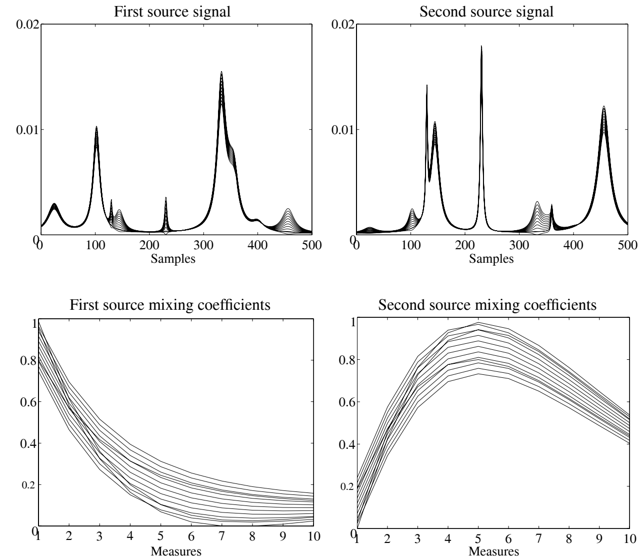

Fig. 2: Admissible solutions

4. CASE OF MORE THAN TWO SOURCES

In this section we consider the case of p source signals. Let

$$\boldsymbol{A} = [\boldsymbol{a}_1\ \cdots\ \boldsymbol{a}_p] \quad \text{and} \quad \boldsymbol{S} = [\boldsymbol{s}_1\ \cdots\ \boldsymbol{s}_p]^T, \tag{23}$$

where $\{\boldsymbol{a}_i\}_{i=1}^p$ are vectors of dimension $(m, 1)$ and $\{\boldsymbol{s}_j\}_{j=1}^p$ are vectors of dimension $(n, 1)$. For notational convenience, in this section, we will note $\boldsymbol{a}_i(\ell)$ the ℓ-th element of vector $\boldsymbol{a}_i$ and similarly, $\boldsymbol{s}_j(k)$ the k-th element of vector $\boldsymbol{s}_j$.

In this case, we are only able to give a necessary condition for the uniqueness of the solution.

Proposition 2 *If the decomposition of $\boldsymbol{X}$ into $\boldsymbol{A}$ and $\boldsymbol{S}$ according to*

$$\boldsymbol{X} = \boldsymbol{A}\,\boldsymbol{S}\ \textit{with}\ \boldsymbol{A}, \boldsymbol{S} \geq 0, \tag{24}$$

is unique, then the following conditions are satisfied:

(A1) $\exists\, k_1, \ldots, k_p$ *such that:*

$$\forall\, i \neq j,\ k_i \neq k_j,\ \boldsymbol{s}_i(k_i) = 0,\ \textit{and}\ \boldsymbol{s}_j(k_i) \neq 0. \tag{25}$$

(A2) $\exists\, \ell_1, \ldots, \ell_p$ *such that:*

$$\forall\, i \neq j,\ \ell_i \neq \ell_j,\ \boldsymbol{a}_i(\ell_i) = 0,\ \textit{and}\ \boldsymbol{a}_j(\ell_i) \neq 0. \tag{26}$$

Proof 2 *The proof of this theorem is achieved by contradiction: suppose that conditions (A1)-(A2) are not satisfied and the decomposition $\boldsymbol{X} = \boldsymbol{A}\,\boldsymbol{S}$ with $\boldsymbol{A}$, $\boldsymbol{S} \geq 0$, is unique.*

Suppose that the condition (A1) is not satisfied and let the $(p \times p)$ elementary transformation $\boldsymbol{T}_{ij}(\lambda)$ defined by

$$\forall\, k = 1, ..., p,\ \forall\, \ell = 1, ..., p,$$
$$\begin{cases} t_{kk} = 1, \\ t_{k\ell} = \lambda\ \textit{if}\ (k, \ell) = (i, j); \\ t_{k\ell} = 0\ \textit{if}\ (k, \ell) \neq (i, j)\ \textit{and}\ (k, \ell) \neq (k, k). \end{cases} \tag{27}$$

We note that $\boldsymbol{T}^{-1}(\lambda) = \boldsymbol{T}(-\lambda)$. *Define*

$$\mathbb{K} = \{k, \boldsymbol{s}_i(k) \neq 0, \boldsymbol{s}_j(k) \neq 0\}\,.$$

The samples where the sources $\boldsymbol{s}_i$ *and* $\boldsymbol{s}_j$ *are simultaneously zero are not taken into account since they are not affected by the possible transformations. The following decomposition*

$$\boldsymbol{X} = \boldsymbol{A}\,\boldsymbol{T}_{ij}(\lambda)\,\boldsymbol{T}_{ij}(-\lambda)\,\boldsymbol{S} \quad (28)$$

with $\lambda > 0$ *ensures the non-negativity of* $\tilde{\boldsymbol{A}} = \boldsymbol{A}\boldsymbol{T}_{ij}(\lambda)$ *and the matrix* $\boldsymbol{T}_{ij}(-\lambda)$ *leads to a transformation of the* i*-th source signal according to*

$$\tilde{\boldsymbol{s}}_i = \boldsymbol{s}_i - \lambda \boldsymbol{s}_j, \quad (29)$$

while the other source signals are unaltered. Defining $(\overline{s}_i, \underline{s}_j)$ *as* $\underline{s}_i = \min_{k \in \mathbb{K}} \boldsymbol{s}_i(k)$ *and* $\overline{s}_j = \max_{k \in \mathbb{K}} \boldsymbol{s}_j(k)$. *There exists* $0 < \lambda < \underline{s}_i / \overline{s}_j$ *such that*

$$\forall k,\ \boldsymbol{s}_i(k) - \lambda \boldsymbol{s}_j(k) \geq \underline{s}_i - \lambda \overline{s}_j \geq 0 \implies \boldsymbol{T}_{ij}(\lambda)\boldsymbol{S} \geq 0.$$

Therefore, the decomposition is not unique. This is in contradiction with the assumptions.

Concerning condition (A2) related to the mixing matrix, the same reasoning is employed using $\lambda < 0$.

This is a necessary but not sufficient condition which shows that, in most cases, the separation using only non-negativity assumptions cannot provide a unique. It would be interesting to state when the separation leads to a unique solution, through the formulation of necessary and sufficient condition for the factorization uniqueness. This point is currently under investigation.

5. CONCLUSION

This paper has shown that under well formulated conditions, the non-negative source separation problem admits a unique solution. These conditions are more flexible than those proposed in previous works [5, 6]. We are currently trying to link this work with the analysis of [7], which gives a geometrical interpretation of the question. The performances of a non-negative source separation algorithm depends on the fulfillment of the uniqueness conditions and the independence assumption. If the uniqueness conditions are satisfied, the independence assumption is not necessary to achieve a correct separation and methods such as ALS [1], NMF [3] will provide very effective results. However, they fail in separating mixtures that do not respect the uniqueness conditions. Similarly, applying the NNICA [9] to non-negative sources whose samples are not independent and/or not well grounded may also lead to wrong decompositions. Finally, the more challenging case is when the source samples are not independent and do not fulfill the uniqueness conditions. In this case, none of the available methods perform successfully the separation. The problem still remains open.

Acknowledgments

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6. REFERENCES

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