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# A Second-Order Statistics Method for Blind Source Separation in Post-Nonlinear Mixtures

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**Abstract**

In the context of nonlinear Blind Source Separation (BSS), the Post-Nonlinear (PNL) model is of great importance due to its suitability for practical nonlinear problems. Under certain mild constraints on the model, Independent Component Analysis (ICA) methods are valid for performing source separation, but requires use of Higher-Order Statistics (HOS). Conversely, regarding the sole use of the Second-Order Statistics (SOS), their study is still in an initial stage. In that sense, in this work, the conditions and the constraints on the PNL model for SOS-based separation are investigated. The study encompasses a time-extended formulation of the PNL problem with the objective of extracting the temporal structure of the data in a more extensive manner, considering SOS-based methods for separation, including the proposition of a new one. Based on this, it is shown that, under some constraints on the nonlinearities and if a

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given number of time delays is considered, source separation can be successfully achieved, at least for polynomial nonlinearities. With the aid of metaheuristics called Differential Evolution and Clonal Selection Algorithm for optimization, the performances of the SOS-based methods are compared in a set of simulation scenarios, in which the proposed method shows to be a promising approach.

*Keywords:* Blind Source Separation, Post-Nonlinear, Second-Order Statistics

## 1. Introduction

In many practical applications, retrieving a set of source signals from some observations that are actually mixtures of these sources can be of great relevance. If there is no (or incomplete) prior knowledge about the sources and mixing transform, the problem is referred to as Blind Source Separation (BSS) [1, 2, 3]. Throughout three decades of existence, this problem has been subject of great attention from the academic community, where the initial efforts were mainly aimed at the standard linear and instantaneous mixing model, with the assumption that the sources are statistically mutually independent. Indeed, the study of this topic contributed to a solid theoretical framework known as Independent Component Analysis (ICA) [1], which provided methods that explicitly use Higher-Order Statistics (HOS), such as FastICA, JADE and Infomax [1, 4].

Although the mutual independence assumption is sufficient for linear separation, the use of the HOS may result in some estimation difficulties. However, in certain cases, additional information about the sources can be explored to lead to simpler methods [5]. For instance, the sources may exhibit temporal structures (i.e., temporal dependence among samples), which can be statistically characterized e.g. by temporal correlations, being thus possible to perform source separation based only on Second-Order Statistics (SOS), if there is sufficient temporal diversity [1]. In this case, even Gaussian sources, which are not separable using HOS methods, can be separated. This perspective motivated the proposal of diverse SOS-based methods, such as SOBI [6], WASOBI [7], AMUSE, TDSEP, among others [1, 4]

Regarding the nonlinear BSS problem, there has been a considerable effort for extending the ICA framework and other BSS methods to nonlinear mixing models, in view of promising applications like smart chemical sensor arrays [8], hyperspectral imaging [9, 10] and quantum bit uncoupling [11]. However, from a general standpoint, mutual independence may not be sufficient for performing nonlinear separation [1]. Thus, except recent works [12] which propose a new general framework for nonlinear source separation, the studies on this topic were focused on a constrained set of nonlinear models in which the ICA methods are still valid [13]. For instance, the Post-Nonlinear (PNL) mixing model is composed of an instantaneous linear stage followed by a set of univariate nonlinear functions, which must obey some constraints (e.g., monotonicity) to enable the use ICA-based methods for separation [14].

However, when dealing with temporally structured sources in nonlinear models, there is still no parallel with the linear case [5, 13], especially because the study based on the sole use of the SOS is very incipient, raising fundamental issues like conditions for identifiability and uniqueness of solutions. In view of this, in this work, we focus on the analysis of SOS-based methods in the PNL mixing problem, prompting to outline the set of constraints and conditions to ensure the validity of the approach. This initial step is made by considering the case in which the nonlinearities belong to a class of cubic polynomials, revealing promising perspectives – including the nonlinear separation of Gaussian sources.

The SOS-based investigation to be followed is performed considering block-structured correlation matrices with a set of time delayed samples, being able to encompass the temporal structure of data more organically [15]. However, the potential nonlinear statistical dependencies it carries demands a suitable treatment of the statistical information, which will be attained through the proposition of a novel SOS-based criterion. Besides these contributions, we consider an extended formulation of the PNL problem, for which the manipulation of the block-structured matrices is more straightforward. This will allow the analytical computation of the considered SOS-based cost functions, providing a rich theoretical analysis.

Although SOS-based methods are usually associated with mathematical simplicity, the nonlinear context may lead to inherent complex multimodal SOS-based cost functions and hence, high computational cost. In that sense, a proper exploration of the search space can be performed by metaheuristics. In this work, the metaheuristics Differential Evolution (DE) [16] and Clonal Selection Algorithm (CLONALG) [17] are considered for parameter optimization in order to avoid local convergence.

This work is organized as follows. In Section 2, the PNL model is presented considering the temporal-extended formulation and the particular nonlinear case. Section 3 describes the SOS-based criteria to be used, introducing the proposed method; the analytical computation of the covariance matrices is presented as well. The identifiability conditions and bounds are analyzed in Section 4 and the performance results are shown in Section 5. Finally, Section 6 concludes the work.

## 2. The Post-Nonlinear Mixing Model

In the problem of Blind Source Separation (BSS), the main objective is to recover the original sources $\mathbf{s}(n)$ from observed mixtures $\mathbf{x}(n) = \mathbf{\Phi}(\mathbf{s}(n))$, with $\mathbf{x}(n) = [x_1(n), \cdots, x_M(n)]^T$ the observation vector with $M$ mixtures, $\mathbf{s}(n) = [s_1(n), \cdots, s_N(n)]^T$ the vector with $N$ source signals at time instant $n$ and $\mathbf{\Phi}(\cdot)$ the mixing mapping [1]. Generally, $\mathbf{\Phi}(\cdot)$ is assumed to be linear and instantaneous, however, this approach may not be adequate for certain applications and a nonlinear model must be considered, such as the Post-Nonlinear (PNL) [14].

The PNL structure is particularly interesting because it sequentially combines linear and nonlinear stages, as shown in Fig. 1. Due to their relative simplicity, the mixtures can be mathematically written as $\mathbf{x}(n) = \mathbf{f}(\mathbf{A}\mathbf{s}(n))$, where $\mathbf{A}$ is an $M \times N$ matrix and $\mathbf{f}(\cdot)$ is a set of $M$ component-wise functions. The separation system is the mirrored version of the mixing system, with output given by $\mathbf{y}(n) = \mathbf{W}\mathbf{g}(\mathbf{x}(n))$, where $\mathbf{W}$ is an $N \times M$ matrix and $\mathbf{g}(\cdot)$ is a set of $M$ component-wise functions [1]. In this work, we focus on the case in which

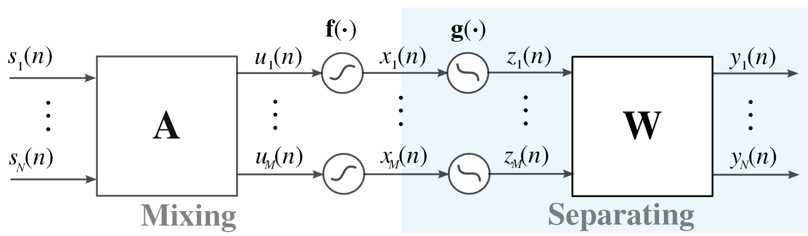



Figure 1: Mixing and separating systems in the PNL model.

$N = M$ (determined case), i.e., when the number of sources and of mixtures are equal (for a single source, the PNL model can establish important analogies with Wiener Hammerstein systems, due to their similarity [18]).

Under certain constraints on the nonlinear functions $\mathbf{f}(\cdot)$ and $\mathbf{g}(\cdot)$, it is known that the (independent) sources can be separated by ICA methods, which requires the use of HOS [1, 19]. However, under the additional assumption that the sources are temporally colored, the viability and the conditions for separation of PNL mixtures using only Second-Order Statistics (SOS) still remain open questions. In that sense, in this work, we search for these answers by considering a class of PNL mixtures to be separated by SOS-based methods. However, the temporal information will be extracted by block-structured correlation matrices with an arbitrary number of time delays. To facilitate the manipulation of these matrices, we formulate a temporal-extended version of the PNL problem, presented in the following.

### *2.1. Time-Dependent Sources in the PNL Model*

The temporal structure in the sources is usually seen as the inherent result of the system which generates them. However, in some applications, it can be modeled as the result of independent and identically distributed (*i.i.d.*) signals processed by linear or nonlinear systems, whose signature is the temporal structure imprinted on the signals. For simplicity, in this work, to investigate the (SOS) features in the PNL models, we restrain ourselves to the case in which the temporal structure is obtained by means of a linear filtering system.

To suitably describe the temporal structure in the sources, we consider vectors with the $N$ sources at time instant $n$ concatenated with $d$ delayed versions of them in the following form (similarly to [15]):

$$\begin{aligned}\underline{\mathbf{s}}(n) &= [s_1(n), \cdots, s_1(n{-}d), s_2(n), \cdots, s_2(n{-}d), \cdots, s_N(n), \cdots, s_N(n{-}d)]^T \\ &= \left[\underline{\mathbf{s}}_1^T(n), \underline{\mathbf{s}}_2^T(n), \cdots, \underline{\mathbf{s}}_N^T(n)\right]^T,\end{aligned} \tag{1}$$

where $d$ is the maximum considered time delay and $\underline{\mathbf{s}}_i(n) = [s_i(n), \cdots, s_i(n{-}d)]^T$, for $i = \{1, \ldots, N\}$. We wish to express the time-extended sources $\underline{\mathbf{s}}(n)$ as functions of $i.i.d$ signals $\underline{\mathbf{r}}(n)$ (note that all the underlined variables are time-extended versions of the classical formulation, similarly to $\underline{\mathbf{s}}(n)$ and $\mathbf{s}(n)$). In order to do so, we consider a set of $N$ Finite Impulse Response (FIR) filters that are responsible for introducing correlation in the signals $\underline{\mathbf{s}}(n)$ (i.e., $\underline{\mathbf{s}}(n)$ are composed of moving average (MA) processes [20]). The coefficients of each FIR filter are arranged in vectors $\mathbf{h}_i$, for $i = \{i, \ldots, N\}$. Hence, for instance, an FIR filter with transfer function $H_i(z) = h_{i,0} + h_{i,1}z^{-1} + \cdots + h_{i,L_{h_i}} z^{-L_{h_i}}$ is represented by the vector $\mathbf{h}_i = [h_{i,0}, h_{i,1}, \cdots, h_{i,L_{h_i}}]$. Based on this, we define

$$\mathbf{H}_i = \mathbf{h}_i \triangleright \mathbf{I}_{d+1} = \begin{bmatrix} h_{i,0} & \cdots & h_{i,L_{h_i}} & 0 & 0 & \cdots & 0 \\ 0 & h_{i,0} & \cdots & h_{i,L_{h_i}} & 0 & \cdots & 0 \\ \vdots & \ddots & & \ddots & & \ddots & \vdots \\ 0 & \cdots & 0 & h_{i,0} & \cdots & h_{i,L_{h_i}} & 0 \\ 0 & \cdots & 0 & 0 & h_{i,0} & \cdots & h_{i,L_{h_i}} \end{bmatrix}, \tag{2}$$

in which $\mathbf{h}_i \triangleright \mathbf{I}_{d+1}$ is the diagonal replication of vector $\mathbf{h}_i$, being the resulting matrix $\mathbf{H}_i$ of dimension $(d{+}1) \times (L_{h_i}{+}d{+}1)$, and $\mathbf{I}_{d+1}$ the identity matrix of size $d{+}1$.

For the sake of simplicity, we assume henceforth $N = 2$ sources without loss of generality. In this case, the sources $\underline{\mathbf{s}}(n)$ can be written as functions of $\underline{\mathbf{r}}(n)$:

$$\underline{\mathbf{s}}(n) = \underline{\mathcal{H}}\underline{\mathbf{r}}(n) = \begin{bmatrix} \mathbf{H}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{H}_2 \end{bmatrix} \underline{\mathbf{r}}(n), \tag{3}$$

where $\underline{\mathcal{H}}$ is a block-diagonal matrix with dimensions $N(d{+}1) \times (\sum_{i=1}^{N}(L_{h_i}{+}d{+}1))$ and $\underline{\mathbf{r}}(n) = [r_1(n), r_1(n{-}1), \cdots, r_1(n{-}L_{h_1}{-}d), r_2(n), r_2(n{-}1), \cdots, r_2(n{-}L_{h_2}{-}d)]^T$

is the temporal-extended *i.i.d.* vector with the original signals $r_1(n)$, $r_2(n)$ and their delayed versions. Note that the samples of each *i.i.d.* signal $r_i(n)$ considered separately will be combined by $\underline{\mathcal{H}}$, but there is no mixing between $r_1(n)$ and $r_2(n)$. Eq. (3) shall be useful for analytically computing certain statistical moments, since it express the sources $s_i(n)$ as functions of *i.i.d.* signals.

Proceeding with the PNL temporal-extended formulation, we can write the linear mixtures as $\underline{\mathbf{u}}(n) = \underline{\mathcal{A}}\underline{\mathbf{s}}(n)$, with the extended linear mixing matrix $\underline{\mathcal{A}}$:

$$\underline{\mathcal{A}} = \begin{bmatrix} a_{11}\mathbf{I}_{d+1} & a_{12}\mathbf{I}_{d+1} \\ a_{21}\mathbf{I}_{d+1} & a_{22}\mathbf{I}_{d+1} \end{bmatrix}, \tag{4}$$

in which each element is replicated along a diagonal of a (sub)matrix of size $d{+}1$. The time-extended observations (mixtures) $\underline{\mathbf{x}}(n)$ can be written as

$$\underline{\mathbf{x}}(n) = \underline{\mathcal{F}}\left(\underline{\mathbf{u}}(n)\right) = \underline{\mathcal{F}}\left(\underline{\mathcal{A}}\underline{\mathbf{s}}(n)\right), \tag{5}$$

where $\underline{\mathcal{F}}(\cdot)$ is a set of functions diagonally positioned as

$$\underline{\mathcal{F}}(\cdot) = \begin{bmatrix} f_1(\cdot)\odot\mathbf{I}_{d+1} & \mathbf{0} \\ \mathbf{0} & f_2(\cdot)\odot\mathbf{I}_{d+1} \end{bmatrix} = \begin{bmatrix} f_1(\cdot) & 0 & 0 & & & \\ 0 & \ddots & 0 & & \mathbf{0} & \\ 0 & 0 & f_1(\cdot) & & & \\ & & & f_2(\cdot) & 0 & 0 \\ & \mathbf{0} & & 0 & \ddots & 0 \\ & & & 0 & 0 & f_2(\cdot) \end{bmatrix}, \tag{6}$$

in which $f(\cdot)\odot\mathbf{I}_{d+1}$ is the diagonal replication of function $f(\cdot)$.

The separating system is a mirrored version of the mixing one, with output

$$\underline{\mathbf{y}}(n) = \underline{\mathcal{W}}\underline{\mathcal{G}}\left(\underline{\mathbf{x}}(n)\right), \tag{7}$$

where $\underline{\mathcal{G}}(\cdot)$ and $\underline{\mathcal{W}}$ have structures similar to $\underline{\mathcal{F}}(\cdot)$ and $\underline{\mathcal{A}}$, respectively.

By combining Eqs. (7), (5) and (3), we are able to directly express the separated sources $\underline{\mathbf{y}}(n)$ as functions of $\underline{\mathbf{r}}(n)$ as

$$\underline{\mathbf{y}}(n) = \underline{\mathcal{W}}\underline{\mathcal{G}}\left(\underline{\mathcal{F}}\left(\underline{\mathcal{A}}\underline{\mathcal{H}}\underline{\mathbf{r}}(n)\right)\right). \tag{8}$$

Undoubtedly, in practical scenarios, the elements $\underline{\mathcal{F}}$, $\underline{\mathcal{A}}$, $\underline{\mathcal{H}}$ and $\underline{\mathbf{r}}(n)$ are considered unknown and the separation task may be performed relying on, for instance, some statistical properties of the sources $\underline{\mathbf{s}}(n)$, like the mutual independence. Notwithstanding, Eq. (8) is of great theoretical importance, since it exposes a direct relation to *i.i.d.* signals and opens the way for the analytical computation of the statistics involved in the separation process, as we intend to show. It is important to note that some additional assumptions may be necessary, for example, the definition of the type of the nonlinearities $\underline{\mathcal{F}}(\cdot)$ and $\underline{\mathcal{G}}(\cdot)$.

### 2.2. A Special Case: The Cubic Nonlinearity

In order to find a subset of constrained PNL models in which the SOS-based methods are sufficient for separation, we start from a simple hypothesis that the combined nonlinear function $\underline{\mathcal{G}} \circ \underline{\mathcal{F}}$ yields as output

$$\underline{\mathbf{z}}(n) = \underline{\mathcal{A}\mathbf{s}}(n) + \underline{\mathbf{\Gamma}}\left(\underline{\mathcal{A}\mathbf{s}}(n)\right)^{\odot 3}, \tag{9}$$

where

$$\underline{\mathbf{\Gamma}} = \begin{bmatrix} \gamma_1 \mathbf{I}_{d+1} & \mathbf{0} \\ \mathbf{0} & \gamma_2 \mathbf{I}_{d+1} \end{bmatrix} \tag{10}$$

and $(\cdot)^{\odot 3}$ is the Hadamard power of 3 (i.e., an element-wise cubic operator). This can be viewed as, for instance, the combination of a cubic nonlinearity $\underline{\mathcal{F}}(\underline{\mathbf{u}}(n)) = \underline{\mathbf{u}}^{\odot 3}(n)$ and a $\underline{\mathcal{G}}(\underline{\mathbf{x}}(n)) = \mathrm{sgn}(\underline{\mathbf{x}}(n)) \odot (|\underline{\mathbf{x}}(n)|)^{\odot 1/3} + \underline{\mathbf{\Gamma}\mathbf{x}}(n)$. Based on Eq. (8), the system output can now be written as

$$\underline{\mathbf{y}}(n) = \underline{\mathcal{W}\mathbf{z}}(n) = \underline{\mathcal{W}\mathcal{A}\mathcal{H}\mathbf{r}}(n) + \underline{\mathcal{W}\mathbf{\Gamma}}\left(\underline{\mathcal{A}\mathcal{H}\mathbf{r}}(n)\right)^{\odot 3}. \tag{11}$$

Hence, according to this model, two observations can be outlined: (*i*) the separated sources can be viewed as the combination of a linear mixing/demixing term and a nonlinear mixing/demixing term; (*ii*) if $\underline{\mathbf{\Gamma}} = \mathbf{0}$, then the second (nonlinear) term vanishes and the problem is reduced to the linear one.

Very interestingly, each element of $\left(\underline{\mathcal{A}\mathcal{H}\mathbf{r}}(n)\right)^{\odot 3}$ can be viewed as a polynomial raised to the power of 3, which can be expanded and rearranged in a matrix form. For instance, in a hypothetical simple case with constants $c_1$ and

$c_2$, we intend to perform the following rearrangement: $(c_1 r_1(n) + c_2 r_1(n-1))^3 = c_1^3 r_1^3(n) + c_2^3 r_1^3(n-1) + 3c_1^2 c_2 r_1^2(n) r_1(n-1) + 3c_1 c_2^2 r_1(n) r_1^2(n-1) = \left[c_1^3, c_2^3, 3c_1^2 c_2, 3c_1 c_2^2\right] \left[r_1^3(n), r_1^3(n-1), r_1^2(n) r_1(n-1), r_1(n) r_1^2(n-1)\right]^T$, where the constant terms and the signals $r_1(n)$ and $r_1(n-1)$ are separated in different vectors. This procedure can be extended to all elements of $(\underline{\mathcal{AH}\mathbf{r}}(n))^{\odot 3}$, but, all considered signals in $\underline{\mathbf{r}}(n)$ (i.e, $r_1(n)$, ..., $r_1(n-L_{h_1}-d)$, $r_2(n)$, ..., $r_2(n-L_{h_2}-d)$) must be taken into account, resulting

$$\begin{aligned}
(\underline{\mathcal{AH}\mathbf{r}}(n))^{\odot 3} &= \begin{bmatrix} (a_{11}h_{1,0})^3 r_1^3(n) + (a_{11}h_{1,1})^3 r_1^3(n-1) + \cdots \\ \vdots \\ (a_{11}h_{1,0})^3 r_1^3(n-d) + (a_{11}h_{1,1})^3 r_1^3(n-d-1) + \cdots \\ (a_{21}h_{1,0})^3 r_1^3(n) + (a_{21}h_{1,1})^3 r_1^3(n-1) + \cdots \\ \vdots \\ (a_{21}h_{1,0})^3 r_1^3(n-d) + (a_{21}h_{1,1})^3 r_1^3(n-d-1) + \cdots \end{bmatrix} \\
&= \begin{bmatrix} [\xi_{11}, \xi_{12}, \ldots] \left[r_1^3(n), r_1^3(n-1), \ldots\right]^T \\ \vdots \\ [\xi_{11}, \xi_{12}, \ldots] \left[r_1^3(n-d), r_1^3(n-d-1), \ldots\right]^T \\ [\xi_{21}, \xi_{22}, \ldots] \left[r_1^3(n), r_1^3(n-1), \ldots\right]^T \\ \vdots \\ [\xi_{21}, \xi_{22}, \ldots] \left[r_1^3(n-d), r_1^3(n-d-1), \ldots\right]^T \end{bmatrix},
\end{aligned} \tag{12}$$

where $\xi_{ij}$ corresponds to the factor that multiplies the term involving the original signals $r_1(n)$, $r_2(n)$ and/or their delayed versions, for $i = 1, \ldots, N$ (recall that it is assumed $N = 2$) and for $j = 1, \ldots, L_v$, with $L_v$ equal to the resulting number of terms after the cubic expansion. The number of elements $L_v$ can be combinatorially obtained: assuming that all FIR filters have the same maximum length $L_h+1$, without loss of generality, we have that $L_v = (N(L_h+1)+2)!/(3!(N(L_h+1)-1)!)$. Due to the excessive length of the vectors, we have shown only the initial terms.

Assuming now that $\boldsymbol{\theta}_i = [\xi_{i1}, \xi_{i2}, \cdots, \xi_{iL_v}]$ is a row vector with $L_v$ elements, and that $\boldsymbol{\rho}(n) = \left[r_1^3(n), r_1^3(n-1), r_2^3(n), r_2^3(n-1), \cdots, r_1^2(n) r_2(n-1), \cdots, r_1(n) r_2(n) r_2(n-1), \cdots\right]^T$ is the column vector with $L_v$ terms involving the signals $r_1(n)$, $r_2(n)$ and their delayed versions, Eq. (12) can be rewritten as

$$(\underline{\mathcal{A}\mathcal{H}\mathbf{r}}(n))^{\odot 3} = \begin{bmatrix} \boldsymbol{\theta}_1 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\theta}_1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & \boldsymbol{\theta}_1 \\ \boldsymbol{\theta}_2 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\theta}_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & \boldsymbol{\theta}_2 \end{bmatrix} \begin{bmatrix} \boldsymbol{\rho}(n) \\ \boldsymbol{\rho}(n-1) \\ \vdots \\ \boldsymbol{\rho}(n-d) \end{bmatrix} = \underline{\boldsymbol{\Theta}}\underline{\boldsymbol{\rho}}(n), \tag{13}$$

where $\underline{\boldsymbol{\rho}}(n)$ is the column vector with $\boldsymbol{\rho}(n)$ and its $d$ delayed versions – so that $\underline{\boldsymbol{\rho}}(n)$ has length $(d+1)(N(L_h+1)+2)!/(3!(N(L_h+1)-1)!)$ – and $\underline{\boldsymbol{\Theta}}$ is a matrix with dimensions $N(d+1) \times (d+1)(N(L_h+1)+2)!/(3!(N(L_h+1)-1)!)$. Note that the computational complexity can increase drastically, depending on the values of $N$ (here chosen to be 2), $d$ and $L_h$.

It is interesting to note in Eq. (13) that $\underline{\boldsymbol{\rho}}(n)$ encompasses elements of $\underline{\mathbf{r}}(n)$ up to the power of 3 (due to the assumed cubic nonlinearity) but we have expressed it by means of a linear matrix multiplication, i.e., $(\underline{\mathcal{A}\mathcal{H}\mathbf{r}}(n))^{\odot 3} = \underline{\boldsymbol{\Theta}}\underline{\boldsymbol{\rho}}(n)$.

As an example, we consider two linear FIR filters $\mathbf{h}_1 = [h_{1,0}, h_{1,1}]$ and $\mathbf{h}_2 = [h_{2,0}, h_{2,1}]$ and the mixtures $\mathbf{x}(n) = (\mathbf{A}\mathbf{s}(n))^{\odot 3}$, with $\mathbf{A} = [a_{11}, a_{12}\,; a_{21}, a_{22}]$. If we consider $d = 1$, the mixtures can be expressed as

$$\begin{aligned} \underline{\mathbf{x}}(n) &= \underline{\mathcal{F}}\left(\underline{\mathcal{A}\mathbf{s}}(n)\right) = (\underline{\mathcal{A}\mathcal{H}\mathbf{r}}(n))^{\odot 3} \\ &= \left( \begin{bmatrix} a_{11} & 0 & a_{12} & 0 \\ 0 & a_{11} & 0 & a_{12} \\ a_{21} & 0 & a_{22} & 0 \\ 0 & a_{21} & 0 & a_{22} \end{bmatrix} \begin{bmatrix} h_{1,0} & h_{1,1} & 0 & 0 & 0 & 0 \\ 0 & h_{1,0} & h_{1,1} & 0 & 0 & 0 \\ 0 & 0 & 0 & h_{2,0} & h_{2,1} & 0 \\ 0 & 0 & 0 & 0 & h_{2,0} & h_{2,1} \end{bmatrix} \cdot \right. \\ &\qquad \left. \cdot \begin{bmatrix} r_1(n), & r_1(n-1), & r_1(n-2), & r_2(n), & r_2(n-1), & r_2(n-2) \end{bmatrix}^T \right)^{\odot 3}. \end{aligned} \tag{14}$$

By proceeding with the cubic (or Volterra) expansion, the vector $\boldsymbol{\rho}(n)$ has $L_v = (N(L_h+1)+2)!/(3!(N(L_h+1)-1)!) = 20$ elements, which are all possible triplets among $r_1(n)$, $r_1(n-1)$, $r_2(n)$ and $r_2(n-1)$, i.e.,

$$
\begin{aligned}
\boldsymbol{\rho}(n) = [\ & r_1^3(n), \quad r_1^3(n-1), \quad r_2^3(n), \quad r_2^3(n-1), \\
& r_1^2(n)r_1(n-1), \quad r_1^2(n)r_2(n), \quad r_1^2(n)r_2(n-1), \quad r_1(n)r_1^2(n-1), \\
& r_1(n)r_2^2(n), \quad r_1(n)r_2^2(n-1), \quad r_1^2(n-1)r_2(n), \quad r_1^2(n-1)r_2(n-1), \\
& r_1(n-1)r_2^2(n), \quad r_1(n-1)r_2^2(n-1), \quad r_2^2(n)r_2(n-1), \quad r_2(n)r_2^2(n-1), \\
& r_1(n)r_1(n-1)r_2(n), \quad r_1(n)r_1(n-1)r_2(n-1), \quad r_1(n)r_2(n)r_2(n-1), \\
& r_1(n-1)r_2(n)r_2(n-1)\ ]^T .
\end{aligned}
\tag{15}
$$

Returning to the (cubic) case with generic FIR filters and arbitrary $d$, it is possible to write a linear-like expression for the separated sources:

$$
\underline{\mathbf{y}}(n) = \underline{\mathcal{W}\mathcal{A}\mathcal{H}\mathbf{r}}(n) + \underline{\mathcal{W}\boldsymbol{\Gamma}\boldsymbol{\Theta}\boldsymbol{\rho}}(n). \tag{16}
$$

Henceforth, we adopt the cubic nonlinearity for our analysis, but it is important to emphasize that the idea of using the Volterra expansion is also valid for other polynomial functions (although this topic will be left for future works). In the following, we present the SOS-based criteria to perform separation and the analytical computation of the covariance matrices involved.

## 3. Joint Diagonalization of Correlation Matrices

The use of SOS in the linear instantaneous BSS problem is known to be effective when it involves sources that present temporal structure [1, 6]. In such a case, the main idea is to jointly diagonalize the correlation matrices between retrieved sources for a given number of delays; in other words, the objective is to mutually decorrelate the outputs $y_i(n)$, for $i = 1, \ldots, N$, but considering different time delays. There are several methods that perform second-order separation, among which we cite the algorithms SOBI [6], WASOBI [7], AMUSE and TDSEP [1, 4]. However, for PNL mixtures, the exclusive use of the SOS for separation has not been addressed yet. In that sense, the temporal-extended formulation of the PNL model may give us important elements to help clarify certain theoretical aspects in this approach. Furthermore, given the complexity of the PNL model, we opt for diversified uses of the SOS, which includes the classical SOBI criterion for separation [6] and an alternative SOS-based separation measure that combines the temporal formulation with the mutual information measure [1], as will be described in the following.

### 3.1. The Block-Diagonalization

Based on the classical SOBI criterion, the following statement can be written: given a number of time delays $d$, it is desired that the correlation matrix

$$\underline{\mathbf{R}}_{\underline{\mathbf{y}}\underline{\mathbf{y}}} = E\left[\underline{\mathbf{y}}(n)\underline{\mathbf{y}}^T(n)\right] = \begin{bmatrix} \underline{\mathbf{R}}_{\underline{y}_1\underline{y}_1} & \underline{\mathbf{R}}_{\underline{y}_1\underline{y}_2} \\ \underline{\mathbf{R}}_{\underline{y}_2\underline{y}_1} & \underline{\mathbf{R}}_{\underline{y}_2\underline{y}_2} \end{bmatrix}. \tag{17}$$

be block-diagonal, i.e., that the cross correlation matrices between outputs (diagonal blocks in Eq. (17)) are all null, where $\underline{\mathbf{R}}_{\underline{y}_i\underline{y}_j} = E\left[\underline{\mathbf{y}}_i(n)\underline{\mathbf{y}}_j^T(n)\right]$, with $\underline{\mathbf{y}}_i(n) = [y_i(n), y_i(n-1), \cdots, \ y_i(n-d)]^T$ and $\underline{\mathbf{y}}(n) = [\underline{\mathbf{y}}_1^T(n), \underline{\mathbf{y}}_2^T(n)]^T$. Hence, we can write the block-diagonalization (BD) criterion as

$$J_{BD} = \min_{\underline{\mathcal{W}},\underline{\mathcal{G}}} \quad \text{blkoff}(\underline{\mathbf{R}}_{\underline{\mathbf{y}}\underline{\mathbf{y}}}), \tag{18}$$

where blkoff$(\cdot)$ is the sum of squared elements in the off-block-diagonal of a square matrix. Note that, as the number of delays $d$ increases, the larger the correlation matrices get and more information can be considered by the criterion. Additionally, a norm constraint can be applied to force the main diagonal of $\underline{\mathbf{R}}_{\underline{\mathbf{y}}\underline{\mathbf{y}}}$ to be unitary (assuming that $y_i(n)$ is stationary, for $i = 1, \ldots, N$), e.g., by summing to the cost (18) the following term:

$$J_c = \min \quad \sum_{i=1}^{N} \left(E\left[y_i^2(n)\right] - 1\right)^2, \tag{19}$$

This constraint is necessary in order to avoid – trivial – null solutions (as a consequence, it is also useful for identifying an unique solution). Different weights can be applied to $J_{BD}$ and $J_c$, causing changes on local minima position – gradient-based optimization methods may be more sensitive to these changes. However, since we are using metaheuristics for parameters optimization (which are intended to be more robust against local minima convergence), we assume equal (unitary) weights for $J_{BD}$ and $J_c$.

### *3.2. The Second-Order Mutual Information Measure*

The mutual information allows an efficient manner of measuring the statistical independence. In order to extract the temporal information in a more complete fashion and also to restrain our analysis to the SOS, we make the following assumption: the sources are mutually independent and (zero-mean) jointly Gaussian distributed for all considered delays and also present a time structure. This will lead to an alternative cost function, when compared to the BD cost, as described bellow.

We start with the definition of mutual independence encompassing the temporal structure of data, i.e.,

$$f_{\underline{\mathbf{y}}}(\underline{\mathbf{v}}) = \prod_{i=1}^{N} f_{\underline{\mathbf{y}}_i}(\underline{\mathbf{v}}_i), \tag{20}$$

where $f_{\underline{\mathbf{y}}}(\underline{\mathbf{v}})$ and $f_{\underline{\mathbf{y}}_i}(\underline{\mathbf{v}}_i)$ are the multivariate probability density functions associated with $\underline{\mathbf{y}}(n)$ and $\underline{\mathbf{y}}_i(n)$, respectively. The temporal structure, in this case, is inherently taken into account by the multivariate densities.

To measure the independence, one can use the mutual information [1] : $I(\mathbf{y}(n), \ldots, \mathbf{y}(n-d)) = -H(\underline{\mathbf{y}}) + \sum_{i=1}^{N} H(\underline{\mathbf{y}}_i)$, where $H(\cdot)$ is Shannon's entropy, defined as $H(\underline{\mathbf{y}}) = -\int_D p(\underline{\mathbf{y}}) \log(p(\underline{\mathbf{y}}))d\underline{\mathbf{y}}$, with $D \subseteq \mathbb{R}^{N(d+1)}$, and $H(\underline{\mathbf{y}}_i) = -\int_{D_i} p(\underline{\mathbf{y}}_i) \log(p(\underline{\mathbf{y}}_i))d\underline{\mathbf{y}}_i$, with $D_i \subseteq \mathbb{R}^{d+1}$, for the marginal entropies. The mutual information is always non-negative and, when independence is reached for all delays, $I(\mathbf{y}(n), \ldots, \mathbf{y}(n-d)) = 0$. In its strict form, $I(\mathbf{y}(n), \ldots, \mathbf{y}(n-d))$ is difficult to be calculated since it demands the estimation of the densities (which is critical in our case, where all densities are multivariate). However, under the supposition of a successful separation, it is expected that the recovered sources be jointly Gaussian as well, i.e., $f_{\underline{\mathbf{y}}}(\mathbf{v}) \sim \mathcal{N}\left(\mathbf{0}, \underline{\mathbf{R}}_{\underline{\mathbf{yy}}}\right)$ or

$$f_{\underline{\mathbf{y}}}(\mathbf{v}) = \frac{1}{\sqrt{|2\pi \underline{\mathbf{R}}_{\underline{\mathbf{yy}}}|}} \exp\left(\frac{-1}{2} \mathbf{v}^T \underline{\mathbf{R}}_{\underline{\mathbf{yy}}}^{-1} \mathbf{v}\right), \tag{21}$$

where $\underline{\mathbf{R}}_{\underline{\mathbf{y}}\underline{\mathbf{y}}}$ is as defined by Eq. (17) and $|\cdot|$ is the determinant operator.

It can be shown that, by combining Eq. (21) with $I(\mathbf{y}(n), \ldots, \mathbf{y}(n-d))$, the separation criterion associated with the mutual information reduces to [21]

$$J_{SOMI} = \min_{\underline{\mathcal{W}}, \underline{\mathcal{G}}} \quad \frac{1}{2} \log \left( \frac{\prod_{i=1}^{N} \left| \underline{\mathbf{R}}_{\underline{y}_i \underline{y}_i} \right|}{\left| \underline{\mathbf{R}}_{\underline{\mathbf{y}}\underline{\mathbf{y}}} \right|} \right). \tag{22}$$

It is important to mention that a similar expression was already obtained through the spectral density of Gaussian sources, being named Gaussian Mutual Information (GMI) [1, 21, 22], and the temporal-extended covariance matrices were used in the convolutive mixing problem [15], but its application to the PNL problem is novel. Hence, we refer to Eq. (22) as the Second-Order Mutual Information (SOMI). As the BD cost, Eq. (22) uses only the SOS information, but instead of using summation of quadratic terms (Eq. (18)), the determinants of matrices $\underline{\mathbf{R}}_{\underline{y}_i \underline{y}_i}$ and $\underline{\mathbf{R}}_{\underline{\mathbf{y}}\underline{\mathbf{y}}}$ are considered (note, however, that the computational complexity is increased by $O(n^3)$ due to the determinant operator).

The objective of the SOMI criterion is to minimize the cost $J_{SOMI}$ so that $J_{SOMI} = 0$. However, the norm constraint given by Eq. (19) is necessary to avoid null (trivial) solutions.

### *3.3. The Quadratic SOMI Cost*

A closer observation on Eq. (22) reveals that, in fact, a matching between the determinant terms $\prod_{i=1}^{N} |\underline{\mathbf{R}}_{\underline{y}_i \underline{y}_i}|$ and $|\underline{\mathbf{R}}_{\underline{\mathbf{y}}\underline{\mathbf{y}}}|$ would lead the cost $J_{SOMI}$ to be equal to zero (i.e., the mutual information is null). In that sense, a similar cost can be written without relying on the logarithm properties, but on the simplicity of a quadratic difference:

$$J_{SOMIq} = \min_{\underline{\mathcal{W}}, \underline{\mathcal{G}}} \left( \prod_{i=1}^{N} |\underline{\mathbf{R}}_{\underline{y}_i \underline{y}_i}| - |\underline{\mathbf{R}}_{\underline{\mathbf{y}}\underline{\mathbf{y}}}| \right)^2, \tag{23}$$

where the minimal (and desired) cost value is zero. Note that the norm constraint (Eq. (19)) is also necessary to avoid null solutions. This cost is named SOMIq due to its quadratic term.

For SOMI and SOMIq, when the correlation matrix $\underline{\mathbf{R}}_{\mathbf{yy}}$ is block-diagonal, we have that $|\underline{\mathbf{R}}_{\mathbf{yy}}| = \prod_{i=1}^{N} |\underline{\mathbf{R}}_{\underline{y}_i\underline{y}_i}|$ and the costs are both null. In that sense, we expect that the solutions for SOMI and SOMIq be the same. However, the quadratic relation in SOMIq may be able to provide a desirable cost shape in the optimization process – we will discuss this point in more detail ahead.

### *3.4. The Analytical Calculation of the Cost Functions*

As usual in SOS-based approaches, the main entity is the correlation matrix and, if one considers the mixing and separating model given by Eq. (16), the expanded correlation matrix $\underline{\mathbf{R}}_{\mathbf{yy}}$ can be computed analytically:

$$\begin{aligned}
\underline{\mathbf{R}}_{\mathbf{yy}} &= E\left[\underline{\mathbf{y}}(n)\underline{\mathbf{y}}^T(n)\right] \\
&= E\left[\underline{\mathcal{WAH}\mathbf{r}}(n)\underline{\mathbf{r}}^T(n)\underline{\mathcal{H}}^T\underline{\mathcal{A}}^T\underline{\mathcal{W}}^T\right] + E\left[\underline{\mathcal{WAH}\mathbf{r}}(n)\underline{\boldsymbol{\rho}}^T(n)\underline{\boldsymbol{\Theta}}^T\underline{\boldsymbol{\Gamma}}^T\underline{\mathcal{W}}^T\right] \\
&\quad + E\left[\underline{\mathcal{W}\boldsymbol{\Gamma\Theta\rho}}(n)\underline{\mathbf{r}}^T(n)\underline{\mathcal{H}}^T\underline{\mathcal{A}}^T\underline{\mathcal{W}}^T\right] + E\left[\underline{\mathcal{W}\boldsymbol{\Gamma\Theta\rho}}(n)\underline{\boldsymbol{\rho}}^T(n)\underline{\boldsymbol{\Theta}}^T\underline{\boldsymbol{\Gamma}}^T\underline{\mathcal{W}}^T\right] \\
&= \underline{\mathcal{WAH}\mathbf{R}_{rr}}\underline{\mathcal{H}}^T\underline{\mathcal{A}}^T\underline{\mathcal{W}}^T + \underline{\mathcal{WAH}\mathbf{R}_{r\rho}}\underline{\boldsymbol{\Theta}}^T\underline{\boldsymbol{\Gamma}}^T\underline{\mathcal{W}}^T + \underline{\mathcal{W}\boldsymbol{\Gamma\Theta}\mathbf{R}_{\rho r}}\underline{\mathcal{H}}^T\underline{\mathcal{A}}^T\underline{\mathcal{W}}^T \\
&\quad + \underline{\mathcal{W}\boldsymbol{\Gamma\Theta}\mathbf{R}_{\rho\rho}}\underline{\boldsymbol{\Theta}}^T\underline{\boldsymbol{\Gamma}}^T\underline{\mathcal{W}}^T,
\end{aligned} \tag{24}$$

where $\underline{\mathbf{R}}_{rr} = E\left[\underline{\mathbf{r}}(n)\underline{\mathbf{r}}^T(n)\right]$, $\underline{\mathbf{R}}_{r\rho} = E\left[\underline{\mathbf{r}}(n)\underline{\boldsymbol{\rho}}^T(n)\right]$, $\underline{\mathbf{R}}_{\rho r} = E\left[\underline{\boldsymbol{\rho}}(n)\underline{\mathbf{r}}^T(n)\right]$ and $\underline{\mathbf{R}}_{\rho\rho} = E\left[\underline{\boldsymbol{\rho}}(n)\underline{\boldsymbol{\rho}}^T(n)\right]$ are the correlation matrices as a function of $\underline{\mathbf{r}}(n)$ and $\underline{\boldsymbol{\rho}}(n)$ – in which $\underline{\boldsymbol{\rho}}(n)$ is the Volterra expansion of $\underline{\mathbf{r}}(n)$. Since $\underline{\mathbf{r}}(n)$ is an *i.i.d.* vector, these covariance matrices have, as non-null elements, only the terms involving $E\left[r_i^2(n)\right]$, $E\left[r_i^4(n)\right]$ and $E\left[r_i^6(n)\right]$, which can be easily obtained. This reveals that some HOS are directly encompassed by the correlation matrices, which might be essential to the nonlinear separation process.

In the BD cost function, only the off-block-diagonal elements are considered, so that the matrices $\underline{\mathbf{R}}_{\underline{y}_i\underline{y}_j}$, for $i \neq j$, are the ones effectively used. For the SOMI and SOMIq costs, the block-diagonal elements $\underline{\mathbf{R}}_{\underline{y}_i\underline{y}_i}$ are considered. Based on Eq. (24), we can write:

$$\begin{aligned}
\underline{\mathbf{R}}_{\underline{y}_i\underline{y}_j} = \underline{\mathcal{W}}_i \Big(&\underline{\mathcal{AH}\mathbf{R}_{rr}}\underline{\mathcal{H}}^T\underline{\mathcal{A}}^T + \underline{\mathcal{AH}\mathbf{R}_{r\rho}}\underline{\boldsymbol{\Theta}}^T\underline{\boldsymbol{\Gamma}}^T \\
&+ \underline{\boldsymbol{\Gamma\Theta}\mathbf{R}_{\rho r}}\underline{\mathcal{H}}^T\underline{\mathcal{A}}^T + \underline{\boldsymbol{\Gamma\Theta}\mathbf{R}_{\rho\rho}}\underline{\boldsymbol{\Theta}}^T\underline{\boldsymbol{\Gamma}}^T\Big)\underline{\mathcal{W}}_j^T,
\end{aligned} \tag{25}$$

where $\underline{\mathcal{W}}_i$ is the $i$th block with $d+1$ rows of $\underline{\mathcal{W}}$. It is possible to note that each of the $(d+1)^2$ elements of $\underline{\mathbf{R}}_{\underline{y}_i\underline{y}_j}$ are quadratic polynomials in function of $\underline{\mathbf{\Gamma}}$ and $\underline{\mathcal{W}}_i$ – the separation coefficients – and can contribute with additional information for solving the system. However, there might be redundant equations, since, under the assumption of stationary discrete-time stochastic processes, $\underline{\mathbf{R}}_{\underline{y}_i\underline{y}_i}$ is Toeplitz, and $\underline{\mathbf{R}}_{\underline{y}_i\underline{y}_j} = \underline{\mathbf{R}}^T_{\underline{y}_j\underline{y}_i}$ by definition.

Using the relations (24) and (25), the costs BD, SOMI and SOMIq can be analytically obtained, i.e., the cost functions can be exactly evaluated without any estimation errors. Note that this approach requires the knowledge of the matrices $\underline{\mathcal{H}}$, $\underline{\mathcal{A}}$, $\underline{\mathbf{\Theta}}$ and $\underline{\mathbf{\Gamma}}$, which, in practice, are not known. However, under a theoretical perspective, it may contribute to a better understanding of the PNL mixtures behavior, as shown next.

## 4. Identifiability and Bounds on Number of Delays

The three aforementioned criteria share a common feature when a solution is found: the extended correlation matrix of the output signals $\underline{\mathbf{R}}_{\mathbf{yy}}$ is precisely a block-diagonal matrix, i.e., all the off-block-diagonal elements are null. This observation allows us to point out some general aspects involving the SOS-based costs in the context of the particular PNL mixture case considered.

### *4.1. Blind Identifiability*

In the linear BSS problem, the study of the blind identification conditions for the SOS-based approaches is a well studied topic [6]: it is known that the linear mixing matrix $\mathbf{A}$ can be identified, up to permutation and scale factors, if the source signals have different spectral shapes. Generally, the demonstration is done by ensuring that the diagonalization process of the correlation matrix for different delays yields eigenvalues that are distinct [4, 1]. In the temporal-extended formulation, this means that $\underline{\mathbf{R}}_{\mathbf{yy}}$ should be block-diagonal and that each block of the main diagonal – i.e., $\underline{\mathbf{R}}_{\underline{y}_i\underline{y}_i}$, for $i = 1, \ldots, N$ – present, at least, two distinct eigenvalues.

The extension of this idea to the general PNL problem becomes more complex, since the identification conditions must be valid for $\mathbf{A}$ and $\mathbf{f}(\cdot)$. In the studied case, the problem may be posed in a simpler manner, since we are able to express the nonlinear mixing functions by means of a linear matrix multiplication (Eq. (16)). In that sense, similarly to the linear case, it is possible to verify the the conditions for identification [1] through the block-diagonalization of $\underline{\mathbf{R}_{\mathbf{yy}}}$ in function of $\underline{\mathcal{W}}$ and $\underline{\mathbf{\Gamma}}$. To solve this problem, we consider two cases: $(i)$ $\underline{\mathbf{\Gamma}}$ is null and $(ii)$ $\underline{\mathbf{\Gamma}}$ has a non-null value.

In case $(i)$, when $\underline{\mathbf{\Gamma}}$ is null, i.e., the case in which the nonlinear part is solved, $\underline{\mathcal{W}}$ must block-diagonalize only $\underline{\mathcal{A}\mathcal{H}\mathbf{R}_{rr}}\underline{\mathcal{H}}^T\underline{\mathcal{A}}^T$ and the conditions are the same as for the linear case [1]: the source signals must have different spectral shapes.

For case $(ii)$, $\underline{\mathbf{\Gamma}}$ is a non-null diagonal matrix (i.e., there remains a nonlinear residual error), the matrices $\underline{\mathbf{R}_{r\rho}}$, $\underline{\mathbf{R}_{\rho r}}$ and $\underline{\mathbf{R}_{\rho\rho}}$ are not block-diagonal (due to inherent HOS encompassed in the process), and $\underline{\mathcal{W}}$ is unable to compensate $\underline{\mathbf{\Theta}}$ by itself. Since the matrices $\underline{\mathbf{R}_{r\rho}}$, $\underline{\mathbf{R}_{\rho r}}$ and $\underline{\mathbf{R}_{\rho\rho}}$ are not block-diagonal, the diagonalization of $\underline{\mathbf{R}_{\mathbf{yy}}}$ would result in non-orthogonal $\underline{\mathcal{W}\mathcal{A}\mathcal{H}}$ or $\underline{\mathcal{W}\mathbf{\Gamma}\mathbf{\Theta}}$, with eigenvalues not unique, which is not a desired solution [1].

Regarding the impossibility of the compensation of $\underline{\mathbf{\Theta}}$ by $\underline{\mathcal{W}}$, we have that $\underline{\mathcal{W}}$ will not be able to jointly diagonalize the linear term as well as the nonlinear ones. For instance, if the linear term $(\underline{\mathcal{A}\mathcal{H}\mathbf{R}_{rr}}\underline{\mathcal{H}}^T\underline{\mathcal{A}}^T)$ is block-diagonalized and $\underline{\mathcal{W}\mathcal{A}\mathcal{H}\mathbf{R}_{rr}}\underline{\mathcal{H}}^T\underline{\mathcal{A}}^T\underline{\mathcal{W}}^T$ is orthogonal (i.e., $\underline{\mathcal{W}} = \underline{\mathcal{A}}^{-1}$), then,

$$\underline{\mathbf{R}_{\mathbf{yy}}} = \underline{\mathcal{H}\mathbf{R}_{rr}}\underline{\mathcal{H}}^T + \underline{\mathcal{H}\mathbf{R}_{r\rho}}\underline{\mathbf{\Theta}}^T\underline{\mathbf{\Gamma}}^T\underline{\mathcal{W}}^T + \underline{\mathcal{W}\mathbf{\Gamma}\mathbf{\Theta}\mathbf{R}_{\rho r}}\underline{\mathcal{H}}^T + \underline{\mathcal{W}\mathbf{\Gamma}\mathbf{\Theta}\mathbf{R}_{\rho\rho}}\underline{\mathbf{\Theta}}^T\underline{\mathbf{\Gamma}}^T\underline{\mathcal{W}}^T, \tag{26}$$

and the nonlinear terms are not block-diagonal for non-null $\underline{\mathbf{\Gamma}}$. On the opposite, if the nonlinear terms are made block-diagonal, the linear term will not be block-diagonal. Hence, the possible orthogonal solution (with distinct eigenvalues) is that with null $\underline{\mathbf{\Gamma}}$. The only exception happens when $\underline{\mathcal{A}} = \mathbf{I}$, i.e., when the linear mixing part is reduced to identity (and all the terms will be block-diagonal). However, this case is not considered, since there is no mixture [19].

Thus, in short, the SOS identifiability conditions are that the signals must present different spectral shapes and that the linear mixing part of the PNL model must effectively occur. However, there is a crucial condition in the separating model: the SOS-based approach requires that $\underline{\mathbf{R}}_{\mathbf{yy}}$ encompasses a linear part, which is equivalent to requiring that the combined nonlinear function $\underline{\mathcal{G}} \circ \underline{\mathcal{F}}$ yields a $\underline{\mathbf{z}}(n)$ with at least one linear term (similarly to Eq. (9)). In other words, $\underline{\mathcal{G}}$ must admit at least one term that compensates the nonlinearities $\underline{\mathcal{F}}$ – yielding the linear term – but can also present a nonlinear residual. The linear term must not vanish, even during the coefficients adaptation. This may be a strong constraint on the PNL separating model, since the choice of $\underline{\mathcal{G}}$ must have a fixed term that compensates $\underline{\mathcal{F}}$; but note that, when it is known that $\underline{\mathcal{F}}$ is composed of polynomial functions, $\underline{\mathcal{G}}$ can be easily constructed by composing several compensating polynomial terms and fixing the promising ones. This general polynomial case, however, will be treated in future works, since, for the moment, the cubic case will be sufficient to provide insightful perspectives.

### *4.2. Bounds on the Number of Delays*

As previously mentioned, each element in the off-block-diagonal of $\underline{\mathbf{R}}_{\mathbf{yy}}$ forms a quadratic polynomial as a function of $\underline{\mathbf{\Gamma}}$ and $\underline{\mathcal{W}}$, which may compose a system of quadratic equations. The number of unknown variables, $k$, in our studied case, is $k = N(N{+}1)$, which are the coefficients of $\underline{\mathbf{\Gamma}}$ and $\underline{\mathcal{W}}$.

Some elements (or equations) of $\underline{\mathbf{R}}_{\mathbf{yy}}$, however, are redundant. For instance, the elements of the main diagonal of $\underline{\mathbf{R}}_{\underline{y}_i\underline{y}_j}$ form the same equation in function of the unknown variables and, hence, they only contribute as a single equation (new information) to the system. In addition, we have that $\underline{\mathbf{R}}_{\underline{y}_i\underline{y}_j} = \underline{\mathbf{R}}^T_{\underline{y}_j\underline{y}_i}$, i.e., the sub-diagonals are equivalent, which also reduces the effective number of equations in the system. In that sense, by removing the redundancy, we have $N(N{-}1)/2$ matrices $\underline{\mathbf{R}}_{\underline{y}_i\underline{y}_j}$, in which the number of effective equations are $d(d{+}1){+}1$ each one, resulting in a total of $N(N{-}1)(d(d{+}1){+}1)/2$ equations in the system. Besides, the normalization given by Eq. (19) also performs a role as a constraint, and can contribute to the system with $N$ equations. Finally, it is possible to state that the number of effective equations in the system is

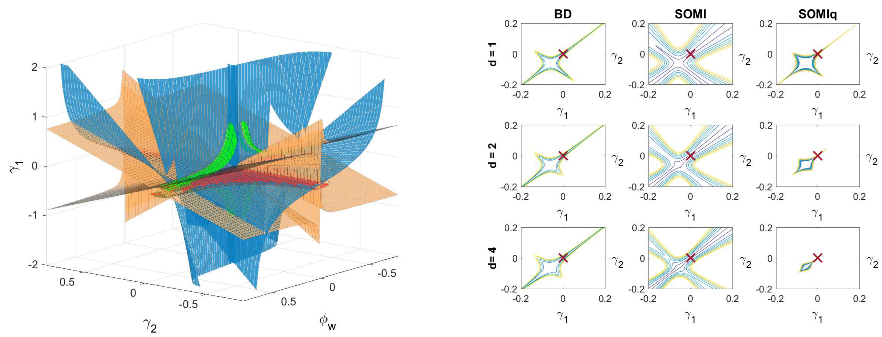
$N(N-1)(d(d+1)+1)/2 + N$. Hence, to obtain valid solutions, it is necessary that $d$ be chosen so that $N(N-1)\left(d(d+1)+1\right)/2+N \geq k$.

Notwithstanding, it is also possible that some of the off-diagonal elements of $\underline{\mathbf{R}}_{\underline{y}_i\underline{y}_j}$ be equivalent, depending on the temporal structure of the mixtures (i.e., $y_i(n)$ and $y_j(n)$ have similar or equal spectral densities) and, in that case, the number of valid equations might be reduced. In that sense, the expression $N(N-1)\left(d(d+1)+1\right)/2+N \geq k$ is only a lower bound for choosing $d$.

In order to illustrate the system of equations, we consider a 2-source and 2-mixture case in which the linear mixing part of the PNL model is a rotation matrix, i.e., $\mathbf{A} = [\cos(\phi_a), -\sin(\phi_a); \sin(\phi_a), \cos(\phi_a)]$. For the separation, based on Eq. (16), we have 2 unknown variables for the joint nonlinear part, $\gamma_1$ and $\gamma_2$, and 1 unknown variable, $\phi_w$, for the linear separating matrix $\mathbf{W}$ (which is a rotation matrix, similar to $\mathbf{A}$). Thus, we have that, for $N$=2 and $d$=1, the number of equations is, at most, $N(N-1)(d(d+1)+1)/2 + N = 5$. Fig. 2(a) shows the surface of each equation for given temporally colored sources, with $\phi_a = 1.02$ rad. In this case, the off-diagonal elements of $\underline{\mathbf{R}}_{\underline{y}_1\underline{y}_2}$ are coincident and we only have 4 valid equations, resulting in 4 surfaces (plotted with different colors) in Fig. 2(a). The intersection points of the surfaces will determine the regions where all equations are satisfied (their intersection occurs for $\gamma_1 = \gamma_2 = 0$ and $\phi_w = k\pi - \phi_a$, $k = 0, \pm1, \pm2, \ldots$ – not observable in Fig. 2(a)). Indeed, any of these points will be a valid solution for the BD, SOMI and SOMIq criteria.

Although the SOS-based criteria are intended to present the same solution, their cost shapes may differ. Consider the previous example but assume that the linear part is has already been solved, leaving just $\gamma_1$ and $\gamma_2$ to be adjusted. In Fig. 2(b), we show the contours as functions of $\gamma_1$ and $\gamma_2$ and for $d$ equal to 1, 2 and 4. In all cases, the global solution is $\gamma_1 = \gamma_2 = 0$ (denoted by an "X" in Fig. 2(b)), which is the desired solution, but local minima also exist. Very interestingly, as $d$ increases, the "weight" of the local optima is reduced, being the global solution more evident (mainly for the SOMIq cost).

Next, we consider the case where $\underline{\mathbf{\Gamma}}$ and $\underline{\mathcal{W}}$ have no constraints – increasing the space of candidate solutions – to evaluate the criteria performance.




(a) Equations surfaces.

(b) Cost Contours.

Figure 2: Number of delays: equations and solutions.

## 5. Performance Analysis

So far, we have verified that the SOS-based criteria share some features, but they might differ in their cost shapes. In fact, when an optimization task is performed, the cost shape might cause a significant impact on the performance. In order to test this effect, we consider simulation scenarios with $N$=$M$=2 and $N$=$M$=3 and with cubic nonlinear mixing functions, i.e., $f_i(u_i(n)) = u_i^3(n)$, for $i = 1, \ldots, N$, or, for the extended-temporal version, $\underline{\mathcal{F}}(\underline{\mathbf{u}}(n)) = \underline{\mathbf{u}}^{\odot 3}(n)$.

As usual in BSS problems, $\mathbf{s}(n)$, $\mathbf{A}$ and $\mathbf{f}(\cdot)$ are not known. Hence, it could be difficult to define a separation structure. For our simulation tests, we assume that the nonlinear compensating function was chosen to be of the form $g_i(x_i(n)) = g_{i,0}\mathrm{sgn}(x_i(n))(|x_i(n)|)^{1/3} + g_{i,1}x_i(n)$, for $i = 1, \ldots, M$. With the objective of obtaining a linear term, which is a separation condition, it is necessary to keep fixed one of the coefficients ($g_{i,0}$ or $g_{i,1}$). Thus, we assume that $g_{i,0} = 1$ remains fixed and $g_{i,1} = \gamma_i$ is allowed to vary (the suitable choice of the fixed coefficients might require some heuristic tests). For the extended-temporal notation, this is equivalent to $\underline{\mathcal{G}}(\underline{\mathbf{x}}(n)) = \mathrm{sgn}(\underline{\mathbf{x}}(n)) \odot (|\underline{\mathbf{x}}(n)|)^{\odot 1/3} + \underline{\mathbf{\Gamma}}\underline{\mathbf{x}}(n)$. Conveniently, this model is exactly as proposed in Eq. (11), where $\underline{\mathbf{\Gamma}}$ and $\underline{\mathcal{W}}$ must be adapted for performing separation.

For the optimization of the weights (linear and nonlinear), we adopt the metaheuristics called Differential Evolution (DE) and Clonal Selection Algorithm (CLONALG), which are efficient techniques to explore the search space and to avoid convergence to local optima [16, 17]. The DE metaheuristic relies on probabilistic vector operations, while CLONALG is based on an artificial immune system inspired by the clonal selection theory and antigen-antibody interactions [17]. Their main difference is the fact that, in DE, the candidate solutions are adapted by mechanisms that exploit the information about the search space that is available in the current population, while, in CLONALG, conventional operators based on random perturbations are used (for more details, please refer to [16, 17]). In simulations, the metaheuristics parameters were adjusted to: the DE parameters were chosen to be $F = 0.5$ (adaptation step) and $CR = 0.9$ (crossover constant), and the CLONALG parameters were $N_c = 10$ (number of clones), $\beta = 5$ (decay of mutation), 15% of new random cells, $T = 50$ (period of cells insertion). For the $N$=$M$=2 case (6 weights: 2 for $\underline{\mathbf{\Gamma}}$ and 4 for $\underline{\mathcal{W}}$), we set $N_P = 500$ (population size/number of cells) and 5000 iterations for both DE and CLONALG, whereas, for the $N$=$M$=3 case (12 weights: 3 for $\underline{\mathbf{\Gamma}}$ and 9 for $\underline{\mathcal{W}}$), we used $N_P = 700$ (the other parameters were kept the same). These parameters were constant for all simulation cases (however, for scenarios with more sources and/or more complex nonlinearities, it is recommended that the search power of the optimization strategy be increased for a higher global convergence rate). In the end of the adaptation, the individual with the best fitness (lower SOS-based cost) is selected to provide the solution. The general steps of the optimization method are as shown in Alg. 1

The performance of the found solutions can be measured in terms of the Signal-to-Interference Ratio (SIR) (after permutation, sign and variance correction), which is defined as $\text{SIR} = 10 \log \left( E[y_i(n)^2]/E[(s_i(n) - y_i(n))^2] \right)$. In that sense, higher SIR values mean better performance solutions.

### 5.1. Performance Using the Analytical Covariance Matrices

In the first scenario, we wish to investigate the effect of the number of delays $d$ in the SOS-based separation criteria using the analytical covariance matrices, i.e., by obtaining $\underline{\mathbf{R}_{\mathbf{yy}}}$ directly from Eq. (24), without estimation errors. For

**Algorithm 1** SOS-based method for optimization using DE/CLONALG

Initialization of DE/CLONALG parameters;

Randomly initialize all $N_P$ individuals in the $\underline{\mathbf{\Gamma}}$ and $\underline{\mathcal{W}}$ search space;

**while** Maximum number of iterations is not reached **do**

  **for** Each individual $i \in N_P$ **do**

    **if** Using DE [16]: **then**

      Generate mutated vector by randomly picking 3 different individuals;

      Combination with the original individual ($F$,$CR$);

    **end if**

    **if** Using CLONALG [17]: **then**

      Generate $N_c$ clones;

      Mutation of the clones ($\beta$);

    **end if**

    Selection:

    Obtain $\underline{\mathbf{R}}_{\underline{yy}}$ analytically (Eq. (25)) or via sample estimation;

    Performance Evaluation, according to

    BD (Eq. (18)), SOMI (Eq. (22)) or SOMIq (Eq. (23))

    Keep the best (original or combination/mutated) individual;

    **if** Using CLONALG: **then**

      Insertion of new individuals at period $T$;

    **end if**

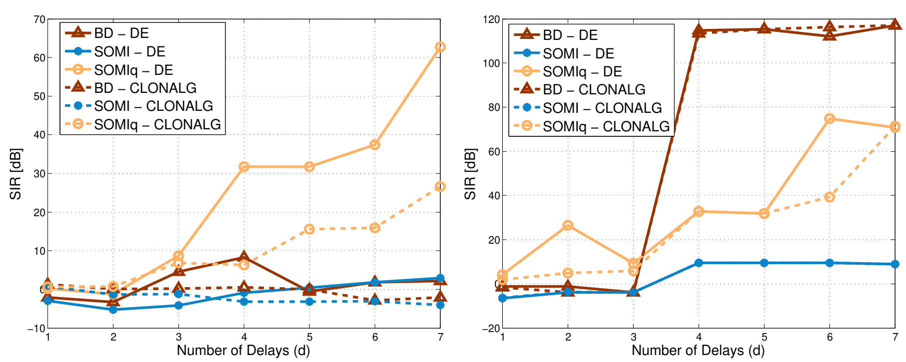
  **end for**

  Pick the best individual of the population and present as best found candidate for solution at this stage

**end while**

$N$=2 sources, two *i.i.d.* Gaussian signals ($r_1(n)$ and $r_2(n)$) are generated and temporally colored by the FIR filters $\mathbf{h}_1 = [1, 0.6, -0.3, 0.1, 0.4, 0.3, -0.22, 0.18, 0.5]$ and $\mathbf{h}_2 = [1, -0.2, -0.8, 0.2, 0.1, -0.41, 0.5, 0.1]$, separately. Note that the temporal structures provided by $\mathbf{h}_1$ and $\mathbf{h}_2$ are of finite length and, hence, there is a limited amount of temporal information to be extracted. The linear mixing matrix is $\mathbf{A} = [0.25, 0.86; -0.86, 0.25]$ and we wish to adapt $\underline{\mathbf{\Gamma}}$ and $\underline{\mathcal{W}}$. Supposing that $r_1(n)$ and $r_2(n)$ are zero-mean and unit variance Gaussian processes and that $\mathbf{h}_1$ and $\mathbf{h}_2$ as well as the mixing coefficients are known, the covariance matrices can be analytically computed with (24).

We considered that the number of delays $d$ can vary from 1 to 7 and, for each value of $d$, we performed 50 independent runs of the DE and CLONALG with the aim of minimizing the BD, SOMI and SOMIq costs (separately). The found solutions were evaluated in terms of SIR for 700,000 test samples (used only for evaluation). Fig. 3(a) shows the mean SIR values for each considered delay, while Fig. 3(b) shows the SIR values for the best solution found by DE and CLONALG throughout the 50 runs. From the mean SIR values, one can

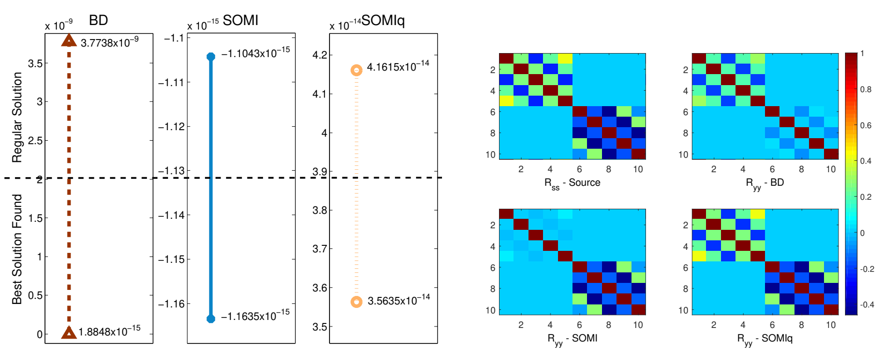



(a) Mean SIR values. (b) SIR performance - Best solution.

Figure 3: Mean and Best Performance - Analytical Costs.

note that the found solutions for the BD and SOMI criteria led to a low value of SIR for all considered delays, for both DE and CLONALG, indicating that their solutions might not be adequate for performing BSS. However, in terms of the best found solution, the BD criterion shows an intriguing result: for $d \geq 4$, the solutions for the BD are able to separate the sources with the highest level of SIR. This indicates that, although we have employed a huge search resource for DE and CLONALG, they have presented difficulties in finding the best solution for BD. For the SOMI criterion, the best found solution shows an improved performance for $d \geq 4$, but it remains around the 10 dB level. On the other hand, for the SOMIq criterion, the DE and CLONALG found good solutions more easily, without great discrepancies between Figs. 3(a) and 3(b), and, from a general perspective, it is possible to say that the solutions SIR level tends to increase with $d$, being the sources successfully separated. Note that, for $d < 2$, the SOMIq best solutions found by DE are not able to separate the sources, which is in accordance with the bound on the number of delays (Section 4.2).

In order to clarify the obtained results, we compare in Fig. 4(a) the lowest attained costs values of BD, SOMI and SOMIq for a 'regular' solution (a randomly picked solution) and the best solution throughout 50 runs of the DE, all for $d = 4$. It is possible to note that, for the BD cost, the difference between




(a) Costs - Regular and best cases.

(b) Extended Correlation Matrices

Figure 4: Cost Comparison and Correlation matrices.

the two cases is larger, being clear that DE is presenting difficulties to find the global optima, differently from the other costs, where the differences were relatively small. This indicates that the BD cost shape may impose some difficulties in finding the global optima, being necessary to increase the search power of the DE metaheuristic. For SOMI, the minimization of Eq. (22) led to small values of the cost, but, due to precision issues, the cost values were negative (ideally positive), which contributed to its poorer performance in comparison with the other criteria. The SOMIq cost, on the other hand, solves the SOMI drawback and converges to close and positive small values.

A more intuitive comparison can be obtained from Fig. 4(b), where we illustrate a colored version of the extended correlation matrix of the sources $\underline{\mathbf{R}}_{\underline{\mathbf{ss}}}$ and of the outputs $\underline{\mathbf{R}}_{\underline{\mathbf{yy}}}$ for the BD, SOMI and SOMIq solutions in one of the executions (the same solution picked as 'regular') of the DE metaheuristic, all for $d$=4. It is possible to note that, for $\underline{\mathbf{R}}_{\underline{\mathbf{ss}}}$, the main diagonal blocks are colored in different patterns, which reveals the temporal structure of the sources, whereas the off-diagonal blocks correspond to uncorrelated values and present a single color. Ideally, the objective is to obtain $\underline{\mathbf{R}}_{\underline{\mathbf{yy}}}$ as close as possible to $\underline{\mathbf{R}}_{\underline{\mathbf{ss}}}$. For the BD solution found by DE, the temporal structure of only one of the sources was preserved, while the other source presented small temporal correlation. A similar result also applies to SOMI, whereas, for the SOMIq output, the found solution was the desired one, whose sources are mutually uncorrelated and with their temporal structure preserved. The observations outlined here were similar to the results found by the CLONALG, hence, we decided to omit them. These results reveal that, although encompassing different searching mechanisms, both metaheuristics were able to identify better solutions with SOMIq, indicating that its cost is able to express the required SOS more efficiently.

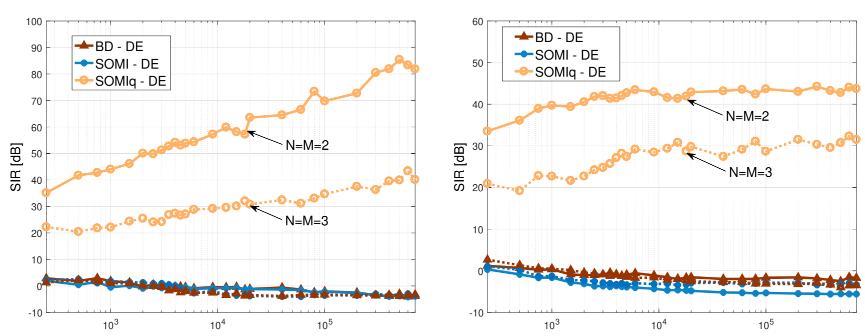
### *5.2. Performance Using Estimated Covariance Matrices*

For real-world problems, the covariance matrices are generally estimated from samples (via sample mean), which certainly leads to approximated values with reduced accuracy. This could be of major importance for the algorithms performance with tendency of converging to local solutions, which, as indicated in the previous analysis, is the case of the BD cost. This issue will be investigated now along with the cases in which the sources are Gaussian and non-Gaussian.

We consider the $N$=$M$=2 and $N$=$M$=3 cases. For $N$=$M$=2, the mixing matrix is $\mathbf{A} = [0.55, -0.92; -0.82, 0.38]$, while, for $N$=$M$=3, $\mathbf{A} = [0.55, -0.92, 0.20;$

$-0.82, 0.38, -0.24; -0.52, -0.27, 0.79]$. For both, the nonlinearity is the cubic function, given by Eq. (9), as adopted throughout this paper. The temporal coloration is obtained through FIR filters, chosen to be $\mathbf{h}_1 = [1, 0.6, -0.3, 0.1, 0.4]$, $\mathbf{h}_2 = [1, -0.2, -0.8, 0.2, 0.1]$ and $\mathbf{h}_3 = [1, 0.4, -0.7, 1.3, 0.2]$ (for $N$=2, only $\mathbf{h}_1$ and $\mathbf{h}_2$ are used). Now, we assume two types of distributions for $r_i(n)$: in the first case, for all $i$=1, …,$N$, $r_i(n)$ is an *i.i.d.* Gaussian signal with zero mean and variance equal to 2 and, in the second case, for all $i$=1, …,$N$, $r_i(n)$ is an *i.i.d.* signal uniformly distributed between $-1$ and $+1$. We consider that the number of samples of $y_i(n)$, may vary from 250 up to 700,000 for the covariance matrices estimation, being used, in the sequel, for obtaining BD, SOMI and SOMIq costs. A test set with 700,000 samples will be used for SIR estimation. The number of considered delays is $d = 4$.

To adapt the coefficients $\underline{\mathbf{\Gamma}}$ and $\underline{\mathcal{W}}$, we use the DE metaheuristic with the same previously defined parameters and perform 100 independent runs (CLONALG was not considered in this case, since its performance is similar to DE). For each number of samples considered in the covariance matrices estimation, the resulting mean SIR performance for the BD, SOMI and SOMIq solutions found by the DE are exhibited in Fig. 5 for the Gaussian and uniform sources (solid lines for the $N$=2 case and dotted lines for the $N$=3 case). It is possible




(a) Gaussian sources. (b) Uniform sources.

Figure 5: Mean SIR [dB] vs. Number of Samples (log).

to note that the BD and SOMI solutions found by the DE presented similar but lower values of SIR in all cases, while the SOMIq solutions achieved the best results: for the Gaussian sources, the higher the number of samples, the higher the SIR level obtained; however, for uniform sources, the number of samples causes less impact on the SIR performance (this limitation might be a consequence of the Gaussianity assumption in the SOMIq cost derivation). In addition, in comparison with the $N$=2 case, SOMIq is still able to perform separation for $N$=3 but with lower SIR values – since, with 12 adjustable coefficients, the DE convergence to local solutions is higher.

## 6. Conclusion

In this work, the problem of BSS was investigated in the context of PNL mixtures from an SOS-based perspective. In order to identify the constraints and conditions for the SOS-based approach, a temporal-extended formulation and a PNL model with cubic polynomial nonlinear functions were considered. Within this context, the classical SOS-based SOBI and GMI criteria were written under this temporal-extended standpoint, being named BD and SOMI, respectively. Moreover, to reduce the mathematical complexity of SOMI, a quadratic-like expression was proposed and named SOMIq.

Due to the simplicity of the SOS-based methods and the assumed cubic nonlinear functions (and also their Volterra expansion), the covariance matrices could be analytically computed. Based on this, a theoretical analysis on the costs defined the identifiability conditions and a lower bound on the number of delays that must be considered for separation: the number of delays will depend on the degrees of freedom of the separation system, from which a resulting linear term must always exist. Interestingly, the analysis might be extended to any polynomial functions. To evaluate the performance of the criteria in the considered PNL model, some simulations were held in scenarios using analytical and estimated versions of the covariance matrices, being the optimization process made by the DE and CLONALG metaheuristics. In the analytical case, the results indicated that the BD cost shape caused some difficulties for the metaheuristics to find the global optima; the SOMI criterion presented some issues in its cost minimization, which led to solutions that were not able to establish mutual independent sources with the desired precision; on the other hand, the SOMIq criterion presented higher global convergence than BD, with solutions that preserved the mutual independence (from an SOS point of view) and the temporal structure of data – also, by increasing the number of delays above the lower bound, we observed an improvement of the performance in terms of SIR. For the case with estimated covariance matrices, the SOMIq criterion again presented the best SIR performance for scenarios with Gaussian and uniformly distributed sources. However, a better performance can be achieved in the Gaussian case, since the SOMIq assumes Gaussian sources.

Although the present analysis focuses on a specific case of the PNL mixtures, it can be viewed as a relevant step towards the use of the SOS framework in the nonlinear BSS problem. In that sense, for future works, we consider the extension of this analysis to other polynomial nonlinearities, other nonlinear mixing models and the investigation of possible computational improvement based on the covariance matrices structure.

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