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Blind Source Separation of a Class of Nonlinear Mixtures

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Abstract. In this work, we deal with blind source separation of a class of nonlinear mixtures. The proposed method can be regarded as an adaptation of the solutions developed in [1, 2] to the considered mixing system. Also, we provide a local stability analysis of the employed learning rule, which permits us to establish necessary conditions for an appropriate convergence. The validity of our approach is supported by simulations.

1 Introduction

The problem of blind source separation (BSS) concerns the retrieval of an unknown set of source signals by using only samples that are mixtures of these original signals. A great number of methods has been proposed for the case wherein the mixture process is of linear nature. The cornerstone of the majority of these techniques is the independent component analysis (ICA) [3]. In contrast to the linear case, the recovery of the independence, which is the very essence of ICA, does not guarantee, as a rule, the separation of the sources when the mixture model is nonlinear. In view of this limitation, a more reasonable approach is to consider constrained mixing systems as, for example, post-nonlinear (PNL) mixtures [4] and linear-quadratic mixtures [2].

In this work, we investigate the problem of BSS in a particular class of nonlinear systems which is related to a chemical sensing application. More specifically, the contributions of this paper are the adaptation of the ideas presented in [1, 2] to the considered mixing system, as well as a study on some necessary conditions for a proper operation of the obtained separating method. Concerning the organization of the document, we begin, in Section 2, with a brief description of the application that has motivated us. After that, in Section 3, we expose the separation method and also a stability analysis of the learning rule. In Section 4, simulations are carried out in order to verify the viability of the proposal. Finally, in Section 5, we state our conclusions and remarks.

2 Motivation and Problem Statement

The classical methods for chemical sensing applications are generally based on the use of an unique high-selective sensor. As a rule, these techniques demand

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sophisticated laboratory analysis, which makes them expensive and time consuming. An attractive alternative to these methods relies on the use of an array of less-selective sensors combined with a post-processing stage whose purpose is exactly to extract the relevant information from the acquired data.

In [5, 6], post-processing stages based on BSS methods were considered in the problem of estimating the concentrations of several ions in a solution. In this sort of application, a device called ion-sensitive field-effect transistor (ISFET) [5] may be employed as sensor. In short, the ISFET is built on a MOSFET by replacing the metallic gate with a membrane sensitive to the ion of interest, thus permitting the conversion of chemical information into electrical one.

The Nikolsky-Eisenman (NE) model [5] provides a very simple and yet adequate description of the ISFET operation. According to this model, the response of the i -th ISFET sensor is given by:

$$x_i = c_{i1} + c_{i2} \log \left(s_i + \sum_{j, j \neq i} a_{ij} s_j^{\frac{z_i}{z_j}} \right), \quad (1)$$

where s_i and s_j are the concentration of the ion of interest and of the concentration of the j -th interfering ion, respectively, and where z_i and z_j denote the valence of the ions i and j , respectively. The selective coefficients a_{ij} model the interference process; c_{i1} and c_{i2} are constants that depends on some physical parameters. Note that when the ions have the same valence, then the model (1) can be seen as a particular case of the class of PNL systems, as described in [6].

In the present work, we envisage the situation in which $z_i \neq z_j$. According to the NE model, one obtains a tough nonlinear mixing model in this case. For the sake of simplicity, we assume, in this paper, that the coefficients c_{i1} and c_{i2} are known (even if their estimations are not so simple). Considering a mixture of two ions, such simplification leads to the following nonlinear mixing system that will be considered in this work

$$\begin{aligned} x_1 &= s_1 + a_{12} s_2^k, \\ x_2 &= s_2 + a_{21} s_1^{\frac{1}{k}}, \end{aligned} \quad (2)$$

where $k = z_1/z_2$ and is known. We consider that k takes only positive integer values. Indeed, in many actual applications, typical target ions are H_3O^+ , NH_4^+ , Ca^{2+} , K^+ , etc. Consequently, many cases correspond to $k \in \mathbb{N}$ and, in this paper, we will focus on this case. Also, the sources are supposed positives, since they represent concentrations. Finally, it is assumed that s_i are mutually independent, which is equivalent to assume that there is no interaction between the ions.

3 Separation Method

For separating sources s_i from mixtures (2), we propose a parametric recursive model (see (3) below), whose parameters w_{ij} will be adjusted by a simple ICA algorithm. Consequently, equilibrium points and their stability are depending both on a structural condition (due to the recursive nature of (3)) and on the learning algorithm, as explained in subsection 3.3.

3.1 Separating Structure

In this work, we adopted the following recurrent network as separating system:

$$\begin{aligned} y_1(m+1) &= x_1 - w_{12}y_2(m)^k \\ y_2(m+1) &= x_2 - w_{21}y_1(m)^{\frac{1}{k}}, \end{aligned} \quad (3)$$

where $[w_{12} \ w_{21}]^T$ are the parameters to be adjusted. In order to understand how this structure works, let $\mathbf{s} = [s_1 \ s_2]^T$ denote a sample of the sources. By considering (2), one can easily check that when $[w_{12} \ w_{21}]^T = [a_{12} \ a_{21}]^T$, then \mathbf{s} corresponds to an equilibrium point of (3). This wise approach to counterbalance the action of the mixing system without relying on its direct inversion was firstly developed in [1] regarding linear BSS. Its extension to the nonlinear case was proposed in [2], in the context of source separation of linear-quadratic mixtures.

Naturally, an ideal operation of (3) as a separating system requires that $\mathbf{s} = [s_1 \ s_2]^T$ be the only equilibrium point when $[w_{12} \ w_{21}]^T = [a_{12} \ a_{21}]^T$. Unfortunately, this is not the case as can be checked by setting $y_1(m+1) = y_1(m) = y_1$ and $y_2(m+1) = y_2(m) = y_2$ in (3). From this, one observes that the determination of the equilibrium points of (3) leads to the following equation:

$$y_1 = x_1 - a_{12} \left(x_2 - a_{21}y_1^{(1/k)} \right)^k. \quad (4)$$

After straightforward calculation, including a binomial expansion, (4) becomes

$$(1 + a_{12}b_0)y_1 + a_{12} \sum_{i=1}^{k-1} b_i y_1^{1-\frac{i}{k}} + (a_{12}b_k - x_1) = 0, \quad (5)$$

where $b_i = \binom{k}{i} x_2^i (-a_{21})^{(k-i)}$.

By considering the transformation $u = y_1^{\frac{1}{k}}$ in (5), one can verify that the solution of this expression is equivalent to the determination of the roots of a polynomial of order k and, as a consequence, the number of equilibrium points grows linearly as k increases. Thus, it becomes evident that the use of (3) is appropriate only for small values of k . For instance, when $k = 2$ there are just two equilibrium points: one corresponds to the sources themselves and the other one corresponds to a mixture of these sources. In the next step of our investigation, we shall verify the conditions to be satisfied so that the equilibrium point associated with the sources be stable.

In view of the difficulty embedded in a global analyze of stability, we consider the study of the local stability in the neighborhood of the equilibrium point $\mathbf{s} = [s_1 \ s_2]^T$ based on the first-order approximation of the nonlinear system (3). This linearization can be expressed by using a vectorial notation as follows:

$$\mathbf{y}(m+1) \approx \mathbf{c} + \mathbf{J}\mathbf{y}(m), \quad (6)$$

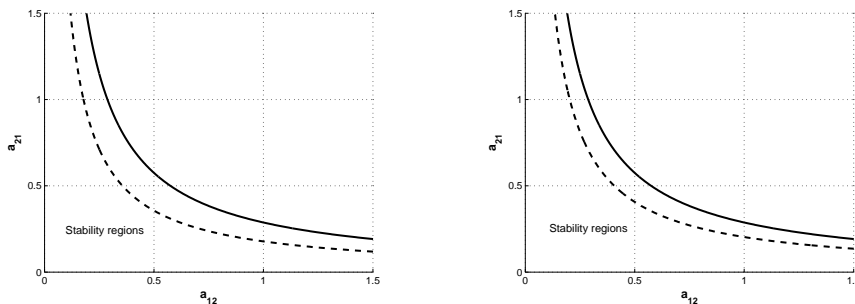
where $\mathbf{y}(m) = [y_1(m) \ y_2(m)]^T$, \mathbf{c} is a constant vector and \mathbf{J} is the Jacobian matrix of (3) evaluated at $[s_1 \ s_2]^T$, which is given by:

$$\mathbf{J} = \begin{bmatrix} 0 & -a_{12}k s_2^{(k-1)} \\ -\frac{1}{k} a_{21} s_1^{(\frac{1}{k}-1)} & 0 \end{bmatrix}. \quad (7)$$

It can be proved that a necessary and sufficient condition for local stability of a discrete system is that the absolute values of the eigenvalues of the Jacobian matrix evaluated at the equilibrium point of interest be smaller than one [7]. Applying this result on (7), the following condition of local stability is obtained:

$$|a_{12}a_{21}s_1^{(\frac{1}{k}-1)}s_2^{k-1}| < 1. \quad (8)$$

This is a first constraint of our strategy, given that this condition must be satisfied for each sample $[s_1 \ s_2]^T$. In order to illustrate this limitation, the stability boundaries in the (a_{12}, a_{21}) plane for several cases are depicted in Figure 1.



(a) Influence of k : sources distributed between $(0.1, 1.1)$ with $k = 2$ (solid) and $k = 3$ (dash).

(b) For $k = 2$: sources distributed between $(0.1, 1.1)$ (solid) and between $(0.2, 2.2)$ (dash).

Fig. 1. Stability boundaries in the (a_{12}, a_{21}) plane.

3.2 Learning Algorithm

We consider a learning rule founded on the cancellation of nonlinear correlations, given by $E\{f(y_i)g(y_j)\}$, between the retrieved sources [1]. The following nonlinear functions were chosen: $f(\cdot) = (\cdot)^3$ and $g(\cdot) = (\cdot)$. Therefore, at each time n , the iteration of the separating method consists of: 1) the computation of y_i , for each sample of the mixtures, according to the dynamics (3) and 2) the update of the parameters w_{ij} according to:

$$\begin{aligned} w_{12}(n+1) &= w_{12}(n) + \mu E\{y_1^3 \bar{y}_2\} \\ w_{21}(n+1) &= w_{21}(n) + \mu E\{y_2^3 \bar{y}_1\}, \end{aligned} \quad (9)$$

where μ corresponds to the learning rate, $[y_1 \ y_2]^T$ denotes the equilibrium point of (3) and \bar{y}_i is a centering version of y_i ^{1,2}. One can check³ that (9) converges

¹ More specifically, we adopt the following notation $\bar{y}_i^r = y_i^r - E\{y_i^r\}$.

² Given that the signals are not supposed zero-mean, the centering of one of the variables in (9) is necessary, so that it converges when y_1 and y_2 are mutually independent.

³ Note that (9) converges when $E\{y_i^3 \bar{y}_j\} = E\{y_i^3 y_j\} - E\{y_i^3\} E\{y_j\} = 0$.

when $E\{y_1^3 y_2\} = E\{y_1^3\}E\{y_2\}$ and $E\{y_2^3 y_1\} = E\{y_2^3\}E\{y_1\}$. Obviously, these conditions are only necessary ones for the statistical independence between the sources and, as a consequence, there may be particular sources for which such strategy fails. On the other hand, this strategy provides a less complex algorithm than those that deal directly with a measure of statistical independence.

In the last section, a stability condition concerning the separation structure was provided. Likewise, as it will be seen in the sequel, it is possible to analyze the stability of the learning rule (9). This study will permit us to determine whether the separating equilibrium point, i.e., $[w_{12} \ w_{21}]^T = [a_{12} \ a_{21}]^T$, corresponds to a stable one and, as a consequence, whether it is attainable for the learning rule.

3.3 Stability Analysis of the Learning Rule

According to the ordinary differential equation theory, it is possible, by assuming that μ is sufficiently small, to rewrite (9) as:

$$\begin{aligned}\frac{dw_{12}}{dt} &= E\{y_1^3 \bar{y}_2\} \\ \frac{dw_{21}}{dt} &= E\{y_2^3 \bar{y}_1\}.\end{aligned}\quad (10)$$

A first point to be stressed is that the determination of all equilibrium points of (10) is a rather difficult task. Even when $k = 1$ in (2), which corresponds to the linear BSS problem, this calculation demands a great deal of effort [8].

Secondly, we are interested in the stability of the point $[w_{12} \ w_{21}]^T = [a_{12} \ a_{21}]^T$, but one must keep in mind that there are structural conditions to be assured so that it corresponds to an equilibrium point of (10). For example, when $k = 2$, we observed through simulations that this ideal adjustment of the separating system usually guarantees the separation of the sources when the local condition (8) is satisfied. Thus, in this situation and under the hypothesis of independent sources, it is assured that $E\{y_i^3 \bar{y}_j\} = E\{s_i^3 \bar{s}_j\} = 0$.

As in Section 3.1, the local stability analysis is based on a first-order approximation of (10). However, since we are dealing with a continuous dynamics in this case, a given equilibrium point of the learning rule is locally stable when the real parts of all eigenvalues of the Jacobian matrix are negatives [7]. After straightforward calculations, one obtains the Jacobian matrix evaluated at the equilibrium point $[a_{12} \ a_{21}]^T$

$$\mathbf{J} = \begin{bmatrix} (3E\{y_1^2 \bar{y}_2 \frac{\partial y_1}{\partial a_{12}}\} + E\{\bar{y}_1^3 \frac{\partial y_2}{\partial a_{12}}\}) & (3E\{y_1^2 \bar{y}_2 \frac{\partial y_1}{\partial a_{21}}\} + E\{\bar{y}_1^3 \frac{\partial y_2}{\partial a_{21}}\}) \\ (3E\{y_2^2 \bar{y}_1 \frac{\partial y_2}{\partial a_{12}}\} + E\{\bar{y}_2^3 \frac{\partial y_1}{\partial a_{12}}\}) & (3E\{y_2^2 \bar{y}_1 \frac{\partial y_2}{\partial a_{21}}\} + E\{\bar{y}_2^3 \frac{\partial y_1}{\partial a_{21}}\}) \end{bmatrix}. \quad (11)$$

Note that, assuming an ideal operation of the separating system, $[y_1 \ y_2]^T$ could be replaced by $[s_1 \ s_2]^T$, which permits us to express the stability conditions of (9) in terms of some statistics of the sources.

The entries of the Jacobian matrix can be calculated by applying the chain rule property on (3). For instance, it is not difficult to verify from that:

$$\frac{\partial y_1}{\partial a_{12}} = -(y_2^k + a_{12} k y_2^{k-1} \frac{\partial y_2}{\partial a_{12}}). \quad (12)$$

Given that

$$\frac{\partial y_2}{\partial a_{12}} = -\frac{1}{k} a_{21} y_1^{\frac{1}{k}-1} \frac{\partial y_1}{\partial a_{12}}, \quad (13)$$

and substituting this expression in (12), one obtains:

$$\frac{\partial y_1}{\partial a_{12}} = \frac{-y_2^k}{1 - a_{12} a_{21} y_1^{\frac{1}{k}-1} y_2^{k-1}}. \quad (14)$$

By conducting similar calculations, one obtains the other derivatives:

$$\frac{\partial y_2}{\partial a_{12}} = \frac{a_{21} y_1^{\frac{1}{k}-1} y_2^k}{k(1 - a_{12} a_{21} y_1^{\frac{1}{k}-1} y_2^{k-1})} \quad (15)$$

$$\frac{\partial y_1}{\partial a_{21}} = \frac{k a_{12} y_1^{\frac{1}{k}} y_2^{k-1}}{1 - a_{12} a_{21} y_1^{\frac{1}{k}-1} y_2^{k-1}} \quad (16)$$

$$\frac{\partial y_2}{\partial a_{21}} = \frac{-y_1^{\frac{1}{k}}}{1 - a_{12} a_{21} y_1^{\frac{1}{k}-1} y_2^{k-1}} \quad (17)$$

As it would be expected, when $k = 1$, one obtains from the derived expressions the same conditions developed in [8] and [9] for the stability of the Héroult-Jutten algorithm for linear source separation.

4 Experimental Results

Aiming to assess the performance of the proposed solution, experiments were conducted for the cases $k = 2$ and $k = 3$. In both situations, the efficacy of the obtained solutions was quantified according to the following index:

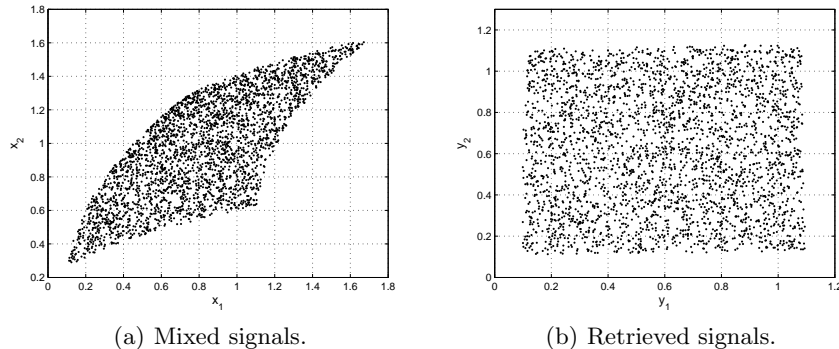
$$SNR_i = 10 \log \left(\frac{E\{s_i^2\}}{E\{(s_i - y_i)^2\}} \right). \quad (18)$$

From this, a global index can be defined as $SNR = 0.5(SNR_1 + SNR_2)$.

k = 2. In a first scenario, we consider the separation of two sources uniformly distributed between $[0.1, 1.1]$. The mixing parameters are given by $a_{12} = 0.5$ and $a_{21} = 0.5$; a set of 3000 samples of the mixtures was considered and the number of iterations regarding the learning algorithm (9) was defined to 3500 with $\mu = 0.05$. The initial conditions of the dynamics (3) were chosen as $[y_1(1) \ y_2(1)]^T = [0 \ 0]^T$. The results of this first case are expressed in the first row of Table 1. In Figure 2, the joint distributions of the mixtures and of the retrieved signals are depicted for a typical case ($SNR = 35\text{dB}$). Note that the outputs of the separating system are almost uniformly distributed, which indicates that the separation task was fulfilled. Also, we performed experiments by considering on each sensor

Table 1. Average SNR results over 100 experiments and standard deviation (STD).

	SNR_1	SNR_2	SNR	$STD(SNR)$
$k = 2$ (Scenario 1)	37.18	33.05	35.12	8.90
$k = 2$ (Scenario 2)	17.98	15.35	16.67	1.72
$k = 2$ (Scenario 3)	36.49	31.84	34.17	4.92
$k = 3$ (Scenario 1)	22.46	21.04	21.75	5.02

**Fig. 2.** First scenario - $k = 2$.

an additive white Gaussian noise with a signal-to-noise ratio of $17dB$. The results for this second scenario are depicted in the second row of Table 1.

A third scenario was composed by a uniformly distributed source between $[0.3, 1.3]$ and a sinusoidal source varying in the range $[0.2, 1.2]$. In this case, the mixing parameters are given by $a_{12} = 0.6$ and $a_{21} = 0.6$ and the constants related to the separating system were adjusted as in the first experiment. Again, the separation method was able to separate the original sources, as can be seen in the third row of Table 1.

$k = 3$. The problem becomes more tricky when $k = 3$. Firstly, we observed through simulations that, even for a separating point $[w_{12} \ w_{21}]^T = [a_{12} \ a_{21}]^T$ that satisfies the equilibrium condition (8), the structure (3) does not guarantee source separation, since there can be another stable equilibrium solution that has no relation with the sources. In this particular case, we observed, after performing some simulations, that the adopted network may be attracted by a stable limit cycle and, also, that it is possible to overcome this problem by changing the initial conditions of (3) when a periodic equilibrium solution occurs.

A second problem in this case is related to the convergence of the learning rule. Some simulations suggested the existence of spurious minima in this case. These two problems result in a performance degradation of the method when compared to the case $k = 2$, as can be seen in the last row of Table 1. In this case, we considered a scenario with two sources uniformly distributed between $[0.3, 1.3]$ and mixing parameters given by $a_{12} = 0.5$ and $a_{21} = 0.5$. The initial

conditions of (3) were defined as $[0.5 \ 0.5]^T$. Also, we considered 3000 samples of the mixtures and 10000 iterations of the learning algorithm with $\mu = 0.01$.

5 Conclusions

The aim of this work was to design a source separation strategy for a class of nonlinear systems that is related to a chemical sensing application. Our approach was based on the ideas presented in [1, 2] in such a way that it may be viewed as an extension of these works to the particular model considered herein. Concerning the proposed technique, we investigated the stability of the separation structure as well as the stability of the learning algorithm. This study permitted us to obtain necessary conditions for a proper operation of the separation method. Finally, the viability of our approach was attested by simulations.

A first perspective of this work concerns its application in a real problem of chemical sensing. Also, there are several questions that deserve a detailed study as, for example, the design of algorithms that minimizes a better measure of independence between the retrieved sources (e.g. mutual information), including an investigation of the separability of the considered model. Another envisaged extension is to provide a source separation method for the most general case of the Nikolsky-Eisenman model, which is given by (1): 1) by considering the logarithmic terms; and 2) by considering the cases $k \in \mathbb{Q}$. Actually, preliminary simulations show that our proposal works for simple cases in $k \in \mathbb{Q}$, such as $k = 1/3$ and $k = 2/3$. However, there are tricky points in the theoretical analysis conducted in this paper that are not appropriate to this new situation.

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