An Overview of Blind Source Separation Methods for Linear-Quadratic and Post-nonlinear Mixtures

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Abstract. Whereas most blind source separation (BSS) and blind mixture identification (BMI) investigations concern linear mixtures (instantaneous or not), various recent works extended BSS and BMI to nonlinear mixing models. They especially focused on two types of models, namely linear-quadratic ones (including their bilinear and quadratic versions, and some polynomial extensions) and post-nonlinear ones. These works are particularly motivated by the associated application fields, which include remote sensing, processing of scanned images (show-through effect) and design of smart chemical and gas sensor arrays. In this paper, we provide an overview of the above two types of mixing models and of the associated BSS and/or BMI methods and applications.

Keywords: Blind source separation · Blind mixture identification · Linear-quadratic mixing model · Post-nonlinear mixing model · Survey

1 Introduction

Blind source separation (BSS) methods aim at estimating a set of source signals from a set of observed signals which are mixtures of these source signals [17]. It has been shown that, if the mixing function applied to the source signals is completely unknown, the BSS problem (or its ICA solution) leads to unacceptable indeterminacies. Therefore, in most investigations the mixing function is requested to belong to a known class and only the values of its parameters are to be estimated. Many of these works are restricted to the simplest class of mixtures, namely linear ones (instantaneous or not) [17]. However, various more advanced studies dealing with *nonlinear* mixtures have also been reported. Two

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nonlinear mixing models have especially been considered. The first one consists of linear-quadratic (LQ) mixtures (and, to some extent, polynomial ones). It forms a natural extension of linear mixtures, by also including second-order (and possibly higher-order) terms. It may thus first be seen as a generic model, to be used as an approximation (truncated polynomial series) of various, possibly unknown, models faced in practical applications. Moreover, LQ mixing has been shown to *actually* occur in some applications. It has thus mainly been used for unmixing of remote sensing data [32,40,46–49], processing of scanned images involving the show-through effect [5,27,45,50] and analysis of gas sensor array data [10]. The other main nonlinear mixing model is the post-nonlinear (PNL) one. In this case, the mixing process comprises an initial linear mixing stage followed by a set of component-wise nonlinear functions. Therefore, such a model is useful in applications where the first stage of the mixing process is of linear nature but the sensors then exhibit a nonlinear response, due to saturation or more complex nonlinear transducer phenomena. The main field of application for PNL models is the design of smart chemical sensor arrays [11,12,25]. PNL models were also applied in the context of remote sensing data [6].

In this paper, we provide an overview of the two above-defined nonlinear mixing models and associated BSS and/or blind mixture identification (BMI) methods reported so far. We first define both mixing models in Sect. 2. We then present BSS/BMI methods for LQ mixtures in Sect. 3, and methods for PNL mixtures in Sect. 4. To conclude, related topics are briefly discussed in Sect. 5.

2 Considered Nonlinear Mixing Models

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

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

where $x_i(n)$ are the values of the P observed mixed signals for the sample index n and $s_j(n)$ are the values of the M unknown source signals which yield these observations, whereas a_{ij} and b_{ijk} are respectively the linear and quadratic mixing coefficients (with unknown values in the blind case) which define the considered source-to-observation transform. The specific version of this model which contains no second-order auto-terms (i.e. $b_{ijk} = 0$ when $k = j$) is called the bilinear mixing model. It corresponds to replacing the second sum in (1) by $\sum_{j=1}^{M-1} \sum_{k=j+1}^{M}$ (additional constant terms are considered in [5]). Similarly, the quadratic version of this model is obtained when all coefficients a_{ij} are zero.

A first matrix form of that model (1) reads

$$x(n) = As(n) + Bp(n) \tag{2}$$

where the source and observation vectors are

$$s(n) = [s_1(n), \ldots, s_M(n)]^T, \qquad x(n) = [x_1(n), \ldots, x_P(n)]^T, \tag{3}$$

where ^{T} stands for transpose and matrix A consists of the mixing coefficients a_{ij}. The column vector $p(n)$ is composed of all source products $s_j(n)s_k(n)$ of (1), i.e. with $1 \leq j \leq k \leq M$, arranged in a fixed, arbitrarily selected, order (see e.g. [49] for the natural order). The matrix B is composed of all entries b_{ijk} arranged so that i is the row index of B and the columns of B are indexed by (j,k) and arranged in the same order as the source products $s_j(n)s_k(n)$ in $p(n)$.

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

$$\tilde{s}(n) = \begin{bmatrix} s(n) \\ p(n) \end{bmatrix} \tag{4}$$

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

$$\tilde{A} = [A \ B]\,. \tag{5}$$

The LQ mixing model (2) then yields

$$x(n) = \tilde{A}\tilde{s}(n). \tag{6}$$

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

$$\tilde{S} = [\tilde{s}(1), \ldots, \tilde{s}(N)], \qquad X = [x(1), \ldots, x(N)]. \tag{7}$$

The single-sample model (6) thus yields its overall matrix version

$$X = \tilde{A}\tilde{S}. \tag{8}$$

Some LQ BSS methods are based on the "original sources" $s_1(n), \ldots, s_M(n)$ contained in $s(n)$, whereas other methods are based on the signals contained in $\tilde{s}(n)$, which are called the "*extended* sources" hereafter.

We also consider a second class of nonlinear mixing models known as post-nonlinear (PNL) models, in which each observed mixture corresponds to a univariate nonlinear function of a linear mixture of the sources. In its scalar form, the PNL model is given by

$$x_i(n) = f_i\left(\sum_{j=1}^{M} a_{ij} s_j(n)\right) \qquad \forall\ i \in \{1, \cdots, P\} \tag{9}$$

where a_{ij} and $f_i(\cdot)$ denote the linear mixing coefficients and the univariate nonlinear functions, respectively. In the blind case, both a_{ij} and $f_i(\cdot)$ are unknown. However, one often assumes that $f_i(\cdot)$ are strictly monotonic functions and, thus, admit inverse functions.

3 BSS/BMI Methods For Linear-Quadratic Mixtures

3.1 Independent Component Analysis (ICA) and Statistical Methods

(A) Methods for i.i.d Sources: Various LQ BSS methods were developed for i.i.d and mutually statistically independent sources, by **exploiting the mutual independence of the outputs of a separating system**. A first class of such methods is intended for the version of the LQ model which is determined with respect to the *original* sources, i.e. such that $P = M$. Their separating systems are nonlinear recurrent networks, which were described e.g. in [20,36] (and then extended e.g. in [14,20,50], including to much broader classes of nonlinear mixtures than LQ ones). The first of these LQ BSS methods [36] may be seen as an LQ extension of the linear Hérault-Jutten method, since it adapts the parameters of the above nonlinear recurrent networks so as to achieve an approximation of output independence, more precisely so as to cancel the (3,1) and (2,1) centered output cross-moments. The second reported method [51] is the LQ extension of Comon's linear approach, since it adapts the above parameters so as to minimize the mutual information of the network outputs, thus completely ensuring output independence.

The above recurrent separating systems are attractive because they only require one to know the analytical expression of the mixing model. On the contrary, direct structures require one to know the analytical expression of the *inverse* of the mixing model, which cannot be derived for *nonlinear* mixing models, except in simple situations such as bilinear models with 2 original sources [5,36]. However, nonlinear recurrent structures may yield some limitations: (i) they may be unstable at equilibrium points of interest or they may even lead to chaotic behavior [20] (see also [19–21] for extended networks which solve such problems; such networks have therefore also been used in [7] as original tools for solving nonlinear equations), (ii) they may have spurious equilibrium points and (iii) they require one to iteratively compute each output vector.

The situation becomes simpler when the number of observations can be increased up to the number of *extended* sources in $\tilde{s}(n)$. The mixing model is then determined and linear with respect to these extended sources, as shown by (6) or (8). Especially, performing M *linear* combinations of all these observations, with adequate coefficient values, then makes it possible to restore all M original sources. These coefficients may be adapted so as to enforce the statistical independence of the restored signals. In [26], this is achieved by a two-stage procedure based on minimizing the mutual information of these restored signals.

Still for mutually statistically independent and i.i.d sources, other reported LQ BSS and extended methods are based on **estimating the mixing model** (thus firstly achieving BMI). The first approach is based on maximizing the likelihood of the observations [15,37,38,50]. These investigations deal with determined mixtures of original sources and use the above-defined recurrent separating networks. The link between BSS methods based on likelihood maximization and mutual information minimization was established in [22] for *nonlinear* mixtures, including LQ ones.

The second reported approach for estimating the mixing model consists in starting from the relationships which define the observed signals with respect to the source signals and mixing coefficients, and deriving resulting expressions of some cumulants or moments of the observed signals with respect to those of the source signals and to the mixing coefficients. Solving these equations for known (estimated) values of the observation cumulants or moments then especially yields the values of the mixing coefficients (up to some indeterminacies). This approach was applied to quadratic mixtures in [16]. Also using cumulants, a quite different BMI method was proposed in [42] for complex-valued sources.

Finally, other LQ BSS methods for i.i.d sources **jointly estimate the sources** *and* **mixing model**, whereas the above-defined methods put more emphasis on *one* of these two types of unknowns of the BSS/BMI problem. This joint approach especially includes LQ Bayesian methods [24,27]. Unlike above-described approaches, Bayesian methods do not explicitly use a separating system and thus avoid the associated potential issues, mainly for determined mixtures of original sources. However, the development of the use of Bayesian methods is limited by the complexity of their implementation and their high computational cost, as compared with the most popular ICA-related methods.

(B) Methods for Non-i.i.d Sources: Other LQ BSS methods have been developed by considering non-i.i.d random source signals and exploiting their autocorrelation (when each source is not independently distributed for different samples n) and/or their non-stationarity (when each source is not identically distributed for different samples). Both properties were used in the extension of the above likelihood-based method proposed in [39]. Similarly, the above-mentioned Bayesian approach [24,27] has been applied to autocorrelated sources. A BMI method for LQ mixtures of autocorrelated and mutually independent source signals was also proposed in [1], using a joint diagonalization of a set of observation correlation matrices. Using similar tools, a method for extracting source products was also presented in [33] for uncorrelated sources with distinct autocorrelations.

3.2 Extensions of Nonnegative Matrix Factorization (NMF)

Although the considered observations (1) are nonlinear mixtures of the original sources, the reformulated mixing model (8) shows that they are linear mixtures of the associated extended sources and that, from the point of view of the latter sources, they follow the matrix-form mixing model encountered in *linear* NMF. When $\tilde{A}$ and $\tilde{S}$ (and thus X) are nonnegative, this allows one to develop LQ BSS/BMI methods for jointly estimating them by extending linear NMF methods, especially by adapting (estimates of) $\tilde{A}$ and the linear part of $\tilde{S}$ so as to minimize the Frobenius norm $||X - \tilde{A}\tilde{S}||_F$. Resulting gradient-based and/or Hessian-based algorithms have more complex forms than for linear mixtures, because they also involve derivatives of the second-order terms of $\tilde{S}$ with respect to the original sources. Several such methods are detailed in [47] (which also addresses polynomial mixtures) and [49] (the application of a standard NMF algorithm to the *extended* sources is also considered in [46,47]). A similar approach, dedicated to the case when both the sources and mixing coefficients follow bilinear models, is described in [32]. Besides, [45] deals with a very specific configuration involving 2 mixtures of 2 original sources, with the same quadratic contribution in both mixtures.

3.3 Sparse Component Analysis (SCA)

For linear mixtures, two major principles used in the literature for performing SCA may be briefly defined as follows. The first one consists in minimizing a sparsity-based cost function, such as the L0 norm of an "error term". The second one consists in taking advantage of zones (i.e. adjacent samples) in the sources where only one source is active, i.e. non-zero. These two principles have been extended to LQ mixtures, respectively in [28] and [18]. Besides, [40] describes an approach which also takes advantage of small parts of the observed data where only one "contribution" is non-zero, more precisely pixels which correspond to only one pure material (i.e. pure pixels) in the considered application to unmixing of remote sensing spectra. However, the proposed criterion is only guaranteed to yield a *necessary* condition for detecting pure pixels.

4 BSS Methods for Post-nonlinear Mixtures

There are basically two approaches to develop BSS methods for the mixing model expressed in (9). In the first one, which will be referred to as the *joint approach*, the nonlinear functions $f_i(\cdot)$ and the mixing matrix are jointly counterbalanced by means of a single criterion. Alternatively, in the *two-stage approach*, an initial stage aims at estimating the nonlinear functions $f_i(\cdot)$ or their inverses. Once these functions are estimated, the second stage simply becomes a linear BSS problem. In the sequel, we shall review methods for the joint and the two-stage approaches.

4.1 Joint Approaches

As in linear BSS, most of the works in PNL separation consider the determined case ($P = M$) and an adaptation framework based on ICA. An important reason for that comes from the theoretical results ensuring ICA-separability in PNL models. Indeed, the seminal work of Taleb and Jutten [59] showed that, by considering the following mirrored version of (9) as separating system

$$y_i(n) = \sum_{j=1}^{P} w_{ij} g_j(x_j(n)) \qquad \forall\, i \in \{1, \cdots, P\}, \tag{10}$$

where w_{ij} and $g_j(\cdot)$ denote, respectively, the separating coefficients and the inverting functions, the recovery of independent components $y_1(n), \cdots, y_P(n)$ leads to source separation under conditions very close to those established for the linear case. Eventually, other works [3,8,61] extended [59] by providing more rigorous and less restrictive proofs.

By relying on the ICA-separability of PNL models, several works, starting from [59], proposed strategies to jointly adapt w_{ij} and $g_j(\cdot)$ by minimizing measures of statistical dependence. Most of these works considered a gradient-based framework for minimizing the mutual information [4,9,59] in the case of i.i.d sources. However, in [43], a joint method based on mutual information was set up to deal with non-i.i.d sources. It is also worth mentioning that alternative criteria of statistical dependence can be considered, as, for instance, in [2].

In the mutual information approach, a first issue is the estimation of the score functions of $y_i(n)$, which was addressed by several works of Pham (see [53], for instance) — these works dealt with general BSS models but were fundamental to many PNL algorithms. A second issue is the risk of local convergence to non-separating minima. In order to overcome this problem, several works proposed learning algorithms based on meta-heuristics [23,56]. Finally, another issue that must be handled in joint PNL ICA algorithms is the parametrization of the inverting functions $g_j(\cdot)$. Indeed, since the ICA-separability results for (10) require bijective pairs $f_j(\cdot)$ and $g_j(\cdot)$, one aims at defining parametric functions $g_j(\cdot)$ that are bijective but flexible enough to compensate $f_j(\cdot)$. Possible solutions considered monotonic polynomials [23], splines [57], functions based on quantiles [54] and monotonic neural networks [31].

As in linear and LQ mixtures, an important class of joint PNL methods are obtained by formulating BSS as a Bayesian estimation problem. A Bayesian approach provides a natural framework to take into account prior information that can be expressed through a probabilistic modeling. On the other hand, the challenging aspect here is related to the practical resolution of the resulting inference problem. In [35], the authors introduced a variational learning scheme in order to perform inference. Alternatively, in [25], a Markov chain Monte Carlo (MCMC) strategy was set up to deal with a special class of PNL models that arises in chemical sensing applications. Such an approach has allowed the incorporation of non-negative priors for the sources and the mixing coefficients [25]. More recently, an MCMC-based Bayesian method was also proposed, but now for a special class of PNL models related to hyperspectral imagery [6]. A Bayesian approach was also considered for dealing with the underdetermined case ($P < M$) [63].

4.2 Two-Stage Approaches

The first two-stage PNL approach [8] addressed the separation of two bounded sources under geometrical arguments. Indeed, since the scatter plot of bounded PNL mixtures presents nonlinear borders, [8] proposed to identify $g_j(\cdot)$ by recovering signals $g_1(x_1)$, $g_2(x_2)$ that provide linear borders in the scatter plot. A similar geometrical approach was proposed in [52] and was able to deal with the case of more than two sources.

Another idea to identify $g_j(\cdot)$ is to exploit prior information related to the sparsity of the sources. This idea is similar to the geometrical approach—indeed, when the sources are sparse, it becomes easier to identify the borders associated with the scatter plot of the mixtures. For instance, in [55], the authors proposed a SCA-based scheme to identify $g_j(\cdot)$ by assuming that there are, for each source $s_i(n)$, a temporal (or spatial) zone in which only $s_i(n)$ is active — such an idea is similar to that previously described for LQ mixtures. Similar SCA schemes were also developed for dealing with the case of underdetermined PNL mixtures [60, 62] — here, of course, the resulting linear BSS problem is more challenging than the determined linear BSS problem.

The underlying criteria for inverting $g_j(\cdot)$ in the two-stage methods presented so far are based on a joint processing of the mixtures. Alternatively, there are two-stage methods that process each mixture in a separate fashion — this approach will be referred to as *independent two-stage methods*. In this case, the resulting method thus comprises P independent executions of an algorithm that blindly compensates each $f_i(\cdot)$ followed by the application of a linear BSS method.

The first independent PNL two-stage methods make use of a well-known property involving probability distributions and nonlinear functions: it is possible to blindly estimate a univariate random variable that underwent a nonlinear distortion by setting up a nonlinear compensating function that provides a new random variable having the same probability distribution as that of the original random variable. This idea of matching the probability distributions of the input and its estimated version was firstly applied in signal processing by White [64].

In the context of PNL methods, it is possible to adapt the strategy proposed in [64] by observing that, after the linear mixing stage, the signals tend to Gaussian variables — this is a consequence of the central limit theorem. Moreover, due to the action of $f_j(\cdot)$, the observations $x_j(n)$ have non-Gaussian distributions. Therefore, a natural idea to counterbalance $f_j(\cdot)$ is to adapt $g_j(\cdot)$ so that its output becomes again Gaussian. Implementations of this strategy can be found in [58,66,67]. Interestingly, these Gaussianization-based methods provide better results as the number of sources increases, since the hypothesis of Gaussian linear mixtures is more realistic as P grows. However, even for a small number of sources they can provide at least an initial approximation of $g_j(\cdot)$ [58].

Alternative independent two-stage methods were proposed by taking into account other prior information than the gaussianity of the linear mixtures. For instance, [29] introduced a novel method that is tailored to the case of bandlimited sources. More recently, by considering the assumption that the sources admit a sparse representation in a known domain, [30] extended [29] and introduced a method for blind compensation of nonlinear functions that can be directly applied to PNL separation problems. Note that, differently from the above-discussed PNL methods based on sparsity priors, the introduced method in [30] operates in an independent fashion.

5 Conclusion

In this overview, we especially focused on practical BSS/BMI methods intended for two major types of nonlinear mixtures. Due to space limitations, we hereafter first only briefly mention closely related topics, i.e. the case of finite-alphabet sources [13], the invertibility of the considered mixing models (see e.g. [36]) the extension of LQ mixtures to polynomial ones (see e.g. [13,47,65]), the separability of these models with given separation principles, such as ICA (see [5] for bounded sources), the approaches based on non-blind and semi-blind BSS methods (see e.g. [20,34]). There are also interesting works that deal with PNL models and were not discussed in this overview paper. For instance, some effort has been put on the case of convolutive PNL mixtures [9,41] and on the problem of blind source extraction in PNL mixtures [44]. Finally, let us stress that other types of nonlinear mixing models have also recently been considered in the literature. All this shows that nonlinear BSS is currently a quite active research field, that we plan to present in more detail in a future publication.

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