

Provably robust blind source separation of linear-quadratic near-separable mixtures*

Christophe Kervazo[†], Nicolas Gillis[‡], and Nicolas Dobigeon[§]

Abstract. In this work, we consider the problem of blind source separation (BSS) by departing from the usual linear model and focusing on the linear-quadratic (LQ) ones. We propose two provably robust and computationally tractable algorithms to tackle this problem under separability assumptions which require the sources to appear as samples in the data set. The first algorithm, referred to as SNPALQ, generalizes the successive nonnegative projection algorithm (SNPA), designed for linear BSS. By explicitly modeling the product terms inherent to the LQ model along the iterations of the SNPA scheme, the nonlinear contributions of the mixing are mitigated, thus improving the separation quality. SNPALQ is shown to be able to recover the ground truth factors that generated the data, even in the presence of noise. The second algorithm is a brute-force (BF) algorithm, which can be used as a post-processing step for SNPALQ. It then enables to discard the spurious (mixed) samples extracted by SNPALQ, thus broadening its applicability. The BF is in turn shown to be robust to noise (under potentially easier-to-check conditions than SNPALQ). We show that SNPALQ with and without the BF postprocessing is relevant in realistic numerical experiments.

Key words. non-linear blind source separation, nonnegative matrix factorization, non-linear hyperspectral unmixing, linear-quadratic models, separability, pure-pixel assumption.

AMS subject classifications. 15A23, 65F55, 68Q25, 65D18

1. Introduction. Blind source separation (BSS) [8, 7, 29] is a powerful paradigm with a wide range of applications such as remote sensing [42], biomedical and pharmaceutical imaging [1, 41], and astronomy [44]. BSS aims at decomposing a given data set into a set of unknown elementary signals to be recovered, generally referred to as the *sources*. Because it is simple and easily interpretable, many works [8] have focused on the *linear* mixing model (LMM) which assumes that the i th data set sample $\bar{\mathbf{x}}_i \in \mathbb{R}^m$, $i \in \llbracket n \rrbracket$, can be written as

$$\bar{\mathbf{x}}_i = \sum_{k=1}^r h_{ki} \mathbf{w}_k + \mathbf{n}_i,$$

where \mathbf{w}_k is the k th source for $k \in \llbracket r \rrbracket = \{1, 2, \dots, r\}$, and h_{ki} its the associated mixing coefficient in the i th (mixed) observation. The vector \mathbf{n}_i accounts for any additive noise and/or slight mismodelings in the i th pixel. Using a standard matrix formulation, the LMM

*
Funding: CK and NG acknowledge the support by the European Research Council (ERC starting grant no 679515), and NG by the Fonds de la Recherche Scientifique - FNRS and the Fonds Wetenschappelijk Onderzoek - Vlaanderen (FWO) under EOS Project no O005318F-RG47. ND is partly supported by the AI Interdisciplinary Institute ANITI funded by the French "Investing for the Future - PIA3" program under the Grant agreement number ANR-19-PI3A-0004.

[†]Télécom Paris, Institut Polytechnique de Paris, France (christophe.kervazo@telecom-paris.fr).

[‡]University of Mons, Mons, Belgium (nicolas.gillis@umons.ac.be, <https://sites.google.com/site/nicolasgillis/>).

[§]University of Toulouse, IRIT/INP-ENSEEIH, Toulouse, France & Institut Universitaire de France (IUF) (nicolas.dobigeon@enseeiht.fr, <http://dobigeon.perso.enseeiht.fr/fr/>).

can thus be rewritten as

$$\bar{\mathbf{X}} = \mathbf{W}\mathbf{H} + \mathbf{N},$$

where $\bar{\mathbf{X}} = [\bar{\mathbf{x}}_1, \bar{\mathbf{x}}_2, \dots, \bar{\mathbf{x}}_m] \in \mathbb{R}^{m \times n}$ is the data set, $\mathbf{W} = [\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_r] \in \mathbb{R}^{m \times r}$ the sources, $\mathbf{H} \in \mathbb{R}^{r \times n}$ the mixing matrix containing the coefficients h_{ki} 's, and $\mathbf{N} = [\mathbf{n}_1, \mathbf{n}_2, \dots, \mathbf{n}_m] \in \mathbb{R}^{m \times n}$ the noise. We denote by $\mathbf{X} = \mathbf{W}\mathbf{H}$ the noiseless version of $\bar{\mathbf{X}}$.

The goal of BSS is to recover \mathbf{W} and \mathbf{H} from the sole knowledge of $\bar{\mathbf{X}}$. This is in general an ill-posed problem [8]. Hence, in most works, additional constraints are imposed on the unknown matrices \mathbf{W} and \mathbf{H} to make the problem better posed: for instance, orthogonality in principal component analysis (PCA – [27]), independence in independent component analysis (ICA – [8]), and sparsity in sparse component analysis (SCA – [46, 7, 29]). We will here focus on nonnegativity constraints, akin to nonnegative matrix factorization (NMF) [31]. Although NMF is NP-hard in general [45], and its solution non-unique [16], Arora et al. [4, 5] have introduced the subclass of near-separable non-negative matrices for which NMF can be solved in a polynomial time with weak indeterminacies. This subclass corresponds to data sets in which each source appears purely in at least one data sample. Building on near-separable NMF, several provably robust algorithms have been proposed [4, 14, 40, 21]. Among them, one can cite the successive projection algorithm (SPA) [3], which is a fast greedy algorithm provably robust to noise [22], or an enhanced version, the successive nonnegative projection algorithm (SNPA) [18], which is more efficient when \mathbf{W} is ill-conditioned and is even applicable when \mathbf{W} is rank deficient.

1.1. LQ mixing model. In various applications, the LMM may however suffer from some limitations and can only be considered as a first-order approximation of non-linear mixing models [6, 13, 11]. In such situations, linear-quadratic (LQ) [9] models can for instance better account for the physical mixing processes by including termwise products of the sources [12, 24]. This model can be written as follows

$$(1.1) \quad \bar{\mathbf{x}}_i = \sum_{k=1}^r h_{ki} \mathbf{w}_k + \sum_{p=1}^r \sum_{l=p}^r \beta_{ipl} (\mathbf{w}_p \odot \mathbf{w}_l) + \mathbf{n}_i.$$

In (1.1), the linear contribution associated to the LMM is complemented by a set of second-order interactions $\mathbf{w}_p \odot \mathbf{w}_l$ between the sources, where \odot denotes the Hadamard product, and β_{ipl} is the amount of the interaction $\mathbf{w}_p \odot \mathbf{w}_l$ within the i th observation. It is worth mentioning the closely-related so-called bilinear mixing model [13, 9], which is a particular instance of the LQ mixing model, from which the *squared* terms $\mathbf{w}_p \odot \mathbf{w}_p$ for $p \in \llbracket r \rrbracket$ in (1.1) are removed; see Application 1.1 below for a discussion in the context of blind hyperspectral unmixing where the LQ and bilinear models are widely used.

The LQ mixing model (1.1) can also be rewritten in a matrix form

$$(1.2) \quad \bar{\mathbf{X}} = \Pi_2(\mathbf{W})\mathbf{H} + \mathbf{N},$$

where $\Pi_2(\mathbf{W}) \in \mathbb{R}^{m \times \tilde{r}}$ is the extended source matrix containing the sources and their second-order products as its columns, with $\tilde{r} = r(r+3)/2$, and $\mathbf{H} \in \mathbb{R}^{\tilde{r} \times n}$ is the matrix gathering all the mixing coefficients associated with the linear (h_{ki} 's) and nonlinear (β_{ipl} 's) contributions.

Written in such a matrix form, the similarity between the LQ and linear models is easily visible: the LQ mixings can be written in a linear form by considering the quadratic terms $\mathbf{w}_p \odot \mathbf{w}_l$ as new sources, additional to the usual ones \mathbf{w}_k . Following this line of thought, the $\mathbf{w}_p \odot \mathbf{w}_l$ terms are often called *virtual sources*. In the sequel of this paper, this terminology will be adopted and the non-virtual sources \mathbf{w}_i will be referred to as *primary*.

Application 1.1 (Hyperspectral imaging). *To illustrate the BSS of LQ-mixtures (LQ-BSS), we consider throughout this paper the example of hyperspectral (HS) imaging. Despite having a finer spectral resolution than conventional natural images, HS images often suffer from a limited spatial resolution. Therefore, several materials are generally present in each pixel, and thus the acquired spectra correspond to mixtures of the different pure material spectra, called endmembers. This mandates the use of BSS methods – more specifically of NMF – to perform spectral unmixing. To be more precise, using the terminology of HS unmixing [13], \mathbf{w}_k in (1.1) corresponds to the spectral signature of the k th endmember, and h_{ki} to the abundance of the k th endmember in the i th pixel. The spectral signature of a source is the fraction of light reflected by that source depending on the wavelength, and hence $0 \leq \mathbf{w}_k \leq 1$ for $k \in \llbracket r \rrbracket$. Concerning the model choice, the linear BSS model is often a too rough approximation in HS: in particular, when the light arriving on the sensor interacts with several materials, nonlinear mixing effects may occur [6, 13, 11]. Specifically, this is often the case when the scene is not flat, for instance in the presence of large geometric structures, such as in urban [34] or forest [12] scenes. In such a context, it has been shown [12, 24] that LQ models enable to better account for multiple scatterings. While it is further possible to include higher-order terms, most of the works neglect the interactions of order larger than two since they are expected to be of significantly lower magnitudes [2, 33] as $0 \leq \mathbf{W} \leq 1$.*

1.2. Identifiability issue in LQ-BSS. Despite source identifiability issues in the general context of non-linear BSS problems [8, 10, 28], it was recently showed [9] that the non-linearity inherent to bilinear mixtures leads to an *essentially unique* solution in the noiseless case. More precisely, it was shown that for a data matrix \mathbf{X} following the bilinear model in the absence of noise (and under some appropriate assumptions, see below), any $\hat{\mathbf{W}}$ and $\hat{\mathbf{H}}$ such that $\mathbf{X} = \Pi_2(\hat{\mathbf{W}})\hat{\mathbf{H}}$ satisfy $\hat{\mathbf{W}} = \mathbf{W}$ and $\hat{\mathbf{H}} = \mathbf{H}$ up to a scaling and permutation of the columns of $\hat{\mathbf{W}}$ and the rows of $\hat{\mathbf{H}}$. However, this identifiability result suffers from some limitations:

- It relies on two strong assumptions:

1. $\text{rowrank}(\mathbf{X}) = \frac{r(r+1)}{2}$, requiring that $\hat{\mathbf{H}}$ has full row rank and hence that every extended source is present in the data set. In other words, all possible interactions of two primary sources must be present in some observation. This is unlikely to happen in practice.
2. the products of the sources up to order four must be linearly independent. It requires the family

$$(1.3) \quad \left(\mathbf{W}, (\mathbf{w}_i \odot \mathbf{w}_j)_{\substack{i,j \in \llbracket r \rrbracket \\ j < i}}, (\mathbf{w}_i \odot \mathbf{w}_j \odot \mathbf{w}_k)_{\substack{i,j,k \in \llbracket r \rrbracket \\ k < j < i}}, (\mathbf{w}_i \odot \mathbf{w}_j \odot \mathbf{w}_k \odot \mathbf{w}_l)_{\substack{i,j,k,l \in \llbracket r \rrbracket \\ l < k < j < i}} \right),$$

to be linearly independent. As its size is $\frac{r(r+1)}{24}((r-1)(r-2) + 12)$, such a

linear independence assumption might not be satisfied in real-world scenarios, since the number of observations m must be of order $\Theta(r^4)$.

- It does not apply to mixings with squared terms [9, section 7], that is, LQ mixings instead of bilinear ones.
- No guarantee is given in the presence of noise. Moreover, finding an exact factorization $\Pi_2(\hat{\mathbf{W}})\hat{\mathbf{H}}$ of \mathbf{X} is a difficult problem. The algorithm used in [9] is a heuristic and does not find an exact solution (see [9, Fig. 4]), leading to errors on the recovered sources.

Application 1.2 (Hyperspectral imaging (cont'd)). *In HS imaging, the assumption that \mathbf{H} has full row rank is unlikely to be satisfied as many endmembers do not interact, because they are located far apart in the image.*

For the second assumption, even with $r = 10$ endmembers, which is a relatively small number, at least $m \geq 385$ spectral bands would be required to ensure the linear independence of the family (1.3). This is not satisfied for typical HS sensors dedicated to Earth observation. As an example, the Airborne Visible / Infrared Imaging Spectrometer (AVIRIS) operated by the Jet Propulsion Laboratory (JPL, NASA), acquires HS images composed of $m = 224$ spectral bands, among them several dozens are inexploitable due to low signal-to-noise ratios.

1.3. Near-separable LQ mixings. To overcome the above identifiability issues, we propose in this work to tackle BSS problems of the form (1.1) under a near-separable NMF-like paradigm. In particular, the rationale is to convert the linear independence condition on the family (1.3) into a non-negative independence condition, which is significantly less restrictive. Consider for instance the family of points located on a sphere within the unit simplex in three dimensions, that is, distinct points within the set $\{\mathbf{x} \in \mathbb{R}_+^3 \mid \|\mathbf{x}\|_1 = 1, \|\mathbf{x}\|_2 = q\}$ for some $q < 1$. Although the rank of this family is 3, no point is within the convex cone of other points, and hence this family is non-negatively independent.

More specifically, denoting $\Delta = \{\mathbf{x} \in \mathbb{R}^{\tilde{r}} \mid x \geq 0, \sum_{i=1}^{\tilde{r}} x_i \leq 1\}$ and $\Pi_2(\mathbf{W})_{\setminus \{j\}}$ the submatrix of $\Pi_2(\mathbf{W})$ excluding \mathbf{w}_j , we assume the following constraints:

$$\begin{aligned}
 & h_{ki} \geq 0 \text{ for all } i \in \llbracket n \rrbracket \text{ and } k \in \llbracket \tilde{r} \rrbracket \text{ (nonnegativity condition),} \\
 (1.4) \quad & \sum_{k=1}^r h_{ki} + \sum_{p=1}^r \sum_{l=p}^r \beta_{ipl} \leq 1 \text{ for all } i \in \llbracket n \rrbracket \text{ (sum-to-at-most-one condition),} \\
 & \alpha_{\Pi_2(\mathbf{W})}(\mathbf{W}) = \min_{j \in \llbracket r \rrbracket} \min_{\mathbf{x} \in \Delta} \|\mathbf{w}_j - \Pi_2(\mathbf{W})_{\setminus \{j\}} \mathbf{x}\|_2 > 0 \text{ (order-2 } \alpha\text{-robust simplicial).}
 \end{aligned}$$

The two first constraints ensure the mixing coefficients for each pixel to be nonnegative and to sum to at most one, and can be equivalently written as $\mathbf{h}_i \in \Delta$ for all $i \in \llbracket \tilde{r} \rrbracket$. The last one ensures that no source lies within the convex hull formed by the other ones, their second order product and the origin. It is thus an extension of the α -robust simplicial¹ definition of [5] which requires that $\alpha_{\mathbf{W}}(\mathbf{W}) = \min_{j \in \llbracket r \rrbracket} \min_{\mathbf{x} \in \Delta} \|\mathbf{w}_j - \mathbf{W}_{\setminus \{j\}} \mathbf{x}\|_2 > 0$.

In addition, we hereafter extend the subclass of r separable mixings of [17] to the LQ model.

¹The denomination “ α -robust simplicial” is slightly abusive here, as the coefficients of \mathbf{x} sum to *at most* one, in contrast to [5] in which they sum to exactly one.

Definition 1.3 (r -LQ separability). The matrix \mathbf{X} is said to be r -LQ separable if it can be written as

$$\mathbf{X} = \Pi_2(\mathbf{W}) \underbrace{\begin{bmatrix} \mathbf{I}_r & \\ \mathbf{0}_{\frac{r(r-1)}{2} \times r} & \mathbf{H}' \end{bmatrix}}_{\mathbf{H}} \mathbf{P},$$

where $\mathbf{W} \in \mathbb{R}^{m \times r}$ is order-2 α -robust simplicial, \mathbf{I}_r is the r -by- r identity matrix, $\mathbf{0}_{p \times q}$ is the p -by- q matrix of zeros, \mathbf{P} is a permutation matrix, $\mathbf{H}' \in \mathbb{R}^{\tilde{r} \times m-r}$ is a matrix satisfying the sum to at most one and nonnegativity conditions.

It is important to note that r -LQ separability requires that all primary sources appear as some samples (that is, as columns of \mathbf{X}), which is not required for the virtual sources. In this work, to take into account the presence of noise in the mixtures, we will more specifically assume the mixing to be (ϵ, r) -LQ near-separable, which is defined as follows.

Definition 1.4 ((ϵ, r) -LQ near-separability). The matrix $\bar{\mathbf{X}}$ is said to be (ϵ, r) -LQ near-separable if it can be written as $\bar{\mathbf{X}} = \mathbf{X} + \mathbf{N}$,

where \mathbf{X} is r -LQ separable (see Definition 1.3), and the noise matrix $\mathbf{N} \in \mathbb{R}^{m \times n}$ satisfies $\max_{i \in [n]} \|\mathbf{n}_i\|_2 \leq \epsilon$.

Application 1.5 (Hyperspectral imaging (cont'd)). It has been shown [13] that bilinear and LQ models enable to better account for multiple scatterings. Examples of such models include the Fan model [15], the generalized bilinear model [23], the polynomial post-nonlinear model [2]; see [13] and the references therein for more details. In this work, we will focus on the so-called Nascimento model [37, 43], which is a bilinear-based model that naturally extends the classical linear model and the sum-to-at-most-one constraint on the abundances.

The near-separable assumption in HS is referred to as the pure-pixel assumption, as it requires each endmember to appear at least once purely within a pixel. This hypothesis is common and realistic [22, 32], provided that the spatial resolution is not too low.

1.4. Contributions. In this paper, we introduce two algorithms which, given a (ϵ, r) -LQ near separable mixture (Definition 1.4), approximately recover the factors \mathbf{W} and \mathbf{H} . As such, our results are (i) theoretical: we show the identifiability of this problem even in the presence of noise, and (ii) practical: the two algorithms run in polynomial time. More specifically, the contributions – graphically summarized in Figure 1 – are the following:

- We introduce the successive nonnegative projection algorithm for linear-quadratic mixtures (SNPALQ), which generalizes SNPA [18] to linear-quadratic (LQ) mixings by explicitly modeling the presence of quadratic products within its greedy search process.
- The conditions under which SNPALQ is provably robust to noise are detailed in Section 3.1.2. In particular, such conditions encompass the linear case (see Section 3.1.1), which is important as the LQ model we consider generalizes the linear one.
- To further mitigate the robustness conditions of SNPALQ and broaden its applicability, we introduce a second algorithm dubbed brute force (BF), that we use as a post-processing step to enhance SNPALQ results (which we denote SNPALQ+BF). In Section 3.2, we prove that BF lead to robustness guarantees under weaker conditions

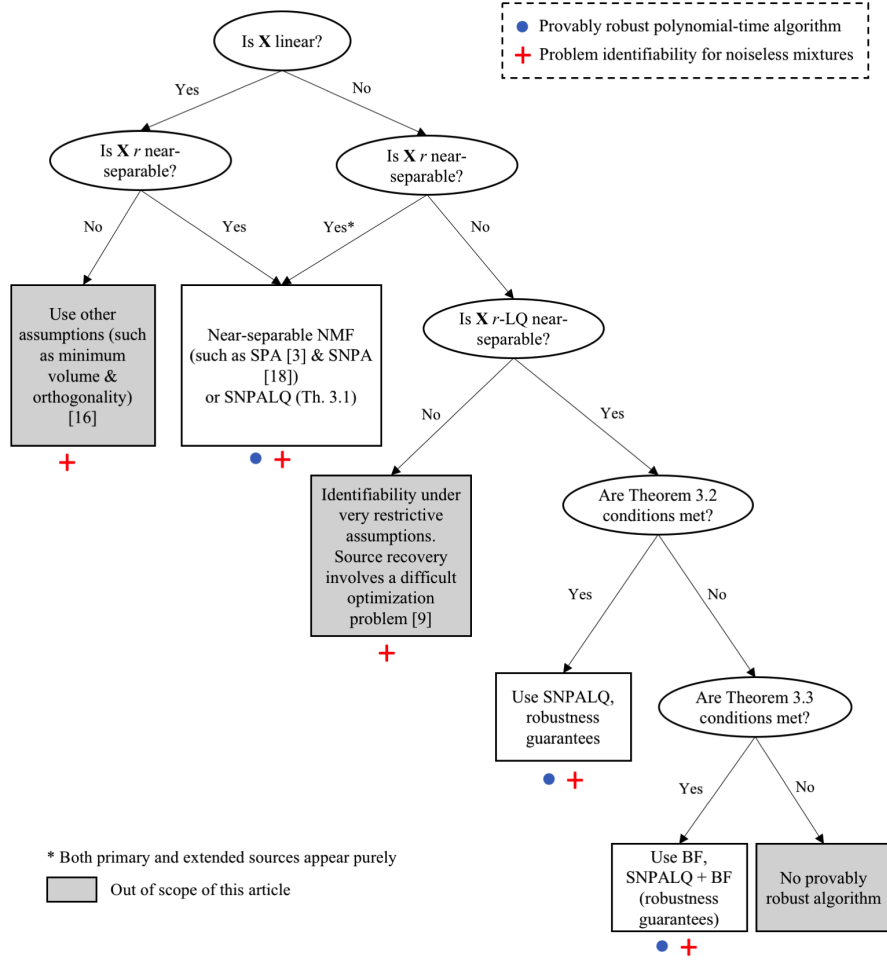


Figure 1. Graphical summary of the contributions, explaining which algorithm to use in which setting. We call a provably robust algorithm an algorithm which is proved to recover the sources even in the presence of noise.

than SNPALQ.

- In Section 4, the effectiveness of the proposed algorithms is attested through extensive numerical experiments, in which among others SNPALQ is shown to obtain better results than SNPA on LQ mixings, and the SNPALQ+BF to obtain a very high rate of perfect recovery of the ground truth factors.

Remark 1.6 (Further interest of the proposed algorithm). Near-separable algorithms have often been used to initialize NMF algorithms that do not rely on the separability assumption [18]. In particular, the initializations of many LQ-BSS algorithms are often (and paradoxically) performed with the output of near-separable algorithms assuming linear mixtures; see for example [2, 34]. Therefore, beyond their intrinsic interest for (r, ϵ) -LQ near-separable mixtures, the two algorithms proposed in this work are fast and reasonable (since based on the LQ model) initialization strategies for LQ-BSS algorithms in the absence of the (r, ϵ) -LQ

near-separability assumption.

1.5. Notation. Table 1 summarizes the notations used in this paper. It will be further clarified within the text when appropriate. For the sake of readability, the notations specific to the proof section in the Appendix are not present in this table.

Table 1
Notation summary.

$\llbracket r \rrbracket$	$\{1, 2, \dots, r\}$
$ \mathcal{K} $	Number of elements in the set \mathcal{K}
$\mathcal{K}(i)$	i th element of the set \mathcal{K}
Δ^r	$\{\mathbf{x} \in \mathbb{R}^r \mathbf{x} \geq 0, \sum_{i=1}^r x_i \leq 1\}$ the superscript r is omitted when it is clear from the context
\mathbf{A}	matrix (bold capital letters)
\mathbf{a}	vector (bold lowercase letters)
\mathbf{a}_i	i th column of a matrix \mathbf{A}
$\mathbf{A}_{\mathcal{K}}$	Submatrix of \mathbf{A} formed by the columns indexed by \mathcal{K}
$\mathbf{A}_{\setminus \mathcal{K}}$	Submatrix formed by all the columns of \mathbf{A} except the ones indexed by \mathcal{K}
$\Pi_2(\mathbf{A})$	$[\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n, \mathbf{a}_1 \odot \mathbf{a}_1, \mathbf{a}_2 \odot \mathbf{a}_1, \mathbf{a}_3 \odot \mathbf{a}_1, \mathbf{a}_2 \odot \mathbf{a}_2, \mathbf{a}_3 \odot \mathbf{a}_2, \dots, \mathbf{a}_n \odot \mathbf{a}_n]$ $= (\mathbf{a}_i \odot \mathbf{a}_j)_{i,j \in \llbracket n \rrbracket, i \leq j}$, where $\mathbf{A} \in \mathbb{R}^{m \times n}$. $\Pi_2(\mathbf{A})$ contains the products of the columns of \mathbf{A} up to order 2
$\Pi_q(\mathbf{A})$	Matrix containing the columns of \mathbf{A} , and their Hadamard products up to order $q \in \mathbb{N}^*$
$K(\mathbf{A})$	$\max_i \ \mathbf{a}_i\ _2$ (maximum ℓ_2 norm of the columns of \mathbf{A})
f	A μ -strongly convex function with a L -Lipschitz gradient
$\alpha_{\Pi_2(\mathbf{A})}(\mathbf{A})$	$\min_j \min_{\mathbf{x} \in \Delta} \ \mathbf{a}_j - \Pi_2(\mathbf{A})_{\setminus \{j\}} \mathbf{x}\ _2$
$\mathcal{P}_{\mathbf{A}}^f(\mathbf{x})$	$\mathbf{A}\mathbf{y}^*$ with $\mathbf{y}^* = \operatorname{argmin}_{\mathbf{y} \in \Delta} f(\mathbf{x} - \mathbf{A}\mathbf{y})$.
$\mathcal{R}_{\mathbf{A}}^f(\mathbf{x})$	$\mathbf{x} - \mathcal{P}_{\mathbf{A}}^f(\mathbf{x})$
$\nu_{f, \Pi_2(\mathbf{A})}(\mathbf{A})$	$\min_j \left\ \mathcal{R}_{\Pi_2(\mathbf{A}) \setminus \{j\}}^f(\mathbf{a}_j) \right\ _2$
$\gamma_{f, \Pi_2(\mathbf{A})}(\mathbf{A})$	$\min_{i \neq j} \left\ \mathcal{R}_{\Pi_2(\mathbf{A}) \setminus \{i, j\}}^f(\mathbf{a}_j) - \mathcal{R}_{\Pi_2(\mathbf{A}) \setminus \{i, j\}}^f(\mathbf{a}_i) \right\ _2$
$\beta_{\Pi_2(\mathbf{A})}^{\text{Lin}}(\mathbf{A})$	$\min \left(\nu_{f, \Pi_2(\mathbf{A})}(\mathbf{A}), \frac{\sqrt{2}}{2} \gamma_{f, \Pi_2(\mathbf{A})}(\mathbf{A}) \right)$
$\beta_{\Pi_2(\mathbf{W})}^{\text{LQ}}(\mathbf{A})$	$\min \left(\frac{\nu_{f, \Pi_2(\mathbf{W})}(\mathbf{A})}{2} \sqrt{\frac{\mu}{L}} \left[1 - \frac{1}{G} \right], \gamma_{f, \Pi_2(\mathbf{W})}(\mathbf{A}) \right)$ with $G > 1$

2. Two algorithms for LQ-BSS: SNPALQ and BF. To perform near-separable BSS of LQ mixtures, a first (naive) approach is to use an LMM-based near-separable NMF algorithm to identify the \tilde{r} extended sources. Since the quadratic terms $(\mathbf{w}_i \odot \mathbf{w}_j)_{i,j \in \llbracket r \rrbracket, j \leq i}$ can be considered as *virtual* sources (see Eq. (1.2)), they could be retrieved along with the columns of \mathbf{W} , provided that they appear purely in the data set. One could for instance resort to SNPA [18], an LMM-based algorithm which has shown to yield very good separation performances compared to state-of-the-art LMM-based algorithms such as VCA [36] and SPA [3], and admits robustness

guarantees. SNPA is a greedy algorithm: it iteratively constructs the near-separable NMF solution, \mathcal{K} , by sequentially adding a new source to the current set of sources already identified. More precisely, after initializing the index set $\mathcal{K} = \emptyset$ and a residual matrix $\mathbf{R} = \bar{\mathbf{X}}$, each iteration of SNPA consists of the following two steps:

- *selection*: the index of the column of \mathbf{R} maximizing a score function f is added to \mathcal{K} .
- *projection*: the residual is updated by projecting the columns of $\bar{\mathbf{X}}$ onto the convex hull formed by the columns of $\bar{\mathbf{X}}_{\mathcal{K}}$ and the origin.

During the *selection* step, the function f aims at selecting the most relevant column of \mathbf{R} to be identified as a source. This function f , applied on the columns of the residual \mathbf{R} at each step, can for example be the ℓ_2 -norm. It needs to fulfill the following assumption:

Assumption 2.1. The function $f: \mathbb{R}^m \mapsto \mathbb{R}_+$ is μ -strongly convex, its gradient is L -Lipschitz and its global minimizer is the all zero vector $\mathbf{0}_m$, that is, $f(\mathbf{0}_m) = 0$.

The *projection* step is a convex optimization problem and can be solved for example using a fast gradient method [38]. We refer the reader to [18, Appendix A] for more details.

Nevertheless, the bottleneck of the above naive approach consisting in using SNPA for LQ mixtures is that the presence of all the *virtual* sources as pure data samples is a too strong assumption. Indeed, all *virtual* sources are not likely to be observed purely in the data set. As such, the recovery of the extended sources by SNPA is not guaranteed, calling for algorithms specifically designed for LQ mixtures.

To overcome this limitation, we propose two new algorithms enabling to tackle LQ mixtures. The first algorithm, referred to as SNPALQ, is a variant of SNPA specifically designed to handle LQ mixings; see Section 2.1. The second one is a brute-force (BF) algorithm, extending the work of [5] to LQ mixtures and exhibiting better practical results than SNPALQ in some experiments; see Section 2.2. As BF is however computationally more expensive than SNPALQ, we propose to use it as a post-processing of the output provided by SNPALQ. Combining both algorithms in a single method, which we refer to as SNPALQ+BF, allows us to benefit from the best of each of these algorithms.

2.1. SNPALQ. The rationale behind SNPALQ is that we are interested in recovering the primary sources only, \mathbf{w}_i for $i \in \llbracket r \rrbracket$. The virtual sources $\mathbf{w}_i \odot \mathbf{w}_j$ ($i, j \in \llbracket r \rrbracket$) can be considered as a nuisance. Therefore, we propose to take them into account in the separation process only to improve the extraction of the primary sources. Specifically, at each iteration of SNPALQ, we perform the following two steps (see Algorithm 2.1):

- *Selection step* (unchanged compared to SNPA): the column of the residual matrix \mathbf{R} maximizing a function f fulfilling Assumption 2.1 is selected.
- *Projection step* (different from SNPA): SNPALQ performs the projection onto the convex hull formed by the origin, the sources extracted so far *and their second-order products*. Therefore, if two sources \mathbf{w}_i and \mathbf{w}_j ($i \neq j$) are extracted during the iterative process of SNPALQ, the contribution of the virtual sources $\mathbf{w}_i \odot \mathbf{w}_j$, $\mathbf{w}_i \odot \mathbf{w}_i$ and $\mathbf{w}_j \odot \mathbf{w}_j$ are removed. Beyond the advantage that these virtual sources will not be extracted in the subsequent steps, their non-linear contribution is reduced, giving more weight to the linear part.

The primary sources \mathbf{W} are more likely to be extracted by SNPALQ than SNPA. Indeed,

recall that SNPA projects each column of $\bar{\mathbf{X}}$ onto the convex hull formed by the origin and all the sources extracted so far, and does not take into account the virtual sources. In contrast, SNPALQ also projects onto virtual sources, cancelling their contributions; see Figure 2 for an illustration.

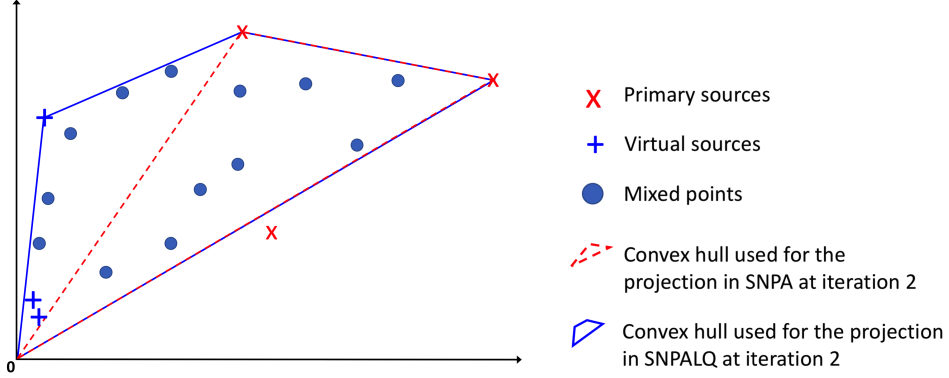


Figure 2. Example of a bilinear mixing for which SNPALQ is successful at recovering \mathbf{W} but SNPA is not (the principle is the same for LQ, except that there are more virtual sources). There are three primary sources, represented with the red X markers, and three virtual sources, namely $\mathbf{w}_i \odot \mathbf{w}_j$ for $i \neq j$ and $1 \leq i, j \leq 3$, represented with the blue + markers. The columns of $\bar{\mathbf{X}}$ are made of the primary sources and the mixed points represented with the blue circles. The red dashed line is the convex hull of the origin and the sources extracted after two iterations of SNPA. The plain blue line is the convex hull of the origin and the sources extracted by SNPALQ after two iterations, as well as the corresponding virtual source. Only the last primary source lies outside of the blue convex hull. Therefore, SNPALQ extracts it in its third iteration and then stops, returning the primary sources only. On the other hand, at the third iteration, SNPA fails to extract the last primary source because some of the (mixed) columns of $\bar{\mathbf{X}}$ lie further away from the red dashed convex hull. Moreover, it will need in total 8 iterations to terminate because the convex hull of the columns of $\bar{\mathbf{X}}$ has 8 vertices (we assume the virtual sources do not appear purely in the data set).

SNPALQ will be proved in Section 3.1.2 to extract the primary sources in the first r steps, under specific conditions.

Concerning the stopping criterion, SNPALQ alternates the two above steps until one of the following two criteria is met:

- A maximum of r_{\max} columns have been extracted. If an upper bound is not available, one can take $r_{\max} = n$ so that SNPALQ relies on the second stopping criterion only.
- $K(\mathbf{R}) \leq t$: the algorithm stops when the relative reconstruction error is sufficiently small. The choice of a good value for the tolerance parameter t is important: if t is too large, SNPALQ could stop before the extraction of all the sources. If t is too low, SNPALQ could extract too many source candidates in the presence of noise, making the whole algorithm computationally expensive. If the noise level ϵ is known, it can be shown that $t = \epsilon [1 + \epsilon \max(1, 2K(\mathbf{X}) + \epsilon)]$ enables to extract all the primary sources².

²The demonstration follows directly from Lemma B.8 and B.14: 1) if SNPALQ has extracted all the canonical columns (that is, the sources up to an approximation error related to the noise – we refer the reader to definition B.7 for more details), then the residual must be smaller than $\epsilon [1 + \epsilon \max(1, 2K(\mathbf{X}) + \epsilon)]$ due to lemma B.8. 2) Reciprocally, if $\max_{j \in [n]} \|\mathbf{r}_j\|_F \leq \epsilon [1 + \epsilon \max(1, 2K(\mathbf{X}) + \epsilon)]$, then all the canonical columns must have been extracted due to Lemma B.14.

Algorithm 2.1 Successive Nonnegative Projection Algorithm for LQ mixtures (SNPALQ)

-
- 1: **Input:** $\bar{\mathbf{X}} \in \mathbb{R}^{m \times \tilde{r}}$: a (ϵ, r) -LQ near-separable matrix following Definition 1.4 and Constraints (1.4), f : a strongly convex function satisfying Assumption 2.1, r_{\max} : number of sources, $t \geq 0$: stopping criterion on the norm of the residual.
 - 2: **Initialization:** $\mathbf{R} = \bar{\mathbf{X}}$, $\mathcal{K} = \{\}$, $k = 1$
 - 3: **while** $K(\mathbf{R}) > t$ and $k \leq r_{\max}$ **do**
 - 4: $p = \operatorname{argmax}_{j \in [n]} f(\mathbf{r}_j)$;
 - 5: $\mathcal{K} = \mathcal{K} \cup \{p\}$;
 - 6: **for** $j \in [n]$ **do**
 - 7: $\mathbf{h}_j = \operatorname{argmin}_{\mathbf{h} \in \Delta_{\frac{|\mathcal{K}|(|\mathcal{K}|+3)}{2}}} f(\bar{\mathbf{x}}_j - \Pi_2(\bar{\mathbf{X}}_{\mathcal{K}})\mathbf{h})$
 - 8: $\mathbf{r}_j = \bar{\mathbf{x}}_j - \Pi_2(\bar{\mathbf{X}}_{\mathcal{K}})\mathbf{h}_j$
 - 9: **end for**
 - 10: $k = k + 1$
 - 11: **end while**
 - 12: **Output:** A set \mathcal{K} of indices such that $\bar{\mathbf{X}}_{\mathcal{K}} \simeq \mathbf{W}$ up to a permutation.
-

Remark 2.2 (Choice of f). The choice of the score function f is nontrivial. In the linear case, that is, for separable NMF, this issue has been discussed in details in [22, Section 4]. For example, using ℓ_p norms with $1 < p < 2$ is more robust to outliers than using the ℓ_2 norm. Investigating the choice of f in the case of LQ mixtures is out of the scope of this paper. We leave it as a direction of further research.

Remark 2.3 (Computing \mathbf{H}). This paper mainly focuses on computing the basis matrix \mathbf{W} so that $\mathbf{X} \approx \Pi_2(\mathbf{W})\mathbf{H}$ for some $\mathbf{H} \geq 0$. The estimation of \mathbf{H} can be generally conducted in a second step by solving the nonnegative least squares (NNLS) problem $\min_{\mathbf{H} \geq 0} \|\mathbf{X} - \Pi_2(\mathbf{W})\mathbf{H}\|_F^2$. In the particular context of unmixing images, this step is usually referred to as *inversion*. To exploit the very nature of the images, this NNLS can be complemented by incorporating an additional regularization to exploit the expected spatial correlations between the pixels, see, e.g., [26].

2.2. Brute force algorithm. The conditions ensuring SNPALQ to recover the sources might not be satisfied in practice (see Sections 3.1.3 and 4.2.3). Therefore, we propose here a second algorithm, BF, inspired by the algorithm of Arora et al. [5] for linear mixtures. As we will see in Section 4, it can enhance the source recovery in some numerical experiments.

Noise-free mixtures – For the sake of simplicity, the rationale underlying BF is first exposed in the absence of noise. Let us assume w.l.o.g. that there are no duplicated columns in the data set \mathbf{X} . Due to the separable assumption, \mathbf{X} can be written as:

$$(2.1) \quad \mathbf{X} = [\mathbf{W}, \tilde{\mathbf{X}}] \mathbf{P} \in \mathbb{R}^{m \times n},$$

where \mathbf{P} is a permutation and $\tilde{\mathbf{X}}$ contains the LQ mixings of \mathbf{W} . Let us consider a column

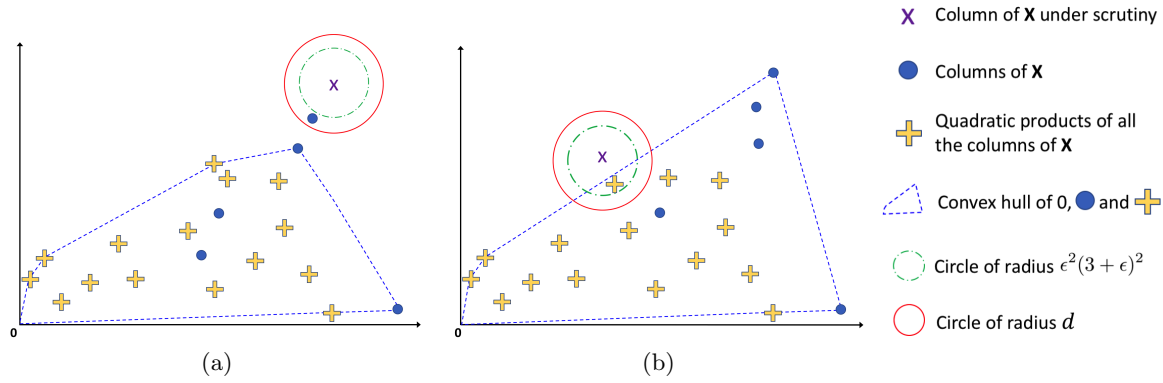


Figure 3. Illustration of condition (2.3) with $f(\cdot) = \|\cdot\|_2$. The point under scrutiny $\bar{\mathbf{x}}_k$ is represented in violet ('X' marker). The dots are the columns of $\mathbf{X} \setminus \{k\}$, and the yellow cross ('+' marker) correspond to the quadratic products of the columns of \mathbf{X} . The plain line ball of radius d and center $\bar{\mathbf{x}}_k$ contains the columns of $\bar{\mathbf{X}}$ which are discarded in (2.3). The dotted polygon is the convex hull of the origin and the columns of $\Pi_2(\mathbf{X}) \setminus \{k\}$ that are not contained in the ball of radius d around $\bar{\mathbf{x}}_k$. The dashed circle of radius $\epsilon^2(3 + \epsilon)^2$ indicates the distance at which the point must be located from the dotted convex hull to be considered an LQ-robust loner. On the figure (a), the dashed circle does not intersect the convex hull, and hence the cross is an LQ-robust loner. On figure (b), the dashed circle overlaps the convex hull, making that its center point is not a robust loner.

of \mathbf{X} , \mathbf{x}_k for $k \in \llbracket n \rrbracket$. We can check whether it is contained in the convex hull of the other columns of \mathbf{X} , their LQ mixtures and the origin by solving

$$s_k = \min_{\mathbf{h} \in \Delta^{\frac{n(n+3)}{2}-1}} \|\mathbf{x}_k - \Pi_2(\mathbf{X}) \setminus \{k\} \mathbf{h}\|_2.$$

If \mathbf{x}_k is not a column of \mathbf{W} , we have $s_k = 0$ under the r -LQ separable mixing model (Definition 1.3: \mathbf{x}_k is inside of the convex hull generated by the origin, the columns of \mathbf{W} and their second-order products). Moreover, under the assumption that \mathbf{W} is order-2 α -robust simplicial, that is $\alpha_{\Pi_2(\mathbf{W})}(\mathbf{W}) > 0$, \mathbf{x}_k is a source, that is a column of \mathbf{W} , if and only if $s_k > 0$.

For sake of consistency with SNPALQ, this condition can be generalized to any function f fulfilling Assumption 2.1. Adopting this generalization, \mathbf{x}_k is as primary source if and only if

$$(2.2) \quad \min_{\mathbf{h} \in \Delta^{\frac{n(n+3)}{2}-1}} f(\mathbf{x}_k - \Pi_2(\mathbf{X}) \setminus \{k\} \mathbf{h}) > 0.$$

Noisy mixtures – The above principles can be extended to make the BF algorithm able to recover an approximation of \mathbf{W} from noisy mixtures $\bar{\mathbf{X}} = \mathbf{X} + \mathbf{N}$ for a bounded noise fulfilling $\max_{i \in \llbracket n \rrbracket} \|\mathbf{n}_i\|_2 \leq \epsilon$ for some $\epsilon \geq 0$; see Algorithm 2.2. To do so, we need to modify (2.2) in two ways.

- In the noise-free case, we assumed that no duplicated columns are present within \mathbf{X} , and it is easy to discard such duplicates. In the noisy setting, when evaluating the residual (2.2), not only the column $\bar{\mathbf{x}}_k$ should be removed from $\Pi_2(\bar{\mathbf{X}})$ but also all columns close to $\bar{\mathbf{x}}_k$ (see Figure 3 for an illustration).
- Moreover, as the noise might shift mixed data points outside the convex hull formed by $\Pi_2(\mathbf{W})$ and the origin, s_k might be nonzero for a mixed column $\bar{\mathbf{x}}$ (that is, $\bar{\mathbf{x}}_k = \tilde{\mathbf{x}}_j$ for some $j \in \llbracket n - r \rrbracket$); see Figure 3 for an illustration.

Therefore, the condition (2.2) in the noiseless case should be modified to

$$(2.3) \quad \min_{\mathbf{h} \in \Delta} f(\bar{\mathbf{x}}_k - \Pi_2(\bar{\mathbf{X}})_{\setminus \{i \in [n] \mid f(\bar{\mathbf{x}}_i - \bar{\mathbf{x}}_k) > d\}} \mathbf{h}) > \frac{L}{2} \epsilon^2 (1 + \max(1, 2K(\mathbf{X}) + \epsilon))^2,$$

with L the Lipschitz constant of f and d a threshold parameter discussed in Appendix B; see (B.14) for an explicit value. The right-hand side stems from the fact that the noise is corrupting both the data columns (with a maximum energy of ϵ) and their quadratic products (with a maximum energy of $\epsilon \max(1, 2K(\mathbf{X}) + \epsilon)$); see Definition B.6.

Following [5], the columns of $\bar{\mathbf{X}}$ satisfying the condition (2.3) are called the *LQ-robust loners*. Section 3.2 will show that these columns exactly correspond to good approximations of the sources. To approximately recover the sources, the BF algorithm then amounts to check which columns of $\bar{\mathbf{X}}$ are LQ-robust loners. However, due to the noise, different LQ-robust loners may be candidates for estimating the *same* source. Therefore, at the end of BF, the LQ-robust loners need to be clustered to obtain a single estimate of each source. Fortunately, such a clustering – described in Algorithm 2.2 – is easy and does not lead to any indeterminacy as the LQ-robust loners are located close to the sources, which are comparatively located further away from each others.

Remark 2.4. If the noise level is unknown, the clustering step described in Algorithm 2.2 can be replaced by any clustering algorithm, such a k -means, although our theoretical robustness guarantee does not cover such an approach.

BF algorithm as a post-processing – Even if the BF algorithm can be used *per se* to perform the separation of (ϵ, r) -LQ near-separable mixtures, it can also serve as a post-processing to refine the results provided by SNPALQ. This strategy is particularly appealing when SNPALQ robustness conditions are not met, in which case SNPALQ may extract mixed data columns or virtual sources in addition to the sought-after primary sources. Given an SNPALQ solution $\bar{\mathbf{X}}_{\mathcal{K}}$, assume that r columns correspond to the primary sources \mathbf{W} , and the $|\mathcal{K}| - r$ remaining ones to (spurious) columns in which the primary sources are mixed along with their quadratic products. Up to a permutation, the SNPALQ solution can be written as

$$(2.4) \quad \bar{\mathbf{X}}_{\mathcal{K}} \simeq [\mathbf{W}, \tilde{\mathbf{X}}] \in \mathbb{R}^{m \times |\mathcal{K}|},$$

where $\tilde{\mathbf{X}} \in \mathbb{R}^{m \times (|\mathcal{K}| - r)}$ are mixed data points. This matches the form of (2.1). Therefore, instead of using the BF algorithm directly on the data set $\bar{\mathbf{X}}$, it can be applied on the SNPALQ solution $\bar{\mathbf{X}}_{\mathcal{K}}$, which has in practice a significantly smaller number of columns, that is, $|\mathcal{K}| \ll n$. Using BF as a post-processing step significantly reduces the computational cost; see Section 2.3. Furthermore, it is worth noting that SNPALQ already identifies as sources columns of $\bar{\mathbf{X}}$ lying far from each other. Thus, in our experiments, the clustering step in BF, whenever used as a post-processing, was most often unnecessary since each cluster contained exactly one point.

Remark 2.5 (Interpretation as post-processing). While we advocate BF as a post-processing enhancing SNPALQ results, the reciprocal point of view can be also adopted: SNPALQ can be seen as a *screening* (or *pruning*) method, enabling to select only a few number of potential candidates and lightening the computational burden of BF.

Algorithm 2.2 Brute force (BF)

-
- 1: **Input:** A (ϵ, r) -LQ near-separable matrix $\bar{\mathbf{X}} \in \mathbb{R}^{m \times n}$ following Definition 1.4 and the constraints 1.4, the number of sources r , and f a strongly convex function satisfying Assumption 2.1, d given by Equation (B.14).
 - 2: **Initialization:** $\mathcal{K} = \{\}$
 - 3: **for** $k \in \llbracket n \rrbracket$ **do**
 - 4: $\mathbf{h}_k = \operatorname{argmin}_{\mathbf{h} \in \Delta} f(\bar{\mathbf{x}}_k - \Pi_2(\bar{\mathbf{X}})_{\setminus \{i \in \llbracket n \rrbracket \mid f(\bar{\mathbf{x}}_i - \bar{\mathbf{x}}_k) > d\}} \mathbf{h})$
 - 5: **if** $f(\bar{\mathbf{x}}_k - \Pi_2(\bar{\mathbf{X}}_{\mathcal{N}})_{\setminus \{i \in \llbracket n \rrbracket \mid f(\bar{\mathbf{x}}_i - \bar{\mathbf{x}}_k) > d\}} \mathbf{h}_k) > \frac{L}{2} \epsilon^2 (1 + \max(1, 2K(\mathbf{X}) + \epsilon))^2$ **then**
 - 6: $\mathcal{K} = \mathcal{K} \cup \{k\}$
 - 7: **end if**
 - 8: **end for**
 - 9: **Clustering on $\bar{\mathbf{X}}_{\mathcal{K}}$:**
 - Compute the clusters : assign two columns $\bar{\mathbf{x}}_i$ and $\bar{\mathbf{x}}_j$ of $\bar{\mathbf{X}}_{\mathcal{K}}$ to the same cluster if and only if $\|\bar{\mathbf{x}}_j - \bar{\mathbf{x}}_i\|_2 \leq 2\sqrt{\frac{2}{\mu}(d + \epsilon L(2K(\mathbf{X}) + \epsilon))}$;
 - Keep in \mathcal{K} a single column per cluster: for each cluster, keep the column of $\bar{\mathbf{X}}_{\mathcal{K}}$ which is the closest to the center of the cluster. Update \mathcal{K} accordingly.
 - 10: **Output:** A set \mathcal{K} of indices such that $\bar{\mathbf{X}}_{\mathcal{K}} \simeq \mathbf{W}$ up to a permutation.
-

2.3. Computational cost. The computational costs of the proposed algorithms are as follows:

- *SNPALQ*: The complexity of the k th iteration is dominated by computing the projection step, which requires the projection of a m -by- n matrix onto a convex hull with $k(k+3)/2 + 1$ vertices, requiring $\mathcal{O}(mnk^2)$ operations with a first-order method [18, Appendix A].
- *BF*: Solving (2.3) for the n data points with a first-order method (as for SNPALQ) requires $\mathcal{O}(mn^2)$ operations. This is computationally rather heavy. For example, for HS images, n is the number of pixels and typically of the order of millions.
- *SNPALQ+BF*: Assuming SNPALQ extracts $|\mathcal{K}|$ indices, it requires $\mathcal{O}(mn|\mathcal{K}|^2)$ operations for SNPALQ, and $\mathcal{O}(m|\mathcal{K}|^2)$ operations for the post-processing with BF. Hence BF used as a post-processing has a smaller computational cost than SNPALQ which further justifies its use.

Remark 2.6 (Handling simpler models). As the LQ mixing model encompasses in particular the linear and bilinear ones, both SNPALQ and BF can be employed to separate these (simpler) mixtures. However, in practice, SNPALQ+BF should be specifically tailored in agreement with the target mixing model. For instance, bilinear mixtures can be handled by SNPALQ+BF by removing the projections on the squared sources in the projection steps, reducing the computational burden while improving the separation performance, avoiding the projections on the non-existing quadratic terms.

3. Theoretical results. This section reports the theoretical results associated with the recovery of the sources by SNPALQ and BF, even in the presence of noise. More specifically, in Section 3.1.1, we first derive robustness guarantees for SNPALQ when applied to *linear* mixings. These guarantees are then extended to LQ mixings in Section 3.1.2. The required conditions for these recovery results are discussed in Section 3.1.3. In Section 3.2, we derive and discuss the recovery guarantees for BF. For the sake of simplicity, the results derived in this section are stated for the particular choice $f(\cdot) = \|\cdot\|_2$. Our results are presented in a more general setting for any function $f(\cdot)$ satisfying Assumption 2.1 in Appendix B, where the proofs are given. The specific proof of SNPALQ robustness for linear mixtures is reported in the supplementary material.

3.1. Robustness of SNPALQ. As the LQ model is a generalization of the linear one (see Section 1), we first prove robustness of SNPALQ with respect to (w.r.t.) noise for *linear* mixings in Section 3.1.1. However, as expected, we will see that the derived bounds on the admissible noise levels and the corresponding error on the source estimates are slightly worse than those associated with SNPA because of the additional projections on the (non-existing) virtual sources. In Section 3.1.2, robustness of SNPALQ is proved in the case of LQ mixings.

3.1.1. Linear mixtures. Before stating the main result of this section in Theorem 3.1, let us introduce additional notations. For a matrix $\mathbf{A} \in \mathbb{R}^{m \times r}$, we define³

$$K(\mathbf{A}) = \|\mathbf{A}\|_{1,2} = \max_{i \in [r]} \|\mathbf{a}_i\|_2,$$

which is the maximum of the ℓ_2 norm of the columns of a matrix \mathbf{A} . We denote $\mathcal{P}_{\mathbf{A}}^f(\mathbf{x})$ the projection of \mathbf{x} onto the convex hull formed by the columns of \mathbf{A} and the origin w.r.t. the semimetric induced by the function f :

$$\mathcal{P}_{\mathbf{A}}^f(\mathbf{x}) = \mathbf{A}\mathbf{y}^* \quad \text{with } \mathbf{y}^* = \underset{\mathbf{y} \in \Delta}{\operatorname{argmin}} f(\mathbf{x} - \mathbf{A}\mathbf{y}).$$

Note that this projection is unique because f is assumed to be strongly convex; see Assumption 2.1. The residual of the projection is denoted $\mathcal{R}_{\mathbf{A}}^f$, that is,

$$\mathcal{R}_{\mathbf{A}}^f(\mathbf{x}) = \mathbf{x} - \mathcal{P}_{\mathbf{A}}^f(\mathbf{x}).$$

When used on matrices, both the projection and residual operators are applied column-wise (that is, $\mathcal{R}_{\mathbf{A}}^f(\mathbf{X})_i = \mathcal{R}_{\mathbf{A}}^f(\mathbf{x}_i)$ for all i). Furthermore, we define the following quantities associated with the minimal norm of the residuals

$$\begin{aligned} \nu_{f, \Pi_2(\mathbf{A})}(\mathbf{A}) &= \min_{j \in [r]} \left\| \mathcal{R}_{\Pi_2(\mathbf{A}) \setminus \{j\}}^f(\mathbf{a}_j) \right\|_2, \\ \gamma_{f, \Pi_2(\mathbf{A})}(\mathbf{A}) &= \min_{\substack{i, j \in [r] \\ i \neq j}} \left\| \mathcal{R}_{\Pi_2(\mathbf{A}) \setminus \{i, j\}}^f(\mathbf{a}_j) - \mathcal{R}_{\Pi_2(\mathbf{A}) \setminus \{i, j\}}^f(\mathbf{a}_i) \right\|_2, \\ \beta_{\Pi_2(\mathbf{A})}^{\text{Lin}}(\mathbf{A}) &= \min \left(\nu_{f, \Pi_2(\mathbf{A})}(\mathbf{A}), \frac{\sqrt{2}}{2} \gamma_{f, \Pi_2(\mathbf{A})}(\mathbf{A}) \right). \end{aligned}$$

³Note that in the signal processing literature, such a norm is sometimes denoted as $\|\mathbf{A}\|_{\infty, 2}$, see for instance [30]. We prefer to keep the original notation of [18].

As such, $\beta_{\Pi_2(\mathbf{A})}^{\text{Lin}}(\mathbf{A})$ is the minimum between the smallest residual of the column of \mathbf{A} and the smallest difference between the residuals of the columns of \mathbf{A} after the projection onto $\Pi_2(\mathbf{A})$.

The following theorem states the robustness of SNPALQ in the case of linear mixtures. As mentioned earlier, it is here presented in a simplified formulation by assuming that $f(\cdot) = \|\cdot\|_2$. Its generalized counterpart for any $f(\cdot)$ satisfying Assumption 2.1, as well as the corresponding detailed proof, are reported in the supplementary material (Theorem SM2.6).

Theorem 3.1 (Robustness of SNPALQ when applied on linear mixings – Simplified version).

Let

$$\bar{\mathbf{X}} = \mathbf{W}\mathbf{H} + \mathbf{N} \in \mathbb{R}^{m \times n}$$

be a near-separable [17] linear mixing with $\alpha_{\Pi_2(\mathbf{W})}(\mathbf{W}) > 0$ and $\beta_{\Pi_2(\mathbf{W})}^{\text{Lin}}(\mathbf{W}) > 0$. Let $K(\mathbf{N}) \leq \epsilon$ with $\epsilon < \mathcal{O}\left(\frac{\beta_{\Pi_2(\mathbf{W})}^{\text{Lin}}(\mathbf{W})^4}{K(\mathbf{W})^2}\right)$. Then SNPALQ (Algorithm 2.1) with $f = \|\cdot\|_2$ identifies in r steps all the columns of \mathbf{W} up to error $\mathcal{O}\left(\epsilon \frac{K(\mathbf{W})^2}{\beta_{\Pi_2(\mathbf{W})}^{\text{Lin}}(\mathbf{W})^2}\right)$.

As in [18], Theorem 3.1 can be proved by induction: we show in the supplementary material that SNPALQ extracts a new column of \mathbf{W} at each iteration.

3.1.2. LQ mixings. We now extend the above result to the case of LQ mixings. Similarly to the linear case, we define

$$\beta_{\Pi_2(\mathbf{W})}^{\text{LQ}}(\mathbf{A}) = \min \left(\frac{\nu_{f, \Pi_2(\mathbf{W})}(\mathbf{A})}{2} \sqrt{\frac{\mu}{L}} \left[1 - \frac{1}{G} \right], \gamma_{f, \Pi_2(\mathbf{W})}(\mathbf{A}) \right),$$

for some constant $G > 1$ upper-bounded by a quantity depending on the mixtures; see (3.1) below. The robustness of SNPALQ when analyzing LQ mixings is stated below for $f(\cdot) = \|\cdot\|_2$. In Appendix B, Theorem B.5 generalizes this statement to any $f(\cdot)$ satisfying Assumption 2.1.

Theorem 3.2 (Robustness of SNPALQ when applied on LQ mixings – Simplified version). Let

$$\bar{\mathbf{X}} = \Pi_2(\mathbf{W})\mathbf{H} + \mathbf{N} \in \mathbb{R}^{m \times n}$$

be an (ϵ, r) -LQ near-separable mixing (see Definition 1.4) with $\alpha_{\Pi_2(\mathbf{W})}(\mathbf{W}) > 0$, $\beta_{\Pi_2(\mathbf{W})}^{\text{LQ}}(\mathbf{W}) > 0$, and $\epsilon < \mathcal{O}\left(\frac{\beta_{\Pi_2(\mathbf{W})}^{\text{LQ}}(\mathbf{W})^4}{K(\Pi_2(\mathbf{W}))^2}\right)$. Furthermore, let us assume that at each iteration of SNPALQ the following condition is fulfilled:

$$(3.1) \quad K\left(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^{\|\cdot\|_2}(\mathbf{A})\right) \geq 2GK \left(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^{\|\cdot\|_2} \left(\left(\mathbf{b}_i \right)_{i \in \llbracket s \rrbracket}, \left(\mathbf{a}_i \odot \mathbf{a}_j \right)_{\substack{i \leq j \\ i \in \llbracket k \rrbracket \\ j \in \llbracket k \rrbracket}}, \left(\mathbf{b}_i \odot \mathbf{b}_j \right)_{\substack{i \leq j \\ i \in \llbracket s \rrbracket \\ j \in \llbracket s \rrbracket}}, \left(\mathbf{a}_i \odot \mathbf{b}_j \right)_{i \in \llbracket k \rrbracket, j \in \llbracket s \rrbracket} \right) \right),$$

where \mathbf{B} contains the columns of \mathbf{W} already extracted by SNPALQ and $\bar{\mathbf{B}}$ the corresponding columns with noise, \mathbf{A} contains the remaining columns of \mathbf{W} still-to-be extracted, and $G > 1$ is a constant. Then, SNPALQ (Algorithm 2.1) with $f = \|\cdot\|_2$ identifies in r steps the columns of \mathbf{W} up to an error $\mathcal{O}\left(\epsilon \frac{K(\Pi_2(\mathbf{W}))^2}{\beta_{\Pi_2(\mathbf{W})}^{\text{LQ}}(\mathbf{W})^2}\right)$.

Similarly to the robustness result for linear mixtures, the above theorem is shown by induction. The main difference is that, in the LQ case, the *virtual* sources (and the mixed data columns for which their contribution is nonzero) might have a large residual and hence be extracted, whereas we would like to extract only the primary sources. Therefore, we must introduce the additional condition (3.1). Roughly speaking, it requires the energy of the residual of a non-already extracted source to be higher than twice the maximum of (i) the largest energy of the virtual sources, which prevents SNPALQ to extract a virtual source, and (ii) the largest energy of the already-extracted sources, which precludes extracting two columns of $\bar{\mathbf{X}}$ corresponding to the same source.

Remark 3.3 (Condition (3.1)). The condition (3.1) is *data and algorithm* dependent. Indeed, it depends on the order in which the columns of $\bar{\mathbf{X}}$ have been extracted. It is possible to provide a data and algorithm independent condition as follows. For $J \subset \llbracket r \rrbracket$, let *us* define

$$\mathbf{M}_J = \left\{ (\mathbf{w}_i)_{i \in J}, (\mathbf{w}_i \odot \mathbf{w}_j)_{\substack{i \leq j \\ i, j \in \llbracket r \rrbracket \setminus J}}, (\mathbf{w}_i \odot \mathbf{w}_j)_{\substack{i \leq j \\ i, j \in J}}, (\mathbf{w}_i \odot \mathbf{w}_j)_{\substack{i \in \llbracket r \rrbracket \setminus J \\ j \in \llbracket J \rrbracket}} \right\}.$$

In Theorem 3.2, Condition (3.1) can be replaced with the following *one*: for all $J \subset \llbracket r \rrbracket$,

$$(3.2) \quad K \left(\mathcal{R}_{\Pi_2(\mathbf{w}_J)}^{\|\cdot\|_2}(\mathbf{W}_{\llbracket r \rrbracket \setminus J}) \right)^2 \geq 4G^2 K \left(\mathcal{R}_{\Pi_2(\mathbf{w}_J)}^{\|\cdot\|_2}(\mathbf{M}_J) \right)^2 \\ + 2 \left(K(\mathbf{W}_{\llbracket r \rrbracket \setminus J}) + [1 + 4G^2] K(\Pi_2(\mathbf{W}_J)) + 4G^2 K(\mathbf{M}_J) \right).$$

Using similar inequalities as in Lemma B.2, it is straightforward to show that condition (3.2) implies condition (3.1). However, the converse does not hold and hence condition (3.2) is more restrictive.

Remark 3.4 (Bounds in Theorem 3.2). The bounds on ϵ and the error on recovering \mathbf{W} in Theorem 3.2 are not easy to interpret. Clearly, these bounds can be weak for some data sets, since $\beta_{\Pi_2(\mathbf{w})}^{\text{LQ}}(\mathbf{W})$ is small as soon as some column of \mathbf{W} , say the j th, is close to the convex hull of $\Pi_2(\mathbf{W})_{\setminus \{j\}}$. Moreover, whether these bounds are tight or not is an open question: a direction of further research would be to improve these bounds or prove they are tight. Note that a similar comment applies to the linear case, where the tightness of SNPA bounds is also an open problem.

3.1.3. Interpretation of SNPALQ recovery conditions. In addition to the mixing constraints described in Section 1.3, among which (ϵ, r) -LQ near-separability, we here give more insights concerning some of the conditions for SNPALQ robustness when applied on LQ mixtures.

Condition on $\alpha_{\Pi_2(\mathbf{w})}(\mathbf{W})$ – The condition $\alpha_{\Pi_2(\mathbf{w})}(\mathbf{W}) > 0$ is of uttermost importance. It ensures that no column of \mathbf{W} lies within the convex hull of the other columns of \mathbf{W} , the origin, and the second order products of the columns of \mathbf{W} . On the contrary, $\alpha_{\Pi_2(\mathbf{w})}(\mathbf{W}) = 0$ would mean that at least one columns of \mathbf{W} would be indistinguishable from the mixed data columns. Compared to SNPA, this condition is more restrictive for *linear* mixings. For example, let us

consider the noiseless mixtures $\mathbf{X} = \mathbf{W}\mathbf{H}$ with

$$\mathbf{W} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

for which $\alpha_{\Pi_2(\mathbf{W})}(\mathbf{W}) = 0$. During its two first iterations, SNPALQ extracts the two first columns of \mathbf{W} . But as $\mathbf{w}_1 \odot \mathbf{w}_2 = \mathbf{w}_3$, all data columns in \mathbf{X} can be written as a nonnegative combination of $[\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_1 \odot \mathbf{w}_2]$, and hence SNPALQ stops after the second iteration (the residual being zero) without extracting \mathbf{w}_3 . On the contrary, SNPA is able to extract the three columns of \mathbf{W} since $\text{rank}(\mathbf{W}) = 3$.

On the other hand, even if the virtual sources appear purely in the mixture, trying to solve the LQ problem using the naive approach explained at the beginning of Section 2, namely applying SNPA on a LQ-mixing with the hope to extract both sources and virtual sources and then rejecting the virtual ones, would require $\alpha_{\Pi_2(\mathbf{W})}(\Pi_2(\mathbf{W})) > 0$, which is a stronger condition than the one of SNPALQ. Indeed, this would require all the virtual sources not to lie within the convex hull of the other columns of $\Pi_2(\mathbf{W})$ and the origin, which should not be required as we do not need to estimate them.

Condition on $\beta_{\Pi_2(\mathbf{W})}^{\text{LQ}}(\mathbf{W})$ – The condition $\beta_{\Pi_2(\mathbf{W})}^{\text{LQ}}(\mathbf{W}) > 0$ is stronger than the corresponding condition of SNPA for linear mixtures which requires $\beta_{\mathbf{W}}^{\text{Lin}}(\mathbf{W}) > 0$. This condition is typically satisfied as long as $\alpha_{\Pi_2(\mathbf{W})}(\mathbf{W}) > 0$. Actually, except for some pathological cases, the residuals of two columns of \mathbf{W} after projection on the convex hull of other columns of \mathbf{W} are expected to be pairwise different, i.e., $\mathcal{R}_{\Pi_2(\mathbf{W}) \setminus \{i,j\}}^f(\mathbf{w}_j) \neq \mathcal{R}_{\Pi_2(\mathbf{W}) \setminus \{i,j\}}^f(\mathbf{w}_i)$ for all $i \neq j$; see the discussion in [18].

Condition on the noise level ϵ – When applied to linear mixings, the admissible noise levels are lower with SNPALQ than SNPA, which requires $\epsilon < \mathcal{O}\left(\frac{\beta_{\mathbf{W}}^{\text{Lin}}(\mathbf{W})^2}{K(\mathbf{W})^2}\right)$. This is expected, and will be confirmed in the numerical experiments of Section 4, since SNPALQ then performs useless additional projections on non-existing virtual sources. On the other hand, when applied to LQ mixings, the admissible noise levels are larger with SNPALQ than SNPA, since the recovery conditions of SNPA involve $\beta_{\Pi_2(\mathbf{W})}(\Pi_2(\mathbf{W}))$. Moreover, SNPALQ does not need the virtual sources to be present in the data set, while SNPA would require each virtual source to appear as a column of $\bar{\mathbf{X}}$.

Condition on $K(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^{\|\cdot\|_2}(\mathbf{A}))$ – At each iteration of SNPALQ, the following condition is required:

$$K(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^{\|\cdot\|_2}(\mathbf{A})) \geq 2GK \left(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^{\|\cdot\|_2} \left((\mathbf{b}_i)_{i \in \llbracket s \rrbracket}, (\mathbf{a}_i \odot \mathbf{a}_j)_{\substack{i \in \llbracket k \rrbracket \\ j \in \llbracket k \rrbracket}}, (\mathbf{b}_i \odot \mathbf{b}_j)_{\substack{i \in \llbracket s \rrbracket \\ j \in \llbracket s \rrbracket}}, (\mathbf{a}_i \odot \mathbf{b}_j)_{\substack{i \in \llbracket k \rrbracket \\ j \in \llbracket s \rrbracket}} \right) \right),$$

with \mathbf{B} the columns of \mathbf{W} already extracted by SNPALQ ($\bar{\mathbf{B}}$ their noisy approximation) and \mathbf{A} the other columns of \mathbf{W} . This means that at each iteration, a new column of \mathbf{W} must have a larger residual than the already extracted sources and the virtual sources. This condition is the most difficult one to fulfil. In particular the difficulties might arise for a large number of

sources, as more terms are present in the right-hand side (see Section 4.2.3), or when \mathbf{W} has large entries. However,

- The condition is sufficient but not necessary (see Section 4.2.3), making that SNPALQ can work even if it is not fulfilled.
- Some terms in the right-hand side are or might be negligible, as

$$K \left(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^{\|\cdot\|_2} ((\mathbf{b}_i)_{i \in [s]}) \right) \leq K \left(\mathcal{R}_{\bar{\mathbf{B}}}^{\|\cdot\|_2} ((\mathbf{b}_i)_{i \in [s]}) \right)$$

and

$$K \left(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^{\|\cdot\|_2} \left((\mathbf{b}_i \odot \mathbf{b}_j)_{\substack{i \leq j \\ i \in [s] \\ j \in [s]}} \right) \right) \leq K \left(\mathcal{R}_{(\bar{\mathbf{b}}_i \odot \bar{\mathbf{b}}_j)_{i \leq j}}^{\|\cdot\|_2} \left((\mathbf{b}_i \odot \mathbf{b}_j)_{\substack{i \leq j \\ i \in [s] \\ j \in [s]}} \right) \right),$$

and the norm of the two right-hand side terms are of the order of the noise level ϵ and $\epsilon + \epsilon^2$, respectively.

- The two remaining terms are driven by the correlation of the columns of \mathbf{W} . If such a correlation is limited, the condition is expected to be more likely fulfilled.
- Even if SNPALQ extracts spurious columns of $\bar{\mathbf{X}}$, the post-processing with BF will discard them as it does not need this condition to be satisfied.

3.2. Robustness of BF on LQ mixings. We now study the robustness of the BF step. First, Theorem 3.5 below states that BF identifies the columns of \mathbf{W} , provided some bounds on the admissible noise levels. The maximum corresponding source estimation error is also given. Then the recovery conditions are discussed.

3.2.1. Main result. The following theorem characterizes the robustness of BF. It is stated in a simplified form by considering $f(\cdot) = \|\cdot\|_2$. Its generalized counterpart handling any $f(\cdot)$ satisfying Assumption 2.1 is reported in Appendix B (see Theorem B.15).

Theorem 3.5 (Robustness of BF when applied on LQ mixings – Simplified version). *Let $\bar{\mathbf{X}} = \Pi_2(\mathbf{W}) + \mathbf{N}$ be an (ϵ, r) -LQ near-separable mixing (Definition 1.4) with ϵ satisfying*

$$4\sqrt{d + 2\epsilon(2K(\mathbf{X}) + \epsilon)} < \alpha_{\mathbf{W}}(\mathbf{W}),$$

where $d = \mathcal{O}\left(\frac{\epsilon}{\alpha_{\Pi_4(\mathbf{W})}(\mathbf{W})^2}\right)$ (see Equation (B.14) in Appendix B for the full expression). Then, BF (Algorithm 2.2) applied on $\bar{\mathbf{X}}$ with $f = \|\cdot\|_2$ identifies the columns of \mathbf{W} up to a ℓ_2 error of $\sqrt{d + 2\epsilon(2K(\mathbf{X}) + \epsilon)}$.

The proof of the above theorem closely follows the proof in the linear case of [5]. In particular it extends two definitions of [5] to LQ mixtures: *i)* the *LQ-robust loners* (see condition (2.3)) and *ii)* the *canonical columns* which are, roughly speaking, the columns corresponding to the sources (up to the noise) in the data set. It then amounts to show that the LQ-robust loners are approximately the canonical columns, which is done by Lemma B.10 (showing that all the robust loners are close to a canonical column) and B.14 (showing that all canonical columns are robust loners). Extracting the robust loners thus enables to approximately recover the sources, as shown by Theorem B.15.

3.2.2. Discussion on the BF recovery conditions. Let us discuss the conditions to ensure the source recovery by BF.

Condition on $\alpha_{\Pi_4(\mathbf{W})}(\mathbf{W})$ – Assuming $\alpha_{\Pi_4(\mathbf{W})}(\mathbf{W}) > 0$ is the counterpart of Deville’s result in [9], which required the family (1.3), containing the products up to order four of the sources, to be linearly independent. Here, this condition is turned into a nonnegative independence, which is significantly less restrictive in general. In fact, this condition is most likely a necessary condition for LQ unmixing since $\alpha_{\Pi_4(\mathbf{W})}(\mathbf{W}) = 0$ implies that some columns of \mathbf{W} can be written as mixtures of other observations.

Condition on ϵ – The condition $4\sqrt{d + 2\epsilon(2 + \epsilon)} < \alpha_{\mathbf{W}}(\mathbf{W})$ with $d = \mathcal{O}\left(\frac{\epsilon}{\alpha_{\Pi_4(\mathbf{W})}(\mathbf{W})^2}\right)$ is a limit on the admissible noise level. Roughly speaking, the better some sources can be approximated by a non-negative combination of the other terms of family (1.3), the smaller the noise power can be.

Comparison with SNPALQ – The conditions of recovery of BF are different from the ones of SNPALQ and can be milder in some cases. For example, in the noiseless case, BF only requires $\alpha_{\Pi_4(\mathbf{W})}(\mathbf{W}) > 0$, in contrast to SNPALQ, which needs in particular the condition (3.1) to be fulfilled. The interest of the BF algorithm will be confirmed in the numerical experiments in Section 4. However, BF is computationally much more demanding (see Section 2.3), which motivates its use as a post-processing for SNPALQ.

4. Numerical results. We here study the behaviors of SNPALQ and BF as a post-processing on simulated yet realistic data sets in the specific applicative context of HS unmixing. The observed mixtures are supposed to follow the Nascimento model [37]. The function $f(\cdot)$ used by the algorithms is here chosen as $f(\cdot) = \|\cdot\|_2$. The code is available from <https://bit.ly/SNPALQv1>.

Section 4.2 dwells on noiseless mixtures. More precisely, we show in Section 4.2.1 that SNPALQ yields very good practical results in this setting, which are enhanced by the BF postprocessing in Section 4.2.2. We further show in Section 4.2.3 that the condition (3.1) is only sufficient: it does not need to be fulfilled for SNPALQ to provide reliable results. In Section 4.3, the robustness of SNPALQ in the presence of noise is studied for different non-linearity levels. Furthermore, in the supplementary material, a first experiment confirms that, beyond the usual Nascimento model involving bilinear mixtures, both SNPALQ and the BF generalize well to LQ models. A second one is also detailed, showing that our results extend with larger numbers of observations m .

SNPA [18] and SPA [3, 22], two well-known algorithms for near-separable NMF, are used to benchmark the results of the proposed algorithm. Note that plenty of non-linear unmixing methods have been proposed in the literature, exploiting parametric models [13, 24] or data-driven models [39, 25]. However, these algorithms have not been considered here for performance comparison since none of them specifically tackle the separation of near-separable mixtures. Moreover, contrary to SPA and SNPA, they are not accompanied by theoretical recovery guarantees, which is one of the main objective of this paper.

4.1. Experimental setting and metrics. Experiments are conducted on realistic (ϵ, r) -LQ near-separable nonnegative data sets \mathbf{X} following Definition 1.4. The parameters of the model are chosen as follows.

- The primary sources (referred to as *endmember* signatures in the HS literature) defin-

ing the columns of \mathbf{W} are defined as spectral signatures extracted from the USGS database⁴. They correspond to reflectance spectra associated with materials from diverse origins (such as minerals, soils, and plants) and naturally follow $0 \leq \mathbf{W} \leq 1$.

- The matrix \mathbf{H}' is generated in the following way:
 - The columns of a first matrix \mathbf{H} of the same dimension as \mathbf{H}' are generated randomly using a Dirichlet distribution $\mathcal{D}(\alpha, \dots, \alpha)$ with $\alpha = 0.5$, which is standard in HS imaging [35].
 - The r first rows (corresponding to the linear contribution) are multiplied by $1 - \nu$, while the remaining rows (corresponding to the virtual endmembers) are multiplied by ν to enable various non-linearity levels:

$$(4.1) \quad \mathbf{H}' = \begin{bmatrix} \mathbf{H}^{[r]} \times (1 - \nu) \\ \mathbf{H}^{[r+1, \tilde{r}]} \times \nu \end{bmatrix}.$$

Note that, accordingly to the Nascimento model [37] we consider here, we mostly focus on bilinear mixtures in this experimental section. In this case, the lines of $\mathbf{H}^{[r+1, \tilde{r}]}$ corresponding to squared sources $(\mathbf{s}_j \odot \mathbf{s}_j)_{j \in [r]}$ are enforced to be all-zero lines.

- The previous transformation does not preserve the sums of the entries in each column of \mathbf{H} which were equal to one (Dirichlet distribution). Since the columns are assumed to sum to (at most) one, the last step divides each column of \mathbf{H}' by its ℓ_1 norm.
- The elements of the matrix \mathbf{N} are independently and identically drawn from a centered Gaussian distribution with a variance corresponding to a given signal-to-noise ratio (SNR).
- The matrix $\bar{\mathbf{X}}$ is finally created ensuring all the entries to be non-negative: $\bar{\mathbf{X}} = [\Pi_2(\mathbf{W})\mathbf{H} + \mathbf{N}]_+$, where $[\cdot]_+$ is the elementwise projection on the non-negative orthant.

The quality of an algorithm is assessed using the minimum spectral angle distance (SAD) between the true and the estimated endmembers:

$$\theta_{\min} = \max_{\pi, \text{permutation of } [r]} \min_{i \in [r]} \text{SAD}(\mathbf{w}_{\pi(i)}, \mathbf{x}_{\mathcal{K}(i)}),$$

where $\text{SAD}(\mathbf{u}, \mathbf{v}) = \frac{\mathbf{u}^T \mathbf{v}}{\|\mathbf{u}\|_2 \|\mathbf{v}\|_2}$. We consider a perfect separation is achieved if $\theta_{\min} > 0.999$.

Remark 4.1 (Real data sets). Although the columns of \mathbf{W} we use are true spectral signatures, the mixtures considered in this work are partially synthetic. Indeed, due to the few works in LQ hyperspectral unmixing, there is a limited amount of relevant data sets with associated ground truth, that is, for which quadratic terms are known to be present and properly quantified. Moreover, when considering real data sets, further challenges might arise, which are not currently tackled by the algorithms herein proposed: for instance, the presence of spectral variability in the endmembers or the presence of outliers [19, 22]. The primary objective of this article is to establish the first theoretical results on LQ near-separable NMF. Tackling such further practical questions is left for future research.

⁴<https://www.usgs.gov/>

4.2. Numerical results on noiseless mixtures.

4.2.1. Study of SNPALQ. We first explore the behavior of SNPALQ as a function of the number of endmembers r in a noiseless setting. We consider $n = 1000$ mixed pixels with $m = 20$ and the non-linearity parameter is chosen as $\nu = 0.5$. We conducted 100 Monte-Carlo experiments, each time generating a new dataset.

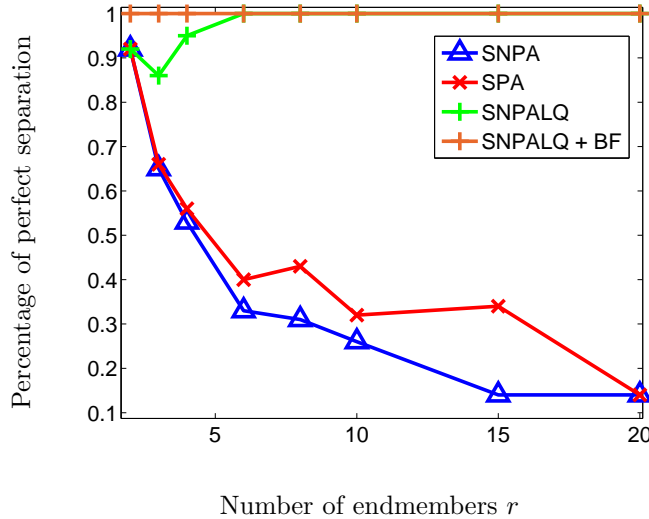


Figure 4. Percentage of experiments in which a perfect separation is achieved, among 100 Monte-Carlo of noiseless bilinear synthetic data sets. The parameters are: $m = 20$ observations, $n = 1000$ pixels and $\nu = 0.5$.

Fig. 4 reports the percentage of full recovery by the different algorithms. In this experiment, SNPALQ obtains much better results than SNPA or SPA, and achieves in more than 90% of the experiments a perfect separation. While an initial improvement of the results when r increases might look surprising, it is probably not to be linked directly with the r value itself, but rather with the generated \mathbf{H}' . Indeed, when r is small, the data columns are more spread within the convex hull formed by the endmembers and these are therefore more difficult to extract; see Section 4.2.3.

On the other hand, the results of SNPA and SPA are rather bad on this non-linear data set, and deteriorate quickly when the number of endmembers increases. While both algorithms obtain close results, it is interesting to note that SPA becomes worse than SNPA when r becomes closer to m , which is expected as SNPA has an interest over SPA mainly when the matrices \mathbf{W} are either not full-rank or ill conditioned [18].

4.2.2. Study of BF as a post-processing step. In this section, we analyze the relevance of the introduction of BF as a post-processing conducted after SNPALQ. Figure 4 displays in orange the separation quality when applying the BF to SNPALQ. This result shows that BF enables to achieve perfect results for all experiments by improving SNPALQ results, especially for low r values.

A natural question is however the *cost* of such a post-processing; see Section 2.2. Table 2 thus

Table 2

1st line: *actual r value*. 2nd line: *average number $|\mathcal{K}|$, over 100 Monte-Carlo experiments, of endmembers extracted by SNPALQ before the BF step*.

r	2	3	4	6	8	10	15	20
$ \mathcal{K} $ SNPALQ before BF	2.08	3.16	4.05	6	8	10	15	20

displays the number of columns extracted by SNPALQ (2nd line) as a function of the actual number r of sources. These columns are the input of the BF, and therefore they determine its computational time. Interestingly enough, on average, SNPALQ does not need to extract more than $r + 1$ components to extract all the columns of \mathbf{W} . As such, the post-processing step is applied on a small number of columns of $\tilde{\mathbf{X}}$ and is cheap.

4.2.3. Discussion about condition (3.1). The introduction of condition (3.1) is one of the major difference compared to the linear case, for which it does not appear explicitly⁵. As such, we here aim at discussing its validity on real noiseless HS data. It is important to notice that this context might be favorable, since \mathbf{W} naturally fulfills $0 \leq \mathbf{W} \leq 1$. To do so, we propose the following complementary experiment: for each of the 100 Monte-Carlo experiments, we draw a new \mathbf{W} matrix from the USGS database and split the columns of \mathbf{W} into two disjoint matrices: $\mathbf{A} = [(\mathbf{w}_i)_{i \in \mathcal{J}, \mathcal{J} \subseteq [r]}]$ and $\mathbf{B} = [(\mathbf{w}_i)_{i \in [r] \setminus \mathcal{J}}]$. We then check whether these matrices \mathbf{A} and \mathbf{B} fulfill condition (3.1). By repeating the process with all the possible \mathbf{A} and \mathbf{B} , we can thus obtain a percentage of subsets \mathbf{A} and \mathbf{B} for which condition (3.1) is fulfilled in the USGS database. In this experiment, we consider $n = 1\,000$ samples with $m = 50$ observations.

Figure 5 (dashed lines) depicts, as a function of the number of endmembers r , the proportion of the different realizations of \mathbf{W} for which condition 3.1 is fulfilled. This proportion of sub-matrices \mathbf{A} and \mathbf{B} fulfilling condition (3.1) decreases with r , which was expected as the number of elements in the right-hand side increases. Then, as exemplified in Figure 2, the condition is observed to be slightly less restrictive in general for SNPALQ than for SNPA.

Most importantly, the results become quite bad for relatively small r values: for $r = 10$, the condition is fulfilled for only slightly more than 5% of the tested subsets \mathbf{A} and \mathbf{B} . Thus it might be surprising that SNPALQ algorithm achieves perfect results in almost all experiments. The reason of such a discrepancy is twofold:

- The dashed lines of Figure 5 consider all the possible ways to split the matrix \mathbf{W} into two submatrices \mathbf{A} and \mathbf{B} . Thus, they do not take into account the order in which the columns of \mathbf{W} are extracted by SNPALQ. In practice however, SNPALQ only needs condition (3.1) to be satisfied for the order in which it extracts the indices, which is easier to fulfil.
- The virtual endmembers typically do not appear purely, which makes condition (3.1) too conservative (recall that this condition is not necessary in the linear case; see Theorem 3.1). In other words, Condition 3.1 considers the worst case scenario for any possible mixing matrix \mathbf{H} while, in practice, the non-linearity can be mild.

⁵More exactly, in the linear case this condition is replaced by one on the admissible noise levels; see [18].

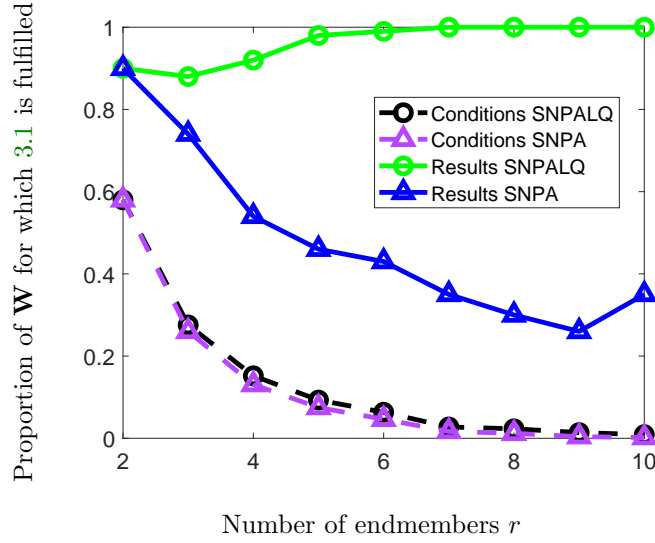


Figure 5. Comparison between theoretical conditions ensuring endmember recovery by SNPALQ (resp. SNPA) and actual results. The dashed line correspond to the percentage of submatrices \mathbf{A} and \mathbf{B} for which condition 3.1 is fulfilled and the plain lines correspond to the actual proportion of perfect recovery by SNPALQ (resp. SNPA).

In summary, while Condition 3.1 might seem restrictive, SNPALQ can yield excellent results in settings in which it is not fulfilled. In particular, it could be of interest to include the non-linearity level ν in a study of necessary conditions for SNPALQ, which is left for future work.

4.3. Robustness study: noisy mixtures. The impact of the noise and non-linearity levels is now studied. We generated bilinear data sets $\tilde{\mathbf{X}}$ with 7 different SNR levels and 12 values for the non-linearity parameter ν . For each pair of SNR and ν values, 24 Monte-Carlo experiments are conducted on nonlinear mixtures characterized by $m = 50$ spectral bands, $r = 10$ endmembers and $n = 1\,000$ pixels.

Figure 6 depicts the recovery performances of SNPALQ and SNPA. For low non-linearity levels, the mixtures approximately follow the LMM: in agreement with their robustness guarantees, the results of SNPALQ+BF are then perfect when the SNR is high ($\text{SNR} \geq 40\text{dB}$); see the upper-left corner of Figure 6a. However, SNPALQ+BF performs worse than SNPA in the presence of a stronger noise ($\text{SNR} \in [25\text{dB}, 30\text{dB}]$), which is expected as it projects the residual onto non-existing virtual endmembers, leading to a loss of information (the norm of the residual decreases faster).

SNPALQ+BF shows its benefit over SNPA when the non-linearity level increases and the noise level is not too large (upper-right corner of the figures). More precisely, when $\nu \geq 0.3$ and $\text{SNR} \geq 40\text{ dB}$, SNPALQ+BF always obtains a perfect recovery, which represents a significant improvement over SNPA, up to 20%. In the lower-right corner of the figure, when the SNR decreases, the results of both algorithms deteriorate as the problem is highly difficult.

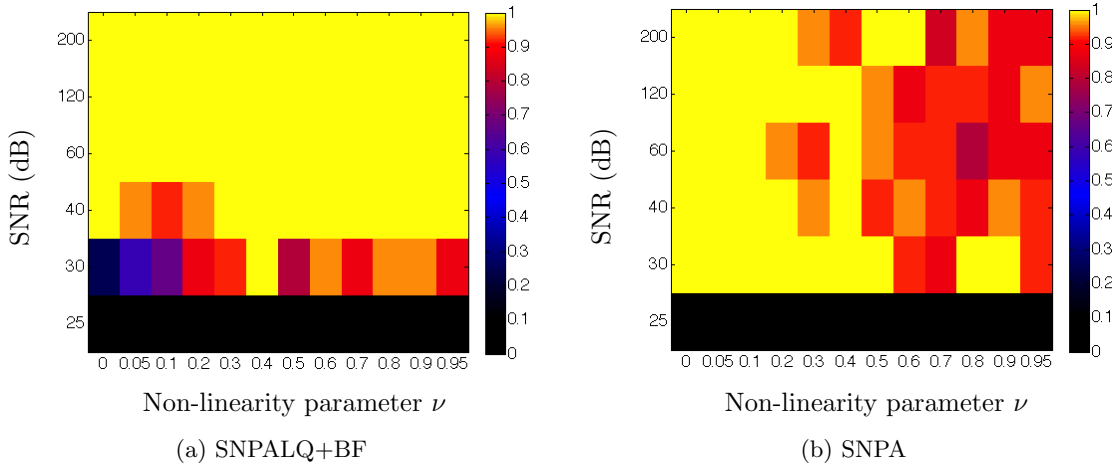


Figure 6. As a function of SNR and non-linearity level ν , percentage of perfect separation using (a) SNPALQ+BF, (b) SNPA.

5. Conclusion. In this paper, we have considered the problem of linear-quadratic blind source separation, under the (r, ϵ) -LQ near-separable assumption which requires the primary sources to appear purely in the data set. We first introduced SNPALQ, an extension of SNPA [18], which takes into account the presence of quadratic terms in the projection step. SNPALQ is guaranteed to recover the sources for linear-quadratic under appropriate conditions. We then introduced a second algorithm, namely brute-force (BF), an extension of the algorithm of Arora et al [5], which provably recovers the sources under often practically-milder conditions than SNPALQ. It is recommended to use BF as a post-processing of SNPALQ (denoted by SNPALQ+BF) due to its high computational cost. Finally, we illustrated the performance of SNPALQ and SNPALQ+BF in various settings, and showed that they obtained good separation results on synthetic data sets, and for various experimental settings, including linear, bilinear and linear quadratic mixtures. Improving SNPALQ+BF results for low SNR while still alleviating recovery conditions of both algorithms is left for future work.

To conclude, let us mention some particularly promising directions of further research:

- *Relaxing near-separability.* In the linear case, near-separability can be relaxed to the so-called sufficiently scattered condition (SSC) which requires \mathbf{H} to be sufficiently sparse. Under the SSC, identifiability is achieved using an NMF formulation minimizing the volume of the convex hull of the columns of \mathbf{W} ; see [16] and [20, Chapter 4] and the references therein. One interesting question would be: can we generalize this result to LQ mixtures?
- *Generalizing to other types of nonlinear mixtures.* Depending on the applicative context, several non-linear mixing models can be considered. In this work, we focused on LQ mixtures and more specifically on the so-called Nascimento model. It would be interesting to extend the algorithms we proposed in this work to other types of non-linear mixtures such as the Fan model [15] and the generalized bilinear model [23].
- *Other applications.* We have focused in this paper on hyperspectral imaging. How-

ever, the LQ model could be meaningful in other applications. For example, in topic modeling, the input matrix is a word-by-document count matrix, and the columns of \mathbf{W} represent topics [31]. The quadratic terms would mean that a word that is used by two topics is more likely to appear in a document discussing these two topics.

Acknowledgment. The authors are thankful to the anonymous reviewers for their insightful comments that helped to improve the paper significantly.

Appendix A. A few useful results of [22, 18].

Lemma A.1 (Lemma 3.3 in [18]). *For any $\mathbf{B} \in \mathbb{R}^{m \times s}$, $\mathbf{x} \in \mathbb{R}^m$, and f satisfying Assumption 2.1, we have $\|\mathcal{R}_{\mathbf{B}}^f(\mathbf{x})\|_2 \leq \sqrt{\frac{L}{\mu}} \|\mathbf{x}\|_2$.*

Lemma A.2 (Lemma 3.13 in [18]). *Let $\mathbf{B} \in \mathbb{R}^{m \times s}$, $\mathbf{A} \in \mathbb{R}^{m \times k}$, $\mathbf{n} \in \mathbb{R}^m$, and $z \in \Delta^k$, and let f satisfy Assumption 2.1. Then,*

$$f\left(\mathcal{R}_{\mathbf{B}}^f(\mathbf{A}\mathbf{z} + \mathbf{n})\right) \leq f\left(\mathcal{R}_{\mathbf{B}}^f(\mathbf{A}\mathbf{z}) + \mathbf{n}\right) \quad \text{and} \quad f\left(\mathcal{R}_{\mathbf{B}}^f(\mathbf{A}\mathbf{z} + \mathbf{n})\right) \leq f\left(\mathcal{R}_{\mathbf{B}}^f(\mathbf{A})\mathbf{z} + \mathbf{n}\right).$$

Lemma A.3 (Lemma 3.14 in [22]). *Let the function f satisfy Assumption 2.1. Then, for any $\|\mathbf{x}\|_2 \leq K$ and $\|\mathbf{n}\|_2 \leq \epsilon \leq K$,*

$$f(\mathbf{x}) - \epsilon KL \leq f(\mathbf{x} + \mathbf{n}) \leq f(\mathbf{x}) + \frac{3}{2}\epsilon KL.$$

Appendix B. Proofs of our main results: SNPALQ and BF are provably robust in the presence of noise.

In this section, we study the robustness of SNPALQ (Section B.1) and of BF (Section B.2) for LQ mixtures. Note that the robustness proof of SNPALQ for linear mixtures, which is comparatively less central to our contribution, is provided in the supplementary material.

Let us introduce some additional notations. For two matrices $\mathbf{A} \in \mathbb{R}^{m \times r_A}$ and $\mathbf{B} \in \mathbb{R}^{m \times r_B}$, we define

$$\alpha_{\mathbf{B}}(\mathbf{A}) = \min_{\substack{j \in [r_A] \\ \mathbf{x} \in \Delta}} \|\mathbf{a}_j - \mathbf{B}_{\setminus\{j\}} \mathbf{x}\|_2.$$

For instance, in the special case $\mathbf{A} = \mathbf{B}$, $\alpha_{\mathbf{A}}(\mathbf{A})$ is the minimum distance between a column of \mathbf{A} and the convex hull formed by the other columns of \mathbf{A} and the origin. Let us also denote $\nu(\mathbf{A}) = \min_{i \in [r_A]} \|\mathbf{a}_i\|_2$, $\gamma(\mathbf{A}) = \min_{\substack{i, j \in [r_A] \\ i \neq j}} \|\mathbf{a}_i - \mathbf{a}_j\|_2$, $\omega(\mathbf{A}) = \min\left(\nu(\mathbf{A}), \frac{\sqrt{2}}{2}\gamma(\mathbf{A})\right)$, and $\Omega(\mathbf{A}) = \min\left(\frac{K(\mathbf{A})}{2}\sqrt{\frac{\mu}{L}}\left[1 - \frac{1}{G}\right], \gamma(\mathbf{A})\right)$, where μ , L and G are some constants that will be specified later.

B.1. Proof of SNPALQ robustness for LQ mixtures. After stating a few useful lemmas, the induction step of the proof of SNPALQ robustness for LQ mixtures is given in Theorem B.4 and the main result is stated in Theorem B.5.

Lemma B.1 ([18]-Lemma 15 extended). *Let $\mathbf{Z} = [\mathbf{P}, \mathbf{Q}]$, where $\mathbf{P} \in \mathbb{R}^{m \times k}$ and $\mathbf{Q} \in \mathbb{R}^{m \times r-k}$, and let f satisfy Assumption 2.1. If*

$$(B.1) \quad K(\mathbf{P}) \geq 2G \sqrt{\frac{L}{\mu}} K(\mathbf{Q}) \quad \text{with} \quad G > \sqrt{\frac{L}{\mu}} \geq 1,$$

then, for any $\delta \in [0, \frac{1}{2}]$,

$$(B.2) \quad f^* = \max_{\mathbf{x} \in \Delta} f(\mathbf{Z}\mathbf{x}) \quad \text{such that } \mathbf{x}_i \leq 1 - \delta \text{ for } 1 \leq i \leq k$$

satisfies

$$(B.3) \quad f^* \leq \max_i f(\mathbf{p}_i) - \frac{1}{2} \mu (1 - \delta) \delta \Omega(\mathbf{P})^2$$

with $\Omega(\mathbf{P}) = \min \left(\gamma(\mathbf{P}), \frac{K(\mathbf{P})}{2} \sqrt{\frac{\mu}{L}} \left[1 - \frac{1}{G} \right] \right)$.

Proof. First, let us provide a lower bound for f^* . Remember that due to the strong convexity of f with parameter μ , its gradient Lipschitz continuity and the fact that $f(\mathbf{0}_m) = 0$, we have that for all $\mathbf{y} \in \mathbb{R}^m$

$$(B.4) \quad \frac{\mu}{2} \|\mathbf{y}\|_2^2 \leq f(\mathbf{y}) \leq \frac{L}{2} \|\mathbf{y}\|_2^2.$$

Consequently, since $(1 - \delta)\mathbf{p}_i$ is an admissible solution, we have that

$$(B.5) \quad f^* \geq f((1 - \delta)\mathbf{p}_i) \geq \frac{1}{2} \mu (1 - \delta)^2 \|\mathbf{p}_i\|_2^2 \geq \frac{\mu}{8} \|\mathbf{p}_i\|_2^2,$$

where the last inequality is due to the assumption $\delta \leq 1/2$.

Let us now discuss upperbounds of f . By strong convexity of f , the optimal solution x^* of (B.2) is attained at a vertex of the feasible domain $\{\mathbf{x} \in \mathbb{R}_+^r \mid \sum_{i=1}^r \mathbf{x}_i \leq 1 \text{ and } \mathbf{x}_i \leq 1 - \delta \text{ for } 1 \leq i \leq r\}$. Here are the different cases

- a) $\mathbf{x}^* = \mathbf{0}_r$;
- b) $\mathbf{x}^* = \mathbf{e}_i$ for $k + 1 \leq i \leq r$;
- c) $\mathbf{x}^* = (1 - \delta)\mathbf{e}_j$ for $1 \leq j \leq k$;
- d) $\mathbf{x}^* = \delta\mathbf{e}_i + (1 - \delta)\mathbf{e}_j$ for $1 \leq i, j \leq k$;
- e) $\mathbf{x}^* = \delta\mathbf{e}_i + (1 - \delta)\mathbf{e}_j$ for $k + 1 \leq i \leq r$ and $1 \leq j \leq k$

Let us analyze them separately.

- a) This first case is clearly impossible, as $f(\mathbf{0}_m) = 0$ and $f(\mathbf{y}) > 0$ for all $\mathbf{y} \neq \mathbf{0}$; see Eq. (B.4).
- b) $\mathbf{Z}\mathbf{x}^* = \mathbf{q}_i$ for some i . Using Eq. (B.4), we obtain

$$(B.6) \quad f^* = f(\mathbf{q}_i) \leq \frac{L}{2} K(\mathbf{Q}) \underset{\text{Hyp. (B.1)}}{\leq} \frac{\mu}{8G^2} K(\mathbf{P})^2 \underset{\text{Eq. (B.5)}}{<} f^*,$$

which is a contraction.

c) $\mathbf{Zx}^* = (1 - \delta)\mathbf{p}_i$ for some i . Let us then distinguish two subcases:

- If $\|\mathbf{p}_j\|_2^2 \leq \frac{\mu}{4L}K(\mathbf{P})^2$, then:

$$\begin{aligned} f^* = f((1 - \delta)\mathbf{p}_j) &\stackrel{\substack{f(\mathbf{0}_m)=0 \\ f \text{ strongly convex}}}{\leq} (1 - \delta)f(\mathbf{p}_j) \stackrel{\text{Eq. (B.4)}}{\leq} (1 - \delta)\frac{L}{2}\|\mathbf{p}_j\|_2^2 \\ &\stackrel{\|\mathbf{p}_j\|_2^2 \leq \frac{\mu}{4L}K(\mathbf{P})^2}{\leq} (1 - \delta)\frac{\mu}{8}K(\mathbf{P})^2 \\ &< \frac{\mu}{8}K(\mathbf{P})^2 \leq f^*, \end{aligned}$$

which is a contradiction.

- If $\|\mathbf{p}_j\|_2^2 > \frac{\mu}{4L}K(\mathbf{P})^2$, then, by strong convexity of f ,

$$f^* \leq (1 - \delta)f(\mathbf{p}_j) - \frac{1}{2}\mu\delta(1 - \delta)\|\mathbf{p}_j\|_2^2 = f(\mathbf{p}_j) - \delta f(\mathbf{p}_j) - \frac{1}{2}\mu\delta(1 - \delta)\|\mathbf{p}_j\|_2^2.$$

$$\text{Since } f(\mathbf{p}_j) \stackrel{\text{Eq. (B.4)}}{\geq} \frac{\mu}{2}\|\mathbf{p}_j\|_2^2 \geq \frac{1}{2}\mu(1 - \delta)\|\mathbf{p}_j\|_2^2,$$

$$\begin{aligned} f^* &< f(\mathbf{p}_j) - \mu\delta(1 - \delta)\|\mathbf{p}_j\|_2^2 \\ &\leq f(\mathbf{p}_j) - \frac{1}{2}\mu\delta(1 - \delta)\left[\frac{1}{2}\sqrt{\frac{\mu}{L}}K(\mathbf{P})\right]^2 \\ &\leq f(\mathbf{p}_j) - \frac{1}{2}\mu\delta(1 - \delta)\left[\frac{K(\mathbf{P})}{2}\sqrt{\frac{\mu}{L}}\left(1 - \frac{1}{G}\right)\right]^2, \end{aligned}$$

which satisfies the bound of the theorem.

d) $\mathbf{Zx}^* = \delta\mathbf{p}_i + (1 - \delta)\mathbf{p}_j$ for some $i \neq j$. Then, by strong convexity of f ,

$$f^* \leq \delta f(\mathbf{p}_i) + (1 - \delta)f(\mathbf{p}_j) - \frac{1}{2}\mu\delta(1 - \delta)\|\mathbf{p}_i - \mathbf{p}_j\|_2^2 \leq K(\mathbf{P}) - \frac{1}{2}\mu\delta(1 - \delta)\gamma(\mathbf{P})^2$$

e) $\mathbf{Yx}^* = \delta\mathbf{q}_i + (1 - \delta)\mathbf{p}_j$ for some i, j . First (similarly to case c), let us distinguish two subcases:

- Let us assume $\|\mathbf{p}_j\|_2^2 \leq \frac{\mu}{4L}K(\mathbf{P})^2$. Then,

$$\begin{aligned} f^* = f(\delta\mathbf{q}_i + (1 - \delta)\mathbf{p}_j) &\stackrel{\text{Strong convexity}}{<} \delta f(\mathbf{q}_i) + (1 - \delta)f(\mathbf{p}_j) \\ &\stackrel{\text{Eq. (B.4)}}{\leq} \delta\frac{L}{2}\|\mathbf{q}_i\|_2^2 + (1 - \delta)\frac{L}{2}\|\mathbf{p}_j\|_2^2 \\ &\stackrel{\text{Hyp. (B.1)}}{<} \delta\frac{\mu}{8}K(\mathbf{P})^2 + (1 - \delta)\frac{\mu}{8}K(\mathbf{P})^2 \\ &= \frac{\mu}{8}K(\mathbf{P})^2 \stackrel{\text{B.5}}{\leq} f^*, \end{aligned}$$

a contradiction.

- If $\|\mathbf{p}_j\|_2^2 > \frac{\mu}{4L} K(\mathbf{P})^2$, then, by strong convexity of f ,

$$f^* \leq \delta f(\mathbf{q}_i) + (1 - \delta) f(\mathbf{p}_j) - \frac{1}{2} \mu \delta (1 - \delta) \|\mathbf{q}_i - \mathbf{p}_j\|_2^2$$

Using the triangle inequality, we obtain

$$\|\mathbf{q}_i - \mathbf{p}_j\|_2 \geq \|\mathbf{p}_j\|_2 - \|\mathbf{q}_i\|_2,$$

since $\|\mathbf{q}_i\|_2 \leq K(\mathbf{Q}) \stackrel{\text{Hyp. (B.1)}}{<} \frac{1}{G} \sqrt{\frac{\mu}{4L}} K(\mathbf{P}) \leq \|\mathbf{p}_j\|_2$. Thus,

$$\|\mathbf{q}_i - \mathbf{p}_j\|_2 \geq \frac{1}{2} \sqrt{\frac{\mu}{L}} K(\mathbf{P}) - \frac{1}{2G} \sqrt{\frac{\mu}{L}} K(\mathbf{P}) = \frac{1}{2} \sqrt{\frac{\mu}{L}} K(\mathbf{P}) \left(1 - \frac{1}{G}\right).$$

Furthermore,

$$\begin{aligned} f(\mathbf{q}_i) &\leq \frac{L}{2} \|\mathbf{q}_i\|_2^2 \leq \frac{L}{2} K(\mathbf{Q})^2 \leq \frac{\mu}{8G^2} K(\mathbf{P})^2 \\ &< \frac{L}{2G^2} \|\mathbf{p}_j\|_2^2 \\ &\leq \frac{L}{\mu G^2} f(\mathbf{p}_j). \end{aligned}$$

Putting the above expressions altogether, we have

$$\begin{aligned} f^* &< f(\mathbf{p}_j) + \delta \frac{L}{\mu G^2} f(\mathbf{p}_j) - \delta f(\mathbf{p}_j) - \frac{1}{2} \mu \delta (1 - \delta) \left[\frac{1}{2} \sqrt{\frac{\mu}{L}} K(\mathbf{P}) \left(1 - \frac{1}{G}\right) \right]^2 \\ &\leq f(\mathbf{p}_j) + \left(\frac{L}{\mu G^2} - 1 \right) \delta f(\mathbf{p}_j) - \frac{1}{2} \mu \delta (1 - \delta) \left[\frac{1}{2} \sqrt{\frac{\mu}{L}} K(\mathbf{P}) \left(1 - \frac{1}{G}\right) \right]^2 \\ &\leq f(\mathbf{p}_j) - \frac{1}{2} \mu \delta (1 - \delta) \left[\frac{1}{2} \sqrt{\frac{\mu}{L}} K(\mathbf{P}) \left(1 - \frac{1}{G}\right) \right]^2 \end{aligned}$$

where the last line, which satisfies the bound of the theorem, requires $L < \mu G^2$. ■

Lemma B.2. Let $\mathbf{A} \in \mathbb{R}^{m \times k}$ and $\bar{\mathbf{B}} \in \mathbb{R}^{m \times s}$ be such that $\bar{\mathbf{B}} - \mathbf{B} = \mathbf{N}$ and $\|\mathbf{N}\|_2 < \epsilon$, and let f satisfy Assumption 2.1. Then,

$$\Omega(\mathcal{R}_{\bar{\mathbf{B}}}^f(\mathbf{A}))^2 \geq \Omega(\mathcal{R}_{\mathbf{B}}^f(\mathbf{A}))^2 - 4\epsilon(K(\mathbf{A}) + K(\mathbf{B})).$$

Proof. Let us look at the two terms of $\Omega(\mathcal{R}_{\bar{\mathbf{B}}}^f(\mathbf{A}))$:

- Denoting $\mathbf{z}_{\mathbf{a}_j} = \operatorname{argmin}_{\mathbf{x} \in \Delta} \|\mathbf{a}_j - \bar{\mathbf{B}}\mathbf{x}\|_2$, we have, for $j \in \llbracket k \rrbracket$,

$$\left\| \mathcal{R}_{\bar{\mathbf{B}}}^f(\mathbf{a}_j) \right\|_2 = \|\mathbf{a}_j - \bar{\mathbf{B}}\mathbf{z}_{\mathbf{a}_j}\|_2 = \|\mathbf{a}_j - (\mathbf{B} + \mathbf{N})\mathbf{z}_{\mathbf{a}_j}\|_2 \geq \left| \|\mathbf{a}_j - \mathbf{B}\mathbf{z}_{\mathbf{a}_j}\|_2 - \|\mathbf{N}\mathbf{z}_{\mathbf{a}_j}\|_2 \right|$$

Thus, for $j \in \llbracket k \rrbracket$,

$$\begin{aligned} \left\| \mathcal{R}_{\mathbf{B}}^f(\mathbf{a}_j) \right\|_2^2 &\geq (\|\mathbf{a}_j - \mathbf{B}\mathbf{z}_{\mathbf{a}_j}\|_2 - \|\mathbf{N}\mathbf{z}_{\mathbf{a}_j}\|_2)^2 \\ &\geq \|\mathbf{a}_j - \mathbf{B}\mathbf{z}_{\mathbf{a}_j}\|_2^2 - 2\|\mathbf{a}_j - \mathbf{B}\mathbf{z}_{\mathbf{a}_j}\|_2 \|\mathbf{N}\mathbf{z}_{\mathbf{a}_j}\|_2 + \|\mathbf{N}\mathbf{z}_{\mathbf{a}_j}\|_2^2 \\ &\geq \left\| \mathcal{R}_{\mathbf{B}}^f(\mathbf{a}_j) \right\|_2^2 - 2(K(\mathbf{A}) + K(\mathbf{B}))\epsilon, \end{aligned}$$

where the last line is obtained since $\mathbf{z}_{\mathbf{a}_j} \in \Delta$. This yields

$$K(\mathcal{R}_{\mathbf{B}}^f(\mathbf{A}))^2 \geq K(\mathcal{R}_{\mathbf{B}}^f(\mathbf{A}))^2 - (K(\mathbf{A}) + K(\mathbf{B}))\epsilon,$$

and, as $0 \leq \frac{\mu}{L} \left[1 - \frac{1}{G}\right]^2 \leq 1$,

$$\frac{K(\mathcal{R}_{\mathbf{B}}^f(\mathbf{A}))^2}{4} \frac{\mu}{L} \left[1 - \frac{1}{G}\right]^2 \geq \frac{K(\mathcal{R}_{\mathbf{B}}^f(\mathbf{A}))^2}{4} \frac{\mu}{L} \left[1 - \frac{1}{G}\right]^2 - \frac{\epsilon(K(\mathbf{A}) + K(\mathbf{B}))}{2}.$$

- Denoting

$$\mathbf{z}_{\mathbf{a}_i} = \operatorname{argmin}_{\mathbf{x} \in \Delta} \|\mathbf{a}_i - \bar{\mathbf{B}}\mathbf{x}\|_2 \quad \text{and} \quad \mathbf{z}_{\mathbf{a}_j} = \operatorname{argmin}_{\mathbf{x} \in \Delta} \|\mathbf{a}_j - \bar{\mathbf{B}}\mathbf{x}\|_2,$$

we have, for $i \neq j, i, j \in \llbracket k \rrbracket$,

$$\left\| \mathcal{R}_{\bar{\mathbf{B}}}^f(\mathbf{a}_i) - \mathcal{R}_{\bar{\mathbf{B}}}^f(\mathbf{a}_j) \right\|_2 \geq \left| \|\mathbf{a}_i - \bar{\mathbf{B}}\mathbf{z}_{\mathbf{a}_i} - (\mathbf{a}_j - \bar{\mathbf{B}}\mathbf{z}_{\mathbf{a}_j})\|_2 - \|\mathbf{N}(\mathbf{z}_{\mathbf{a}_i} - \mathbf{z}_{\mathbf{a}_j})\|_2 \right|.$$

This yields

$$\left\| \mathcal{R}_{\bar{\mathbf{B}}}^f(\mathbf{a}_i) - \mathcal{R}_{\bar{\mathbf{B}}}^f(\mathbf{a}_j) \right\|_2^2 \geq \gamma(\mathcal{R}_{\bar{\mathbf{B}}}^f(\mathbf{A}))^2 - 4\epsilon(K(\mathbf{A}) + K(\mathbf{B})),$$

which gives the result. ■

Lemma B.3. *Let $\mathbf{A} \in \mathbb{R}^{m \times k}$ such that $\bar{\mathbf{B}} \in \mathbb{R}^{m \times s}$ be such that $\mathbf{B} - \bar{\mathbf{B}} = \mathbf{N}$ and $\|\mathbf{N}\|_2 < \epsilon$, and let f satisfy Assumption 2.1. Then,*

$$\Omega(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\mathbf{A}))^2 \geq \Omega(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A}))^2 - 4(K(\mathbf{A}) + K(\Pi_2(\mathbf{B}))) \max(\epsilon, 2\epsilon K(\mathbf{B}) + \epsilon^2).$$

Proof. The result follows directly from the previous Lemma B.2, by noting that ■

$$\|\Pi_2(\bar{\mathbf{B}}) - \Pi_2(\mathbf{B})\|_2 \leq \max(\epsilon, 2\epsilon K(\mathbf{B}) + \epsilon^2).$$

Theorem B.4 (Robustness of SNPAB when applied on linear-quadratic mixings - induction step). *Let the following hold:*

- \mathbf{X} follows a (r, ϵ) -LQ near-separable mixing model. Precisely, $\bar{\mathbf{X}}$ satisfies Definition 1.4 with

$$\begin{aligned} \bar{\mathbf{X}} &= \Pi_2(\mathbf{W})\mathbf{H} + \mathbf{N}, \quad \mathbf{W} = [\mathbf{A}, \mathbf{B}] \quad \text{and} \quad \mathbf{A} \in \mathbb{R}^{m \times k}, \quad \mathbf{B} \in \mathbb{R}^{m \times s}, \\ \mathbf{H} &\in \mathbb{R}_+^{\frac{r(r+1)}{2} \times n} \quad \text{with } \forall j \in \llbracket n \rrbracket, \mathbf{h}_j \in \Delta. \end{aligned}$$

Let us further assume the noise to be bounded as $\|\mathbf{N}\|_{1,2} \leq \epsilon$, and denote by $\mathbf{X} = \Pi_2(\mathbf{W})\mathbf{H}$ the noiseless version of $\bar{\mathbf{X}}$. Note that, with these notations,

$$\Pi_2(\mathbf{W}) = \begin{bmatrix} (\mathbf{a}_i)_{i \in \llbracket k \rrbracket}, (\mathbf{b}_i)_{i \in \llbracket s \rrbracket}, (\mathbf{a}_i \odot \mathbf{a}_j)_{\substack{i \leq j \\ i \in \llbracket k \rrbracket \\ j \in \llbracket k \rrbracket}}, (\mathbf{b}_i \odot \mathbf{b}_j)_{\substack{i \leq j \\ i \in \llbracket s \rrbracket \\ j \in \llbracket s \rrbracket}}, (\mathbf{a}_i \odot \mathbf{b}_j)_{\substack{i \in \llbracket k \rrbracket \\ j \in \llbracket s \rrbracket}} \end{bmatrix}.$$

- $\bar{\mathbf{B}} \in \mathbb{R}^{m \times s}$ satisfies $K(\mathbf{B} - \bar{\mathbf{B}}) \leq C\epsilon$ for some $C > 0$.
- $\mathbf{W} = [\mathbf{A}, \mathbf{B}]$ is such that $\alpha_{\Pi_2(\mathbf{B})}(\mathbf{A}) > 0$, $\gamma(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A})) > 0$.
- For some $G > 1$, the matrix \mathbf{W} and the considered \mathbf{A} and \mathbf{B} satisfy:

(B.7)

$$K(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\mathbf{A})) \geq 2GK \left(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f \left((\mathbf{b}_i)_{i \in \llbracket s \rrbracket}, (\mathbf{a}_i \odot \mathbf{a}_j)_{\substack{i \leq j \\ i \in \llbracket k \rrbracket \\ j \in \llbracket k \rrbracket}}, (\mathbf{b}_i \odot \mathbf{b}_j)_{\substack{i \leq j \\ i \in \llbracket s \rrbracket \\ j \in \llbracket s \rrbracket}}, (\mathbf{a}_i \odot \mathbf{b}_j)_{\substack{i \in \llbracket k \rrbracket \\ j \in \llbracket s \rrbracket}} \right) \right).$$

- f satisfies Assumption 2.1 with strong convexity parameter μ and gradient Lipschitz constant L such that $L < \mu G^2$.
- ϵ is sufficiently small so that

(B.8)

$$C\epsilon < \min \left(\frac{-40L^{3/2} - 16\mu^{3/2}CK(\mathbf{W}) + \sqrt{(40L^{3/2} + 16\mu^{3/2}CK(\mathbf{W}))^2 + \frac{32\mu^3C^2\Omega(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A}))^2}{K(\Pi_2(\mathbf{W}))}}}{16\mu^{3/2}C}, \right. \\ \left. \frac{\mu^{3/2}C\Omega(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A}))^2}{K(\Pi_2(\mathbf{W}))(40L^{3/2} + 8C\mu^{3/2})}, \frac{\min(M, \Omega(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A})))^2}{8K(\Pi_2(\mathbf{W}))}, \right. \\ \left. \sqrt{K(\mathbf{W})^2 + \frac{\min(M, \Omega(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A})))^2}{8K(\Pi_2(\mathbf{W}))}} - K(\mathbf{W}) \right)$$

with $M \geq 0$ a constant and

$$\Omega(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A})) = \min \left(\gamma(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A})), \frac{K(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A}))}{2} \sqrt{\frac{\mu}{L}} \left[1 - \frac{1}{G} \right] \right).$$

Then the index i corresponding to a column $\bar{\mathbf{x}}_i$ of $\bar{\mathbf{X}}$ maximizing the function $f(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\cdot))$ satisfies

$$(B.9) \quad \mathbf{x}_i = \Pi_2(\mathbf{W})\mathbf{h}_i \quad \text{with} \quad h_{il} \geq 1 - \delta \quad \text{for some } l \in \llbracket k \rrbracket,$$

and

$$(B.10) \quad \delta = \frac{20\epsilon K(\Pi_2(\mathbf{W}))}{\Omega(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A}))^2 - 8K(\Pi_2(\mathbf{W}))C\epsilon \max(1, 2K(\mathbf{W}) + C\epsilon)} \frac{L^{3/2}}{\mu^{3/2}} \leq \frac{1}{2}.$$

This implies

$$(B.11) \quad \|\bar{\mathbf{x}}_i - \mathbf{w}_l\|_2 = \|\bar{\mathbf{x}}_i - \mathbf{a}_l\|_2 \leq \epsilon \left[1 + \frac{40K(\Pi_2(\mathbf{W}))^2}{\Omega(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A}))^2 - M^2} \frac{L^{3/2}}{\mu^{3/2}} \right].$$

Proof. The robustness is proved by contradiction. Let us assume that the column of $\bar{\mathbf{X}}$ maximizing $f(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\cdot))$ satisfies $\bar{\mathbf{x}}_i = \Pi_2(\mathbf{W})\mathbf{h}_i + \mathbf{n}_i$ with $h_{il} < 1 - \delta$ for $1 \leq l \leq k$. We have

$$\begin{aligned} f(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\bar{\mathbf{x}}_i)) &\stackrel{\text{Lemma A.2}}{\leq} f(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\Pi_2(\mathbf{W})\mathbf{h}_i + \mathbf{n}_i)) \\ &\stackrel{\text{Lemma A.3}}{\leq} f(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\Pi_2(\mathbf{W})\mathbf{h}_i)) + \frac{3}{2}\epsilon K(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\Pi_2(\mathbf{W})\mathbf{h}_i))L. \end{aligned}$$

Using Lemma A.1,

$$\left\| \mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\Pi_2(\mathbf{W})\mathbf{h}_i) \right\|_2 \leq \max_i \left\| \mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\Pi_2(\mathbf{W})\mathbf{h}_i) \right\|_2 \stackrel{\text{Lemma A.1}}{\leq} \sqrt{\frac{L}{\mu}} K(\Pi_2(\mathbf{W})),$$

we obtain

$$\begin{aligned} (B.12) \quad f(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\bar{\mathbf{x}}_i)) &\leq f(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\Pi_2(\mathbf{W})\mathbf{h}_i)) + \frac{3}{2}\epsilon K(\Pi_2(\mathbf{W})) \frac{L^{3/2}}{\mu^{1/2}} \\ &\leq \max_{\substack{\mathbf{x} \in \Delta^r \\ \mathbf{x}_l \leq 1-\delta \\ 1 \leq l \leq k}} f(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\Pi_2(\mathbf{W})\mathbf{x})) + \frac{3}{2}\epsilon K(\Pi_2(\mathbf{W})) \frac{L^{3/2}}{\mu^{1/2}} \\ &\stackrel{\substack{\text{Lem (B.1)} \\ \text{Eq. (B.7)}}}{\leq} \max_j f(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\mathbf{a}_j)) - \frac{1}{2}\mu\delta(1-\delta)\Omega(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\mathbf{A}))^2 + \frac{3}{2}\epsilon K(\Pi_2(\mathbf{W})) \frac{L^{3/2}}{\mu^{1/2}} \\ &\stackrel{\text{Lemma A.2}}{\leq} \max_j f(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\bar{\mathbf{a}}_j) - \mathbf{n}_j) - \frac{1}{2}\mu\delta(1-\delta)\Omega(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\mathbf{A}))^2 \\ &\quad + \frac{3}{2}\epsilon K(\Pi_2(\mathbf{W})) \frac{L^{3/2}}{\mu^{1/2}} \\ &\stackrel{\text{Lemma A.3}}{\leq} \max_j f(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\bar{\mathbf{a}}_j)) - \frac{1}{2}\mu\delta(1-\delta)\Omega(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\mathbf{A}))^2 + \frac{9}{2}\epsilon K(\Pi_2(\mathbf{W})) \frac{L^{3/2}}{\mu^{1/2}} \\ &\stackrel{\text{Lem (B.3)}}{\leq} \max_j f(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\bar{\mathbf{a}}_j)) - \frac{1}{2}\mu\delta(1-\delta) \left[\Omega(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\mathbf{A}))^2 \right. \\ &\quad \left. - 4(K(\mathbf{A}) + K(\Pi_2(\mathbf{B})))C\epsilon \max(1, 2K(\mathbf{B}) + C\epsilon) \right] + \frac{9}{2}\epsilon K(\Pi_2(\mathbf{W})) \frac{L^{3/2}}{\mu^{1/2}} \\ &\stackrel{\text{Lem (B.3)}}{\leq} \max_j f(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\bar{\mathbf{a}}_j)) - \frac{1}{2}\mu\delta(1-\delta) \left[\Omega(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\mathbf{A}))^2 - 8K(\Pi_2(\mathbf{W}))C\epsilon \right. \\ &\quad \left. \times \max(1, 2K(\mathbf{W}) + C\epsilon) \right] + \frac{9}{2}\epsilon K(\Pi_2(\mathbf{W})) \frac{L^{3/2}}{\mu^{1/2}}. \end{aligned}$$

The fifth inequality follows from Lemma A.1 since

$$\left\| \mathcal{R}_{\Pi_2(\mathbf{B})}^f(\bar{\mathbf{a}}_j) \right\|_2 \leq \sqrt{\frac{L}{\mu}} \|\bar{\mathbf{a}}_j\|_2 \leq \sqrt{\frac{L}{\mu}} (K(\Pi_2(\mathbf{W})) + \epsilon) \leq 2\sqrt{\frac{L}{\mu}} K(\Pi_2(\mathbf{W})),$$

if $\epsilon \leq K(\Pi_2(\mathbf{W}))$, which implies that

$$\begin{aligned} f^* &< \max_j f \left(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\bar{\mathbf{a}}_j) \right) \\ &- \frac{1}{2} \mu \delta (1 - \delta) \left[\Omega \left(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A}) \right)^2 - 8K(\Pi_2(\mathbf{W})) C \epsilon \max(1, 2K(\mathbf{W}) + C\epsilon) \right] + \frac{10}{2} \epsilon K(\Pi_2(\mathbf{W})) \frac{L^{3/2}}{\mu^{1/2}}. \end{aligned}$$

Then, replacing δ by its expression (B.10), we obtain

$$\begin{aligned} &\frac{1}{2} \mu \delta (1 - \delta) \left[\Omega \left(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A}) \right)^2 - 8K(\Pi_2(\mathbf{W})) C \epsilon \max(1, 2K(\mathbf{W}) + C\epsilon) \right] \\ &\geq \frac{1}{4} \mu \delta \left[\Omega \left(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A}) \right)^2 - 8K(\Pi_2(\mathbf{W})) C \epsilon \max(1, 2K(\mathbf{W}) + C\epsilon) \right] \\ &= \frac{1}{4} \mu \left(20 \frac{\epsilon K(\Pi_2(\mathbf{W}))}{\Omega \left(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A}) \right)^2 - 8K(\Pi_2(\mathbf{W})) C \epsilon \max(1, 2K(\mathbf{W}) + C\epsilon)} \frac{L^{3/2}}{\mu^{3/2}} \right) \\ &\quad \times \left[\Omega \left(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A}) \right)^2 - 8K(\Pi_2(\mathbf{W})) C \epsilon \max(1, 2K(\mathbf{W}) + C\epsilon) \right] \\ &= \frac{10}{2} \epsilon K(\Pi_2(\mathbf{W})) \frac{L^{3/2}}{\mu^{3/2}}. \end{aligned}$$

Therefore we finally obtain a contradiction since we should have

$$f \left(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\bar{\mathbf{x}}_i) \right) < \max_j f \left(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\bar{\mathbf{a}}_j) \right),$$

which is impossible since $\bar{\mathbf{x}}_i$ should maximize $f \left(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\cdot) \right)$ among the columns of $\bar{\mathbf{X}}$ and the $\bar{\mathbf{a}}_j$ are among these columns.

Note that in the previous reasoning, we have assumed δ to be in $[0, \frac{1}{2}]$, which is satisfied if:

$$\begin{aligned} C\epsilon &< \min \left(\frac{-40L^{3/2} - 16\mu^{3/2}CK(\mathbf{W}) + \sqrt{(40L^{3/2} + 16\mu^{3/2}CK(\mathbf{W}))^2 + \frac{32\mu^3C^2\Omega(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A}))^2}{K(\Pi_2(\mathbf{W}))}}}{16\mu^{3/2}C}, \right. \\ &\quad \left. \frac{C\mu^{3/2}\Omega(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A}))^2}{K(\Pi_2(\mathbf{W}))(40L^{3/2} + 8C\mu^{3/2})}, \frac{\Omega(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A}))^2}{8K(\Pi_2(\mathbf{W}))}, -K(\mathbf{W}) + \sqrt{K(\mathbf{W})^2 + \frac{\Omega(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A}))^2}{8K(\Pi_2(\mathbf{W}))}} \right) \end{aligned}$$

The proof of (B.11) follows from result (B.9). We have

$$\mathbf{x}_i = (1 - \delta') \mathbf{w}_l + \sum_{k \neq l} \gamma_k \mathbf{w}_k + \sum_{i,j} g_{ij} \mathbf{w}_i \odot \mathbf{w}_j \text{ for some } l \text{ and } 1 - \delta' \geq 1 - \delta$$

so that $\sum_{k \neq l} \gamma_k + \sum_{i,j} g_{ij} \leq \delta' \leq \delta$. Hence

$$\begin{aligned} \|\mathbf{x}_i - \mathbf{w}_l\|_2 &= \left\| -\delta' \mathbf{w}_l + \sum_{k \neq l} \gamma_k \mathbf{w}_k + \sum_{i,j} g_{ij} \mathbf{w}_i \odot \mathbf{w}_j \right\|_2 \leq 2\delta' \max_j \|\Pi_2(\mathbf{W})_j\|_2 \\ &= 2\delta' K(\Pi_2(\mathbf{W})) \\ &\leq 2\delta K(\Pi_2(\mathbf{W})), \end{aligned}$$

which gives, when considering the noisy version of \mathbf{X} ,

$$\|\bar{\mathbf{x}}_i - \mathbf{w}_l\|_2 \leq (\|\bar{\mathbf{x}}_i - \mathbf{x}_i\|_2 + \|\mathbf{x}_i - \mathbf{w}_l\|_2) \leq \epsilon + 2K(\Pi_2(\mathbf{W}))\delta\epsilon \text{ for some } 1 \leq l \leq k.$$

To conclude the proof, we use the fact that

$$\epsilon + 2K(\Pi_2(\mathbf{W}))\delta\epsilon \leq \epsilon \left[1 + \frac{40K(\Pi_2(\mathbf{W}))^2}{\Omega(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A}))^2 - M^2} \frac{L^{3/2}}{\mu^{3/2}} \right] = \hat{C}\epsilon,$$

where M^2 is a constant⁶ chosen such that $M^2 > 8K(\Pi_2(\mathbf{W}))C\epsilon \max(1, 2K(\mathbf{W}) + C\epsilon)$, which requires

$$C\epsilon < \frac{M^2}{8K(\Pi_2(\mathbf{W}))}$$

and

$$C\epsilon < -K(\mathbf{W}) + \sqrt{K(\mathbf{W})^2 + \frac{M^2}{8K(\Pi_2(\mathbf{W}))}}.$$

■

Theorem B.5 (Robustness of SNPALQ when applied on LQ mixings). *Let*

$$\bar{\mathbf{X}} = \Pi_2(\mathbf{W})\mathbf{H} + \mathbf{N} \in \mathbb{R}^{m \times n}$$

be an (ϵ, r) -LQ near-separable mixing (Definition 1.4) with

$$\alpha_{\Pi_2(\mathbf{W})}(\mathbf{W}) > 0 \text{ and } \beta_{\Pi_2(\mathbf{W})}^{LQ}(\mathbf{W}) > 0.$$

Let f satisfy Assumption 2.1, and let

(B.13)

$$\begin{aligned} \hat{C}\epsilon &< \min \left(\frac{-40L^{3/2} - 16\mu^{3/2}\hat{C}K(\mathbf{W}) + \sqrt{\left(40L^{3/2} + 16\mu^{3/2}\hat{C}K(\mathbf{W})\right)^2 + \frac{32\mu^3\hat{C}^2\beta_{\Pi_2(\mathbf{W})}^{LQ}(\mathbf{W})^2}{K(\Pi_2(\mathbf{W}))}}}{16\mu^{3/2}\hat{C}}, \right. \\ &\quad \left. \frac{\mu^{3/2}\hat{C}\beta_{\Pi_2(\mathbf{W})}^{LQ}(\mathbf{W})^2}{K(\Pi_2(\mathbf{W}))(40L^{3/2} + 8\hat{C}\mu^{3/2})}, \frac{\min(M, \beta_{\Pi_2(\mathbf{W})}^{LQ}(\mathbf{W}))^2}{8K(\Pi_2(\mathbf{W}))}, \sqrt{K(\mathbf{W})^2 + \frac{\min(M, \beta_{\Pi_2(\mathbf{W})}^{LQ}(\mathbf{W}))^2}{8K(\Pi_2(\mathbf{W}))}} - K(\mathbf{W}) \right) \end{aligned}$$

⁶The reader might wonder why such a constant M does not appear in SNPALQ robustness proof for linear mixings. Actually, it was implicitly chosen as $M^2 = \Omega(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A}))^2/2$.

where

$$\hat{C} = 1 + \frac{40K(\Pi_2(\mathbf{W}))^2}{\beta_{\Pi_2(\mathbf{W})}^{LQ}(\mathbf{W})^2 - M^2} \frac{L^{3/2}}{\mu^{3/2}},$$

with M a constant⁷ (the smaller M , the more restrictive the condition on the noise, but the better the estimation). Furthermore, let us assume that at each iteration of SNPALQ the following condition is fulfilled:

$$K\left(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f(\mathbf{A})\right) \geq 2GK\left(\mathcal{R}_{\Pi_2(\bar{\mathbf{B}})}^f\left(\left(\mathbf{b}_i\right)_{i \in \llbracket s \rrbracket}, \left(\mathbf{a}_i \odot \mathbf{a}_j\right)_{\substack{i \leq j \\ i \in \llbracket k \rrbracket \\ j \in \llbracket k \rrbracket}}, \left(\mathbf{b}_i \odot \mathbf{b}_j\right)_{\substack{i \leq j \\ i \in \llbracket s \rrbracket \\ j \in \llbracket s \rrbracket}}, \left(\mathbf{a}_i \odot \mathbf{b}_j\right)_{\substack{i \in \llbracket k \rrbracket \\ j \in \llbracket s \rrbracket}}\right)\right),$$

where \mathbf{B} contains the columns of \mathbf{W} already extracted by SNPALQ and $\bar{\mathbf{B}}$ the corresponding columns with noise, \mathbf{A} contains the remaining columns of \mathbf{W} still-to-be extracted, and $L < \mu G^2$ is a constant. Then, SNPALQ identifies in r steps the columns of \mathbf{W} up to an error $\hat{C}\epsilon$. Precisely, denoting \mathcal{K} the index set extracted by SNPALQ after r steps, there exists a permutation π of $\llbracket r \rrbracket$ such that:

$$\max_{1 \leq j \leq r} \|\bar{\mathbf{x}}_{\mathcal{K}(j)} - \mathbf{w}_{\pi(j)}\|_2 \leq \hat{C}\epsilon.$$

Proof. The result follows by induction.

- In the initialization step, \mathbf{B} is the empty matrix.
- The induction step is given by Theorem B.4: the \mathbf{B} matrix corresponds to the columns of \mathbf{W} extracted so far by SNPALQ, while the columns of \mathbf{A} the ones still-to-be extracted. Letting

$$\hat{C} = 1 + \frac{40K(\Pi_2(\mathbf{W}))^2}{\beta_{\Pi_2(\mathbf{W})}^{LQ}(\mathbf{W})^2 - M^2} \frac{L^{3/2}}{\mu^{3/2}}$$

in Theorem B.4, we obtain that if the already extracted columns are at a distance at most $\hat{C}\epsilon$ of some columns of \mathbf{W} (more exactly, $\|\bar{\mathbf{B}} - \mathbf{B}\|_2 \leq \hat{C}\epsilon$), then the next extracted column will be at distance at most $\hat{C}\epsilon$ from a new column of \mathbf{W} (that is, a column of \mathbf{A}), provided that ϵ is small enough. ■

B.2. Proofs for the Brute Force algorithm (BF).

Definition B.6 (LQ-robust loner). Let $\bar{\mathbf{X}}$ be an (ϵ, r) -LQ near-separable mixing satisfying Definition 1.4. Let us denote \mathcal{L} the set of indices $k \in \llbracket n \rrbracket$ such that

$$(B.14) \quad f(\bar{\mathbf{x}}_k - \bar{\mathbf{x}}_j) \leq d = \epsilon V,$$

⁷Despite a slight loss of generality, the reader can think of $M^2 = \Omega(\mathcal{R}_{\Pi_2(\mathbf{B})}^f(\mathbf{A}))^2/2$ to create a link with the linear case.

where

$$V = \frac{L^2}{2\mu\alpha_{\Pi_4(\mathbf{W})}(\mathbf{W})^2} K(\mathbf{X})^2 Y^2 [\epsilon(1 + \max(1, 2K(\mathbf{X}) + \epsilon))^2 + 2K(\mathbf{X})Y + 2\max(1, 2K(\mathbf{X}) + \epsilon)(\epsilon + K(\mathbf{X})Y)] \\ + \frac{3}{2}L(4K(\mathbf{X}) + \epsilon),$$

with $Y = 1 + \max(1, K(\mathbf{X}))$. We call $\bar{\mathbf{x}}_j$ a robust loner if

$$\min_{\mathbf{h}^* \in \Delta} f(\bar{\mathbf{x}}_j - \Pi_2(\bar{\mathbf{X}}_{[n] \setminus \mathcal{L}}) \mathbf{h}^*) > \frac{L}{2} \epsilon^2 (1 + \max(1, 2K(\mathbf{X}) + \epsilon))^2.$$

Definition B.7 (Canonical columns). Let $\bar{\mathbf{X}}$ be (ϵ, r) -LQ near-separable; see Definition 1.4. We call canonical columns (associated to $i \in [r]$), the columns $\bar{\mathbf{X}}_{k(i)}$, $k(i) \in [n]$, of $\bar{\mathbf{X}}$ such that all the columns of $\mathbf{H}_{k(i)}$ have a single nonzero entry located in their i th row. Note that by definition of near-separability, there exists at least a canonical column for all $i \in [r]$. Moreover, all the canonical columns $\bar{\mathbf{x}}_{k(i)}$ associated to $i \in [r]$ satisfy $f(\bar{\mathbf{x}}_{k(i)} - \mathbf{w}_i) < \frac{L}{2} \epsilon^2$.

Lemma B.8. Let $\bar{\mathbf{X}}$ be (ϵ, r) -LQ near-separable (Definition 1.4). Considering all the canonical columns, written as $\bar{\mathbf{X}}_{\mathcal{K}}$ (that is, the canonical columns associated to all $i \in [r]$), every column $\bar{\mathbf{x}}_j$ of $\bar{\mathbf{X}}$ is such that

$$\min_{\mathbf{h}^* \in \Delta} f(\bar{\mathbf{x}}_j - \Pi_2(\bar{\mathbf{X}}_{\mathcal{K}}) \mathbf{h}^*) \leq \frac{L}{2} \epsilon^2 (1 + \max(1, 2K(\mathbf{X}) + \epsilon))^2.$$

Proof. For all $\mathbf{h} \in \Delta$, we have:

$$f(\bar{\mathbf{x}}_j - \Pi_2(\bar{\mathbf{X}}_{\mathcal{K}}) \mathbf{h}) \leq \frac{L}{2} \|\bar{\mathbf{x}}_j - \Pi_2(\bar{\mathbf{X}}_{\mathcal{K}}) \mathbf{h}\|_2^2 \\ \leq \frac{L}{2} (\|\bar{\mathbf{x}}_j - \mathbf{x}_j\|_2 + \|\mathbf{x}_j - \Pi_2(\mathbf{X}_{\mathcal{K}}) \mathbf{h}\|_2 \\ + \|(\Pi_2(\mathbf{X}_{\mathcal{K}}) - \Pi_2(\bar{\mathbf{X}}_{\mathcal{K}})) \mathbf{h}\|_2)^2.$$

Moreover

$$\|\bar{\mathbf{x}}_j - \mathbf{x}_j\|_2 + \|\mathbf{x}_j - \Pi_2(\mathbf{X}_{\mathcal{K}}) \mathbf{h}\|_2 + \|(\Pi_2(\mathbf{X}_{\mathcal{K}}) - \Pi_2(\bar{\mathbf{X}}_{\mathcal{K}})) \mathbf{h}\|_2 \\ \leq \epsilon + \|\mathbf{x}_j - \Pi_2(\mathbf{X}_{\mathcal{K}}) \mathbf{h}\|_2 + \max(\epsilon, 2K(\mathbf{X})\epsilon + \epsilon^2).$$

Thus,

$$\min_{\mathbf{h}^* \in \Delta} f(\bar{\mathbf{x}}_j - \Pi_2(\bar{\mathbf{X}}_{\mathcal{K}}) \mathbf{h}^*) \leq \frac{L}{2} \epsilon^2 (1 + \max(1, 2K(\mathbf{X}) + \epsilon))^2.$$

Lemma B.9. Let $\bar{\mathbf{X}} = \Pi_2(\mathbf{W})\mathbf{H} + \mathbf{N}$ be (ϵ, r) -LQ near-separable (Definition 1.4). Let us denote $\bar{\mathbf{x}}_{k(i)}$ any robust loner associated to $i \in [r]$. If $f(\bar{\mathbf{x}}_j - \mathbf{w}_i) > d + \epsilon L(2K(\mathbf{X}) + \epsilon)$ for some $j \in [t]$, then $f(\bar{\mathbf{x}}_j - \bar{\mathbf{x}}_{k(i)}) > d$.

Proof. We have

$$\begin{aligned}
 f(\bar{\mathbf{x}}_j - \bar{\mathbf{x}}_{k(i)}) &= f(\bar{\mathbf{x}}_j - \mathbf{w}_i - \mathbf{n}_{k(i)}) \\
 &\geq f(\bar{\mathbf{x}}_j - \mathbf{w}_i) - \epsilon K(\bar{\mathbf{x}}_j - \mathbf{w}_i)L \\
 &> d + \epsilon L(2K(\mathbf{X}) + \epsilon) - \epsilon(2K(\mathbf{X}) + \epsilon)L \\
 &= d.
 \end{aligned}$$

Lemma B.10. *Let $\bar{\mathbf{X}} = \Pi_2(\mathbf{W})\mathbf{H} + \mathbf{N}$ be (ϵ, r) -LQ near-separable (Definition 1.4). If a column $\bar{\mathbf{x}}_j$ is a robust loner, then there is an index $i \in \llbracket r \rrbracket$ such that*

$$f(\bar{\mathbf{x}}_j - \mathbf{w}_i) \leq d + \epsilon L(2K(\mathbf{X}) + \epsilon).$$

Proof. The result is proved by contraposition. We want to show that

If $\forall i \in \llbracket r \rrbracket, f(\bar{\mathbf{x}}_j - \mathbf{w}_i) > d + \epsilon(2K(\mathbf{X}) + \epsilon)$, then $\bar{\mathbf{x}}_j$ is not a robust loner.

If $\bar{\mathbf{x}}_j$ is such that $\forall i \in \llbracket r \rrbracket, f(\bar{\mathbf{x}}_j - \mathbf{w}_i) > d + \epsilon L(2K(\mathbf{X}) + \epsilon)$, then $\forall i \in \llbracket r \rrbracket, f(\bar{\mathbf{x}}_j - \bar{\mathbf{x}}_{k(i)}) > d$, with $\bar{\mathbf{x}}_{k(i)}$ the canonical columns associated to i ; see lemma B.9. As such, denoting $\bar{\mathbf{X}}_{\mathcal{K}}$ all the canonical columns, to be a robust loner $\bar{\mathbf{x}}_j$ must satisfy

$$\min_{\mathbf{h}^* \in \Delta} f(\bar{\mathbf{x}}_j - \Pi_2(\bar{\mathbf{X}}_{\mathcal{K}})\mathbf{h}^*) > \frac{L}{2}\epsilon^2(1 + \max(1, 2K(\mathbf{X}) + \epsilon))^2.$$

This is however not the case according to Lemma B.8. Thus, by definition, $\bar{\mathbf{x}}_j$ is not a robust loner. ■

Lemma B.11. *Let $\bar{\mathbf{X}} = \Pi_2(\mathbf{W})\mathbf{H} + \mathbf{N}$ be (ϵ, r) -LQ near-separable (Definition 1.4), $i \in \llbracket r \rrbracket$ and $\bar{\mathbf{x}}_{k(i)}$ a canonical column associated to i . If, for some $k \in \llbracket n \rrbracket$, $f(\bar{\mathbf{x}}_k - \mathbf{w}_i) \leq d - \frac{3}{2}\epsilon L(2K(\mathbf{X}) + \epsilon)$, then $f(\bar{\mathbf{x}}_k - \bar{\mathbf{x}}_{k(i)}) \leq d$.*

Proof. We have

$$\begin{aligned}
 f(\bar{\mathbf{x}}_k - \bar{\mathbf{x}}_{k(i)}) &= f(\bar{\mathbf{x}}_k - \mathbf{w}_i - \mathbf{n}_{k(i)}) \\
 &\leq f(\bar{\mathbf{x}}_k - \mathbf{w}_i) + \frac{3}{2}\epsilon LK(\bar{\mathbf{x}}_k - \mathbf{w}_i) \\
 &= d - \frac{3}{2}\epsilon L(2K(\mathbf{X}) + \epsilon) + \frac{3}{2}\epsilon L(2K(\mathbf{X}) + \epsilon) \\
 &= d
 \end{aligned}$$

Lemma B.12. *Let $\bar{\mathbf{X}} = \Pi_2(\mathbf{W})\mathbf{H} + \mathbf{N}$ be (ϵ, r) -LQ near-separable (Definition 1.4). All the columns $\bar{\mathbf{x}}_j$, $j \in \llbracket n \rrbracket$, with $\mathbf{x}_j = \sum_{k=1}^r a_{kj}\mathbf{w}_k + \sum_{l=1}^r \sum_{q=l+1}^r b_{jlq}\mathbf{w}_l \odot \mathbf{w}_q$ and $a_{ij} > 1 - \sqrt{\frac{2d-3\epsilon L(4K(\mathbf{X})+\epsilon)}{LK(\mathbf{X})^2[1+\max(1, K(\mathbf{X}))]^2}}$ for some $i \in \llbracket r \rrbracket$ satisfy $f(\bar{\mathbf{x}}_j - \mathbf{w}_i) \leq d - \frac{3}{2}\epsilon L(2K(\mathbf{X}) + \epsilon)$.*

Proof. We want to prove that

$$\left\{ \bar{\mathbf{x}}_j \mid a_{ij} > 1 - \sqrt{\frac{2d-3\epsilon L(4K(\mathbf{X})+\epsilon)}{LK(\mathbf{X})^2[1+\max(1, K(\mathbf{X}))]^2}} \right\} \subseteq \left\{ \bar{\mathbf{x}}_j \mid f(\bar{\mathbf{x}}_j - \mathbf{w}_i) \leq d - \frac{3}{2}\epsilon L(2K(\mathbf{X}) + \epsilon) \right\}$$

Let us consider a column $\bar{\mathbf{x}}_j \in \left\{ \bar{\mathbf{x}}_j \mid a_{ij} > 1 - \sqrt{\frac{2d-3\epsilon L(4K(\mathbf{X})+\epsilon)}{LK(\mathbf{X})^2[1+\max(1, K(\mathbf{X}))]^2}} \right\}$. We have (looking at the noiseless version \mathbf{x}_j of $\bar{\mathbf{x}}_j$) that

$$\begin{aligned} f(\mathbf{x}_j - \mathbf{w}_j) &\leq \frac{L}{2} \|\mathbf{x}_j - \mathbf{w}_i\|_2^2 \\ &= \frac{L}{2} \left\| \mathbf{w}_i - a_{ij}\mathbf{w}_i - \sum_{k \neq i}^r a_{kj}\mathbf{w}_k - \sum_{l=1}^r \sum_{q=l}^r b_{jlq}\mathbf{w}_l \odot \mathbf{w}_q \right\|_2^2 \\ &= \frac{L}{2} (1 - a_{ij})^2 \left\| \mathbf{w}_i - \frac{1}{1 - a_{ij}} \left(\sum_{k \neq i}^r a_{kj}\mathbf{w}_k + \sum_{l=1}^r \sum_{q=l}^r b_{jlq}\mathbf{w}_l \odot \mathbf{w}_q \right) \right\|_2^2. \end{aligned}$$

Moreover

$$\begin{aligned} &\left\| \mathbf{w}_i - \frac{1}{1 - a_{ij}} \left(\sum_{k \neq i}^r a_{kj}\mathbf{w}_k + \sum_{l=1}^r \sum_{q=l}^r b_{jlq}\mathbf{w}_l \odot \mathbf{w}_q \right) \right\|_2 \\ &\leq \|\mathbf{w}_i\|_2 + \left\| \frac{1}{1 - a_{ij}} \left(\sum_{k \neq i}^r a_{kj}\mathbf{w}_k + \sum_{l=1}^r \sum_{q=l}^r b_{jlq}\mathbf{w}_l \odot \mathbf{w}_q \right) \right\|_2 \\ &\leq K(\mathbf{X}) + \max(K(\mathbf{X}), K(\mathbf{X})^2), \end{aligned}$$

where the second inequality is obtained using $\frac{1}{1-a_{ij}} \left(\sum_{k \neq i}^r a_{kj} + \sum_{l=1}^r \sum_{q=l}^r b_{jlq} \right) = 1$. Therefore,

$$f(\mathbf{x}_j - \mathbf{w}_j) \leq \frac{L}{2} (1 - a_{ij})^2 K(\mathbf{X})^2 [1 + \max(1, K(\mathbf{X}))]^2.$$

To conclude the proof, let us consider the noisy $\bar{\mathbf{x}}_j$, we have

$$\begin{aligned} f(\bar{\mathbf{x}}_j - \mathbf{w}_i) &= f(\mathbf{x}_j + \mathbf{n}_j - \mathbf{w}_i) \\ &\leq f(\mathbf{x}_j - \mathbf{w}_i) + \frac{3}{2} L \epsilon K(\mathbf{x}_j - \mathbf{w}_i) \\ &\leq \frac{L}{2} (1 - a_{ij})^2 K(\mathbf{X})^2 [1 + \max(1, K(\mathbf{X}))]^2 + 3L\epsilon K(\mathbf{X}) \\ &\leq d - \frac{3}{2} \epsilon L (2K(\mathbf{X}) + \epsilon). \end{aligned}$$

Lemma B.13. Let $\bar{\mathbf{X}}$ be (ϵ, r) -LQ near-separable (Definition 1.4), $\mathcal{J} \subseteq \llbracket n \rrbracket$ and $\bar{\mathbf{x}}_{k(i)}$ a canonical column associated to i . If

$$\text{for some } i \in \llbracket r \rrbracket, f(\mathbf{w}_i - \Pi_2(\mathbf{X}_{\mathcal{J}})\mathbf{h}) \geq \frac{\mu}{2L} \frac{2d - 3\epsilon L(4K(\mathbf{X}) + \epsilon)}{K(\mathbf{X})^2[1 + \max(1, K(\mathbf{X}))]^2} \alpha_{\Pi_4(\mathbf{W})}(\mathbf{W})^2,$$

then

$$f(\bar{\mathbf{x}}_{k(i)} - \Pi_2(\bar{\mathbf{X}}_{\mathcal{J}})\mathbf{h}) \geq \frac{L}{2} \epsilon^2 (1 + \max(1, 2K(\mathbf{X}) + \epsilon))^2.$$

Proof. We have

$$\begin{aligned}
f(\bar{\mathbf{x}}_{k(i)} - \Pi_2(\bar{\mathbf{X}}_{\mathcal{J}})\mathbf{h}) &\geq f(\bar{\mathbf{x}}_{k(i)} - \Pi_2(\mathbf{X}_{\mathcal{J}})\mathbf{h}) - L\epsilon \max(1, 2K(\mathbf{X}) + \epsilon)K(\bar{\mathbf{x}}_{k(i)} - \Pi_2(\mathbf{X}_{\mathcal{J}})\mathbf{h}) \\
&\geq f(\mathbf{w}_i - \Pi_2(\mathbf{X}_{\mathcal{J}})\mathbf{h}) - L\epsilon K(\mathbf{w}_i - \Pi_2(\mathbf{X}_{\mathcal{J}})\mathbf{h}) \\
&\quad - L\epsilon \max(1, 2K(\mathbf{X}) + \epsilon)(\epsilon + K(\mathbf{X})[1 + \max(1, K(\mathbf{X}))]) \\
&\geq f(\mathbf{w}_i - \Pi_2(\mathbf{X}_{\mathcal{J}})\mathbf{h}) - L\epsilon K(\mathbf{X})[1 + \max(1, K(\mathbf{X}))] \\
&\quad - L\epsilon \max(1, 2K(\mathbf{X}) + \epsilon)(\epsilon + K(\mathbf{X})[1 + \max(1, K(\mathbf{X}))]) \\
&\geq \frac{L}{2}\epsilon^2(1 + \max(1, 2K(\mathbf{X}) + \epsilon))^2.
\end{aligned}$$

Lemma B.14 (Extension of [5] – Claim 5.10). *All canonical columns are LQ-robust loners.*

Proof. Let $\bar{\mathbf{x}}_{k(i)}$ be a canonical column associated to $i \in \llbracket r \rrbracket$: we have that $f(\bar{\mathbf{x}}_{k(i)} - \mathbf{w}_i) \leq \frac{L}{2}\epsilon^2$. To check whether $\bar{\mathbf{x}}_{k(i)}$ is a robust-loner, we must leave out of consideration the columns $\bar{\mathbf{x}}_k$ such that $f(\bar{\mathbf{x}}_k - \bar{\mathbf{x}}_{k(i)}) \leq d$. This particularly excludes all the columns satisfying

$$f(\bar{\mathbf{x}}_k - \mathbf{w}_i) \leq d - \frac{3}{2}\epsilon L(2K(\mathbf{X}) + \epsilon),$$

see Lemma B.11. In particular, only the columns $\bar{\mathbf{x}}_j$, $j \in \mathcal{J}$ with $\mathbf{x}_j = \sum_{k=1}^r a_{kj}\mathbf{w}_k + \sum_{l=1}^r \sum_{q=l+1}^r b_{jlq}\mathbf{w}_l \odot \mathbf{w}_q$ and $\mathbf{a}_{ij} \leq 1 - \sqrt{\frac{2d-3\epsilon L(4K(\mathbf{X})+\epsilon)}{LK(\mathbf{X})^2[1+\max(1, K(\mathbf{X}))]^2}}$ are taken into account (Lemma B.12).

Since the ℓ_2 distance of \mathbf{w}_i to the convex hull of $\Pi_4(\mathbf{W})$ is at least $\alpha_{\Pi_4(\mathbf{W})}(\mathbf{W})$, the distance between \mathbf{w}_i and the convex hull of the retained $\mathbf{X}_{\mathcal{J}}$ columns and their quadratic product is at least $\sqrt{\frac{2d-3\epsilon L(4K(\mathbf{X})+\epsilon)}{LK(\mathbf{X})^2[1+\max(1, K(\mathbf{X}))]^2}}\alpha_{\Pi_4(\mathbf{W})}(\mathbf{W})$. As for all $\mathbf{h} \in \Delta$

$$f(\mathbf{w}_i - \Pi_2(\mathbf{X}_{\mathcal{J}})\mathbf{h}) \geq \frac{\mu}{2} \|\mathbf{w}_i - \Pi_2(\mathbf{X}_{\mathcal{J}})\|_2^2,$$

we obtain

$$f(\mathbf{w}_i - \Pi_2(\mathbf{X}_{\mathcal{J}})\mathbf{h}) \geq \frac{\mu}{2L} \frac{2d - 3\epsilon L(4K(\mathbf{X}) + \epsilon)}{K(\mathbf{X})^2[1 + \max(1, K(\mathbf{X}))]^2} \alpha_{\Pi_4(\mathbf{W})}(\mathbf{W})^2.$$

Thus, $f(\bar{\mathbf{x}}_{k(i)} - \Pi_2(\bar{\mathbf{X}}_{\mathcal{J}})\mathbf{h}) \geq \frac{L}{2}\epsilon^2(1 + \max(1, 2K(\mathbf{X}) + \epsilon))^2$ (see Lemma B.13) and hence $\bar{\mathbf{x}}_{k(i)}$ is a robust loner. \blacksquare

Theorem B.15 (Robustness of BF when applied on LQ mixings). *Let $\mathbf{X} = \Pi_2(\mathbf{W}) + \mathbf{N}$ satisfying Definition 1.4 with $\|\mathbf{n}_i\|_1 \leq \epsilon$ for $i \in \llbracket n \rrbracket$. Let also ϵ satisfy*

$$4\sqrt{\frac{2}{\mu}(d + \epsilon L(2K(\mathbf{X}) + \epsilon))} < \alpha_{\mathbf{W}}(\mathbf{W}).$$

Then, BF with f satisfying Assumption 2.1 identifies the columns of \mathbf{W} up to a ℓ_2 error of

$$\sqrt{\frac{2}{\mu}(d + \epsilon L(2K(\mathbf{X}) + \epsilon))}.$$

Proof. By Lemma B.14, all canonical columns are robust loners. Moreover, Lemma B.10 shows that every robust-loner $\bar{\mathbf{x}}_j$ satisfies $f(\bar{\mathbf{x}}_j - \mathbf{w}_i) \leq d + \epsilon L(2K(\mathbf{X}) + \epsilon)$ for some $i \in \llbracket r \rrbracket$. As such, identifying the robust loners enables to approximately identify the columns of \mathbf{W} . Since several robust-loners can correspond to the same source, we need to apply a clustering step to regroup them. This is done easily, as two robust loners $\bar{\mathbf{x}}_j$ and $\bar{\mathbf{x}}_k$ correspond to the same source if and only if they satisfy $\|\bar{\mathbf{x}}_j - \bar{\mathbf{x}}_k\|_2 \leq 2\sqrt{\frac{2}{\mu}(d + \epsilon L(2K(\mathbf{X}) + \epsilon))}$. In fact,

- If two robust loners $\bar{\mathbf{x}}_j$ and $\bar{\mathbf{x}}_k$ correspond to the same source (in the sense that $f(\bar{\mathbf{x}}_j - \mathbf{w}_i) \leq d + \epsilon L(2K(\mathbf{X}) + \epsilon)$ and $f(\bar{\mathbf{x}}_k - \mathbf{w}_i) \leq d + \epsilon L(2K(\mathbf{X}) + \epsilon)$), they must satisfy

$$\begin{aligned} \|\bar{\mathbf{x}}_j - \bar{\mathbf{x}}_k\|_2 &= \|\bar{\mathbf{x}}_j - \mathbf{w}_i + \mathbf{w}_i - \bar{\mathbf{x}}_k\|_2 \\ &\leq \|\bar{\mathbf{x}}_j - \mathbf{w}_i\|_2 + \|\bar{\mathbf{x}}_k - \mathbf{w}_i\|_2 \\ &\leq \sqrt{\frac{2}{\mu}} \left[\sqrt{f(\bar{\mathbf{x}}_j - \mathbf{w}_i)} + \sqrt{f(\bar{\mathbf{x}}_k - \mathbf{w}_i)} \right] \\ &\leq 2\sqrt{\frac{2}{\mu}(d + \epsilon L(2K(\mathbf{X}) + \epsilon))}. \end{aligned}$$

- If two robust loners satisfy $\|\bar{\mathbf{x}}_j - \bar{\mathbf{x}}_k\|_2 \leq 2\sqrt{\frac{2}{\mu}(d + \epsilon L(2K(\mathbf{X}) + \epsilon))}$, they must correspond to the same source \mathbf{w}_i . This follows by contradiction: suppose that $\bar{\mathbf{x}}_j$ corresponds to a source \mathbf{w}_i ($f(\bar{\mathbf{x}}_j - \mathbf{w}_i) \leq d + \epsilon L(2K(\mathbf{X}) + \epsilon)$) and $\bar{\mathbf{x}}_k$ to another source \mathbf{w}_l , $l \neq i$ ($f(\bar{\mathbf{x}}_k - \mathbf{w}_l) \leq d + \epsilon L(2K(\mathbf{X}) + \epsilon)$). Then we obtain that:

$$\begin{aligned} \|\bar{\mathbf{x}}_j - \mathbf{w}_i\|_2 &\leq \sqrt{\frac{2}{\mu} f(\bar{\mathbf{x}}_j - \mathbf{w}_i)} \leq \sqrt{\frac{2}{\mu} (d + \epsilon L(2K(\mathbf{X}) + \epsilon))}, \text{ and} \\ \|\bar{\mathbf{x}}_k - \mathbf{w}_l\|_2 &\leq \sqrt{\frac{2}{\mu} f(\bar{\mathbf{x}}_k - \mathbf{w}_l)} \leq \sqrt{\frac{2}{\mu} (d + \epsilon L(2K(\mathbf{X}) + \epsilon))}, \end{aligned}$$

from which it can be deduced that

$$\begin{aligned} \|\bar{\mathbf{x}}_j - \bar{\mathbf{x}}_k\|_2 &= \|\bar{\mathbf{x}}_j - \mathbf{w}_i + \mathbf{w}_i - \mathbf{w}_l + \mathbf{w}_l + \bar{\mathbf{x}}_k\|_2 \\ &\geq \|\mathbf{w}_i - \mathbf{w}_l\|_2 - \|\bar{\mathbf{x}}_j - \mathbf{w}_i\|_2 - \|\bar{\mathbf{x}}_k - \mathbf{w}_l\|_2 \\ &\geq \alpha_{\mathbf{W}}(\mathbf{W}) - 2\sqrt{\frac{2}{\mu} (d + \epsilon L(2K(\mathbf{X}) + \epsilon))} \\ &> 4\sqrt{\frac{2}{\mu} (d + \epsilon L(2K(\mathbf{X}) + \epsilon))} - 2\sqrt{\frac{2}{\mu} (d + \epsilon L(2K(\mathbf{X}) + \epsilon))} \\ &= 2\sqrt{\frac{2}{\mu} (d + \epsilon L(2K(\mathbf{X}) + \epsilon))}, \end{aligned}$$

which is a contradiction.

Therefore, once the robust-loners are found and the clustering described above performed, each source can be identified by picking a point from each cluster. The ℓ_2 -norm error is then at most $\sqrt{\frac{2}{\mu} (d + \epsilon L(2K(\mathbf{X}) + \epsilon))}$. ■

References.

- [1] H. AKBARI, K. UTO, Y. KOSUGI, K. KOJIMA, AND N. TANAKA, *Cancer detection using infrared hyperspectral imaging*, *Cancer science*, 102 (2011), pp. 852–857.
- [2] Y. ALTMANN, A. HALIMI, N. DOBIGEON, AND J.-Y. TOURNERET, *Supervised nonlinear spectral unmixing using a postnonlinear mixing model for hyperspectral imagery*, *IEEE Trans. Image Process.*, 21 (2012), pp. 3017–3025.
- [3] U. ARAÚJO, B. SALDANHA, R. GALVÃO, T. YONEYAMA, H. CHAME, AND V. VISANI, *The successive projections algorithm for variable selection in spectroscopic multicomponent analysis*, *Chemometrics and Intelligent Laboratory Systems*, 57 (2001), pp. 65–73.
- [4] S. ARORA, R. GE, R. KANNAN, AND A. MOITRA, *Computing a nonnegative matrix factorization—provably*, in *Proc. of the 44th Symp. on Theory of Computing (STOC '12)*, 2012, pp. 145–162.
- [5] S. ARORA, R. GE, R. KANNAN, AND A. MOITRA, *Computing a nonnegative matrix factorization—provably*, *SIAM Journal on Computing*, 45 (2016), pp. 1582–1611.
- [6] J. M. BIOUCAS-DIAS, A. PLAZA, N. DOBIGEON, M. PARENTE, Q. DU, P. GADER, AND J. CHANUSSOT, *Hyperspectral unmixing overview: Geometrical, statistical, and sparse regression-based approaches*, *IEEE J. Sel. Topics Appl. Earth Observations Remote Sens.*, 5 (2012), pp. 354–379.
- [7] J. BOBIN, J. RAPIN, A. LARUE, AND J.-L. STARCK, *Sparsity and adaptivity for the blind separation of partially correlated sources.*, *IEEE Transactions on Signal Processing*, 63 (2015), pp. 1199–1213.
- [8] P. COMON AND C. JUTTEN, *Handbook of Blind Source Separation: Independent component analysis and applications*, Academic Press, 2010.
- [9] Y. DEVILLE, *From separability/identifiability properties of bilinear and linear-quadratic mixture matrix factorization to factorization algorithms*, *Digital Signal Processing*, 87 (2019), pp. 21–33.
- [10] Y. DEVILLE AND L. T. DUARTE, *An overview of blind source separation methods for linear-quadratic and post-nonlinear mixtures*, in *International Conference on Latent Variable Analysis and Signal Separation*, Springer, 2015, pp. 155–167.
- [11] N. DOBIGEON, Y. ALTMANN, N. BRUN, AND S. MOUSSAOUI, *Linear and nonlinear unmixing in hyperspectral imaging*, in *Data Handling in Science and Technology*, vol. 30, Elsevier, 2016, pp. 185–224.
- [12] N. DOBIGEON, L. TITS, B. SOMERS, Y. ALTMANN, AND P. COPPIN, *A comparison of nonlinear mixing models for vegetated areas using simulated and real hyperspectral data*, *IEEE J. Sel. Topics Appl. Earth Observations Remote Sens.*, 7 (2014), pp. 1869–1878.
- [13] N. DOBIGEON, J.-Y. TOURNERET, C. RICHARD, J. C. M. BERMUDEZ, S. McLAUGHLIN, AND A. O. HERO, *Nonlinear unmixing of hyperspectral images: Models and algorithms*, *IEEE Signal Process. Mag.*, 31 (2014), pp. 82–94.
- [14] E. ESSER, M. MOLLER, S. OSHER, G. SAPIRO, AND J. XIN, *A convex model for nonnegative matrix factorization and dimensionality reduction on physical space*, *IEEE Transactions on Image Processing*, 21 (2012), pp. 3239–3252.
- [15] W. FAN, B. HU, J. MILLER, AND M. LI, *Comparative study between a new nonlinear model and common linear model for analysing laboratory simulated-forest hyperspectral data*, *International Journal of Remote Sensing*, 30 (2009), pp. 2951–2962.

- [16] X. FU, K. HUANG, N. D. SIDIROPOULOS, AND W.-K. MA, *Nonnegative matrix factorization for signal and data analytics: Identifiability, algorithms, and applications*, IEEE Signal Processing Magazine, 36 (2019), pp. 59–80.
- [17] N. GILLIS, *Sparse and unique nonnegative matrix factorization through data preprocessing*, The Journal of Machine Learning Research, 13 (2012), pp. 3349–3386.
- [18] N. GILLIS, *Successive nonnegative projection algorithm for robust nonnegative blind source separation*, SIAM Journal on Imaging Sciences, 7 (2014), pp. 1420–1450.
- [19] N. GILLIS, *Successive projection algorithm robust to outliers*, in 2019 IEEE 8th International Workshop on Computational Advances in Multi-Sensor Adaptive Processing (CAMSAP), IEEE, 2019, pp. 331–335.
- [20] N. GILLIS, *Nonnegative Matrix Factorization*, SIAM, Philadelphia, 2020.
- [21] N. GILLIS AND R. LUCE, *Robust near-separable nonnegative matrix factorization using linear optimization*, Journal of Machine Learning Research, 15 (2014), pp. 1249–1280.
- [22] N. GILLIS AND S. A. VAVASIS, *Fast and robust recursive algorithms for separable nonnegative matrix factorization*, IEEE Transactions on Pattern Analysis and Machine Intelligence, 36 (2013), pp. 698–714.
- [23] A. HALIMI, Y. ALTMANN, N. DOBIGEON, AND J.-Y. TOURNERET, *Nonlinear unmixing of hyperspectral images using a generalized bilinear model*, IEEE Transactions on Geoscience and Remote Sensing, 49 (2011), pp. 4153–4162.
- [24] R. HEYLEN, M. PARENTE, AND P. GADER, *A review of nonlinear hyperspectral unmixing methods*, IEEE J. Sel. Topics Appl. Earth Observations Remote Sens., 7 (2014), pp. 1844–1868.
- [25] D. HONG, L. GAO, J. YAO, N. YOKOYA, J. CHANUSSOT, U. HEIDEN, AND B. ZHANG, *Endmember-guided unmixing network (egu-net): A general deep learning framework for self-supervised hyperspectral unmixing*, IEEE Transactions on Neural Networks and Learning Systems, (2021).
- [26] M.-D. IORDACHE, J. M. BIOUCAS-DIAS, AND A. PLAZA, *Total variation spatial regularization for sparse hyperspectral unmixing*, IEEE Transactions on Geoscience and Remote Sensing, 50 (2012), pp. 4484–4502.
- [27] I. JOLLIFFE, *Principal component analysis. 1986*, Springer-verlag, New York, 2 (1986), p. 29.
- [28] C. KERVAZO AND J. BOBIN, *Stacked sparse blind source separation for non-linear mixtures*, (2019).
- [29] C. KERVAZO, J. BOBIN, C. CHENOT, AND F. SUREAU, *Use of PALM for ℓ_1 sparse matrix factorization: Difficulty and rationalization of an heuristic approach*, Digital Signal Processing, (in press).
- [30] M. KOWALSKI, *Sparse regression using mixed norms*, Applied and Computational Harmonic Analysis, 27 (2009), pp. 303–324.
- [31] D. D. LEE AND H. S. SEUNG, *Learning the parts of objects by non-negative matrix factorization*, Nature, 401 (1999), p. 788.
- [32] W.-K. MA, J. M. BIOUCAS-DIAS, T.-H. CHAN, N. GILLIS, P. GADER, A. J. PLAZA, A. AMBIKAPATHI, AND C.-Y. CHI, *A signal processing perspective on hyperspectral unmixing: Insights from remote sensing*, IEEE Signal Process. Mag., 31 (2013), pp. 67–81.
- [33] I. MEGANEM, P. DÉLIOT, X. BRIOTTET, Y. DEVILLE, AND S. HOSSEINI, *Linear-*

- quadratic mixing model for reflectances in urban environments*, IEEE Trans. Geosci. Remote Sens., 52 (2013), pp. 544–558.
- [34] I. MEGANEM, Y. DEVILLE, S. HOSSEINI, P. DELIOT, AND X. BRIOTTET, *Linear-quadratic blind source separation using NMF to unmix urban hyperspectral images*, IEEE Trans. Signal Process., 62 (2014), pp. 1822–1833.
 - [35] J. M. NASCIMENTO AND J. M. BIOUCAS-DIAS, *Hyperspectral unmixing based on mixtures of Dirichlet components*, IEEE Transactions on Geoscience and Remote Sensing, 50 (2011), pp. 863–878.
 - [36] J. M. NASCIMENTO AND J. M. DIAS, *Vertex component analysis: A fast algorithm to unmix hyperspectral data*, IEEE transactions on Geoscience and Remote Sensing, 43 (2005), pp. 898–910.
 - [37] J. M. P. NASCIMENTO AND J. M. BIOUCAS-DIAS, *Nonlinear mixture model for hyperspectral unmixing*, in Image and Signal Processing for Remote Sensing XV, L. Bruzzone, C. Notarnicola, and F. Posa, eds., SPIE, sep 2009.
 - [38] Y. NESTEROV, *Introductory lectures on convex optimization: A basic course*, vol. 87, Springer Science & Business Media, 2013.
 - [39] B. PALSSON, M. O. ULFARSSON, AND J. R. SVEINSSON, *Convolutional autoencoder for spatial-spectral hyperspectral unmixing*, in IGARSS 2019-2019 IEEE International Geoscience and Remote Sensing Symposium, IEEE, 2019, pp. 357–360.
 - [40] B. RECHT, C. RE, J. TROPP, AND V. BITTORF, *Factoring nonnegative matrices with linear programs*, in Advances in Neural Information Processing Systems, 2012, pp. 1214–1222.
 - [41] O. Y. RODIONOVA, L. P. HOUMØLLER, A. L. POMERANTSEV, P. GELADI, J. BURGER, V. L. DOROFYEV, AND A. P. ARZAMASTSEV, *Nir spectrometry for counterfeit drug detection: a feasibility study*, Analytica Chimica Acta, 549 (2005), pp. 151–158.
 - [42] M. E. SCHAEPMAN, S. L. USTIN, A. J. PLAZA, T. H. PAINTER, J. VERRELST, AND S. LIANG, *Earth system science related imaging spectroscopy—an assessment*, Remote Sensing of Environment, 113 (2009), pp. S123–S137.
 - [43] B. SOMERS, K. COOLS, S. DELALIEUX, J. STUCKENS, D. V. DER ZANDE, W. W. VERSTRAETEN, AND P. COPPIN, *Nonlinear hyperspectral mixture analysis for tree cover estimates in orchards*, Remote Sensing of Environment, 113 (2009), pp. 1183–1193.
 - [44] K. E. THEMELIS, F. SCHMIDT, O. SYKIOTI, A. A. RONTOGIANNIS, K. D. KOUTROUMBAS, AND I. A. DAGLIS, *On the unmixing of mex/omega hyperspectral data*, Planetary and Space Science, 68 (2012), pp. 34–41.
 - [45] S. A. VAVASIS, *On the complexity of nonnegative matrix factorization*, SIAM Journal on Optimization, 20 (2010), pp. 1364–1377.
 - [46] M. ZIBULEVSKY AND B. A. PEARLMUTTER, *Blind source separation by sparse decomposition in a signal dictionary*, Neural computation, 13 (2001), pp. 863–882.