Sparse Unmixing of Hyperspectral Data

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Abstract

Linear spectral unmixing is a popular tool in remotely sensed hyperspectral data interpretation. It aims at estimating the fractional abundances of pure spectral signatures (also called endmembers) in each mixed pixel collected by an imaging spectrometer. In many situations, the identification of endmember signatures in the original data set may be challenging due to insufficient spatial resolution, mixtures happening at different scales, and unavailability of completely pure spectral signatures in the scene. However, the unmixing problem can also be approached in a semi-supervised fashion, i.e. by assuming that the observed image signatures can be expressed in the form of linear combinations of a number of pure spectral signatures known in advance (e.g. spectra collected on the ground by a field spectro-radiometer). Unmixing then amounts to finding the optimal subset of signatures in a (potentially very large) spectral library that can best model each mixed pixel in the scene. In practice, this is a combinatorial problem which calls for efficient linear sparse regression techniques based on sparsity-inducing regularizers, since the number of endmembers participating in a mixed pixel is usually very small compared with the (ever-growing) dimensionality – and availability – of spectral libraries.

Linear sparse regression is an area of very active research with strong links to compressed sensing, basis pursuit, basis pursuit denoising, and matching pursuit. In this work, we study the linear spectral unmixing problem under the light of recent theoretical results published in those referred to areas. Furthermore, we provide a comparison of several available and new linear sparse regression algorithms with the ultimate goal of analyzing their potential in solving the spectral unmixing problem by resorting to available spectral libraries.

Our experimental results, conducted using both simulated and real hyperspectral data sets collected by the NASA Jet Propulsion Laboratory’s Airborne Visible Infra-Red Imaging Spectrometer (AVIRIS) and spectral libraries publicly available from U.S. Geological Survey (USGS), indicate the potential of sparse regression techniques in the task of accurately characterizing mixed pixels using library spectra. This opens new perspectives for spectral unmixing, since the abundance estimation process no longer depends on the availability of pure spectral signatures in the input data nor on the capacity of a certain endmember extraction algorithm to identify such pure signatures.

Index Terms

Hyperspectral imaging, spectral unmixing, abundance estimation, sparse regression, convex optimization.

I. INTRODUCTION

Hyperspectral imaging has been transformed from being a sparse research tool into a commodity product available to a broad user community [1]. The wealth of spectral information available from advanced hyperspectral imaging
instruments currently in operation has opened new perspectives in many application domains, such as monitoring of environmental and urban processes or risk prevention and response, including – among others – tracking wildfires, detecting biological threats, and monitoring oil spills and other types of chemical contamination. Advanced hyperspectral instruments such as NASA’s Airborne Visible Infra-Red Imaging Spectrometer (AVIRIS) [2] are now able to cover the wavelength region from 0.4 to 2.5 µm using more than 200 spectral channels, at nominal spectral resolution of 10 nm. The resulting hyperspectral data cube is a stack of images (see Fig. 1) in which each pixel (vector) is represented by a spectral signature or fingerprint that characterizes the underlying objects.

Several analytical tools have been developed for remotely sensed hyperspectral data processing in recent years, covering topics like dimensionality reduction, classification, data compression, or spectral unmixing [3], [4]. The underlying assumption governing clustering and classification techniques is that each pixel vector comprises the response of a single underlying material. However, if the spatial resolution of the sensor is not high enough to separate different materials, these can jointly occupy a single pixel. For instance, it is likely that the pixel collected over a vegetation area in Fig. 1 actually comprises a mixture of vegetation and soil. In this case, the measured spectrum may be decomposed into a linear combination of pure spectral signatures of soil and vegetation, weighted by abundance fractions that indicate the proportion of each macroscopically pure signature in the mixed pixel [5].

To deal with this problem, linear spectral mixture analysis techniques first identify a collection of spectrally pure constituent spectra, called endmembers in the literature, and then express the measured spectrum of each mixed pixel as a linear combination of endmembers weighted by fractions or abundances that indicate the proportion of each endmember present in the pixel [6]. It should be noted that the linear mixture model assumes minimal secondary reflections and/or multiple scattering effects in the data collection procedure, and hence the measured spectra can be expressed as a linear combination of the spectral signatures of materials present in the mixed pixel [see Fig.
2(a)]. Quite opposite, the nonlinear mixture model assumes that the endmembers form an intimate mixture inside the respective pixel, so that incident radiation interacts with more than one component and is affected by multiple scattering effects [see Fig. 2(b)]. Nonlinear unmixing generally requires prior knowledge about object geometry and physical properties of the observed objects. In this work we will focus exclusively on the linear mixture model due to its computational tractability and flexibility in different applications.

The linear mixture model assumes that the spectral response of a pixel in any given spectral band is a linear combination of all the endmembers present in the pixel, at the respective spectral band. For each pixel, the linear model can be written as follows:

$$y_i = \sum_{j=1}^{q} m_{ij} \alpha_j + n_i,$$  \hspace{1cm} (1)

where $y_i$ is the measured value of the reflectance at spectral band $i$, $m_{ij}$ is the reflectance of the $j$-th endmember at spectral band $i$, $\alpha_j$ is the fractional abundance of the $j$-th endmember, and $n_i$ represents the error term for the spectral band $i$ (i.e. the noise affecting the measurement process). If we assume that the hyperspectral sensor used in data acquisition has $L$ spectral bands, Eq. (1) can be rewritten in compact matrix form as:

$$y = M\alpha + n,$$  \hspace{1cm} (2)

where $y$ is an $L \times 1$ column vector (the measured spectrum of the pixel), $M$ is an $L \times q$ matrix containing $q$ pure spectral signatures (endmembers), $\alpha$ is a $q \times 1$ vector containing the fractional abundances of the endmembers, and $n$ is an $L \times 1$ vector collecting the errors affecting the measurements at each spectral band. The so-called abundance non-negativity constraint (ANC): $\alpha_i \geq 0$ for $i = 1, \ldots, q$, and the abundance sum-to-one constraint (ASC): $\sum_{i=1}^{q} \alpha_i = 1$, which we respectively represent in compact form by:

$$\alpha \geq 0,$$  \hspace{1cm} (3)

$$1^T \alpha = 1,$$  \hspace{1cm} (4)

where $1^T$ is a line vector of 1’s compatible with $\alpha$, are often imposed into the model described in Eq. (1) [7], owing to the fact that $\alpha_i$, for $i = 1, \ldots, q$, represent the fractions of the endmembers present in the considered pixel.
In a typical hyperspectral unmixing scenario, we are given a set \( Y \equiv \{ y_i \in \mathbb{R}^L, i = 1, \ldots, n \} \) of \( n \) observed \( L \)-dimensional spectral vectors, and the objective is to estimate the mixing matrix \( M \) and the fractional abundances \( \alpha \) for every pixel in the scene. This is a blind source separation problem and, naturally, independent component analysis methods come to mind to solve it. However, the assumption of statistical independence among the sources (the fractional abundances in our application), central to independent component analysis methods, does not hold in hyperspectral applications, since the sum of fractional abundances associated to each pixel is constant. Thus, sources are statistically dependent, which compromises the performance of independent component analysis algorithms in hyperspectral unmixing [8].

We note the constraints (3) and (4) define the set \( S_{q-1} \equiv \{ \alpha \in \mathbb{R}^q | \alpha \geq 0, 1^T \alpha = 1 \} \), which is the probability simplex in \( \mathbb{R}^q \). Furthermore, the set \( S_M \equiv \{ M\alpha \in \mathbb{R}^L | \alpha \in S_{q-1} \} \) is also a simplex whose vertices are the columns of \( M \). Over the last decade, several algorithms have exploited this geometrical property by estimating the “smallest” simplex set containing the observed spectral vectors [9], [10]. Some classic techniques for this purpose assume input data set contains at least one pure pixel for each distinct material present in the scene, and therefore a search procedure aimed at finding the most spectrally pure signatures in the input scene is feasible. Among the endmember extraction algorithms working under this regime we can list some popular approaches such as the pixel purity index (PPI) [11], N-FINDR [12], orthogonal subspace projection (OSP) technique in [13], and vertex component analysis (VCA) [14]. However, the assumption under which these algorithms perform may be difficult to guarantee in practical applications due to several reasons:

1) First, if the spatial resolution of the sensor is not high enough to separate different pure signature classes at a macroscopic level, the resulting spectral measurement can be a composite of individual pure spectra which correspond to materials that jointly occupy a single pixel. In this case, the use of image-derived endmembers may not result in accurate fractional abundance estimations since it is likely that such endmembers may not be completely pure in nature.

2) Second, mixed pixels can also result when distinct materials are combined into a microscopic (intimate) mixture, independently of the spatial resolution of the sensor. Since the mixtures in this situation happen at the particle level, the use of image-derived spectral endmembers cannot accurately characterize intimate spectral mixtures.

In order to overcome the two aforementioned issues, other advanced endmember generation algorithms have also been proposed under the assumption that pure signatures are not present in the input data. Such techniques include optical real-time adaptive spectral identification system (ORASIS) [15], convex cone analysis (CCA) [16], iterative error analysis (IEA) [17], automatic morphological endmember extraction (AMEE) [18], iterated constrained endmembers (ICE) [19], minimum volume constrained non-negative matrix factorization (MVC-NMF) [20], spatial-spectral endmember extraction (SSEE) [21], sparsity-promoting ICE (SPICE) [22], minimum volume simplex analysis (MVSA) [23], and simplex identification via split augmented Lagrangian (SISAL) [24]. A necessary condition for these endmember generation techniques to yield good estimates is the presence in the data set of at
least \( q - 1 \) spectral vectors on each facet of the simplex set \( S_M \) [24]. This condition is very likely to fail in highly mixed scenarios, in which the above techniques generate artificial endmembers, i.e. not necessarily associated to physically meaningful spectral signatures of true materials.

In this work, we adopt a novel semi-supervised approach to linear spectral unmixing which relies on the increasing availability of spectral libraries of materials measured on the ground, for instance, using advanced field spectroradiometers. Our main assumption is that mixed pixels can be expressed in the form of linear combinations of a number of pure spectral signatures known in advance and available in a library, such as a the well-known one publicly available from U.S. Geological Survey (USGS)\(^1\), which contains over 1300 mineral signatures, or the NASA Jet Propulsion Laboratory’s Advanced Spaceborne Thermal Emission and Reflection Radiometer (ASTER) spectral library\(^2\), a compilation of over 2400 spectra of natural and man-made materials. When the unmixing problem is approached using spectral libraries, the abundance estimation process no longer depends on the availability of pure spectral signatures in the input data nor on the capacity of a certain endmember extraction algorithm to identify such pure signatures. Quite opposite, the procedure is reduced to finding the optimal subset of signatures in the library that can best model each mixed pixel in the scene. Despite the appeal of this semi-supervised approach to spectral unmixing, this approach is also subject to a few potential drawbacks:

1) One risk in using library endmembers is that these spectra are rarely acquired under the same conditions as the airborne data. Image endmembers have the advantage of being collected at the same scale as the data and can, thus, be more easily associated with features on the scene. However, such image endmembers may not always be present in the input data. In this work, we rely on the use of advanced atmospheric correction algorithms which convert the input hyperspectral data from at-sensor radiance to reflectance units.

2) The ability to obtain useful sparse solutions for an under-determined system of equations depends, mostly, on the degree of coherence between the columns of the system matrix and the degree of sparseness of original signals (i.e., the abundance fractions) [25], [26], [27], [28]. The most favorable scenarios correspond to highly sparse signals and system matrices with low coherence. Unfortunately, in hyperspectral applications the spectral signatures of the materials tend to be highly correlated. On the other hand, the number of materials present in a given scene is often small, say, less than 20 and, most importantly, the number of materials participating in a mixed pixel is usually on the order of 4–5 [5]. Therefore, the undesirable high coherence of hyperspectral libraries can be mitigated, to some extent, by the highly sparse nature of the original signals.

3) The sparse solutions of under-determined systems are computed by solving optimization problems containing non-smooth terms [26]. The presence of these terms introduces complexity because the standard optimization tools of the gradient and Newton family cannot be directly used. To make the scenario even more complex, a typical hyperspectral image has hundreds or thousands of spectral vectors, implying an equal number of

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\(^1\) Available online: http://speclab.cr.usgs.gov/spectral-lib.html

\(^2\) Available online: http://speclib.jpl.nasa.gov
independent optimizations to unmix the complete scene. To cope with this computational complexity, we resort to recently introduced (fast) algorithms based on the augmented Lagrangian method of multipliers [29].

In this work, we specifically address the problem of sparsity when unmixing hyperspectral data sets using spectral libraries, and further provide a quantitative and comparative assessment of several available and new optimization algorithms in the context of linear sparse problems. The remainder of the paper is organized as follows. Section II formulates the sparse regression problem in the context of hyperspectral unmixing. Section III describes several available and new unmixing algorithms with the ultimate goal of analyzing their potential in solving sparse hyperspectral unmixing problems. Section IV provides an experimental validation of the considered algorithms using simulated hyperspectral mixtures from real and synthetic spectral libraries. The primary reason for the use of simulated data is that all details of the simulated mixtures are known and can be efficiently investigated because they can be manipulated individually and precisely. As a complement to simulated data experiments, Section V presents an experimental validation of the considered sparse regression and convex optimization algorithms using a well-known hyperspectral scene collected by the AVIRIS instrument over the Cuprite mining district in Nevada. The USGS spectral library is used for conducting extensive semi-supervised unmixing experiments on this scene. Finally, Section VI concludes with some remarks and hints at plausible future research. An Appendix is devoted to the description of the parameter settings used in our experiments and to the strategies followed to infer these parameters.

II. SPECTRAL UNMIXING REFORMULATED AS A SPARSE REGRESSION PROBLEM

In this section, we revisit the classic linear spectral unmixing problem and reformulate it as a semi-supervised approach using sparse regression (SR) terminology. Furthermore, we review the SR optimization problems relevant to our unmixing problem, their theoretical characterization, their computational complexity, and the algorithms to solve them exactly or approximately.

Let us assume that the spectral endmembers used to solve the mixture problem are no longer extracted nor generated using the original hyperspectral data as input, but instead selected from a library containing a large number of spectral samples available \textit{a priori}. In this case, unmixing amounts to finding the optimal subset of samples in the library that can best model each mixed pixel in the scene. This means that a searching operation must be conducted in a (potentially very large) library, which we denote by \( A \in \mathbb{R}^{L \times m} \), where \( L \) and \( m \) are the number of spectral bands and the number of materials in the library, respectively. All libraries herein considered correspond to under-determined systems, i.e., \( L < m \). With the aforementioned assumptions in mind, let \( x \in \mathbb{R}^m \) denote the fractional abundance vector with regards to the library \( A \). As usual, we say that \( x \) is a \( k \)-sparse vector if it has at most \( k \) components different from zero. With these definitions in place, we can now write our SR problem as:

\[
\min_x \|x\|_0 \quad \text{subject to} \quad \|y - Ax\|_2 \leq \delta, \quad x \geq 0, \quad 1^T x = 1,
\]  

(5)
where $\|x\|_0$ denotes the number of non-zero components of $x$ and $\delta \geq 0$ is the error tolerance due to noise and modeling errors. A solution of problem (5), if any, belongs to the set of sparsest signals belonging to the $(m-1)$-probability simplex satisfying error tolerance inequality $\|y - Ax\|_2 \leq \delta$. Prior to addressing problem (5), we consider a series of simpler related problems.

A. Exact solutions

Let us first start by assuming that noise is zero and ANC and ASC constraints are not enforced. Our SR optimization problem is then:

$$\begin{equation}
(P_0): \min_x \|x\|_0 \text{ subject to } Ax = y.
\end{equation}$$

If the system of linear equations $Ax = y$ has a solution satisfying $2\|x\|_0 < \text{spark}(A)$, where $\text{spark}(A) \leq \text{rank}(A) + 1$ is the smallest number of linearly dependent columns of $A$, it is necessarily the unique solution of $(P_0)$ [30], [31]. The spark of a matrix gives us a very simple way to check the uniqueness of a solution of the system $Ax = y$. For example, if the elements of $A$ are independent and identically distributed (i.i.d.), then with probability 1 we have $\text{spark}(A) = m + 1$, implying that every solution with no more than $L/2$ entries is unique.

In our SR problem, we would like then to compute the spark of the hyperspectral library being used, to have an idea of what is the minimum level of sparsity of the fractional abundance vectors that can be uniquely determined by solving $(P_0)$. Computing the spark of a general matrix is, however, a hard problem, at least as difficult as solving $(P_0)$. This complexity has fostered the introduction of entities simpler to compute, although providing less tight bounds. The mutual coherence is such an example; denoting the $k^{th}$ column in $A$ by $a_k$ and the $\ell_2$ norm by $\|\cdot\|_2$, the mutual coherence of $A$ is given by:

$$\mu(A) \equiv \max_{1 \leq k, j \leq m, k \neq j} \frac{|a_k^T a_j|}{\|a_k\|_2 \|a_j\|_2},$$

i.e., by the maximum absolute value of the cosine of the angle between any two columns of $A$. The mutual coherence supplies us with a lower bound for the spark given by [30]:

$$\text{spark}(A) \geq 1 + \frac{1}{\mu(A)}.$$

Unfortunately, as it will be shown further, the mutual coherence of hyperspectral libraries is very close to 1 leading to useless bounds for the spark. In the following, we illustrate two relaxed strategies for computing $(P_0)$: pursuit algorithms and nonnegative signals.

1) Pursuit algorithms: The problem $(P_0)$ is NP-hard (meaning that the problem is combinatorial and very complex to solve) [32] and therefore there is little hope in solving it in a straightforward way. Greedy algorithms, such as the orthogonal basis pursuit (OMP) [33], and basis pursuit (BP) [34] are two alternative approaches to compute the sparsest solution. The basis pursuit replaces the $\ell_0$ norm in $(P_0)$ with the $\ell_1$ norm:

$$\begin{equation}
(P_1): \min_x \|x\|_1 \text{ subject to } Ax = y.
\end{equation}$$
Contrary to problem \((P_0)\), problem \((P_1)\) is convex and can be written as a linear programming (LP) problem and solved using LP solvers. What is, perhaps, totally unexpected is that, in given circumstances related with matrix \(A\), problem \((P_1)\) has the same solution as problem \((P_0)\). This result is stated in terms of the restricted isometric constants introduced in [27]. Herein, we use the variant proposed in [35]. Let \(\alpha_k, \beta_k \geq 0\) to be the tightest constants in the inequalities:

\[
\alpha_k \|x\|_2 \leq \|Ax\|_2 \leq \beta_k \|x\|_2, \quad \|x\|_0 \leq k,
\]

and further define:

\[
\gamma_{2s} \equiv \frac{\beta_{2s}^2}{\alpha_{2s}^2} \geq 1.
\]

Then, under the assumption that \(\gamma_{2s} < 4\sqrt{2} - 3 \simeq 2.6569\), every \(s\)-sparse vector is recovered by solving problem \((P_1)\) (see Theorem 2.1 and Corollary 2.1 of [35]). Meanwhile, it has been shown that, in some cases, the OMP algorithm also provides the \((P_0)\) solution in a fashion comparable with the BP alternative, with the advantage of being faster and easier to implement [36], [26].

2) Nonnegative signals: We now consider the problem:

\[
(P_0^+) \colon \min_x \|x\|_0 \quad \text{subject to} \quad Ax = y, \quad x \geq 0.
\]

and follow a line of reasoning close to that of [25]. Hyperspectral libraries generally contain only nonnegative components (i.e. reflectances). Thus, by assuming that the zero vector is not in the columns of \(A\), it is always possible to find a vector \(h\) such that:

\[
h^T A = w^T > 0.
\]

Since all components of \(w\) are nonnegative, the matrix \(W^{-1}\), where \(W \equiv \text{diag}(w)\), is well-defined and has positive diagonal entries. Defining \(z \equiv Wx, \ c \equiv h^Ty, \ D \equiv AW^{-1}\), and noting that:

\[
h^T AW^{-1}z = 1^T z,
\]

the problem \((P_0^+)\) is equivalent to:

\[
(P_0^+) \colon \min_x \|z\|_0 \quad \text{subject to} \quad Dz = y, \quad z \geq 0, \quad 1^T z = c.
\]

We conclude that, when the original signals are nonnegative and the system matrices comply with property (12), then problem (11) enforces the equality constraint \(1^T z = c\). This constraint has very strong connections with the ASC constraint which is so popular in hyperspectral applications. ASC is, however, prone to strong criticisms because, in a real image, there is strong signature variability [37] that, at the very least, introduces positive scaling factors varying from pixel to pixel in the signatures present in the mixtures. As a result, the signatures are defined up to a scale factor and, thus, ASC should be replaced with a generalized ASC of the form \(\sum_i \xi_i x_i = 1\), in which the weights \(\xi_i\) denote the pixel-dependent scale factors. What we conclude from the equivalence between problems (11) and (14) is that the nonnegativity of the sources imposes automatically a generalized ASC. For this reason we do not impose explicitly the ASC constraint.
Similarly to problem \((P_0)\), problem \((P_0^+)\) is NP-hard and impossible to solve exactly for a general matrix \(A\). As in subsection II-A1, we can consider instead the \(\ell_1\) relaxation:

\[
(P_1^+): \min_x \|z\|_1 \text{ subject to } Dz = y \quad z \geq 0.
\]

(15)

Here, we have dropped the equality constraint \(1^Tz = c\) because it is satisfied by any solution of \(Dz = y\). As with problem \((P_0)\), the condition \(\gamma_{2s} < 4\sqrt{2} - 3 \simeq 2.6569\) referred to in subsection II-A1, is now applied to the restricted isometric constants of matrix \(D\) to ensure that any \(s\)-sparse vector solution of \((P_0^+)\) is recovered by solving the problem \((P_1^+)\).

Another way of characterizing the uniqueness of the solution of problem \((P_0^+)\) is via the one-sided coherence introduced in [25]. However, similarly to the mutual coherence, the one-sided coherence of hyperspectral libraries is very close to one leading to useless bounds. The coherence may be increased by left multiplying the system \(Dz = y\) with a suitable invertible matrix \(P\) [25]. This preconditioning tends to improve the performance of greedy algorithms such as OMP. It leads, however, to an optimization problem equivalent to \((P_1^+)\). Thus, a BP solver yields the same solution.

**B. Approximate solutions**

We now assume now that the perturbation \(n\) in the observation model is not zero, and still we want to find an approximate solution for our SR problem. The computation of approximate solutions raises issues parallel to those found for exact solutions as addressed above. Therefore, we go very briefly through the same topics. Again, we start by assuming that the noise is zero and ANC and ASC constraints are not enforced. Our noise-tolerant SR optimization problem is then:

\[
(P_0^\delta): \min_x \|x\|_0 \text{ subject to } \|Ax - y\|_2 \leq \delta.
\]

(16)

The concept of uniqueness of the sparsest solution is now replaced with the concept of stability [38], [39], [35]. For example, in [38] it is shown that, given a sparse vector \(x_0\) satisfying the sparsity constraint \(x_0 < (1 + 1/\mu(A))/2\) such that \(\|Ax_0 - y\| \leq \delta\), then every solution \(x_0^\delta\) of problem \((P_0^\delta)\) satisfies:

\[
\|x_0^\delta - x_0\|^2 \leq \frac{4\delta^2}{1 - \mu(A)(2x_0 - 1)}.
\]

(17)

Notice that, when \(\delta = 0\), i.e., when the solutions are exact, this result parallels those ensuring the uniqueness of the sparsest solution. Again, we illustrate two relaxed strategies for computing \((P_0)\):

1) **Pursuit algorithms:** Problem \((P_0^\delta)\), as \((P_0)\), is NP-hard. We consider here two approaches to tackle this problem. The first is the greedy OMP algorithm with stopping rule \(\|Ax - y\|_2 \leq \delta\). The second consists of relaxing the \(\ell_0\) norm to the \(\ell_1\) norm, thus obtaining a so-called basis pursuit denoising (BPDN) optimization problem [34]:

\[
(P_1^\delta): \min_x \|x\|_1 \text{ subject to } \|Ax - y\|_2 \leq \delta.
\]

(18)
Contrarily to problem \((P^\delta_0)\), problem \((P^\delta_1)\) is convex and, thus, it is very likely to be solved efficiently with convex optimization methods. As in \((P^\delta_0)\), the stability of the solution of problem \((P^\delta_1)\) has also been provided \([28],[35]\). For example, from Theorem 3.1 of \([35]\), we have that, if \(\gamma_{2s} < 4\sqrt{\delta} - 3 \simeq 2.6569\), the \(\ell_2\) error between any \(s\)-sparse solution \(x\) of \(Ax = y\) and any solution \(x^s_i\) of \((P^\delta_1)\) satisfies:
\[
\|x^s_i - x\|_2 \leq C\delta,
\]  
where \(\delta\) is a constant depending on the restricted isometric constants \(\alpha_{2s}\) and \(\beta_{2s}\) defined in \((9)\).

2) Nonnegative signals: We now consider the problem:
\[
(P^\delta_0^+) : \min_{x} \|x\|_0 \quad \text{subject to} \quad \|Ax - y\|_2 \leq \delta, \quad x \geq 0.
\]  
Following the reasoning already put forward in subsection II-A2, we have that problem \((P^\delta_0^+)\) is equivalent to:
\[
\min_{z} \|z\|_0 \quad \text{subject to} \quad \|Dz - y\|_2 \leq \delta, \quad z \geq 0,
\]  
where, as in subsection II-B2, \(D \equiv AW^{-1}\), \(W \equiv \text{diag}(h^T A)\) and \(h\) is chosen such that \(h^T A > 0\). From the observation equation \(y = Dz + n\) and from \(\|n\| \leq \delta\), we may now write \(1^T z = c + h^T n\), where \(c \equiv h^T y\). Therefore, the positivity constraint in problem \((P^\delta_0^+)\) jointly with the property \(h^T A > 0\) impose implicitly a soft constraint \(\|1^T z - c\|_2 \leq \delta_h\), where \(\delta_h\) is such that \(\|h^T n\|_2 \leq \delta_h\).

Similarly to \((P^\delta_1)\), problem \((P^\delta_0^+)\) is NP-hard and impossible to solve exactly for a general matrix \(A\) or \(D\). As in subsection II-B1, we consider instead the \(\ell_1\) relaxation:
\[
(P^\delta_1^+) : \min_{z} \|z\|_1 \quad \text{subject to} \quad \|Dz - y\|_2 \leq \delta, \quad z \geq 0.
\]  
As with problem \((P^\delta_1)\), the condition \(\gamma_{2s} < 4\sqrt{\delta} - 3 \simeq 2.6569\) is now applied to the restricted isometric constants of matrix \(D\), thus ensuring the stability of the solutions of \((P^\delta_1^+)\).

III. ALGORITHMS

In the previous section we have listed a series of optimization problems aimed at computing sparse exact and approximate solutions for our hyperspectral SR problem. In this section, we explain in detail the algorithms we are going to use for experimental validation in the next two sections. Specifically, we considered five unmixing algorithms, of which three do not enforce explicitly the sparseness of the solution, while the other two belong to the sparse unmixing class of algorithms.

A. Orthogonal Matching Pursuit Algorithms

Many variants of the OMP have been published (see \([25]\) and the references therein). Herein, we use the standard implementation shown, for one pixel, in Algorithm 1. The algorithms keeps track of the residual \(y - Ax^i\), where \(x^i\) is the estimate of \(x\) at the \(i\)-th algorithm iteration. At the first iteration, the initial residual is equal to the observed spectrum of the pixel, the vector of fractional abundances is null and the matrix of the indices of selected endmembers is empty. Then, at each iteration, the algorithm finds the member of \(A\) which is best correlated to the
Algorithm 1 Pseudocode of the Classic Orthogonal Matching Pursuit (OMP) Algorithm.

**Initialization:**
- Iteration: $i = 0$
- Initial solution: $x^0 = 0$
- Initial residual: $r^0 = y$
- Initial matrix of selected indices: $Λ^0 = Φ$ (empty)

**Main iteration:**
- Update iteration: $i ← i + 1$
  - Compute the index of the best correlated member of $A$ to the actual residual:
    $$ \text{index} ← \arg \min_{1 ≤ k ≤ m} \| A_k x^{i-1} - r^{i-1} \|_2^2 $$
    where $A_k$ represents the $k^{th}$ column of $A$
  - Update support: $Λ^i ← Λ^{i-1} \cup \{ \text{index} \}$
  - Update solution: $x^i ← \arg \min_x \| A_{Λ^i} x - y \|_2^2$ subject to: $\text{Support} \{ x^i \} = Λ^i$
    (where $A_{Λ^i}$ is the matrix containing the columns of $A$ having the indexes from $Λ^i$)
  - Update residual: $r^i ← y - Ax^i$
- Stop if termination rule: $\| r^i \|_2^2 ≤ T$ is satisfied (the norm of the residual is below a preset threshold $T$)
- Otherwise, repeat from **Main iteration**.

actual residual, adds this member to the matrix of endmembers, updates the residual and computes the estimate of $x$ using the selected endmembers. The algorithm stops when a stop criterion is satisfied (in our case, when the actual residual is smaller than a preset threshold $T$). A member from $A$ cannot be selected more than once, as the residual is orthogonalized with respect to the members already selected.

OMP may be used in any of the problems listed in Section II. We consider, however, the OMP variation proposed in [25] tailored to problems $(P_0^+)$ and $(P_δ^+)$, and which we denote by OMP$^+$. In this variation, the Update solution step in Algorithm 1 is modified to:

$$ z^i = \arg \min_z \| Dz - y \| \text{ subject to } \text{Support} \{ z^i \} = S^i, \ z > 0. $$ (23)

The OMP and OMP$^+$ stopping rule is adapted either to solve exact or approximate problems. Considering that $ε$ represents a measure of the error in the accuracy of the unmixing result, in the former case $ε$ is very small ($ε → 0$), leading to the use of a small $T$ as stopping threshold, whereas in the latter case $ε > 0$, which translates to setting a higher value for the stopping threshold $T$ in Algorithm 1.

**B. Basis Pursuit and Basis Pursuit Denoising Algorithms**

In this work, we also use the recently introduced constrained sparse unmixing algorithm via variable splitting and augmented Lagrangian (CSUnSAL) [29] to solve the linear problems $(P_1^1)$ and $(P_1^+)$ and the quadratic problems $(P_δ^1)$ and $(P_δ^+)$. CSUnSAL is tailored to hyperspectral applications with hundreds of thousands or millions of spectral vectors to unmix. This algorithm exploits the alternating direction method of multipliers (ADMM) [40] in
a way similar to recent works [41] and [42]. Here, we use the acronyms CSUnSAL, CSUnSAL+, CSUnSALδ, and CSUnSALδ+ to denote the variant of CSUnSAL tailored to (P1), (P1+), (Pδ), and (Pδ+) problems, respectively.

C. Unconstrained Basis Pursuit and Basis Pursuit Denoising Algorithms

All the constrained optimization problems (P1), (P1+), (Pδ), and (Pδ+) can be converted into unconstrained versions by minimizing the respective Lagrangian. For example, the problem (Pδ) is equivalent to:

$$\min_x \frac{1}{2} \|Ax - y\|_2^2 + \lambda \|x\|_1. \tag{24}$$

The parameter λ > 0 is the Lagrange multiplier and λ → 0 when δ → 0. This model, sometimes referred to as the least squares (LS) ℓ1 model, is widely used in the signal processing community. It was used before to address the unmixing problem in [43], in which the endmembers were first extracted from the original image using the N-FINDR endmember extraction algorithm [12] and, then, the respective fractional abundances of the endmembers were inferred. However, the N-FINDR algorithm assumes the presence of pure pixels in the original image. According to our best knowledge, this approach was never used before to address the hyperspectral unmixing problem using spectral libraries.

In this work, we use the sparse unmixing algorithm via variable splitting and augmented Lagrangian (SUUnSAL), introduced in [29], to solve problem (24). SUUnSAL, as CSUnSAL, exploits the ADMM method [40] in a way similar to [42] and [41]. SUUnSAL solves the unconstrained versions of (P1), (P1+), (Pδ), and (Pδ+). Hereinafter, we use the acronyms SUUnSAL, SUUnSAL+, SUUnSALδ, and SUUnSALδ+ to denote the respective variant.

It is important to emphasize that, by setting λ = 0 in (24), one can arrive to a LS solution of the system, which is obtained by solving the unconstrained optimization problem:

$$\text{(PLS)}: \min_x \|y - Ax\|_2. \tag{25}$$

The solution of optimization problem (25) has poor behavior in terms of accuracy when the matrix of coefficients is ill-conditioned (as it is always the case in the sparse unmixing problem, in which we deal with fat matrices) or when the observations are affected by noise. However, one can take advantage of the physical constraints usually imposed in the unmixing problem (ANC and ASC) by plugging them into the objective function of (PLS). Using this approach, we can simply arrive to the so-called non-negative constrained LS (NCLS) and fully constrained LS (FCLS) solutions in [44] by first activating the ANC and, then, by activating both the ANC and ASC constraints, respectively. In this paper, we use SUUnSAL to solve the constrained versions of the LS problem because, as mentioned before, they are particular cases of (24) when λ = 0.

D. Iterative Spectral Mixture Analysis (ISMA)

In this work we also use the iterative spectral mixture analysis (ISMA) algorithm [45] to solve the considered problems. The pseudocode of ISMA is shown in Algorithm 2. ISMA is an iterative technique derived from the standard spectral mixture analysis formulation presented in Eq. (2). It finds an optimal endmember set by examining
Algorithm 2 Pseudocode of the Iterative Spectral Mixture Analysis Algorithm.

Part 1:

Initialization:

Iteration: \( i = 1 \)

Initial spectral library: \( A^1 \leftarrow A \)

Main iteration:

Compute solution: \( x^i \leftarrow \arg \min_x \|A^i x - y\|_2^2 \)

Compute RMSE: \( \text{RMSE}^i \leftarrow \frac{1}{\sqrt{L}} \| \hat{y} - y \|_2 \), where \( \hat{y} = A^i x^i \)

Compute the member of \( A^i \) having the lowest abundance: \( \text{index} \leftarrow \min_k (x^i_k) \)

Remove the member having the lowest fractional abundance from the spectral library: \( A^i \leftarrow A^i \backslash A^i_{\text{index}} \)

If \( A \) still contains more than one member, update iteration: \( i \leftarrow i + 1 \) and repeat Main iteration

Part 2:

Compute the variation of the RMSE for all iterations \( i_{\text{min}} \leq i \leq m : \Delta \text{RMSE}_i = 1 - \text{RMSE}_{i-1}/\text{RMSE}_i \)

where \( i_{\text{min}} \) is the minimum number of iterations before stopping the search

Determine the position of the first substantial increase in the \( \Delta \text{RMSE} \) (the critical iteration): \( i_{\text{ARMSE}_{\text{max}}} \)

The final solution is the solution computed in Part 1 at the critical iteration

The change in the root mean square error (RMSE) after reconstructing the original scene using the fractional abundance estimations, as shown in Algorithm 2. The algorithm consists of two parts. In the first one, ISMA initially computes an unconstrained solution of the unmixing problem in Eq. (2), using all the spectral signatures available in a spectral library \( A \). Then, it removes the signature with the lowest estimated fractional abundance in \( x^i \) and repeats the process with the remaining signatures, until only one signature remains. In the second part of the algorithm, a so-called critical iteration is identified as the iteration corresponding to the first abrupt change in the RMSE, computed as follows:

\[
\Delta \text{RMSE} \equiv 1 - \left( \frac{\text{RMSE}_{j-1}}{\text{RMSE}_j} \right),
\]

where \( \text{RMSE}_j \) is the RMSE corresponding to the \( j \)th iteration. The critical iteration corresponds to the optimal set of endmembers. The idea of recovering the true endmember set by analyzing the change in the RMSE is based on the fact that, before finding the optimal set of endmembers, the RMSE varies in certain (small) limits and it has a bigger variation when one endmember from the optimal set is removed, as the remaining endmembers are not sufficient to model with good accuracy the actual observation. It is important to emphasize that ISMA computes, at each iteration, an unconstrained solution instead of a constrained one. This is because is predictable that, when the set of endmembers approaches the optimal one, the estimated fractional abundance vector \( \hat{x} \) will actually approach \( x \), the true one.
IV. EXPERIMENTS WITH SIMULATED DATA

In this section, we run a series of simulated data experiments which are mainly intended to address two fundamental questions:

1) What is the minimum sparsity of signals which are recoverable using hyperspectral libraries?
2) Among the optimization problems and respective algorithms, what are the more suitable ones to address hyperspectral SR problem?

The section is organized as follows. First, we describe the spectral libraries used in our simulated data experiments and the performance discriminators. Then, we compute approximate solutions without imposing the ASC (due to the reasoning showed in subsection II-A2) for simulated mixtures, using the techniques described in section III. We do not address the unmixing problem when the observations are not affected by noise since, in this case, and for the levels of sparsity considered, all the methods were able to recover the correct solution. Further, we present a comparison of the algorithms used to solve the unmixing problem from two viewpoints: their computational complexity, and their behavior with different noise levels. Next, a short example is dedicated to the case when the ASC holds, for one particular library and with observations affected by correlated noise. The last experiment of this section exemplifies the application of sparse unmixing techniques to spectral libraries composed by image-derived endmembers, an approach that can be adopted if no spectral library is available a priori. The section concludes with a summary of the most important aspects observed in our simulated data experiments.

A. Spectral Libraries Used in Simulated Data Experiments

We have considered the following spectral libraries in our experiments:

- \( \mathbf{A}_1 \in \mathbb{R}^{224 \times 498} \): A selection of 498 materials (different mineral types) from the USGS library denoted splib06\(^3\) and released in September 2007. The reflectance values are measured for 224 spectral bands distributed uniformly in the interval 0.4–2.5 \( \mu \)m.
- \( \mathbf{A}_2 \in \mathbb{R}^{224 \times 342} \): Subset of \( \mathbf{A}_1 \), where the angle between any two different columns is larger than 3°. We have made this pruning because there are many signatures in \( \mathbf{A}_1 \) which correspond to very small variations, including scalings, of the same material.
- \( \mathbf{A}_3 \in \mathbb{R}^{224 \times 500} \): A selection of 500 materials generated using a spectral library generator tool, which allows an user to create a spectral library starting from the ASTER library\(^4\), a compilation of over 2400 spectra of natural and man-made materials. Specifically, each of the members has the reflectance values measured for 224 spectral bands distributed uniformly in the interval 3-12 \( \mu \)m. In this library, there were selected spectra corresponding to materials of the following types: man-made (30), minerals (265), rocks (130), soil (40), water (2), vegetation (2), frost/snow/ice (1) and stony meteorites (30). Notice that, in a real scenario, a library like this is not likely to be used, as it is expected that a given mixture does not contain materials of so many

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\(^3\)Available online: http://speclab.cr.usgs.gov/spectral.lib06

\(^4\)Available online: http://speclib.jpl.nasa.gov
different types. Although real hyperspectral images are acquired usually in a narrower range of wavelengths, this library represents an interesting case study since it is highly heterogeneous from the viewpoint of the type of materials that actually compose it, compared to $A_1$ and $A_2$ (which contain only mineral spectra). At the same time, using this library leads to more challenging unmixing problem due to the internal characteristics of the library, as it will be seen further.

- $A_4 \in \mathbb{R}^{224 \times 449}$: Subset of $A_3$, generated following the same reasonings as for $A_2$.

For comparative purposes, we also consider the following two libraries made of i.i.d components:

- $A_5 \in \mathbb{R}^{224 \times 440}$: made of i.i.d. Gaussian components of zero mean and variance one
- $A_6 \in \mathbb{R}^{224 \times 440}$: made of i.i.d. components uniformly distributed in the interval $[0, 1]$.

Fig. 3(a) plots the mean signature and two other signatures randomly chosen from library $A_1$. All the curves shown are non-negative and relatively smooth. These characteristics can also be seen in Fig. 3(b), which plots the mean square value of the DCT coefficients computed over all signatures of the library $A_1$ jointly with their cumulative energy. From this plot, we conclude that 99.9% of the energy is contained in the first 21 coefficients. If we assume that (from a practical point of view) the remaining coefficients are zero, then the spark of $A_1$ should be no larger than 21. This results from the following:

1) Computing the DCT of the columns of $A$ is equivalent to left multiplying $A$ by an unitary $L \times L$ matrix, which, therefore, does not change the spark($A$).

2) Any matrix with zero elements for any line greater that a given natural $l$, has rank no larger than $l$.

Table I characterizes the libraries $A_1$ to $A_6$. We draw attention on the very high values of the coherence for the spectral libraries (both original and pruned versions). The upper limits of the spark values for libraries $A_1$ to $A_4$ anticipate difficulties in the SR. These difficulties are somehow mitigated by the very low level of sparsity of the signal in which we are interested. On the other hand, it is important to emphasize that libraries composed by i.i.d.
components (similar to A$_5$ and A$_6$) have been used extensively in the literature in order to investigate the ability of different algorithms to deal with under-determined systems of equations. In a sparse unmixing context, the use of these libraries is mainly intended to preliminarily validate the algorithms used. This is because these libraries represent ideal situations that are never encountered in real scenarios, as it can be concluded from Table I. In the following subsections we present a series of simulation results based on the aforementioned libraries and aimed at assessing the potential of SR techniques in the context of hyperspectral unmixing applications.

### B. Performance Discriminators

Before presenting our experimental results, it is first important to describe the parameter settings and performance discrimination metrics adopted in our experiments. Regarding parameter settings, the algorithms described in section III have been applied to unmix simulated mixtures containing a number of endmembers (i.e. values of the sparsity level) which ranges from 2 to 20. For each considered cardinality, spectral library and noise level, we generated 100 mixtures containing random members from the library. The fractional abundances were randomly generated following a Dirichlet distribution [14]. ISMA, OMP and OMP+ algorithms were constrained to return solutions having at most 30 endmembers (we assume that it is not plausible that a mixed pixel contains more materials). Also, the RMSE variation for ISMA ($\Delta$RMSE) was simply related to the difference between two consecutive values of the RMSE: $\Delta$RMSE$_i \equiv$ RMSE$_i$ − RMSE$_{i-1}$. We remind that ISMA is a per-pixel optimization method. This means that the stopping criterion should be individually set for each pixel separately, which is impossible in real scenes with thousands or tens of thousands of pixels. In our experiments, the stopping criterion was set for a large number of samples at once. The semi-optimal parameters that we have set empirically in our experiments are reported in an Appendix (see Table IV for additional details). It is important to emphasize that, in Table IV and in all the following figures, the algorithms: OMP, ISMA, SUNSAL and CSUnSAL are used to solve the unmixing problems (P$_1$) and (P$_1^+$), whereas SUNSAL+ and CSUnSAL+ algorithms are used to solve the problems (P$_1^+$) and (P$_1^{+\downarrow}$). Finally, algorithms SUNSAL+D and CSUnSAL+D solve the modified problems shown in (15). SUNSAL solves also the NCLS problem. It is also important to note that algorithms OMP+, SUNSAL+D and CSUnSAL+D were not applied for the library (A$_5$), as the corresponding technique is dedicated to nonnegative signals.

#### Table I

**Mutual Coherence Values and Estimation of the Spark for Different Spectral Libraries.**

<table>
<thead>
<tr>
<th>Spectral library</th>
<th>A$_1$</th>
<th>A$_2$</th>
<th>A$_3$</th>
<th>A$_4$</th>
<th>A$_5$</th>
<th>A$_6$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Description</td>
<td>USGS</td>
<td>USGS pruned</td>
<td>ASTER</td>
<td>ASTER pruned</td>
<td>i.i.d. Gaussian</td>
<td>i.i.d. Uniform</td>
</tr>
<tr>
<td>Number of spectra ($t$)</td>
<td>498</td>
<td>342</td>
<td>500</td>
<td>449</td>
<td>440</td>
<td>440</td>
</tr>
<tr>
<td>Number of spectral bands ($L$)</td>
<td>224</td>
<td>224</td>
<td>224</td>
<td>224</td>
<td>220</td>
<td>220</td>
</tr>
<tr>
<td>Minimum wavelength ($w_{min}$) in µm</td>
<td>0.4</td>
<td>0.4</td>
<td>3</td>
<td>3</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Maximum wavelength ($w_{max}$) in µm</td>
<td>2.5</td>
<td>2.5</td>
<td>12</td>
<td>12</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>spark($\mathbf{A}$) (upper bound)</td>
<td>21</td>
<td>23</td>
<td>30</td>
<td>54</td>
<td>221</td>
<td>221</td>
</tr>
<tr>
<td>Mutual coherence $\mu(S)$</td>
<td>0.99998</td>
<td>0.9986</td>
<td>1</td>
<td>0.9986</td>
<td>0.3141</td>
<td>0.8388</td>
</tr>
</tbody>
</table>
Regarding the adopted performance discriminators, the quality of the reconstruction of a spectral mixture was measured using the signal to reconstruction error: 

$$
SRE \equiv E[\|x\|^2]/E[\|x - \hat{x}\|^2],
$$

measured in dB: 

$$
SRE(dB) \equiv 10 \log_{10}(SRE).
$$

We use this error measure, instead of the classical root-mean-squared error (RMSE), as it gives more information regarding the power of the error in relation with the power of the signal. We also computed a so-called “probability of success”, $p_s$, which is an estimate of the probability that the relative error power be smaller than a certain threshold. This metric is a widespread one in sparse regression literature, and is formally defined as follows: 

$$
p_s \equiv P(\|\hat{x} - x\|^2/\|x\|^2 \leq \text{threshold}).
$$

For example, if we set threshold $= 10$ and get $p_s = 1$ this means that the total relative error power of the fractional abundances is, with probability one, less than \frac{1}{10}. This gives an indication about the stability of the estimation that is not inferable directly from the SRE (which is an average). In our case, the estimation result is considered successful when 

$$
\frac{\|\hat{x} - x\|^2}{\|x\|^2} \geq 3.16 \ (5\text{dB}).
$$

In all the following figures related to the SRE(dB), we plot a dashed blue line representing the 5dB level in all situations in which at least one of the algorithms reaches this value. The main rationale for using this threshold is that, after inspecting the results of different unmixing scenarios, we concluded that a reconstruction attaining $SRE(dB) = 5\text{dB}$ is still useful. To illustrate this situation, we simulated a toy hyperspectral image with dimensions $15 \times 15$ pixels using the spectral library $A_1$. We assumed the presence of 5 randomly selected endmembers in all simulated pixels, with all observations affected by white noise with signal-to-noise ratio (SNR $\equiv \|A x\|^2/\|n\|^2$) given by SNR $= 40\text{dB}$. For better visual perception of the unmixing results, the fractional abundance of one of the endmembers follows a deterministic pattern (say, a staircase shape with fifteen values comprised between 0 and 1) with the other abundances generated randomly (such that the ASC holds in each pixel). Fig. 4 shows the true and the inferred abundance maps obtained for the first endmember when $SRE(dB) = 5.3\text{dB}$ after applying the SUnSAL algorithm. Fig. 4 also shows the true and reconstructed reflectance values at spectral band number 100 (1.28 $\mu$m) of our toy hyperspectral image. Finally, the last row of Fig. 4 shows the difference images (which represent the per-pixel differences between the images in the top and middle rows of the same figure) in order to represent the magnitude of the errors that occurred in the estimation of fractional abundances and in the image reconstruction at the considered spectral band. Note the low values of the errors achieved in both cases. The simple toy example in Fig. 4 indicates that a reconstruction with $SRE(dB) \geq 5\text{dB}$ can be considered of good accuracy. Fig. 5 also shows the true and the reconstructed spectra of a randomly selected pixel in our toy hyperspectral image. In Fig. 5, the reconstructed spectrum was obtained for $SRE(dB) = 4.8\text{dB}$. Moreover, while in this example the noise was set to a low value, in the following tests the observations are affected by higher noise (SNR $= 30\text{dB}$) meaning that the chosen threshold is even more powerful in terms of performance discrimination.

C. Calculation of Approximate Solutions Without Imposing the ASC Constraint

In this subsection, we consider that the observations are affected by noise, i.e. $n \neq 0$. The SNR was set to 30dB. This noise level was chosen after analyzing the SNR estimated using the VCA [14] algorithm\(^5\) in several

\(^5\)Demo available on-line at http://www.lx.it.pt/ bioucas/code.htm
Fig. 4. Toy example illustrating the reconstruction quality obtained for SRE(dB) \( \approx 5 \) dB. The figures at the top respectively represent the abundance fractions of an endmember and the reflectance values of spectral band 100 (1.28 \( \mu m \)) in the toy hyperspectral image, the figures in the middle represent the respective estimations using SUnSAL algorithm, while the figures at the bottom show the corresponding differences between the true and the estimated values in both cases.

real hyperspectral images, and for different values of the number of endmembers assumed to be present in the respective scenes.

It is important to emphasize that the additive perturbation in the model described in Eq. (2) may be motivated by several causes, including system noise, Poisson noise related with the photon counting process, and modeling errors related with deviations in the spectral signatures resulting from atmospheric interferers, or nonlinearities in the observation mechanism. The first two causes usually introduce band uncorrelated noise, whereas the latter one yields band correlated noise. In hyperspectral imaging applications, we argue that correlated noise is a major concern since it is very difficult to calibrate the observations resulting from an airborne/spaceborne sensor with regards to those in a spectral library of signatures acquired in a laboratory and free of atmospheric interferers, let alone spectral variability issues. Taking into account that, in real applications, the noise is highly correlated as it represents mainly modeling noise and the spectra are of low-pass type with respect to the wavelength, in our simulations we considered white noise on the one hand and, on the other, colored noise resulting from low-pass
filtering i.i.d. Gaussian noise, using a normalized cut-off frequency of $\frac{5\pi}{L}$. For a given mixture, the unmixing process was again considered successful when $\text{SRE} > 5 \text{dB}$. In the following, we describe our experiments assuming white and correlated noise, respectively.

1) Experiments Assuming White Noise: Fig. 6 shows the SRE(dB) obtained for our simulated observations affected by white noise. Similarly, Fig. 7 shows the probability of success $p_s$ achieved by each method for the simulated observations affected by white noise. It should be noted that we removed the curves corresponding to algorithms with poor behavior from the plots in Figs. 6 and 7. From these figures, we can conclude that pruning the libraries can improve the performances of the algorithms when the observations are affected by white noise. Fig. 7 shows that the highest probability of success is achieved by SUnSAL (specifically, by its positive constrained version) and NCLS. The library $\mathbf{A}_3$ seems to be the most difficult one to treat for all methods (being the most coherent matrix), but its pruned version is much more accessible. CSUnSAL particularly exhibits a significant performance improvement when pruning the libraries. For the libraries composed by real signatures: $\mathbf{A}_1 \ldots \mathbf{A}_4$, the probability of success is low for all the methods when the cardinality is higher than 10. Nevertheless, in a sparse unmixing framework we are interested in solutions with a smaller number of endmembers, say, up to 5 endmembers per pixel. For the libraries composed by i.i.d. entries, all the methods exhibit good behavior. For the other libraries, ISMA and OMP exhibit poor results.

2) Experiments Assuming Correlated noise: Fig. 8 shows the SRE(dB) obtained for our simulated observations affected by correlated noise. Similarly, Fig. 9 shows the probability of success $p_s$ obtained for our simulated observations affected by correlated noise. From the viewpoint of our considered problem, perhaps this is the most interesting case study since noise in the hyperspectral images is usually correlated. From Figs. 8 and 9, it can be
Fig. 6. Plot of the SRE(dB) values (as a function of the number of endmembers) obtained by the different sparse unmixing methods when applied to the simulated data with white noise (SNR=30dB), using different spectral libraries.

Fig. 7. Plot of the $p_s$ values (as a function of the number of endmembers) obtained by the different sparse unmixing methods when applied to the simulated data with white noise (SNR=30dB), using different spectral libraries.
observed that most considered sparse unmixing methods exhibit better performance when applied to observations affected by colored noise. As in previous (and subsequent) experiments, we removed the curves corresponding to algorithms with poor behavior. For the libraries composed by real signatures, the highest probability of success is achieved by CSUnSAL and/or its variants, followed closely by the unconstrained version of SUnSAL (see the plots for the most difficult cases, corresponding to $A_1$ and $A_3$). This result confirms our introspection that imposing sparsity can lead to improved results in the context of hyperspectral unmixing problems using spectral libraries.

D. Comparison of Unmixing Algorithms with Regards to Computational Complexity

An important issue in the evaluation of sparse unmixing algorithms is their computational complexity, in particular, when large spectral libraries are used to solve the unmixing problem. In this regard, we emphasize that both OMP (and its variations) and ISMA are computationally complex, with cubic running time $O(L^3)$. All remaining algorithms (NCLS, FCLS, SUunSAL and its variations, CSUnSAL and its variations) have the same theoretical complexity, with quadratic running time $O(L^2)$. A more detailed comparison reporting the actual algorithm running times in the task of unmixing a real hyperspectral scene are given (for the same computing environment) in section V.

E. Comparison of Unmixing Algorithms in the Presence of Different Noise Levels

In this subsection we compare the performances of the considered sparse unmixing algorithms with different noise levels. Specifically, we consider SNR levels of 20, 30, 40 and 50dB, both for white and correlated noise. In this

Fig. 8. Plot of the SRE(dB) values (as a function of the number of endmembers) obtained by the different sparse unmixing methods when applied to the simulated data with correlated noise (SNR=30dB), using different spectral libraries.
Fig. 9. Plot of the $p_s$ values (as a function of the number of endmembers) obtained by the different sparse unmixing methods when applied to the simulated data with correlated noise (SNR=30dB), using different spectral libraries.

In the experiment, the observations were generated by assuming a fixed cardinality of the solution: $k = 5$. Fig. 10 shows the SRE(dB) as a function of the noise level affecting the measurements in the case of white noise, while Fig. 11 shows the same plots in the case of measurements affected by correlated noise, for different spectral libraries. Again we removed the curves corresponding to algorithms with poor behavior. The algorithm parameters in this experiment were set using the procedure described in the Appendix (see Table V). From Figs. 10 and 11, we can conclude that the performance of the algorithms decreases when the noise increases, as expected. In general, the algorithm behavior observed in previous simulated scenarios is confirmed here, with the general trend that most considered approaches perform better in the presence of correlated noise rather than in the presence of white noise. For the white noise scenario, both SUnSAL and SUnSAL+ generally provide the highest values of SRE(dB), particularly for high SNR values. For the correlated noise scenario, CSUnSAL and its variation CSUnSAL+ generally provide the highest scores of SRE(dB), with the exception of spectral library $A_6$ for which NCLS provides the highest error scores as it was already the case in previous experiments. To conclude this subsection, it is worth mentioning that we not only evaluated the performance of the proposed method with different libraries and fixed cardinality of the solution (as illustrated in Figs. 10 and 11), but also with a fixed library and variable cardinality of the solution. For instance, extensive experiments conducted using only the library $A_1$ for different cardinalities of the solution (not included here for space considerations) led to the same conclusions obtained using all the libraries.
Fig. 10. Plot of the SRE(dB) values (as a function of the considered SNR) obtained by the different sparse unmixing methods when applied to the simulated data with white noise, using different spectral libraries.

Fig. 11. Plot of the SRE(dB) values (as a function of the considered SNR) obtained by the different sparse unmixing methods when applied to the simulated data with correlated noise, using different spectral libraries.
This subsection discusses the results obtained in a noisy environment by the techniques presented in section III which include the ASC constraint, denoted by SUnSAL$^{ASC}$ (which solves here also the FCLS problem) and CSUnSAL$^{ASC}$. The simulated data were generated as explained in subsection IV-C but this time imposing the ASC constraint, and adding both white and correlated noise to the simulated observations. The spectral library used in this example is $A_1$. When the ASC holds, SUnSAL$^{ASC}$ is equal to FCLS since, no matter how the parameter $\lambda$ is chosen, the sparsity enforcing term does not play any role (it is a constant). As a consequence, we do not plot here the results obtained by SUnSAL$^{ASC}$, but, instead, the results obtained by SUnSAL+ and CSUnSAL+ for white noise and correlated noise, respectively. Fig. 12 shows the values of SRE(dB) and $p_s$ for the two considered cases (white and correlated noise). These results exemplify the behavior of the constrained unmixing algorithms in the hypothetical situation in which the ASC constraint holds, an assumption that is not always true in real unmixing scenarios due to signature variability issues as explained in subsection II-A2. Fig. 12 shows that the performances of SUnSAL+ and FCLS are quite similar (with a small advantage for SUnSAL+) and generally superior to those achieved by CSUnSAL$^{ASC}$ for white noise, while both CSUnSAL+ and CSUnSAL$^{ASC}$ exhibit a significant performance improvement with regards to FCLS when applied to unmix observations affected by correlated noise, especially for high cardinalities of the solution.
G. Application of sparse unmixing techniques to image-derived endmembers

The main goal of this experiment is to analyze the performance of sparse unmixing techniques when a spectral library is not available a priori. In this case, the proposed methods can still be applied by resorting to an artificially generated spectral library constructed using image-derived endmembers. In our experiment, we first derived a subset of 12 members from library $A_1$ (the subset was generated after retaining only the spectral signatures which form a spectral angle larger than $20^\circ$ with all other signatures in the library). Then, we randomly selected five of the spectral signatures in the resulting subset and used them to generate a simulated hyperspectral image with $75 \times 75$ pixels and 224 bands per pixel. The data were generated using a linear mixture model, using the five randomly selected signatures as the endmembers and imposing the ASC in each simulated pixel. In the resulting image, illustrated in Fig. 13(a), there are pure regions as well as mixed regions constructed using mixtures ranging between two and five endmembers, distributed spatially in the form of distinct square regions. Figs. 13(b)–(e) respectively show the true fractional abundances for each of the five endmembers. The background pixels are made up of a mixture of the same five endmembers, but this time their respective fractional abundances values were fixed to 0.5130, 0.1476, 0.1158, 0.1242 and 0.0994, respectively. The simulated data was then contaminated with noise (SNR=20dB).

Once the simulated data set was generated, we used the HySime algorithm [46] to find the signal subspace and projected the data on this subspace. Then, two endmember extraction algorithms: VCA and N-FINDR were used to automatically extract the endmembers from the simulated data. The obtained endmember sets were merged in order to construct the spectral library used in the sparse unmixing process. In this library, only materials with spectral angle of at least $3^\circ$ with regards to other materials in the library were retained in order to avoid strong similarities
between the spectral signatures when conducting the sparse unmixing process. The abundance estimation was then conducted with SUnSAL+, using different values of the parameter \( \lambda \). The same algorithm was used to find the NCLS solution by setting \( \lambda = 0 \). Finally, the estimated and true abundances were aligned and the SRE(dB) was computed. Table II shows the mean SRE(dB) achieved, both for different values of \( \lambda \) and for each different endmember. For illustrative purposes, Fig. 14 also graphically displays the abundance estimation results obtained for one specific endmember (the 5th one used in the simulations). From Table II, it can be seen that sparse techniques can still be successfully applied using image-derived endmembers in case there is no spectral library available \textit{a priori}. Even in the presence of significant noise, SUnSAL+ always performed better than NCLS, no matter the value of \( \lambda \) tested or the endmember considered. The results displayed in Fig. 14 are also in line with these observations. It is also worth noting that, in this experiment, we did not determine \textit{a priori} the optimal parameter for \( \lambda \).

### Table II

<table>
<thead>
<tr>
<th>SRE(dB) Values Achieved after Applying SUnSAL+ to Image-Derived Endmembers from the Simulated Image in Fig. 13.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Results for different values of ( \lambda )</strong></td>
</tr>
<tr>
<td>Mean SRE (dB)</td>
</tr>
<tr>
<td>---------------</td>
</tr>
<tr>
<td>( \times 10^{-1} )</td>
</tr>
<tr>
<td><strong>Results for different endmembers</strong></td>
</tr>
<tr>
<td>Mean SRE (dB)</td>
</tr>
<tr>
<td>---------------</td>
</tr>
<tr>
<td>( \times 10^{-1} )</td>
</tr>
</tbody>
</table>
H. Summary and Main Observations

In summary, our main observation from the experiments conducted in this section is that spectral libraries are indeed suitable for solving the sparse unmixing problem in our simulated analysis scenarios. Although the techniques which do not explicitly enforce the sparsity of the solution exhibit similar performances with regards to sparse techniques when the observations are affected by white noise, our experimental results demonstrated that, by enforcing the sparsity of the solution, unmixing results can significantly improve when the observations are affected by correlated noise, which is the most typical one in real hyperspectral imaging scenarios. It is also worth noting that, according to our experiments, the sparse techniques exhibit better performance when the number of endmembers is low (say, up to 5), which is a reasonable assumption in practice, but also for higher cardinalities when the noise is correlated. Finally, we also demonstrated that sparse unmixing methods can be applied using image-derived endmembers when there is no spectral library available \textit{a priori}. Although our experiments with simulated mixtures are quite encouraging, the complexity of real mixtures is usually quite high and it is difficult to account for all possible issues affecting such mixtures when conducting simulations. For this reason, further experiments using real hyperspectral data sets are highly desirable. These will be conducted in the following section.

V. Experiments with Real Data

The scene used in our real data experiments is the well-known AVIRIS Cuprite data set, available online in reflectance units\(^6\). This scene has been widely used to validate the performance of endmember extraction algorithms. The portion used in experiments corresponds to a 350 \(\times\) 350-pixel subset of the sector labeled as f970619t01p02_r02_sc03.a.rfl in the online data. The scene comprises 224 spectral bands between 0.4 and 2.5 \(\mu\)m, with nominal spectral resolution of 10 nm. Prior to the analysis, bands 1–2, 105–115, 150–170, and 223–224 were removed due to water absorption and low SNR in those bands, leaving a total of 188 spectral bands. The Cuprite site is well understood mineralogically, and has several exposed minerals of interest, all included in the USGS library considered in experiments, denoted splib06\(^7\) and released in September 2007. In our experiments, we use spectra obtained from this library as input to the unmixing methods described in section III. For illustrative purposes, Fig. 15 shows a mineral map produced in 1995 by USGS, in which the Tricorder 3.3 software product [47] was used to map different minerals present in the Cuprite mining district\(^8\). It should be noted that the Tricorder map is only available for hyperspectral data collected in 1995, while the publicly available AVIRIS Cuprite data was collected in 1997. Therefore, a direct comparison between the 1995 USGS map and the 1997 AVIRIS data is not possible. However, the USGS map serves as a good indicator for qualitative assessment of the fractional abundance maps produced by the unmixing algorithms described in section III.

In order to compute approximate solutions and to compare the performances of the algorithms described in Section III, a toy subscene of 70 \(\times\) 30 pixels of the Cuprite data set was first used prior to conducting experiments


\(^7\)http://speclab.cr.usgs.gov/spectral.lib06

\(^8\)http://speclab.cr.usgs.gov/cuprite95.tgif.2.2um_map.gif
Fig. 15. USGS map showing the location of different minerals in the Cuprite mining district in Nevada. The map is available online at: http://speclab.cr.usgs.gov/cuprite95.tgif.2.2um_map.gif.

Fig. 16. AVIRIS Cuprite hyperspectral scene used in our experiments. (a) Spatial localization of a toy 70 × 30-pixel subscene in the considered 350 × 350-pixel data set. (b) Spectral band at 558 nm wavelength of the toy subscene.
Fig. 17. (a) Plot of diagonal values of the correction matrix \( C \). (b) Original (blue) and corrected (red) spectrum of a randomly selected pixel in the AVIRIS Cuprite data set.

with the 350 \( \times \) 350-pixel scene. The position of the toy subscene in the 350 \( \times \) 350 scene is shown in Fig. 16(a), while the spectral band at 558 nm wavelength of the toy subscene is shown in Fig. 16(b). The results obtained for the 350 \( \times \) 350-pixel scene are presented at the end of this section.

In all our experiments with real data, we use library \( A_1 \) to compute approximate solutions. However, before processing the hyperspectral data, we should first focus our attention on calibration issues. As we have already referred to before, even though we are working with atmospherically corrected data in reflectance units, there are always calibration mismatches between the real pixel spectra and the spectra available in the library due to the rather different acquisition conditions of the two data types. In order to minimize these mismatches, we apply a band-dependent correction strategy to the original data set, which amounts at replacing the data set \( Y \) with \( CY \), where \( C \) is a diagonal matrix that minimizes the modeling error, i.e.:

\[
\tilde{C} = \text{arg min}_{C, X \geq 0, \frac{1}{n} \sum X = 1} \| A_1 X - CY \|_2,
\]  

(27)

where \( X \geq 0 \) is the fractional abundance matrix. Problem (27) is non-convex and, thus, very hard to solve exactly. We have computed a sub-optimal solution to this problem by alternating the minimizing with respect to \( C \) and to \( X \). We start the iterative procedure with \( C = I \). The minimization with respect to \( C \) and to \( X \) are, respectively, least squares and constrained least squares problems. To speed up the process and ensure quality in the estimate of \( C \), we removed non-sparse fractional abundances from \( X \) and the respective spectral vectors from \( Y \) after the first iteration. We ran a total of 20 iterations. The plot of the correction factors with regards to the spectral bands is displayed in Fig. 17(a). These factors are always close to one, apart from a few bands in the blue wavelengths. For illustrative purposes, Fig. 17(b) shows a random pixel observation from the original AVIRIS Cuprite data set and its corrected version using the aforementioned strategy.

After correcting the data, the unmixing problem was first solved for the toy subscene, using the sparse unmixing algorithms described in section III. The parameters used were: \( \lambda = 10^{-5} \) for SUnSAL and all its variations, and
\[ \delta = 10^{-4} \] for CSUnSAL and all its variations. Fig. 18 represents the fractional abundance estimations obtained for each endmember material in the \( A_1 \) spectral library (as a function of the pixel index in the considered toy subscene) by the considered sparse unmixing methods. We emphasize that there are a total of \( 70 \times 30 = 2100 \) pixels in the toy subscene. As shown by Fig. 18, the unconstrained version of CSUnSAL leads to highly inaccurate (i.e. physically unrealistic) results since the solutions contain negative values. CSUnSAL+, on the other hand, introduces more reasonable abundance estimates which, in turn, do not comply with the ASC constraint since the sum of all abundance fractions per pixel generally exceed the value 1.0, i.e. these are super-unitary. CSUnSAL+D seems far more realistic than the unconstrained version. Both SUnSAL+D and CSUnSAL+D produce, in some cases, super-unitary fractional abundances. SUnSAL and SUnSAL+ exhibit similar performances, with the general observation that SUnSAL return vectors of fractional abundances which are more dense than SUnSAL+. Another general observation is that the constrained methods show clearly the sparsity of the solution, as the non-zero fractions appear in distinct lines (sometimes grouped in clusters). This is due to the fact that, in the library, there are consecutive members describing similar materials. This general observation is strengthened if we compute the average number of endmembers having fractional abundances higher than 0.05 in one pixel: 44.05 for SUnSAL, 6.07 for SUnSAL+, 6.2 for SUnSAL+D, 68.55 for CSUnSAL, 8.36 for CSUnSAL+ and 11.09 for CSUnSAL+D. For illustrative purposes, Fig. 19 exemplifies the most significant minerals found by SUnSAL+ in the toy subscene.

It is important to note that the constrained results of sparse unmixing algorithms have very similar norms of the reconstruction error, with all of them situated for one randomly selected pixel around 0.05. We have used this observation in order to set the stopping threshold in the OMP and OMP+ algorithms to this value (i.e. by forcing them to achieve exactly the same error). In the case of ISMA we empirically set the algorithm threshold to \( t_3 = 2 \), based on the observed RMSE variation of a small number of randomly selected pixels (10). It is also worth noting that choosing a threshold for ISMA is extremely difficult in this application, since the RMSE has a very smooth variation and the critical iteration is very difficult to identify. For illustrative purposes, the unmixing results after using these three algorithms (OMP, OMP+ and ISMA) are reported in Fig. 21. From Fig. 21, it can be seen that OMP performs poorly (its solution contains many negative fractional abundances). OMP+ performs better and tolerates large super-unitary values, although the sparsity of the solution is quite apparent. The same observation is valid for ISMA. For the sake of completeness, Fig. 20 shows the fractional abundances estimated by NCLS in the toy subscene. The results were obtained using the SUnSAL algorithm, by setting \( \lambda = 0 \) and activating the ANC constraint. Before reporting the abundance estimation results obtained for the \( 350 \times 350 \)-pixel data set, Table III reports the processing times (in seconds) measured after applying the considered unmixing algorithms to the toy \( 70 \times 30 \)-pixel subscene. The algorithms were implemented using MatlabR2009 on a desktop PC equipped with an Intel Core 2 Duo CPU (at 2.33 GHz) and 2GB of RAM memory. As shown by Table III, ISMA is quite slow compared to the other algorithms, while OMP and OMP+ are the fastest ones. NCLS and SUnSAL in all its variants exhibit comparable running times, while CSUnSAL proves to be slower than them. In turn, SUnSAL is very fast in the unconstrained version. Although some of the reported sparse unmixing algorithms needed significant times to complete their calculations in this example, their implementation in the form of parallel algorithms is very
Fig. 18. Fractional abundance estimations obtained for each endmember material in the A_1 spectral library (as a function of the pixel index in the considered toy subscene) by the considered sparse unmixing methods.
Fig. 19. Fractional abundance estimations obtained for each endmember material in the $A_1$ spectral library (as a function of the pixel index in the considered toy subscene) by the SUnSAL+ method. The most significant minerals found by this algorithm are outlined.

Fig. 20. Fractional abundance estimations obtained for each endmember material in the $A_1$ spectral library (as a function of the pixel index in the considered toy subscene) by the NCLS method.

feasible and this strategy (not adopted in this work) can lead to significant reductions in processing time in future developments.

Based on the previous results, which indicate that the ANC-constrained versions of SUnSAL and CSUnSAL exhibit similar performances in this problem and that sparse techniques generally exhibit better performance than those techniques that do not explicitly enforce sparseness, we now apply the SUnSAL+ algorithm to estimate fractional abundances in the $350 \times 350$-pixel AVIRIS Cuprite scene using the spectral library $A_1$ and a pruned version of $A_1$. The pruned version was obtained by simply removing some of the spectral signatures which form
a spectral angle smaller than 2.5°, thus obtaining a library with 390 spectrally distinct signatures denoted by $\mathbf{A}$. Fig. 22 shows a visual (qualitative) comparison between the fractional abundance maps, estimated for 7 highly materials in the AVIRIS Cuprite scene, by applying the SUnSAL+ algorithm. For comparative purposes, the spatial distribution maps of these materials extracted from the Tricorder classification map shown in Fig. 15 are also displayed. From Fig. 22, it can be observed that the SUnSAL+ sparse unmixing technique is able to find a good approximation for the distribution of the materials in the scene, both for the original and also for the pruned version of the spectral library. It should be noted that there are still some differences between our estimated abundance maps and the Tricorder maps, mainly due to the fact that the Tricorder maps are in fact classification maps (i.e., all pixels are considered pure and classified as belonging or not to a class given by the representative mineral in that pixel) and not abundance maps (in which the value assigned to a mixed pixel varies depending on the degree of presence of the mineral in the pixel). Even so, it can be seen visually that the SUnSAL+ sparse unmixing technique generally returns the highest abundances exactly for those pixels classified as belonging to the respective class of materials.

VI. Conclusions and Future Research

In this paper, we have reformulated the spectral unmixing problem under the light of sparse regression, and further evaluated the performance of several (available and new) sparse regression algorithms in spectral unmixing applications. One significant advantage of using sparse regression for spectral unmixing purposes is to take advantage of the increasing availability of spectral libraries of materials measured on the ground, for instance, using advanced field spectro-radiometers. Through the sparse unmixing techniques described in this paper, mixed pixels can be
Fig. 22. Qualitative comparison between the fractional abundance maps estimated by the SUnSAL+ sparse unmixing technique and the classification maps produced by USGS Tricorder algorithm for the 350 x 350-pixel AVIRIS Cuprite scene.
expressed in the form of linear combinations of a number of pure spectral signatures known in advance and available in a library. With this strategy, the abundance estimation process no longer depends on the availability of pure spectral signatures in the input data nor on the capacity of a certain endmember extraction algorithm to identify such pure signatures. Quite opposite, the procedure is reduced to finding the optimal subset of signatures in the library that can best model each mixed pixel in the scene.

Although our experimental results (conducted with both simulated and real data sets) are very encouraging, there are several aspects to be considered in practice and worth being further investigated in future research efforts. One is the fact that the library spectra are rarely acquired under the same conditions as the airborne data. To address this issue, in this work we have adopted a simple correction algorithm to compensate for possible interferers. Another issue is the fact that the ability to obtain useful sparse solutions of an under-determined system of equations depends, mostly, on the degree of coherence between the columns of the system matrix and also on the degree of sparseness of the original signals. As a result, the most favorable scenarios correspond to highly sparse signals and system matrices with low coherence. Unfortunately, in hyperspectral imaging applications the spectral signatures of the materials tend to be highly correlated. This unfavorable aspect is, somehow, balanced by the highly sparse nature of the fractional abundances. A final issue to be explored in future developments is the high computational complexity of sparse unmixing algorithms, addressed in this work by the consideration of fast algorithms based on the augmented Lagrangian method of multipliers but also subject to further improvements related with the inherently parallel nature of such algorithms. In fact, an important advantage of sparse unmixing methods is that their complexity depends more on the cardinality of the solution and on the number of spectra in the library and less on the size of the hyperspectral image to be processed. Since sparse unmixing is conducted in pixel-by-pixel fashion, the procedure could be accelerated by dividing the image into sub-images (or sub-sets of pixels) of any size, and processing the sub-partitions in parallel without the need to establish an optimal size of sub-images or sub-partitions. This feature anticipates high scalability of potential parallel solutions to this approach.

APPENDIX

In this Appendix, we report the parameters used in our simulated data experiments. Specifically, Table IV reports the parameters used when looking for approximate solutions in experiments with SNR = 30dB, for each considered cardinality, unmixing method and spectral library. In order to ensure a fair comparison, we defined near-optimal parameters for groups or levels of sparsity, with each group being described by a representative level for all considered methods. The parameters were denoted as follows: \( t_1, t_2 \) and \( t_3 \) are the thresholds imposed in the stopping criteria for OMP, OMP+ and ISMA; \( \lambda_1, \lambda_2, \lambda_3 \) are the regularization parameters for SUnSAL, SUnSAL+ and SUnSAL+D; and \( \delta_1, \delta_2, \delta_3 \) are the tolerance errors for CSUnSAL, CSUnSAL+ and CSUnSAL+D, respectively. It should be noted that NCLS does not require any input parameter.

In order to find near-optimal parameters in this particular case (SNR = 30dB), the representative levels for the groups of sparsity were chosen as follows: for \( k = 2 \ldots 6 \) the representative level is \( k_1 = 4 \); for \( k = 7 \ldots 13 \) the representative level is \( k_2 = 10 \); and for \( k = 14 \ldots 20 \) the representative level is \( k_3 = 17 \). Table IV (columns (a)
and (b)] show the near-optimal parameters established for the simulated data sets affected by white and correlated noise, respectively. These parameters are near-optimal for the representative cardinalities, but they are applied for all sparsity levels in the respective group and they were inferred by testing the algorithms using toy examples, i.e. by considering a large range of possible discrete values on the basis of a small number of samples (10).

<table>
<thead>
<tr>
<th>TABLE IV</th>
</tr>
</thead>
<tbody>
<tr>
<td>PARAMETER SETTINGS USED IN OUR SIMULATED DATA EXPERIMENTS WHEN THE SNR WAS CONSTANT (SNR = 30dB).</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(a) White noise</th>
<th>(b) Colored noise</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_1 = 4$</td>
<td>$k_2 = 10$</td>
</tr>
<tr>
<td>OMP $\ell_1$</td>
<td></td>
</tr>
<tr>
<td>$A_1$</td>
<td>0.21</td>
</tr>
<tr>
<td>$A_2$</td>
<td>0.035</td>
</tr>
<tr>
<td>$A_3$</td>
<td>0.245</td>
</tr>
<tr>
<td>$A_4$</td>
<td>0.105</td>
</tr>
<tr>
<td>$A_5$</td>
<td>0.365</td>
</tr>
<tr>
<td>$A_6$</td>
<td>0.29</td>
</tr>
</tbody>
</table>

| ISMA $\ell_1$ | | | | | |
| $A_1$ | 0.00 | 0.01 | 0.002 | 0.08 | 0.002 | 0.005 |
| $A_2$ | 0.21 | 0.01 | 0.002 | 0.005 | 0.005 | 0.005 |
| $A_3$ | 0.02 | 0.085 | 0.245 | 0.275 | 0.155 | 0.165 |
| $A_4$ | 0.025 | 0.01 | 0.02 | 0.3 | 0.2 | 0.15 |
| $A_5$ | - | - | - | - | - | - |
| $A_6$ | 0.285 | 0.25 | 0.23 | 0.24 | 0.14 | 0.065 |

| SUNSAL $\lambda_1$ | | | | | |
| $A_1$ | 0.004 | 0.004 | 0.003 | 10^{-5} | 10^{-5} | 10^{-5} |
| $A_2$ | 3 \times 10^{-4} | 3 \times 10^{-4} | 6 \times 10^{-4} | 10^{-5} | 10^{-5} | 10^{-5} |
| $A_3$ | 0.4 | 0.5 | 0.5 | 0.008 | 0.003 | 0.001 |
| $A_4$ | 0.002 | 0.005 | 0.004 | 5 \times 10^{-5} | 5 \times 10^{-5} | 10^{-5} |
| $A_5$ | 0.5 | 0.3 | 0.2 | 0.4 | 0.4 | 0.1 |
| $A_6$ | 0.5 | 0.3 | 0.5 | 0.4 | 0.2 | 0.1 |

| SUNSAL+ $\lambda_1$ | | | | | |
| $A_1$ | 0.04 | 0.04 | 0.01 | 10^{-5} | 10^{-5} | 10^{-5} |
| $A_2$ | 0.003 | 10^{-6} | 10^{-5} | 10^{-5} | 10^{-5} | 10^{-5} |
| $A_3$ | 0.5 | 0.3 | 0.4 | 5 \times 10^{-4} | 6 \times 10^{-4} | 5 \times 10^{-4} |
| $A_4$ | 6 \times 10^{-5} | 5 \times 10^{-6} | 8 \times 10^{-5} | 10^{-4} | 10^{-5} | 10^{-5} |
| $A_5$ | 0.5 | 0.3 | 0.2 | 0.4 | 0.3 | 0.2 |
| $A_6$ | 0.08 | 0.06 | 0.03 | 0.04 | 0.03 | 0.03 |

| SUNSAL+D $\lambda_3$ | | | | | |
| $A_1$ | 0.05 | 0.01 | 0.003 | 7 \times 10^{-4} | 3 \times 10^{-4} | 7 \times 10^{-4} |
| $A_2$ | 0.002 | 5 \times 10^{-4} | 10^{-5} | 3 \times 10^{-6} | 10^{-6} | 5 \times 10^{-7} |
| $A_3$ | 0.4 | 0.3 | 0.3 | 0.001 | 0.004 | 0.001 |
| $A_4$ | 0.003 | 0.001 | 0.001 | 10^{-6} | 5 \times 10^{-6} | 10^{-7} |
| $A_5$ | - | - | - | - | - | - |
| $A_6$ | 0.1 | 0.1 | 0.3 | 0.09 | 0.09 | 0.09 |

| CSUNSAL $\lambda_1$ | | | | | |
| $A_1$ | 0.3 | 0.2 | 0.2 | 0.001 | 0.001 | 5 \times 10^{-5} |
| $A_2$ | 0.09 | 0.04 | 0.03 | 10^{-5} | 2 \times 10^{-4} | 10^{-4} |
| $A_3$ | 10^{-7} | 10^{-7} | 10^{-12} | 0.2 | 0.02 | 0.009 |
| $A_4$ | 0.03 | 0.03 | 0.03 | 10^{-4} | 10^{-5} | 10^{-5} |
| $A_5$ | 0.3 | 0.2 | 0.1 | 0.3 | 0.1 | 0.08 |
| $A_6$ | 0.2 | 0.2 | 0.2 | 0.2 | 0.2 | 0.2 |

| CSUNSAL+ $\lambda_2$ | | | | | |
| $A_1$ | 0.4 | 0.3 | 0.3 | 10^{-5} | 5 \times 10^{-5} | 10^{-5} |
| $A_2$ | 0.03 | 0.03 | 0.03 | 10^{-4} | 10^{-4} | 5 \times 10^{-4} |
| $A_3$ | 0.03 | 0.01 | 0.01 | 10^{-4} | 10^{-4} | 10^{-4} |
| $A_4$ | 0.03 | 0.03 | 0.02 | 10^{-5} | 5 \times 10^{-5} | 5 \times 10^{-5} |
| $A_5$ | 0.3 | 0.2 | 0.1 | 0.3 | 0.2 | 0.09 |
| $A_6$ | 0.2 | 0.2 | 0.2 | 0.3 | 0.2 | 0.1 |

| CSUNSAL+D $\lambda_3$ | | | | | |
| $A_1$ | 0.03 | 0.01 | 0.01 | 10^{-4} | 10^{-4} | 10^{-4} |
| $A_2$ | 10^{-4} | 10^{-5} | 10^{-5} | 10^{-4} | 10^{-5} | 10^{-5} |
| $A_3$ | 10^{-4} | 10^{-4} | 10^{-4} | 10^{-4} | 10^{-4} | 10^{-4} |
| $A_4$ | 10^{-5} | 10^{-5} | 10^{-5} | 10^{-7} | 10^{-7} | 10^{-7} |
| $A_5$ | - | - | - | - | - | - |
| $A_6$ | 0.1 | 0.08 | 0.01 | 0.1 | 0.02 | 0.01 |
On the other hand, Table V reports the parameters used in our simulated data experiments when the true cardinality was $k = 5$ and the SNR varied between 20 and 50dB. These parameters were found in a similar fashion to the ones reported in Table IV, considering two representative levels of the SNR: $k_1 = 25$dB for SNR $= 20 \ldots 30$dB, and $k_2 = 45$dB for $k = 40 \ldots 50$dB. To conclude this section, we would like to emphasize our significant efforts in testing the most suitable parameters in order to report only near-optimal results for each considered method.

**ACKNOWLEDGMENT**

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Dr. Bioucas-Dias is an Associate Editor of the IEEE TRANSACTIONS ON IMAGE PROCESSING, was an Associate Editor of the IEEE TRANSACTIONS ON CIRCUITS AND SYSTEMS, and a Guest Editor of a special issue of the IEEE TRANSACTIONS ON GEOSCIENCE AND REMOTE SENSING. He has been a member of program/technical committees of several international conferences, including CVPR, ICPR, ICIAR, IGARSS, ICIP, SPIE, EMMCVPR, ISVC, and WHISPERS.

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He was a Visiting Researcher with the Remote Sensing Signal and Image Processing Laboratory, University of Maryland Baltimore County, Baltimore; with the Applied Information Sciences Branch, Goddard Space Flight Center, Greenbelt, MD; and with the AVIRIS Data Facility, Jet Propulsion Laboratory, Pasadena, CA. Since 2000, he has been an Associate Professor with the Department of Technology of Computers and Communications, University of Extremadura, Caceres, Spain, where he was an Assistant Professor from 1997 to 1999. He is the Coordinator of the Hyperspectral Imaging Network (Hyper-I-Net), which is a European project designed to build an interdisciplinary research community focused on hyperspectral imaging activities. He has been a Proposal Reviewer with the European Commission, the European Space Agency, and the Spanish Government, and has also served as a Reviewer for more than 40 different journals. He is the author or coauthor of more than 230 publications on remotely sensed hyperspectral imaging, including more than 40 Journal Citation Report papers, book chapters, and conference proceeding papers. He has coedited a book on high-performance computing in remote sensing and several special issues on remotely sensed hyperspectral imaging for different journals. He has served as a Reviewer for more than 130 manuscripts submitted to the IEEE TRANSACTIONS ON GEOSCIENCE AND REMOTE SENSING. His research interests include remotely sensed hyperspectral imaging, pattern recognition, signal and image processing, and efficient implementation of large-scale scientific problems on parallel and distributed computer architectures.

Dr. Plaza is an Associate Editor of the IEEE TRANSACTIONS ON GEOSCIENCE AND REMOTE SENSING on hyperspectral image analysis and signal processing. He is a recipient of the recognition of Best Reviewers of the IEEE GEOSCIENCE AND REMOTE SENSING LETTERS in 2009.
REFERENCES


### TABLE V

Parameter settings used in our simulated data experiments when the SNR varied between 20 and 50 dB.

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