ALTERNATING DIRECTION ALGORITHMS FOR CONSTRAINED SPARSE REGRESSION: APPLICATION TO HYPERSPECTRAL UNMIXING

José M. Bioucas-Dias and *Mário A. T. Figueiredo*

Instituto de Telecomunicações, *Instituto Superior Técnico*, Lisboa, **Portugal**

ABSTRACT

Convex optimization problems are common in hyperspectral unmixing. Examples are the constrained least squares (CLS) problem used to compute the fractional abundances in a linear mixture of known spectra, the constrained basis pursuit (CBP) to find sparse (*i.e.,* with a small number of terms) linear mixtures of spectra, selected from large libraries, and the constrained basis pursuit denoising (CBPDN), which is a generalization of BP to admit modeling errors. In this paper, we introduce two new algorithms to efficiently solve these optimization problems, based on the alternating direction method of multipliers, a method from the augmented Lagrangian family. The algorithms are termed SUnSAL (*sparse unmixing by variable splitting and augmented Lagrangian*) and C-SUnSAL (*constrained SUnSAL*). C-SUnSAL solves the CBP and CBPDN problems, while SUnSAL solves CLS as well as a more general version thereof, called *constrained sparse regression* (CSR). C-SUnSAL and SUnSAL are shown to outperform off-the-shelf methods in terms of speed and accuracy.

1. INTRODUCTION

Hyperspectral unmixing (HU) is a *source separation problem* with applications in remote sensing, analytical chemistry, and other areas [10, 11, 12]. Given a set of observed mixed hyperspectral vectors, HU aims at estimating the number of reference spectra (the *endmembers*), their spectral signatures, and their fractional abundances, usually under the assumption that the mixing is linear [10, 12].

Unlike in a canonical source separation problem, the *sources* in HU (*i.e.*, the fractional abundances of the spectra/materials present in the data) exhibit statistical dependency [15]. This characteristic, together with the high dimensionality of the data, places HU beyond the reach of most standard source separation algorithms, thus fostering active research in the field.

Most HU methods can be classified as statistical or geometrical. In the (statistical) Bayesian framework, all inference relies on the posterior probability density of the unknowns, given the observations. According to Bayes' law, the posterior probability density results from two factors: the observation model (the likelihood), which formalizes the assumed data generation model, possibly including random perturbations such as additive noise; the prior, which may impose natural constraints on the endmembers (*e.g.,* nonnegativity) and on the fractional abundances (*e.g.,* belonging to the probability simplex, since they are relative abundances), as well as model spectral variability [5, 14, 16].

Geometrical approaches exploit the fact that, under the linear mixing model, the observed hyperspectral vectors belong to a simplex set whose vertices correspond to the endmembers. Therefore, finding the endmembers amounts to identifying the vertices of that simplex [18, 16, 3, 13, 20, 1].

Sparse regression is another direction recently explored for HU [9], which has connections with both the statistical and the geometrical frameworks. In this approach, the problem is formulated as that of fitting the observed (mixed) hyperspectral vectors with sparse (*i.e.,* containing a small number of terms) linear mixtures of spectral signatures from a large dictionary available *a priori*. Estimating the endmembers is thus not necessary in this type of methods. Notice that the sparse regression problems in this context are not standard, as the unknown coefficients (the fractional abundances) sum to one (the so-called *abundance sum constraint* – ASC) and are nonnegative (*abundance non-negativity constraint* – ANC). These problems are thus referred to as *constrained sparse regression* (CSR).

Several variants of the CSR problem can be used for HU; some examples follow. In the classical *constrained least squares* (CLS), the fractional abundances in a linear mixture of known spectra are estimated by minimizing the total squared error, under the ANC and the ASC. Although no sparseness is explicitly encouraged in CLS, under some conditions (namely positivity of the spectra) it can be shown that the solutions are indeed sparse [2]. *Constrained basis pursuit* (CBP) is a variant of the well-known *basis pursuit* (BP) criterion [4] under the ANC and the ASC; as in BP, CBP uses the ℓ_1 norm to explicitly encourage sparseness of the fractional abundance vectors. Finally, *constrained basis pursuit denoising* (CBPDN) is a generalization of CBP that admits modeling errors (*e.g.*, observation noise).

1.1. Contribution

In this paper, we introduce a class of alternating direction algorithms to solve several CSR problems (namely CLS, CBP, and CBPDN). The proposed algorithms are based on the *alternating direction method of multipliers* (ADMM) [8, 7, 6], which decomposes a difficult problem into a sequence of simpler ones. Since ADMM can be derived as a variable splitting procedure followed by the adoption of an augmented Lagrangian method to solve the resulting constrained problem, we term our algorithms as SUnSAL (*spectral unmixing by splitting and augmented Lagrangian*) and C-SUnSAL (*constrained SUnSAL*).

The paper is organized as follows. Section 2 introduces notation and formulates the optimization problems. Section 3 reviews the ADMM and the associated convergence theorem. Section 4 introduces the SUnSAL and C-SUnSAL algorithms. Section 5 presents experimental results, and Section 6 ends the paper by presenting a few concluding remarks.

2. PROBLEM FORMULATION: CSR, CLS, CBP, CBPDN

Let $\mathbf{A} \in \mathbb{R}^{k \times n}$ denote a matrix containing the n spectral signatures of the endmembers, $\mathbf{x} \in \mathbb{R}^n$ denote the (unknown) fractional abundance vector, and $\mathbf{y} \in \mathbb{R}^k$ be an (observed) mixed spectral vector.

In this paper, we assume that $\mathbf{A}$ is known; this is the case the CSR approach [9], where it is a library with a large number of spectral signatures, thus usually $n > k$. Matrix $\mathbf{A}$ can also be the output of an endmember extraction algorithm, in which case usually $n \ll k$. The key advantage of the CSR approach is that it avoids the estimation of endmembers, quite often a very hard problem.

The general CSR problem is defined as

$$(\mathrm{P_{CSR}}): \quad \min_{\mathbf{x}} \overbrace{(1/2)\|\mathbf{A}\mathbf{x}-\mathbf{y}\|_2^2 + \lambda\|\mathbf{x}\|_1}^{L(\mathbf{x})} \quad \text{subject to: } \mathbf{x} \geq \mathbf{0}, \ \mathbf{1}^T\mathbf{x} = 1, \tag{1}$$

where $\|\mathbf{x}\|_2$ and $\|\mathbf{x}\|_1$ denote the ℓ_2 and ℓ_1 norms of $\mathbf{x}$, respectively, $\lambda \geq 0$ is a parameter controlling the relative weight between the ℓ_2 and ℓ_1 terms, $\mathbf{1}$ denotes a column vector of 1's, and the inequality $\mathbf{x} \geq \mathbf{0}$ is to be understood in the componentwise sense. The constraints $\mathbf{x} \geq \mathbf{0}$ and $\mathbf{1}^T\mathbf{x} = 1$ correspond to the ANC and ASC, respectively. The CLS problem corresponds to $\mathrm{P_{CSR}}$ with $\lambda = 0$. The CBP and CBPDN problems are also equivalent to particular cases of $\mathrm{P_{CSR}}$, as stated next.

The CBP optimization problem is

$$(\mathrm{P_{CBP}}): \quad \min_{\mathbf{x}} \ \|\mathbf{x}\|_1 \quad \text{subject to: } \mathbf{A}\mathbf{x} = \mathbf{y}, \ \mathbf{x} \geq \mathbf{0}, \ \mathbf{1}^T\mathbf{x} = 1, \tag{2}$$

Notice that $\mathrm{P_{CBP}}$ corresponds to $\mathrm{P_{CSR}}$ with $\lambda \to \infty$.

The CBPDN optimization problem is

$$(\mathrm{P_{CBPDN}}): \quad \min_{\mathbf{x}} \ \|\mathbf{x}\|_1 \quad \text{subject to: } \|\mathbf{A}\mathbf{x}-\mathbf{y}\|_2 \leq \delta, \ \mathbf{x} \geq \mathbf{0}, \ \mathbf{1}^T\mathbf{x} = 1. \tag{3}$$

Problem $\mathrm{P_{CSR}}$ is equivalent to $\mathrm{P_{CBPDN}}$ in the sense that for any choice of δ for which $\mathrm{P_{CBPDN}}$ is feasible, there is a choice of λ for which the solutions of the two problems coincide [19]. Finally, notice that $\mathrm{P_{CBP}}$ corresponds to $\mathrm{P_{CBPDN}}$ with $\delta = 0$.

3. THE ADMM

Consider an unconstrained problem of the form

$$\min_{\mathbf{x}\in\mathbb{R}^n} \ f_1(\mathbf{x}) + f_2(\mathbf{G}\,\mathbf{x}), \tag{4}$$

where $f_1 : \mathbb{R}^n \to \bar{\mathbb{R}}$, $f_2 : \mathbb{R}^p \to \bar{\mathbb{R}}$, and $\mathbf{G} \in \mathbb{R}^{p\times n}$. The ADMM [6, 7, 8], the key tool in this paper, is as shown in Fig. 1. The following is a simplified version of a theorem of Eckstein and Bertsekas stating convergence of ADMM.

Theorem 1 ([6]) *Let $\mathbf{G}$ have full column rank and f_1, f_2 be closed, proper, and convex. Consider arbitrary $\mu > 0$ and $\mathbf{u}_0, \mathbf{d}_0 \in \mathbb{R}^p$. Consider three sequences $\{\mathbf{x}_k \in \mathbb{R}^n, \ k = 0, 1, ...\}$, $\{\mathbf{u}_k \in \mathbb{R}^p, \ k = 0, 1, ...\}$, and $\{\mathbf{d}_k \in \mathbb{R}^p, \ k = 0, 1, ...\}$ that satisfy*

$$\mathbf{x}_{k+1} = \arg\min_{\mathbf{x}} f_1(\mathbf{x}) + \frac{\mu}{2}\|\mathbf{G}\mathbf{x}-\mathbf{u}_k-\mathbf{d}_k\|_2^2 \tag{5}$$

$$\mathbf{u}_{k+1} = \arg\min_{\mathbf{u}} f_2(\mathbf{u}) + \frac{\mu}{2}\|\mathbf{G}\mathbf{x}_{k+1}-\mathbf{u}-\mathbf{d}_k\|_2^2 \tag{6}$$

$$\mathbf{d}_{k+1} = \mathbf{d}_k - (\mathbf{G}\,\mathbf{x}_{k+1} - \mathbf{u}_{k+1}). \tag{7}$$

Then, if (4) has a solution, the sequence $\{\mathbf{x}_k\}$ converges to it; otherwise, at least one of the sequences $\{\mathbf{u}_k\}$ or $\{\mathbf{d}_k\}$ diverges.

Algorithm *ADMM*
1. Set $k = 0$, choose $\mu > 0$, $\mathbf{u}_0$, and $\mathbf{d}_0$.
2. **repeat**
3. $\quad \mathbf{x}_{k+1} \in \arg\min_{\mathbf{x}} f_1(\mathbf{x}) + \frac{\mu}{2}\|\mathbf{G}\,\mathbf{x} - \mathbf{u}_k - \mathbf{d}_k\|_2^2$
4. $\quad \mathbf{u}_{k+1} \in \arg\min_{\mathbf{u}} f_2(\mathbf{u}) + \frac{\mu}{2}\|\mathbf{G}\,\mathbf{x}_{k+1} - \mathbf{u} - \mathbf{d}_k\|_2^2$
5. $\quad \mathbf{d}_{k+1} \leftarrow \mathbf{d}_k - (\mathbf{G}\,\mathbf{x}_{k+1} - \mathbf{u}_{k+1})$
6. $\quad k \leftarrow k + 1$
7. **until** stopping criterion is satisfied.

Fig. 1. The alternating direction method of multipliers (ADMM).

4. APPLICATION OF ADMM

In this section, we specialize the ADMM to each of the optimization problems stated in Section 2.

4.1. ADMM for CSR and CLS: the SUnSAL Algorithm

We start by writing the optimization $\mathrm{P_{CSR}}$ in the equivalent form

$$\min_{\mathbf{x}} \ (1/2)\|\mathbf{A}\mathbf{x}-\mathbf{y}\|_2^2 + \lambda\|\mathbf{x}\|_1 + \iota_{\{1\}}(\mathbf{1}^T\mathbf{x}) + \iota_{\mathbb{R}^n_+}(\mathbf{x}), \tag{8}$$

where ι_S is the indicator function of the set S (*i.e.*, $\iota_S(\mathbf{x}) = 0$ if $\mathbf{x} \in S$ and $\iota_S(\mathbf{x}) = \infty$ if $\mathbf{x} \notin S$). We now apply the ADMM using the following translation table:

$$f_1(\mathbf{x}) \equiv \frac{1}{2}\|\mathbf{A}\mathbf{x}-\mathbf{y}\|_2^2 + \iota_{\{1\}}(\mathbf{1}^T\mathbf{x}) \tag{9}$$

$$f_2(\mathbf{x}) \equiv \lambda\|\mathbf{x}\|_1 + \iota_{\mathbb{R}^n_+}(\mathbf{x}) \tag{10}$$

$$\mathbf{G} \equiv \mathbf{I}. \tag{11}$$

With the current setting, step 3 (Fig. 1) of the ADMM requires solving a quadratic problem with linear equality constraint, the solution of which is

$$\mathbf{x}_{k+1} \leftarrow \mathbf{B}^{-1}\mathbf{w} - \mathbf{C}(\mathbf{1}^T\mathbf{B}^{-1}\mathbf{w} - 1) \tag{12}$$

where

$$\mathbf{B} \equiv \mathbf{A}^T\mathbf{A} + \mu\mathbf{I} \tag{13}$$

$$\mathbf{C} \equiv \mathbf{B}^{-1}\mathbf{1}(\mathbf{1}^T\mathbf{B}^{-1}\mathbf{1})^{-1} \tag{14}$$

$$\mathbf{w} \equiv \mathbf{A}^T\mathbf{y} + \mu(\mathbf{u}_k + \mathbf{d}_k). \tag{15}$$

Step 4 of the ADMM (Fig. 1) is simply

$$\mathbf{u}_{k+1} \leftarrow \arg\min_{\mathbf{u}} \ (1/2)\|\mathbf{u} - \boldsymbol{\nu}_k\|_2^2 + (\lambda/\mu)\|\mathbf{u}\|_1 + \iota_{\mathbb{R}^n_+}(\mathbf{u}) \tag{16}$$

where $\boldsymbol{\nu}_k \equiv \mathbf{x}_{k+1} - \mathbf{d}_k$. Without the term $\iota_{\mathbb{R}^n_+}$, the solution of (16) would be the well-known soft threshold [4]:

$$\mathbf{u}_{k+1} \leftarrow \mathrm{soft}(\boldsymbol{\nu}_k, \lambda/\mu). \tag{17}$$

A straightforward reasoning leads to the conclusion that the effect of the ANC term $\iota_{\mathbb{R}^n_+}$ is to project onto the first orthant, thus

$$\mathbf{u}_{k+1} \leftarrow \max\{\mathbf{0}, \mathrm{soft}(\boldsymbol{\nu}_k, \lambda/\mu)\}, \tag{18}$$

where the maximum is to be understood in the componentwise sense.

Fig. 2 shows the SUnSAL algorithm, which is obtained by replacing lines 3 and 4 of ADMM by (12) and (18), respectively.

The objective function (8) is proper, convex, lower semi-continuous, and coercive, thus it has a non-empty set of minimizers

Algorithm *SUnSAL*
1. Set $k = 0$, choose $\mu > 0$, $\mathbf{u}_0$, and $\mathbf{d}_0$.
2. **repeat**
3. $\quad \mathbf{w} \leftarrow \mathbf{A}^T\mathbf{y} + \mu(\mathbf{u}_k + \mathbf{d}_k)$
4. $\quad \mathbf{x}_{k+1} \leftarrow \mathbf{B}^{-1}\mathbf{w} - \mathbf{C}(\mathbf{1}^T\mathbf{B}^{-1}\mathbf{w} - 1)$
5. $\quad \boldsymbol{\nu}_k \leftarrow \mathbf{x}_{k+1} - \mathbf{d}_k$
6. $\quad \mathbf{u}_{k+1} \leftarrow \max\{\mathbf{0}, \text{soft}(\boldsymbol{\nu}_k, \lambda/\mu)\}$
7. $\quad \mathbf{d}_{k+1} \leftarrow \mathbf{d}_k - (\mathbf{x}_{k+1} - \mathbf{u}_{k+1})$
8. $\quad k \leftarrow k + 1$
9. **until** stopping criterion is satisfied.

Fig. 2. Spectral unmixing by variable slitting and augmented Lagrangian (SUnSAL).

(see [19], for definitions of these convex analysis concepts). Functions f_1 and f_2 in (9) and (10) are closed and $\mathbf{G} \equiv \mathbf{I}$ is obviously of full column rank, thus Theorem 1 can be invoked to ensure convergence of SUnSAL.

Concerning the computational complexity, we refer that, in hyperspectral applications, the rank of matrix $\mathbf{B}$ is no larger that the number of bands, often of the order of a few hundred, thus $\mathbf{B}^{-1}$ can be easily precomputed. The complexity of the algorithm per iteration is thus $O(n^2)$, corresponding to the matrix-vector products.

To solve the CLS problem, we simply run SUnSAL with $\lambda = 0$. Moreover, the ANC (non-negativity constrain) can be turned off by using (17) instead of (18) and the ASC (sum to one constraint) can be deactivated by setting $\mathbf{C} = 0$ in (12).

4.2. ADMM for CBP and CBPDN: the C-SUnSAL Algorithm

Given that the CBP problem corresponds to CBPDN with $\delta = 0$, we address only the latter. Problem P_{CBPDN} is equivalent to

$$\min_{\mathbf{x}} \ \|\mathbf{x}\|_1 + \iota_{B(\mathbf{y},\delta)}(\mathbf{A}\mathbf{x}) + \iota_{\{1\}}(\mathbf{1}^T\mathbf{x}) + \iota_{\mathbb{R}_+}(\mathbf{x}), \tag{19}$$

where $B(\mathbf{y}, \delta) = \{\mathbf{z} : \|\mathbf{z} - \mathbf{y}\|_2 \leq \delta\}$ is a radius-δ closed ball around $\mathbf{y}$. To apply the ADMM we use the following definitions:

$$f_1(\mathbf{x}) = \iota_{\{1\}}(\mathbf{1}^T\mathbf{x}) \tag{20}$$

$$f_2(\mathbf{u}) = \iota_{B(\mathbf{y},\delta)}(\mathbf{u}_1) + \lambda\|\mathbf{u}_2\|_1 + \iota_{\mathbb{R}^n_+}(\mathbf{u}_2) \tag{21}$$

$$\mathbf{G} = [\mathbf{A}^T \ \mathbf{I}]^T. \tag{22}$$

where $\mathbf{u} = [\mathbf{u_1}^T \ \mathbf{u}_2^T]^T$. With the above definitions, the solution of line 3 of ADMM (Fig. 1), a quadratic problem with linear equality constraints, is

$$\mathbf{x}_{k+1} \leftarrow \mathbf{B}^{-1}\mathbf{w} - \mathbf{C}(\mathbf{1}^T\mathbf{B}^{-1}\mathbf{w} - 1), \tag{23}$$

where

$$\mathbf{B} \equiv \mathbf{A}^T\mathbf{A} + \mathbf{I} \tag{24}$$

$$\mathbf{C} \equiv \mathbf{B}^{-1}\mathbf{1}(\mathbf{1}^T\mathbf{B}^{-1}\mathbf{1})^{-1} \tag{25}$$

$$\mathbf{w} \equiv \mathbf{A}^T(\mathbf{u}_{1,k} + \mathbf{d}_{1,k}) + (\mathbf{u}_{2,k} + \mathbf{d}_{2,k}). \tag{26}$$

Because the variables $\mathbf{u}_1$ and $\mathbf{u}_2$ are decoupled, line 4 of ADMM (Fig. 1) consists in solving two separate problems,

$$\mathbf{u}_{1,k+1} \in \arg\min_{\mathbf{u}} \ (1/2)\|\mathbf{u} - \boldsymbol{\nu}_{1,k}\|_2^2 + \iota_{B(\mathbf{y},\delta)}(\mathbf{u}) \tag{27}$$

$$\mathbf{u}_{2,k+1} \in \arg\min_{\mathbf{u}} \ (1/2)\|\mathbf{u} - \boldsymbol{\nu}_{2,k}\|_2^2 + (\lambda/\mu)\|\mathbf{u}\|_1 + \iota_{\mathbb{R}^n_+}(\mathbf{u}) \tag{28}$$

Algorithm *C-SUnSAL*
1. Set $k \leftarrow 0$, choose $\mu > 0$, $\mathbf{u}_{1,0}$, $\mathbf{d}_{1,0}$, $\mathbf{u}_{2,0}$, and $\mathbf{d}_{2,0}$.
2. **repeat**
3. $\quad \mathbf{w} \leftarrow \mathbf{A}^T(\mathbf{u}_{1,k} + \mathbf{d}_{1,k}) + (\mathbf{u}_{2,k} + \mathbf{d}_{2,k})$
4. $\quad \mathbf{x}_{k+1} \leftarrow \mathbf{B}^{-1}\mathbf{w} - \mathbf{C}(\mathbf{1}^T\mathbf{B}^{-1}\mathbf{w} - 1)$
5. $\quad \boldsymbol{\nu}_{1,k} \leftarrow \mathbf{A}\mathbf{x}_{k+1} - \mathbf{d}_{1,k}$
6. $\quad \mathbf{u}_{1,k+1} \leftarrow \psi_B(\mathbf{y}, \delta)(\boldsymbol{\nu}_{1,k})$
7. $\quad \boldsymbol{\nu}_{2,k} \leftarrow \mathbf{x}_{k+1} - \mathbf{d}_{2,k}$
8. $\quad \mathbf{u}_{2,k+1} \leftarrow \max\{\mathbf{0}, \text{soft}(\boldsymbol{\nu}_{2,k}, \lambda/\mu)\}$
9. $\quad \mathbf{d}_{1,k+1} \leftarrow \mathbf{d}_{1,k} - (\mathbf{A}\mathbf{x}_{k+1} - \mathbf{u}_{1,k+1})$
10. $\quad \mathbf{d}_{2,k+1} \leftarrow \mathbf{d}_{2,k} - (\mathbf{x}_{k+1} - \mathbf{u}_{2,k+1})$
11. $\quad k \leftarrow k + 1$
12. **until** stopping criterion is satisfied.

Fig. 3. Constrained spectal unmixing by variable slitting and augmented Lagrangian (C-SUnSAL).

where

$$\boldsymbol{\nu}_{1,k} = \mathbf{A}\mathbf{x}_{k+1} - \mathbf{d}_{1,k} \tag{29}$$

$$\boldsymbol{\nu}_{2,k} = \mathbf{x}_{k+1} - \mathbf{d}_{2,k}. \tag{30}$$

The solution of (27) is the projection onto the ball $B(\mathbf{y}, \delta)$, given by

$$\mathbf{u}_{1,k+1} \leftarrow \psi_B(\mathbf{y}, \delta)(\boldsymbol{\nu}_{1k}) \equiv \begin{cases} \boldsymbol{\nu}_{1k}, & \|\boldsymbol{\nu}_{1,k} - \mathbf{y}\|_2 \leq \delta \\ \mathbf{y} + \frac{\boldsymbol{\nu}_{1,k} - \mathbf{y}}{\|\boldsymbol{\nu}_{1,k} - \mathbf{y}\|_2}\,\delta, & \|\boldsymbol{\nu}_{1,k} - \mathbf{y}\|_2 > \delta. \end{cases} \tag{31}$$

Similarly to (18), the solution of (28) is given by

$$\mathbf{u}_{2,k+1} \leftarrow \max\{\mathbf{0}, \text{soft}(\boldsymbol{\nu}_{2,k}, \lambda/\mu)\}. \tag{32}$$

Fig. 3 shows the C-SUnSAL algorithm for CBPDN, which results from replacing line 3 of ADMM (Fig. 1) by (23) and line 4 of ADMM by (31)–(32). As mentioned above, C-SUnSAL can be used to solve the CBP problem simply by setting $\delta = 0$. As in SUnSAL, the ANC and/or the ASC can be deactivated trivially.

The objective function (19) is proper, convex, lower semi-continuous, and coercive, thus it has a non-empty set of minimizers. Functions f_1 and f_2 in (20) and (21) are closed and $\mathbf{G}$ in (22) is obviously of full column rank, thus Theorem 1 can be invoked to ensure convergence of C-SUnSAL.

Concerning the computational complexity, the scenario is similar to that of SUnSAL, thus complexity of C-SUnSAL is $O(n^2)$ per iteration.

5. EXPERIMENTS

We now report experimental results obtained with simulated data generated according to $\mathbf{y} = \mathbf{A}\mathbf{x} + \mathbf{n}$, where $\mathbf{n} \in \mathbb{R}^k$ models additive perturbations. In hyperspectral applications, these perturbations are mostly model errors dominated by low-pass components. For this reason, we generate the noise by low-pass filtering samples of zero-mean i.i.d. Gaussian sequences of random variables. We define the signal-to-noise ratio (SNR) as

$$\text{SNR} \equiv 10\log_{10}\left(\frac{\mathbb{E}[\|\mathbf{A}\mathbf{x}\|_2^2]}{\mathbb{E}[\|\mathbf{n}\|_2^2]}\right).$$

The expectations in the above definition are approximated with sample means over 10 runs. The original fractional abundance vectors $\mathbf{x}$ are generated in the following way: given s, the number of non-zero components in $\mathbf{x}$, we generate random samples uniformly in the $(s-1)-$simplex and distribute randomly these s values among the

Table 1. RSNR values and execution times for the Gaussian library defined in the text (average over 10 runs).

	SUnSAL		C-SUnSAL		`lsqnonneg`	
SNR (dB)	RSNR (dB)	time (sec)	RSNR (dB)	time (sec)	RSNR	time (sec)
20	**10**	0.12	3	0.12	3	31
30	**32**	0.12	27	0.12	25	32
40	**37**	0.12	30	0.12	27	48
50	**48**	0.12	47	0.12	42	57

Table 2. RSNR values and execution times for the USGS library (average over 10 runs).

	SUnSAL		C-SUnSAL		`lsqnonneg`	
SNR (dB)	RSNR (dB)	time (sec)	RSNR (dB)	time (sec)	RSNR	time (sec)
30	**6**	0.13	1.5	0.13	-7	22
40	**17**	0.13	12.2	0.13	10	32
50	**23**	0.13	14.5	0.13	15	47

components of $\mathbf{x}$. We considered two libraries (*i.e.,* matrices $\mathbf{A}$): a 200×400 matrix with zero-mean unit variance i.i.d. Gaussian entries and a 224×498 matrix with a selection of 498 materials (different mineral types) from the USGS library denoted splib06[1].

As far as we know, there are no special purpose algorithms for solving the CSR, CBP, and CBPDN problems. Of course these are canonical convex problems, thus they can be tackled with standard convex optimization techniques. Namely, the CLS, which is a particular case of CSR, can be solved with the MATLAB function `lsqnonneg`, which we use as baseline in our comparisons.

Tables 1 and 2 report reconstruction SNR (RSNR), defined as

$$\text{RSNR} = 10 \log_{10} \left(\frac{\mathbb{E}[\|\mathbf{x}\|_2^2]}{\mathbb{E}[\|\mathbf{x} - \widehat{\mathbf{x}}\|_2^2]} \right),$$

where $\widehat{\mathbf{x}}$ is the estimated fractional abundance vector, and execution times, for the two libraries referred above. The `lsqnonneg` is run with its default options. SUnSAL and C-SUnSAL run 200 iterations, which was found to be more than enough to achieve convergence.

We highlight the following conclusions: (**a**) the proposed algorithms achieve higher accuracy in about two orders of magnitude shorter time. This is a critical issue in imaging application where an instance of the problem has to be solved for each pixel; (**b**) the lower accuracy obtained with the USGS matrix is due to the fact that the spectral signatures are highly correlated resulting in a much harder problem than with the Gaussian matrix.

6. CONCLUDING REMARKS

In this paper, we introduced new algorithms to solve a class of optimization problems arising in spectral unmixing. The proposed algorithms are based on the *alternating direction method of multipliers*, which decomposes a difficult problem into a sequence of simpler ones. We showed that sufficient conditions for convergence are satisfied. In limited set of experiments, the proposed algorithms were shown to clearly outperform an off-the-shelf optimization tool. Ongoing work includes a comprehensive experimental evaluation of the proposed algorithms.

[1] http://speclab.cr.usgs.gov/spectral.lib06

7. REFERENCES

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