A perturbed linear mixing model accounting for spectral variability

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ABSTRACT

Hyperspectral unmixing aims at determining the reference spectral signatures composing a hyperspectral image, their abundance fractions and their number. In practice, the spectral variability of the identified signatures induces significant abundance estimation errors. To address this issue, this paper introduces a new linear mixing model explicitly accounting for this phenomenon. In this setting, the extracted endmembers are interpreted as possibly corrupted versions of the true endmembers. The parameters of this model can be estimated using an optimization algorithm based on the alternating direction method of multipliers. The performance of the proposed unmixing method is evaluated on synthetic and real data.

Index Terms—Hyperspectral imagery, linear unmixing, endmember variability, Alternating Direction Method of Multipliers (ADMM).

1. INTRODUCTION

Hyperspectral unmixing consists of identifying the spectral signatures from which the data are derived—referred to as endmembers—their abundances and their number according to a predefined mixing model. Assuming no microscopic interaction between the materials of the imaged scene, a linear mixing model (LMM) is known to be adapted to describe the data structure [1]. However, the spectral signatures contained in a reference pixel can vary spectrally from a pixel to another due to the varying acquisition conditions. This can result in significant estimation errors being propagated throughout the unmixing process. Various models either derived from a statistical or a deterministic point of view have been designed to address this issue [2].

Since the identified signatures can be considered as variable instances of reference endmembers, we introduce an extended version of the classical LMM to model the spectral variability. In [3], the variability is assumed to only result from scaling factors. Conversely, in this paper, inspired by a model designed in [4], each endmember is represented by a “pure” spectral signature corrupted by an additive perturbation accounting for spectral variability. The perturbation is allowed to vary from a pixel to another to represent spatial-spectral variability within the image. To the best of our knowledge, it is the first time endmember variability has been explicitly modeled as an additive perturbation. Finally, the results obtained with the ADMM in hyperspectral imagery [5] and in image deblurring [6, 7] have motivated the use of a similar framework for spectral unmixing using a perturbed LMM (PLMM).

The paper is organized as follows. The proposed PLMM is introduced in Section 2. Section 3 describes an ADMM-based algorithm to estimate the parameters of this model. Experimental results obtained on synthetic and real data are reported in Section 4 and 5 respectively. Section 6 finally concludes this work.

2. PROBLEM STATEMENT

2.1. Perturbed linear mixing model (PLMM)

Each pixel $y_n$ of a hyperspectral image is represented by a linear combination of $K$ endmembers—denoted by $m_k$—affected by a spatially varying perturbation vector $d m_{n,k}$ accounting for endmember variability. The resulting PLMM can be written

$$ y_n = \sum_{k=1}^{K} a_{kn} (m_k + d m_{n,k}) + b_n \quad \text{for} \quad n = 1, \ldots, N \quad (1) $$

where $L$ is the number of spectral bands, $N$ is the number of pixels, $y_n$ denotes the $n$th image pixel, $m_k$ is the $k$th endmember, $a_{kn}$ is the proportion of the $k$th endmember in the $n$th pixel, and $d m_{n,k}$ denotes the perturbation of the $k$th endmember in the $n$th pixel. The term $b_n$ represents the noise resulting from the data acquisition and the modeling errors.

In matrix form, the PLMM (1) can be written as follows

$$ Y = MA + \left[ \begin{array}{c} \Delta \end{array} \right] + B \quad (2) $$

where $Y = [y_1, \ldots, y_N]$ is an $L \times N$ matrix containing the image pixels, $M$ is an $L \times K$ matrix containing the endmembers $m_k$, $A$ is a $K \times N$ matrix composed of the abundance vectors $a_n$, $dM_n$ is an $L \times K$ matrix whose columns are
the perturbation vectors \( d_{n,k} \) associated with the \( n \)th pixel, and \( B \) is an \( L \times N \) matrix accounting for the noise. The non-negativity and sum-to-one constraints usually considered to reflect physical considerations are

\[
\mathbf{A} \succeq \mathbf{0}_{K,N}, \quad \mathbf{A}^T \mathbf{1}_K = 1_N \\
\mathbf{M} \succeq \mathbf{0}_{L,K}, \quad \mathbf{M} + \mathbf{dM}_n \succeq \mathbf{0}_{L,K}, \quad \forall n = 1, \ldots, N. \tag{3}
\]

where \( \succeq \) denotes term-wise inequality. When compared to models found in the literature to mitigate the variability impact [2], the model (1) presents the advantage to explicitly address the variability phenomenon. Besides, the variability is not assumed to only result from scaling factors as in [3].

2.2. Problem formulation

The PLMM (1) and constraints (3) can be combined to form a constrained optimization problem. We propose to define the data fitting term as the Frobenius distance between the observations and the reconstructed data. Since the problem is ill-posed, we introduce penalization functions \( \Phi, \Psi \) and \( \Upsilon \) to reflect the a priori knowledge on \( \mathbf{M}, \mathbf{A} \) and \( \mathbf{dM} \) respectively. As a result, the optimization problem is expressed as

\[
(\mathbf{M}^*, \mathbf{dM}^*, \mathbf{A}^*) = \arg \min_{\mathbf{M}, \mathbf{dM}, \mathbf{A}} \left\{ J(\mathbf{M}, \mathbf{dM}, \mathbf{A}) \text{ s.t. } (3) \right\} \tag{4}
\]

with

\[
J(\mathbf{M}, \mathbf{dM}, \mathbf{A}) = \frac{1}{2} \| \mathbf{Y} - \mathbf{MA} - \Delta \|_F^2 + \alpha \Phi(\mathbf{A}) + \beta \Psi(\mathbf{M}) + \gamma \Upsilon(\mathbf{dM}) \tag{5}
\]

where the penalization parameters \( \alpha, \beta, \gamma \) control the trade-off between the data fitting term and the penalties \( \Phi(\mathbf{A}), \Psi(\mathbf{M}) \) and \( \Upsilon(\mathbf{dM}) \). In addition, we assume that the penalization functions are separable, leading to

\[
\Phi(\mathbf{A}) = \sum_{n=1}^N \phi(a_n), \quad \Psi(\mathbf{M}) = \sum_{\ell=1}^L \psi(\tilde{\mathbf{m}}_\ell), \quad \Upsilon(\mathbf{dM}) = \sum_{n=1}^N \upsilon(\mathbf{dM}_n) \tag{6}
\]

where \( \phi, \psi \) and \( \upsilon \) are non-negative differentiable convex functions, and \( \tilde{\mathbf{m}}_\ell \) denotes the \( \ell \)th row of \( \mathbf{M} \). This assumption is used to decompose (4) into a collection of sub-problems described in Section 3. All these penalizations are described in the next paragraphs.

2.2.1. Abundance penalization

The abundance penalization \( \Phi \) has been chosen to promote spatially smooth abundances as in [8]. More precisely, the abundance spatial smoothness penalization is written in matrix form as

\[
\Phi(\mathbf{A}) = \frac{1}{2} \| \mathbf{AH} \|_F^2 \tag{7}
\]

where \( \mathbf{H} \in \mathbb{R}^{N \times 4N} \) is a matrix computing the differences between the abundances of a given pixel and those of its 4 nearest neighbors [8]. The only terms depending on the \( n \)th abundance vector \( a_n \) are

\[
\phi(a_n) = \frac{1}{2} \left( \sum_{k=0}^3 h_k a_{n,k} \right) \| a_n \|_2^2 + \left( \sum_{k=0}^3 h_k a_{n,k} \right) \sum_{i=0}^N \sum_{j=0}^N g_{n,k} a_{i,j} \right) a_n. \tag{8}
\]

2.2.2. Endmember penalization

As for \( \Psi \), classical penalizations found in the literature consist of constraining the size of the simplex whose vertices are the endmember signatures. The mutual distance between each endmember introduced in [9] approximates the volume occupied by the \((K-1)\)-simplex and is expressed as

\[
\Psi(\mathbf{M}) = \frac{1}{2} \sum_{i \neq j} \| m_i - m_j \|_2^2 = \frac{1}{2} \sum_{k=1}^K \| \mathbf{MG}_k \|_F^2 \tag{9}
\]

where

\[
\mathbf{G}_k = -\mathbf{I}_K + e_k \mathbf{I}_K^T \tag{10}
\]

for \( k = 1, \ldots, K \) and \( e_k \) denotes the \( k \)th canonical basis vector of \( \mathbb{R}^K \). Hence

\[
\psi(\tilde{\mathbf{m}}_\ell) = \frac{1}{2} \sum_{k=1}^K \| \tilde{\mathbf{m}}_\ell \mathbf{G}_k \|_2^2. \tag{11}
\]

2.2.3. Variability penalization

The function \( \Upsilon \) has been designed to limit the norm of the spectral variability in order to capture a reasonable endmember variability level. In this paper, we propose to consider

\[
\upsilon(\mathbf{dM}_n) = \frac{1}{2} \| \mathbf{dM}_n \|_2^2. \tag{12}
\]

3. AN ADMM-BASED ALGORITHM

Since the problem (4) is non-convex, the cost function \( J \) has been successively minimized with respect to each variable \( \mathbf{A}, \mathbf{M} \) and \( \mathbf{dM} \) until a stopping criterion is satisfied [6]. The assumptions made on \( \Phi, \Psi, \Upsilon \) in Section 2 allow the global optimization problem to be further decomposed into a collection of convex sub-problems exclusively involving differentiable functions. These sub-problems are finally solved using ADMM steps. The resulting algorithmic scheme is summarized in Algo 1. Some considerations about the convergence of the proposed algorithm are provided in an extended version of this paper [10].
3.1. Optimization with respect to $A$

With the assumptions made in paragraph 2.2, optimizing $J$ with respect to $A$ under the constraints (3) is equivalent to solving

$$a_n^* = \arg \min_{a_n} \left\{ \frac{1}{2} \| y_n - (M + dM_n)a_n \|_2^2 + \alpha \phi(a_n) \right\}, \quad \text{s.t. } a_n \geq 0, \quad a_n^T 1_K = 1$$

(13)

After introducing the splitting variables $w_n^{(A)} \in \mathbb{R}^K$ for $n = 1, \ldots, N$ such that

$$\begin{pmatrix} 1_K \\ 0_K \end{pmatrix} a_n + \begin{pmatrix} -1_K \\ I_K \end{pmatrix} w_n = \begin{pmatrix} 0_K \\ 1 \end{pmatrix},$$

(14)

the resulting scaled augmented Lagrangian is expressed as

$$\mathcal{L}_{\mu_n}^{(A)}(a_n, w_n^{(A)}, \lambda_n^{(A)}) = \frac{1}{2} \| y_n - (M + dM_n)a_n \|_2^2 + \frac{\mu_n^{(A)}}{2} \| Qa_n + R w_n^{(A)} - s + \lambda_n^{(A)} \|_2^2 + \alpha \phi(a_n) + I_{K,1}^+ \left( w_n^{(A)} \right)$$

(15)

where $\mu_n^{(A)} > 0$ and $I_{K,1}^+$ is the indicator function on $(\mathbb{R}^+)^K$. Thus, for $n = 1, \ldots, N$,

$$a_n^* = \left[ (M + dM_n)^T (M + dM_n) + \mu_n^{(A)} Q^T Q + \alpha c_n I_K \right]^{-1} \begin{pmatrix} (M + dM_n)^T y_n - \alpha c_n + \mu_n^{(A)} Q^T (s - R w_n^{(A)} - \lambda_n^{(A)}) \end{pmatrix}$$

(16)

and

$$w_n^{(A)*} = \max \left( a_n + \lambda_n^{(A)}_{n,1,K}, 0 \right)$$

(17)

where $\lambda_n^{(A)}_{n,1,K}$ is the vector composed of the $K$ first elements of $\lambda_n^{(A)}$ and the max should be understood as a term-wise operator. In the absence of any penalization, the solution is obtained by making $\alpha = 0$ in the previous equations.

3.2. Optimization with respect to $M$

Similarly, optimizing $J$ with respect to $M$ under the constraints (3) is equivalent to solving

$$\mathcal{L}_{\mu}^{(M)}(\tilde{m}_\ell, W_{\ell}^{(M)}, dM_{\ell}) = \frac{1}{2} \| \tilde{y}_\ell - \tilde{m}_\ell A - \tilde{\delta}_\ell \|_2^2 + \beta \psi(\tilde{m}_\ell)$$

(18)

the associated scaled augmented Lagrangian can be written

$$\mathcal{L}_{\mu}^{(M)}(\tilde{m}_\ell, W_{\ell}^{(M)}, dM_{\ell}) = \frac{1}{2} \| \tilde{y}_\ell - \tilde{m}_\ell A - \tilde{\delta}_\ell \|_2^2 + \frac{\mu_{\ell}^{(M)}}{2} \left( \| \tilde{m}_\ell - W_{\ell}^{(M)} \|_F^2 + F_{\ell} \right)$$

(19)

$$+ \beta \psi(\tilde{m}_\ell) + I_{N+1,K}^+(W_{\ell}^{(M)})$$

with $\mu_{\ell}^{(M)} > 0$ and $I_{N+1,K}^+$ the indicator function on $(\mathbb{R}^+)^{N+1 \times K}$. Thus

$$\tilde{m}_\ell^* = \left[ \tilde{y}_\ell - \tilde{\delta}_\ell, A^T + \mu_{\ell}^{(M)} e^T (W_{\ell}^{(M)} - F_{\ell} - \Lambda_{\ell}^{(M)}) \right]$$

(20)

$$\left[ A A^T + \beta \sum_{k=1}^K G_k G_k^T + \mu_{\ell}^{(M)} (e^T e) I_K \right]^{-1}$$

(21)

and

$$W_{\ell}^{(M)*} = \max \left( \epsilon \tilde{m}_\ell + F_{\ell} + \Lambda_{\ell}^{(M)}, O_{(N+1),K} \right).$$

In the absence of any endmember penalization, the solution is obtained by making $\beta = 0$ in the previous equation.

3.3. Optimization with respect to $dM$

Finally, optimizing $J$ with respect to $dM$ under the constraint (3) is equivalent to solving

$$dM_n^* = \arg \min_{dM_n} \left\{ \frac{1}{2} \| y_n - (M + dM_n)a_n \|_2^2 \right\}_{\gamma}$$

(23)

$$+ \gamma \psi(dM_n) \quad \text{s.t. } M + dM_n \succeq O_{L,K}$$

where $O_{L,K}$ is the identity matrix of size $L \times K$. The solution is obtained by making $\gamma = 0$ in the previous equation.
for \( n = 1, \ldots, N \). Introducing the splitting variables
\[
W_n^{(dM)} = M + dM_n,
\]
the resulting scaled augmented Lagrangian is given by
\[
L_{\mu_n^{(dM)}} \left( dM, W_n^{(dM)}, \Lambda_n^{(dM)} \right) = I_{L,K}^+ \left( W_n^{(dM)} \right)
+ \frac{1}{2} \| y_n - (M + dM_n) a_n \|_2^2 + \gamma \tau (dM_n)
+ \frac{\mu_n^{(dM)}}{2} \| dM_n + M - W_n^{(dM)} + \Lambda_n^{(dM)} \|_F^2
\]
with \( \mu_n^{(dM)} > 0 \) and \( I_{L,K}^+ \) the indicator function on \((\mathbb{R}_+)^{L \times K}\).

Hence
\[
dM_n = \left[ (y_n - Ma_n)^T + \mu_n^{(dM)} \left( W_n^{(dM)} - M - \Lambda_n^{(dM)} \right) \right] a_n a_n^T + (\mu_n^{(dM)} + \gamma) I_{K}^{-1}
\]
and
\[
W_n^{(dM)*} = \max \left( dM_n + M + \Lambda_n^{(dM)}, O_{L,K} \right).
\]

4. EXPERIMENTS WITH SYNTHETIC DATA

The method is first evaluated on a 128 × 64-pixel image resulting from linear mixtures of 3 endmembers with \( L = 160 \) spectral bands, without any pure pixel to evaluate the method in a challenging situation. Any mixture has been corrupted by an additive white Gaussian noise to ensure a signal-to-noise ratio of 30dB. The corrupted endmembers involved in the mixture have been generated using the product of reference endmembers with randomly generated piecewise-affine functions. Different affine functions have been considered for each endmember in each pixel, which provides realistic endmembers with controlled variability 1.

4.1. State-of-the-art methods

The proposed method is compared to the VCA [11] / FCLS [12] algorithms and to the automated endmember bundles (AEB, [13]). For the proposed method, the endmembers and abundances have been initialized with VCA/FCLS and the variability matrices have been initialized with all their entries equal to \( \epsilon_{ps}^2 \). The algorithm is stopped when the relative difference between two successive values of the objective function is less than \( 10^{-3} \). The regularization parameters associated with the augmented Lagrangians have been initialized with the following values: \( \mu_n^{(A)}(0) = \mu_n^{(dM)}(0) = 10^{-4} \), \( \mu_n^{(M)}(0) = 10^{-8} \), and adjusted using the rule described in [14, p. 20] with \( \tau_{\text{incr}} = \tau_{\text{decr}} = 1.1, \mu = 10, \epsilon_{\text{abs}} = 10^{-1} \) and \( \epsilon_{\text{rel}} = 10^{-4} \).

\[1\] More simulations results are available in [10].

\[2\] MATLAB constant \( \epsilon_{ps} = 2.22 \times 10^{-16} \).

### Table 1. Simulation results for synthetic data (GMSE(A)×10^{-2}, GMSE(dM)×10^{-4}, RE×10^{-4}).

<table>
<thead>
<tr>
<th>Method</th>
<th>VCA/FCLS</th>
<th>AEB</th>
<th>Proposed method</th>
</tr>
</thead>
<tbody>
<tr>
<td>aSAM(M)</td>
<td>5.0639</td>
<td>5.1104</td>
<td>4.1543</td>
</tr>
<tr>
<td>GMSE(A)</td>
<td>2.07</td>
<td>2.11</td>
<td>1.44</td>
</tr>
<tr>
<td>GMSE(dM)</td>
<td>/</td>
<td>/</td>
<td>4.36</td>
</tr>
<tr>
<td>RE</td>
<td>2.66</td>
<td>2.66</td>
<td>0.38</td>
</tr>
<tr>
<td>time (s)</td>
<td>1</td>
<td>33</td>
<td>1990</td>
</tr>
</tbody>
</table>

The performance of the algorithm has been assessed in terms of endmember estimation using the average spectral angle mapper (aSAM). In terms of abundance and perturbation estimations, global mean square errors (GMSEs) have been computed. Finally, the reconstruction error (RE) detailed in the following lines has been considered as a measure of fit.

\[
aSAM(M) = \frac{1}{K} \sum_{k=1}^{K} \frac{\| m_k - \hat{m}_k \|}{\| m_k \|} \| \hat{m}_k \|_2
\]

\[
\text{GMSE}(dM) = \frac{1}{NLK} \sum_{n=1}^{N} \| dM_n - \hat{dM}_n \|_F^2
\]

\[
\text{GMSE}(A) = \frac{1}{KN} \| A - \hat{A} \|_F^2
\]

\[
\text{RE} = \frac{1}{LN} \| Y - \hat{Y} \|_F^2
\]

where \( \hat{Y} \) is the matrix formed by the pixels reconstructed with the estimated parameters \( \hat{A}, \hat{M} \) and \( \hat{dM}_n \).

4.2. Results

The performance measures returned by the unmixing methods are provided in Table 1. The proposed method provides competitive results when compared to other methods and exhibits lower REs, at the price of a higher computational cost.

### Table 2. Experiments conducted on real data (Madonna) (RE ×10^{-6}).

<table>
<thead>
<tr>
<th>Method</th>
<th>VCA/FCLS</th>
<th>AEB</th>
<th>ADMM</th>
</tr>
</thead>
<tbody>
<tr>
<td>RE</td>
<td>8.64</td>
<td>5.25</td>
<td>0.43</td>
</tr>
<tr>
<td>time (s)</td>
<td>0.41</td>
<td>1.77</td>
<td>1.88</td>
</tr>
</tbody>
</table>

5. EXPERIMENTS WITH REAL DATA

Keeping the same parameters as in Section 4, the proposed algorithm has been applied to a data-set (31 × 30) composed of 160 spectral bands extracted from an image acquired in 2010 by the Hyspex hyperspectral scanner over Villelongue, France. The image is composed of forested and urban areas.
Since there is no ground truth for this data set, we present the unmixing performance in terms of reconstruction error (see Table 2). The results depicted in Figs. 1 and 2 are consistent with those of VCA/FCLS. Moreover, regular vertical patterns almost surely due to a sensor defect or miscalibration during the data post-processing appear on the energy map of the variability terms. This observation is consistent with the remark made in [15].

6. CONCLUSION AND FUTURE WORK

This paper introduced a new linear mixing model including an additive spatially varying perturbation matrix to capture endmember variability. Hyperspectral unmixing was performed by alternating minimization of an appropriately regularized cost function, each minimization being performed by ADMM. Simulations conducted on synthetic and real data enabled the interest of the proposed solution to be appreciated. The choice of the penalization parameters $\alpha, \beta$ and $\gamma$ was performed by cross validation. The development of automatic strategies to estimate these parameters remains an open problem.

REFERENCES


