

Multi-Band Image Fusion Based on Spectral Unmixing

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Abstract

This paper presents a multi-band image fusion algorithm based on unsupervised spectral unmixing for combining a high-spatial low-spectral resolution image and a low-spatial high-spectral resolution image. The widely used linear observation model (with additive Gaussian noise) is combined with the linear spectral mixture model to form the likelihoods of the observations. The non-negativity and sum-to-one constraints resulting from the intrinsic physical properties of the abundances are introduced as prior information to regularize this ill-posed problem. The joint fusion and unmixing problem is then formulated as maximizing the joint posterior distribution with respect to the endmember signatures and abundance maps. This optimization problem is attacked with an alternating optimization strategy. The two resulting sub-problems are convex and are solved efficiently using the alternating direction method of multipliers. Experiments are conducted for both synthetic and semi-real data. Simulation results show that the proposed unmixing based fusion scheme improves both the abundance and endmember estimation comparing with the state-of-the-art joint fusion and unmixing algorithms.

Index Terms

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Multi-band image fusion, Bayesian estimation, block circulant matrix, Sylvester equation, alternating direction method of multipliers, block coordinate descent.

I. INTRODUCTION

Fusing multiple multi-band images enables a synergetic exploitation of complementary information obtained by sensors of different spectral ranges and different spatial resolutions. In general, a multi-band image can be represented as a three-dimensional data cube indexed by three exploratory variables (x, y, λ) , where x and y are the two spatial dimensions of the scene, and λ is the spectral dimension (covering a range of wavelengths). Typical examples of multi-band images include hyperspectral (HS) images [2], multi-spectral (MS) images [3], integral field spectrographs [4], magnetic resonance spectroscopy images [5]. However, multi-band images with high spectral resolution generally suffers from the limited spatial resolution of the data acquisition devices, mainly due to physical and technological reasons. These limitations make it infeasible to acquire a high spectral resolution multi-band image with a spatial resolution comparable to those of MS and panchromatic (PAN) images (which are acquired in much fewer bands) [6]. For example, HS images benefit from excellent spectroscopic properties with several hundreds or thousands of contiguous bands but are limited by their relatively low spatial resolution [7]. As a consequence, reconstructing a high-spatial and high-spectral multi-band image from multiple and complementary observed images, although challenging, is a crucial inverse problem that has been addressed in various scenarios. In particular, fusing a high-spatial low-spectral resolution image and a low-spatial high-spectral image is an archetypal instance of multi-band image reconstruction, such as pansharpening (MS+PAN) [8] or HS pansharpening (HS+PAN) [9]. The interested reader is invited to consult the references [8] and [9] for an overview of the HS pansharpening problems and corresponding fusion algorithms.

In general, the degradation mechanisms in HS, MS, and PAN imaging, with respect to (w.r.t.) the target high-spatial and high-spectral image can be summarized as spatial and spectral transformations. Thus, the multi-band image fusion problem can be interpreted as restoring a three dimensional data-cube from two degraded data-cubes, which is an inverse problem. As this inverse problem is generally ill-posed, introducing prior distributions (reg-

ularizers in the the regularization framework) to regularize the target image has been widely explored [10]–[12]. Regarding regularization, the usual high spectral and spatial correlations of the target images imply that they admit sparse or low rank representations, which has in fact been exploited in, for example, [10]–[17].

In [14], a *maximum a posterior* (MAP) estimator incorporating a stochastic mixing model has been designed for the fusion of HS and MS images. In [18], a non-negative sparse promoting algorithm for fusing HS and RGB images has been developed by using an alternating optimization algorithm. However, both approaches developed in [14] and [18] require a very basic assumption that a low spatial resolution pixel is obtained by averaging the high resolution pixels belonging to the same area, whose size depends the downsampling ratio. This nontrivial assumption implies that the fusion of two multi-band images can be divided into fusing small blocks, which greatly decreases the complexity of the overall problem. Note that this assumption has also been used in [17], [19], [20]. However, this averaging assumption can be violated easily as the area in a high resolution image corresponding to a low resolution pixel can be arbitrarily large (depending on the spatial blurring) and the downsampling ratio is generally fixed (depending on the sensor physical characteristics).

To overcome this limitation, a more general forward model, which formulates the blurring and downsampling as two separate operations, has been recently developed and widely used [9], [10], [12], [15], [21], [22]. Based on this model, a non-negative matrix factorization pansharpener of HS image has been proposed in [21]. Similar works have been developed independently in [16], [23], [24]. Later, Yokoya *et al.* have proposed to use a coupled nonnegative matrix factorization (CNMF) unmixing for the fusion of low-spatial-resolution HS and high-spatial-resolution MS data, where both HS and MS data are alternately unmixed into endmember and abundance matrices by the CNMF algorithm [15]. Though this algorithm is rooted in physical principles and easy to implement owing to its simple update rules, it does not use the abundances estimated from the HS image and the endmember signatures estimated from the MS image, which makes the spectral and spatial information in both images not fully exploited. It is worthy to note that a similar fusion and unmixing framework was recently introduced in [25], in which the alternating NMF steps in CNMF were replaced by alternating proximal forward-backward steps.

In this work, we formulate the unmixing based multi-band image fusion problem as an inverse problem in which the regularization is implicitly imposed by a low rank representation inherent to the linear spectral mixture model and by non-negativity and sum-to-one constraints resulting from the intrinsic physical properties of the abundances. In the proposed approach, the endmember signatures and abundances are jointly estimated from the observed multi-band images. The optimization w.r.t. the endmember signatures and the abundances are both constrained linear regression problems, which can be solved efficiently by the alternating direction method of multipliers (ADMM).

The remaining of this paper is organized as follows. Section II gives a short introduction of the widely used linear mixture model and forward model for multi-band images. Section III formulates the unmixing based fusion problem as an optimization problem, which is solved using the Bayesian framework by introducing the popular constraints associated with the endmembers and abundances. The proposed fast alternating optimization algorithm is presented in Section IV. Section V presents experimental results assessing the accuracy and the numerical efficiency of the proposed method. Conclusions are finally reported in Section VI.

II. PROBLEM STATEMENT

To better distinguish spectral and spatial properties, the pixels of the target multi-band image, which is of high-spatial and high-spectral resolution, can be rearranged to build an $m_\lambda \times n$ matrix \mathbf{X} , where m_λ is the number of spectral bands and $n = n_r \times n_c$ is the number of pixels in each band (n_r and n_c represent the numbers of rows and columns respectively). In other words, each column of the matrix \mathbf{X} consists of a m_λ -valued pixel and each row gathers all the pixel values in a given spectral band.

A. Linear Mixture Model

This work exploits an intrinsic property of multi-band images, according to which each spectral vector of an image can be represented by a linear mixture of several spectral signatures, referred to as endmembers. Mathematically, we have

$$\mathbf{X} = \mathbf{MA} \tag{1}$$

where $\mathbf{M} \in \mathbb{R}^{m_\lambda \times p}$ is the endmember matrix whose columns are spectral signatures and $\mathbf{A} \in \mathbb{R}^{p \times n}$ is the corresponding abundance matrix whose columns are abundance fractions. This linear mixture model has been widely used in HS unmixing (see [26] for a detailed review).

B. Forward Model

Based on the pixel ordering introduced at the beginning of Section II, any linear operation applied to the left (resp. right) side of \mathbf{X} describes a spectral (resp. spatial) degradation action. In this work, we assume that two complementary images of high-spectral or high-spatial resolutions, respectively, are available to reconstruct the target high-spectral and high-spatial resolution target image. These images result from linear spectral and spatial degradations of the full resolution image \mathbf{X} , according to the popular models

$$\begin{aligned}\mathbf{Y}_M &= \mathbf{R}\mathbf{X} + \mathbf{N}_M \\ \mathbf{Y}_H &= \mathbf{X}\mathbf{B}\mathbf{S} + \mathbf{N}_H\end{aligned}\tag{2}$$

where

- $\mathbf{X} \in \mathbb{R}^{m_\lambda \times n}$ is the full resolution target image as described in Section II-A.
- $\mathbf{Y}_M \in \mathbb{R}^{n_\lambda \times n}$ and $\mathbf{Y}_H \in \mathbb{R}^{m_\lambda \times m}$ are the observed spectrally degraded and spatially degraded images.
- $\mathbf{R} \in \mathbb{R}^{n_\lambda \times m_\lambda}$ is the spectral response of the MS sensor, which can be *a priori* known or estimated by cross-calibration [27].
- $\mathbf{B} \in \mathbb{R}^{n \times n}$ is a cyclic convolution operator acting on the bands.
- $\mathbf{S} \in \mathbb{R}^{n \times m}$ is a d uniform downsampling operator (it has $m = n/d$ ones and zeros elsewhere), which satisfies $\mathbf{S}^T\mathbf{S} = \mathbf{I}_m$.
- \mathbf{N}_M and \mathbf{N}_H are additive terms that include both modeling errors and sensor noises.

The noise matrices are assumed to be distributed according to the following matrix normal distributions¹

$$\begin{aligned}\mathbf{N}_M &\sim \mathcal{MN}_{m_\lambda, m}(\mathbf{0}_{m_\lambda, m}, \mathbf{\Lambda}_M, \mathbf{I}_m) \\ \mathbf{N}_H &\sim \mathcal{MN}_{n_\lambda, n}(\mathbf{0}_{n_\lambda, n}, \mathbf{\Lambda}_H, \mathbf{I}_n)\end{aligned}$$

where $\mathbf{0}_{a,b}$ is an $a \times b$ matrix of zeros and \mathbf{I}_a is the $a \times a$ identity matrix. The column covariance matrices are assumed to be the identity matrix to reflect the fact that the noise is pixel-independent. The row covariance matrices $\mathbf{\Lambda}_M$ and $\mathbf{\Lambda}_H$ are assumed to be diagonal matrices, whose diagonal elements can vary depending on the noise powers in the different bands. More specifically, $\mathbf{\Lambda}_H = \text{diag}[s_{H,1}^2, \dots, s_{H,m_\lambda}^2]$ and $\mathbf{\Lambda}_M = \text{diag}[s_{M,1}^2, \dots, s_{M,n_\lambda}^2]$, where diag is an operator transforming a vector into a diagonal matrix, whose diagonal terms are the elements of this vector.

The matrix equation (2) has been widely advocated for the pansharpening and HS pansharpening problems, which consist of fusing a PAN image with an MS or an HS image [9], [28], [29]. Similarly, most of the techniques developed to fuse MS and HS images also rely on a similar linear model [11], [15], [30]–[34]. From an application point of view, this model is also important as motivated by recent national programs, e.g., the Japanese next-generation space-borne HS image suite (HISUI), which acquires and fuses the co-registered HS and MS images for the same scene under the same conditions, following this linear model [35].

C. Composite Fusion Model

Combining the linear mixture model (1) and the forward model (2) leads to

$$\begin{aligned}\mathbf{Y}_M &= \mathbf{RMA} + \mathbf{N}_M \\ \mathbf{Y}_H &= \mathbf{MABS} + \mathbf{N}_H\end{aligned}\tag{3}$$

where all matrix dimensions and their respective relations are summarized in Table I.

Note that the matrix \mathbf{M} can be selected from a known spectral library [36] or estimated

¹The probability density function $p(\mathbf{X}|\mathbf{M}, \mathbf{\Sigma}_r, \mathbf{\Sigma}_c)$ of a matrix normal distribution $\mathcal{MN}_{r,c}(\mathbf{M}, \mathbf{\Sigma}_r, \mathbf{\Sigma}_c)$ is defined by

$$p(\mathbf{X}|\mathbf{M}, \mathbf{\Sigma}_r, \mathbf{\Sigma}_c) = \frac{\exp\left(-\frac{1}{2}\text{tr}\left[\mathbf{\Sigma}_c^{-1}(\mathbf{X} - \mathbf{M})^T \mathbf{\Sigma}_r^{-1}(\mathbf{X} - \mathbf{M})\right]\right)}{(2\pi)^{rc/2} |\mathbf{\Sigma}_c|^{r/2} |\mathbf{\Sigma}_r|^{c/2}}$$

where $\mathbf{M} \in \mathbb{R}^{r \times c}$ is the mean matrix, $\mathbf{\Sigma}_r \in \mathbb{R}^{r \times r}$ is the row covariance matrix and $\mathbf{\Sigma}_c \in \mathbb{R}^{c \times c}$ is the column covariance matrix.

TABLE I: Matrix dimension summary

Notation	Definition	Relation
m	no. of pixels in each row of \mathbf{Y}_H	$m = n/d$
n	no. of pixels in each row of \mathbf{Y}_M	$n = m \times d$
d	decimation factor	$d = n/m$
m_λ	no. of bands in \mathbf{Y}_H	$m_\lambda \gg n_\lambda$
n_λ	no. of bands in \mathbf{Y}_M	$n_\lambda \ll m_\lambda$

a priori from the HS data [37]. Also, it can be estimated jointly with the abundance matrix \mathbf{A} [38]–[40], which will be the case in this work.

D. Statistical Methods

To summarize, the problem of fusing and unmixing high-spectral and high-spatial resolution images can be formulated as estimating the unknown matrices \mathbf{M} and \mathbf{A} from (3), which can be regarded as a joint non-negative matrix factorization (NMF) problem. As is well known, the NMF problem is non-convex and has no unique solution, leading to an ill-posed problem. Thus, it is necessary to incorporate some intrinsic constraints or prior information to regularize this problem, improving the conditioning of the problem.

Various priors have been already advocated to regularize the multi-band image fusion problem, such as Gaussian priors [10], [41], sparse representations [11] or total variation (TV) priors [12]. The choice of the prior usually depends on the information resulting from previous experiments or from a subjective view of constraints affecting the unknown model parameters [42], [43]. The inference of \mathbf{M} and \mathbf{A} (whatever the form chosen for the prior) is a challenging task, mainly due to the large size of \mathbf{X} and to the presence of the downsampling operator \mathbf{S} , which prevents any direct use of the Fourier transform to diagonalize the blurring operator \mathbf{B} . To overcome this difficulty, several computational strategies, including Markov chain Monte Carlo (MCMC) [10], block coordinate descent method (BCD) [44], and tailored variable splitting under the ADMM framework [12], have been proposed, both applied to different kinds of priors, e.g., the empirical Gaussian prior [10], [41], the sparse presentation based prior [11], or the TV prior [12]. More recently, contrary to the algorithms described above, a much more efficient method, named *Robust Fast fUision based on Sylvester Equation (R-FUSE)* has been proposed to solve explicitly an underlying Sylvester equation associated

with the fusion problem derived from (3) [45]. This solution can be implemented *per se* to compute the maximum likelihood estimator in a computationally efficient manner, which has also the great advantage of being easily generalizable within a Bayesian framework when considering various priors.

In our work, we propose to form priors by exploiting the intrinsic physical properties of abundances and endmembers, which is widely used in conventional unmixing, to infer \mathbf{A} and \mathbf{M} from the observed data \mathbf{Y}_M and \mathbf{Y}_H . More details will be given in following sections.

III. PROBLEM FORMULATION

Following the Bayes rule, the posterior distribution of the unknown parameters \mathbf{M} and \mathbf{A} can be obtained by the product of their likelihoods and prior distributions, which are detailed in what follows.

A. Likelihoods (Data Fidelity Term)

Using the statistical properties of the noise matrices \mathbf{N}_M and \mathbf{N}_H , \mathbf{Y}_M and \mathbf{Y}_H have matrix Gaussian distributions, i.e.,

$$\begin{aligned} p(\mathbf{Y}_M|\mathbf{M}, \mathbf{A}) &= \mathcal{MN}_{n_\lambda, n}(\mathbf{RMA}, \mathbf{\Lambda}_M, \mathbf{I}_n) \\ p(\mathbf{Y}_H|\mathbf{M}, \mathbf{A}) &= \mathcal{MN}_{m_\lambda, m}(\mathbf{MABS}, \mathbf{\Lambda}_H, \mathbf{I}_m). \end{aligned} \quad (4)$$

As the collected measurements \mathbf{Y}_M and \mathbf{Y}_H have been acquired by different (possibly heterogeneous) sensors, the noise matrices \mathbf{N}_M and \mathbf{N}_H are sensor-dependent and can be generally assumed to be statistically independent. Therefore, \mathbf{Y}_M and \mathbf{Y}_H are independent conditionally upon the unobserved scene $\mathbf{X} = \mathbf{MA}$. As a consequence, the joint likelihood function of the observed data is

$$p(\mathbf{Y}_M, \mathbf{Y}_H|\mathbf{M}, \mathbf{A}) = p(\mathbf{Y}_M|\mathbf{M}, \mathbf{A}) p(\mathbf{Y}_H|\mathbf{M}, \mathbf{A}). \quad (5)$$

The negative logarithm of the likelihood is

$$\begin{aligned}
& -\log p(\mathbf{Y}_M, \mathbf{Y}_H | \mathbf{M}, \mathbf{A}) \\
&= -\log p(\mathbf{Y}_M | \mathbf{M}, \mathbf{A}) - \log p(\mathbf{Y}_H | \mathbf{M}, \mathbf{A}) + C \\
&= \frac{1}{2} \|\boldsymbol{\Lambda}_H^{-\frac{1}{2}} (\mathbf{Y}_H - \mathbf{MABS})\|_F^2 + \frac{1}{2} \|\boldsymbol{\Lambda}_M^{-\frac{1}{2}} (\mathbf{Y}_M - \mathbf{RMA})\|_F^2 \\
&+ C
\end{aligned}$$

where $\|\mathbf{X}\|_F = \sqrt{\text{trace}(\mathbf{X}^T \mathbf{X})}$ is the Frobenius norm of \mathbf{X} and C is a constant.

B. Priors (Regularization Term)

1) *Abundances*: As the mixing coefficient $a_{i,j}$ (the element located in the i th row and j th column of \mathbf{A}) represents the proportion (or probability of occurrence) of the i th endmember in the j th measurement [26], [46], the abundance vectors satisfy the following *abundance non-negativity constraint* (ANC) and *abundance sum-to-one constraint* (ASC)

$$\mathbf{a}_j \geq 0 \quad \text{and} \quad \mathbf{1}_p^T \mathbf{a}_j = 1, \forall j \in \{1, \dots, n\} \quad (6)$$

where \mathbf{a}_j is the j th column of \mathbf{A} , \geq means “element-wise greater than” and $\mathbf{1}_p^T$ is a $p \times 1$ vector with all ones. Accounting for all the image pixels, the constraints (6) can be rewritten in matrix form

$$\mathbf{A} \geq 0 \quad \text{and} \quad \mathbf{1}_p^T \mathbf{A} = \mathbf{1}_n^T. \quad (7)$$

Moreover, the ANC and ASC constraints can be converted into a uniform distribution for \mathbf{A} on the feasible region \mathcal{A} , i.e.,

$$p(\mathbf{A}) = \begin{cases} c_{\mathcal{A}} & \text{if } \mathbf{A} \in \mathcal{A} \\ 0 & \text{elsewhere} \end{cases} \quad (8)$$

where $\mathcal{A} = \{\mathbf{A} | \mathbf{A} \geq 0, \mathbf{1}_p^T \mathbf{A} = \mathbf{1}_n^T\}$, $c_{\mathcal{A}} = 1/\text{vol}(\mathcal{A})$ and $\text{vol}(\mathcal{A}) = \int_{\mathbf{A} \in \mathcal{A}} d\mathbf{A}$ is the volume of the set \mathcal{A} .

2) *Endmembers*: As the endmember signatures represent the reflectances of different materials, each element of the matrix \mathbf{M} should be between 0 and 1. Thus, the constraints for \mathbf{M} can be written as

$$0 \leq \mathbf{M} \leq 1. \quad (9)$$

Similarly, these constraints for the matrix \mathbf{M} can be converted into a uniform distribution on the feasible region \mathcal{M}

$$p(\mathbf{M}) = \begin{cases} c_{\mathbf{M}} & \text{if } \mathbf{M} \in \mathcal{M} \\ 0 & \text{elsewhere} \end{cases}$$

where $\mathcal{M} = \{\mathbf{M} | 0 \leq \mathbf{M} \leq 1\}$ and $c_{\mathbf{M}} = 1/\text{vol}(\mathcal{M})$.

C. Posteriors (Constrained Optimization)

Combining the likelihoods (5) and the priors $p(\mathbf{M})$ and $p(\mathbf{A})$, the Bayes theorem provides the posterior distribution of \mathbf{M} and \mathbf{A}

$$\begin{aligned} & p(\mathbf{M}, \mathbf{A} | \mathbf{Y}_H, \mathbf{Y}_M) \\ & \propto p(\mathbf{Y}_H | \mathbf{M}, \mathbf{A}) p(\mathbf{Y}_M | \mathbf{M}, \mathbf{A}) p(\mathbf{M}) p(\mathbf{A}) \end{aligned}$$

where \propto means ‘‘proportional to’’. Thus, the unmixing based fusion problem can be interpreted as maximizing the joint posterior distribution of \mathbf{A} and \mathbf{M} . Moreover, by taking the negative logarithm of $p(\mathbf{M}, \mathbf{A} | \mathbf{Y}_H, \mathbf{Y}_M)$, the MAP estimator of (\mathbf{A}, \mathbf{M}) can be obtained by solving the minimization

$$\begin{aligned} \min_{\mathbf{M}, \mathbf{A}} L(\mathbf{M}, \mathbf{A}) \quad \text{s.t.} \quad & \mathbf{A} \geq 0 \quad \text{and} \quad \mathbf{1}_p^T \mathbf{A} = \mathbf{1}_n^T \\ & 0 \leq \mathbf{M} \leq 1 \end{aligned} \tag{10}$$

where

$$\begin{aligned} L(\mathbf{M}, \mathbf{A}) = & \frac{1}{2} \left\| \Lambda_H^{-\frac{1}{2}} (\mathbf{Y}_H - \mathbf{M} \mathbf{A} \mathbf{B} \mathbf{S}) \right\|_F^2 \\ & + \frac{1}{2} \left\| \Lambda_M^{-\frac{1}{2}} (\mathbf{Y}_M - \mathbf{R} \mathbf{M} \mathbf{A}) \right\|_F^2. \end{aligned}$$

In this formulation, the fusion problem can be regarded as a generalized unmixing problem, which includes two data fidelity terms. Thus, both images contribute to the estimation of the endmember signatures (endmember extraction step) and the high-resolution abundance maps (inversion step). For the endmember estimation, a popular strategy is to use a subspace transformation as a preprocessing step, such as in [39], [47]. In general, the subspace transformation is learned *a priori* from the high-spectral resolution image empirically, e.g., from

the HS data. This empirical subspace transformation alleviates the computational burden greatly and can be incorporated in our framework easily.

IV. ALTERNATING OPTIMIZATION SCHEME

Even though problem (10) is convex w.r.t. \mathbf{A} and \mathbf{M} separately, it is non-convex w.r.t. these two matrices jointly and has more than one solution. We propose an optimization technique that alternates optimizations w.r.t. \mathbf{A} and \mathbf{M} , which is also referred to as a BCD algorithm. The optimization w.r.t. \mathbf{A} (resp. \mathbf{M}) conditional on \mathbf{M} (resp. \mathbf{A}) can be achieved efficiently with the ADMM algorithm [48], which converges to a solution of the respective convex optimization under some mild conditions. The resulting alternating optimization algorithm, referred to as Fusion based on Unmixing for Multi-band Images (FUMI), is detailed in Algorithm 1, where $\text{EEA}(\mathbf{Y}_H)$ in line 1 represents an endmember extraction algorithm to estimate endmembers from HS data. The optimization steps w.r.t. \mathbf{A} and \mathbf{M} are detailed below.

Algorithm 1: Multi-band Image Fusion based on Spectral Unmixing (FUMI)

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Input:  $\mathbf{Y}_M, \mathbf{Y}_H, \Lambda_M, \Lambda_H, \mathbf{R}, \mathbf{B}, \mathbf{S}$ 
/* Initialize  $\mathbf{M}$  */
1  $\mathbf{M}^{(0)} \leftarrow \text{EEA}(\mathbf{Y}_H)$ ;
2 for  $t = 1, 2, \dots$  to stopping rule do
   /* Optimize w.r.t.  $\mathbf{A}$  using ADMM (see Algorithm 2) */
3    $\mathbf{A}^{(t)} \in \arg \min_{\mathbf{A} \in \mathcal{A}} L(\mathbf{M}^{(t-1)}, \mathbf{A})$ ;
   /* Optimize w.r.t.  $\mathbf{M}$  using ADMM (see Algorithm 5) */
4    $\mathbf{M}^{(t)} \in \arg \min_{\mathbf{M} \in \mathcal{M}} L(\mathbf{M}, \mathbf{A}^{(t)})$ ;
5 end
6 Set  $\hat{\mathbf{A}} = \mathbf{A}^{(t)}$  and  $\hat{\mathbf{M}} = \mathbf{M}^{(t)}$ ;
Output:  $\hat{\mathbf{A}}$  and  $\hat{\mathbf{M}}$ 

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A. Convergence Analysis

To analyze the convergence of Algorithm 1, we recall a convergence criterion for the BCD algorithm stated in [44, p. 273].

Theorem 1 (Bertsekas, [44]; Proposition 2.7.1). *Suppose that L is continuously differentiable w.r.t. \mathbf{A} and \mathbf{M} over the convex set $\mathcal{A} \times \mathcal{M}$. Suppose also that for each $\{\mathbf{A}, \mathbf{M}\}$, $L(\mathbf{A}, \mathbf{M})$*

viewed as a function of \mathbf{A} , attains a unique minimum $\bar{\mathbf{A}}$. The similar uniqueness also holds for \mathbf{M} . Let $\{\mathbf{A}^{(t)}, \mathbf{M}^{(t)}\}$ be the sequence generated by the BCD method as in Algorithm 1. Then, every limit point of $\{\mathbf{A}^{(t)}, \mathbf{M}^{(t)}\}$ is a stationary point.

The target function defined in (10) is continuously differentiable. Note that it is not guaranteed that the minima w.r.t. \mathbf{A} or \mathbf{M} are unique. We may however argue that a simple modification of the objective function, consisting in adding the quadratic term $\alpha_1 \|\mathbf{A}\|_F^2 + \alpha_2 \|\mathbf{M}\|_F^2$, where α_1 and α_2 are very small thus obtaining a strictly convex objective function, ensures that the minima of (11) and (15) are uniquely attained and thus we may invoke the Theorem (1). In practice, even without including the quadratic terms, we have systematically observed convergence of Algorithm 1.

B. Optimization w.r.t. the Abundance Matrix \mathbf{A} (\mathbf{M} fixed)

The minimization of $L(\mathbf{M}, \mathbf{A})$ w.r.t. the abundance matrix \mathbf{A} conditional on \mathbf{M} can be formulated as

$$\begin{aligned} \min_{\mathbf{A}} \quad & \frac{1}{2} \|\Lambda_{\mathbf{H}}^{-\frac{1}{2}} (\mathbf{Y}_{\mathbf{H}} - \mathbf{M}\mathbf{A}\mathbf{B}\mathbf{S})\|_F^2 + \frac{1}{2} \|\Lambda_{\mathbf{M}}^{-\frac{1}{2}} (\mathbf{Y}_{\mathbf{M}} - \mathbf{R}\mathbf{M}\mathbf{A})\|_F^2 \\ \text{s.t.} \quad & \mathbf{A} \geq 0 \quad \text{and} \quad \mathbf{1}_p^T \mathbf{A} = \mathbf{1}_n^T. \end{aligned} \quad (11)$$

This constrained minimization problem can be solved by introducing an auxiliary variable to split the objective and the constraints, which is the spirit of the ADMM algorithm. More specifically, by introducing the splitting $\mathbf{V} = \mathbf{A}$, the optimization problem (11) w.r.t. \mathbf{A} can be written as

$$\min_{\mathbf{A}, \mathbf{V}} L_1(\mathbf{A}) + \iota_{\mathcal{A}}(\mathbf{V}) \quad \text{s.t.} \quad \mathbf{V} = \mathbf{A}$$

where $L_1(\mathbf{A}) =$

$$\frac{1}{2} \|\Lambda_{\mathbf{H}}^{-\frac{1}{2}} (\mathbf{Y}_{\mathbf{H}} - \mathbf{M}\mathbf{A}\mathbf{B}\mathbf{S})\|_F^2 + \frac{1}{2} \|\Lambda_{\mathbf{M}}^{-\frac{1}{2}} (\mathbf{Y}_{\mathbf{M}} - \mathbf{R}\mathbf{M}\mathbf{A})\|_F^2$$

and

$$\iota_{\mathcal{A}}(\mathbf{V}) = \begin{cases} 0 & \text{if } \mathbf{V} \in \mathcal{A} \\ +\infty & \text{otherwise.} \end{cases}$$

Recall that $\mathcal{A} = \{\mathbf{A} | \mathbf{A} \geq 0, \mathbf{1}_p^T \mathbf{A} = \mathbf{1}_n^T\}$.

The augmented Lagrangian associated with the optimization of \mathbf{A} can be written as

$$\begin{aligned} \mathcal{L}(\mathbf{A}, \mathbf{V}, \mathbf{G}) &= \frac{1}{2} \left\| \Lambda_{\mathbf{H}}^{-\frac{1}{2}} (\mathbf{Y}_{\mathbf{H}} - \mathbf{MABS}) \right\|_F^2 + \iota_{\mathcal{A}}(\mathbf{V}) \\ &+ \frac{1}{2} \left\| \Lambda_{\mathbf{M}}^{-\frac{1}{2}} (\mathbf{Y}_{\mathbf{M}} - \mathbf{RMA}) \right\|_F^2 + \frac{\mu}{2} \left\| \mathbf{A} - \mathbf{V} - \mathbf{G} \right\|_F^2 \end{aligned} \quad (12)$$

where \mathbf{G} is the so-called scaled dual variable and $\mu > 0$ is the augmented Lagrange multiplier, weighting the augmented Lagrangian term [48]. The ADMM summarized in Algorithm 2, consists of an \mathbf{A} -minimization step, a \mathbf{V} -minimization step and a dual variable \mathbf{G} update step (see [48] for further details about ADMM). Note that the operator $\Pi_{\mathcal{X}}(\mathbf{X})$ in Algorithm 2 represents projecting the variable \mathbf{X} onto a set \mathcal{X} , which is defined as

$$\Pi_{\mathcal{X}}(\mathbf{X}) = \arg \min_{\mathbf{Z} \in \mathcal{X}} \left\| \mathbf{Z} - \mathbf{X} \right\|_F^2.$$

Algorithm 2: ADMM sub-iterations to estimate \mathbf{A}

Input: $\mathbf{Y}_{\mathbf{M}}, \mathbf{Y}_{\mathbf{H}}, \Lambda_{\mathbf{M}}, \Lambda_{\mathbf{H}}, \mathbf{R}, \mathbf{B}, \mathbf{S}, \mu > 0$
1 Initialization: $\mathbf{V}^{(0)}, \mathbf{G}^{(0)}$;
2 for $k = 0$ **to stopping rule do**
 /* Optimize w.r.t \mathbf{A} (Algorithm 3) */
3 $\mathbf{A}^{(t,k+1)} \in \arg \min_{\mathbf{A}} \mathcal{L}(\mathbf{A}, \mathbf{V}^{(k)}, \mathbf{G}^{(k)})$;
 /* Optimize w.r.t \mathbf{V} (Algorithm 4) */
4 $\mathbf{V}^{(k+1)} \leftarrow \Pi_{\mathcal{A}}(\mathbf{A}^{(t,k+1)} - \mathbf{G}^{(k)})$;
 /* Update Dual Variable \mathbf{G} */
5 $\mathbf{G}^{(k+1)} \leftarrow \mathbf{G}^{(k)} - (\mathbf{A}^{(t,k+1)} - \mathbf{V}^{(k+1)})$;
6 end
7 Set $\mathbf{A}^{(t+1)} = \mathbf{A}^{(t,k+1)}$;
Output: $\mathbf{A}^{(t+1)}$

Given that the functions $L_1(\mathbf{A})$ and $\iota_{\mathcal{A}}(\mathbf{V})$ are both closed, proper, and convex, thus, invoking the Eckstein and Bertsekas theorem [49, Theorem 8], the convergence of Algorithm 2 to a solution of (11) is guaranteed.

1) *Updating \mathbf{A} :* In order to minimize (12) w.r.t. \mathbf{A} , we solve the equation $\partial \mathcal{L}(\mathbf{A}, \mathbf{V}^{(k)}, \mathbf{G}^{(k)}) / \partial \mathbf{A} = \mathbf{0}$, which is equivalent to the generalized Sylvester equation

$$\mathbf{C}_1 \mathbf{A} + \mathbf{A} \mathbf{C}_2 = \mathbf{C}_3 \quad (13)$$

where

$$\begin{aligned}\mathbf{C}_1 &= (\mathbf{M}^T \boldsymbol{\Lambda}_H^{-1} \mathbf{M})^{-1} \left((\mathbf{R}\mathbf{M})^T \boldsymbol{\Lambda}_M^{-1} \mathbf{R}\mathbf{M} + \mu \mathbf{I}_p \right) \\ \mathbf{C}_2 &= \mathbf{B}\mathbf{S}(\mathbf{B}\mathbf{S})^T \\ \mathbf{C}_3 &= (\mathbf{M}^T \boldsymbol{\Lambda}_H^{-1} \mathbf{M})^{-1} (\mathbf{M}^T \boldsymbol{\Lambda}_H^{-1} \mathbf{Y}_H (\mathbf{B}\mathbf{S})^T \\ &\quad + (\mathbf{R}\mathbf{M})^T \boldsymbol{\Lambda}_M^{-1} \mathbf{Y}_M + \mu(\mathbf{V}^{(k)} + \mathbf{G}^{(k)})).\end{aligned}$$

Eq. (13) can be solved analytically by exploiting the properties of the circulant and down-sampling matrices \mathbf{B} and \mathbf{S} , as summarized in Algorithm 3 and demonstrated in [45]. Note that the matrix \mathbf{F} represents the FFT operation and its conjugate transpose (or Hermitian transpose) \mathbf{F}^H represents the iFFT operation. The matrix $\mathbf{D} \in \mathbb{C}^{n \times n}$ is a diagonal matrix, which has eigenvalues of the matrix \mathbf{B} in its diagonal line and can be rewritten as

$$\mathbf{D} = \begin{bmatrix} \mathbf{D}_1 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{D}_2 & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{D}_d \end{bmatrix}$$

where $\mathbf{D}_i \in \mathbb{C}^{m \times m}$. Thus, we have $\bar{\mathbf{D}}^H \bar{\mathbf{D}} = \sum_{t=1}^d \mathbf{D}_t^H \mathbf{D}_t = \sum_{t=1}^d \mathbf{D}_t^2$, where $\bar{\mathbf{D}} = \mathbf{D}(\mathbf{1}_d \otimes \mathbf{I}_m)$. Similarly, the diagonal matrix $\boldsymbol{\Lambda}_C$ has eigenvalues of the matrix \mathbf{C}_1 in its diagonal line (denoted as $\lambda_1, \dots, \lambda_{\tilde{m}_\lambda}$ and $\lambda_i \geq 0, \forall i$). The matrix \mathbf{Q} contains eigenvectors of the matrix \mathbf{C}_1 in its columns. The auxiliary matrix $\bar{\mathbf{A}} \in \mathbb{C}^{m_\lambda \times n}$ is decomposed as $\bar{\mathbf{A}} = [\bar{\mathbf{a}}_1^T, \bar{\mathbf{a}}_2^T, \dots, \bar{\mathbf{a}}_p^T]^T$.

2) *Updating V*: The update of \mathbf{V} can be made by simply computing the Euclidean projection of $\mathbf{A}^{(t,k+1)} - \mathbf{G}^{(k+1)}$ onto the canonical simplex \mathcal{A} , which can be expressed as follows

$$\begin{aligned}\hat{\mathbf{V}} &= \arg \min_{\mathbf{V}} \frac{\mu}{2} \|\mathbf{V} - (\mathbf{A}^{(t,k+1)} - \mathbf{G}^{(k+1)})\|_F^2 + \iota_{\mathcal{A}}(\mathbf{V}) \\ &= \Pi_{\mathcal{A}}(\mathbf{A}^{(t,k+1)} - \mathbf{G}^{(k+1)})\end{aligned}$$

where $\Pi_{\mathcal{A}}$ denotes the projection (in the sense of the Euclidean norm) onto the simplex \mathcal{A} . This classical projection problem has been widely studied and can be achieved by numerous methods [50]–[53]. In this work, we adopt the popular strategy first proposed in [50] and

Algorithm 3: A closed-form solution of (13) w.r.t. \mathbf{A}

Input: $\mathbf{Y}_M, \mathbf{Y}_H, \mathbf{\Lambda}_M, \mathbf{\Lambda}_H, \mathbf{R}, \mathbf{B}, \mathbf{S}, \mathbf{V}^{(k)}, \mathbf{G}^{(k)}, \mu > 0$
 /* Circulant matrix decomposition: $\mathbf{B} = \mathbf{FDF}^H$ */

- 1 $\mathbf{D} \leftarrow \text{EigDec}(\mathbf{B});$
- 2 $\bar{\mathbf{D}} \leftarrow \mathbf{D}(\mathbf{1}_d \otimes \mathbf{I}_m);$
 /* Calculate \mathbf{C}_1 */
- 3 $\mathbf{C}_1 \leftarrow (\mathbf{M}^T \mathbf{\Lambda}_H^{-1} \mathbf{M})^{-1} \left((\mathbf{R}\mathbf{M})^T \mathbf{\Lambda}_M^{-1} \mathbf{R}\mathbf{M} + \mu \mathbf{I}_p \right);$
 /* Eigen-decomposition of \mathbf{C}_1 : $\mathbf{C}_1 = \mathbf{Q}\mathbf{\Lambda}_C \mathbf{Q}^{-1}$ */
- 4 $(\mathbf{Q}, \mathbf{\Lambda}_C) \leftarrow \text{EigDec}(\mathbf{C}_1);$
 /* Calculate \mathbf{C}_3 */
- 5 $\mathbf{C}_3 \leftarrow (\mathbf{M}^T \mathbf{\Lambda}_H^{-1} \mathbf{M})^{-1} (\mathbf{M}^T \mathbf{\Lambda}_H^{-1} \mathbf{Y}_H (\mathbf{B}\mathbf{S})^T + (\mathbf{R}\mathbf{M})^T \mathbf{\Lambda}_M^{-1} \mathbf{Y}_M + \mu(\mathbf{V}^{(k)} + \mathbf{G}^{(k)}));$
 /* Calculate $\bar{\mathbf{C}}_3$ */
- 6 $\bar{\mathbf{C}}_3 \leftarrow \mathbf{Q}^{-1} \mathbf{C}_3 \mathbf{F};$
 /* Calculate $\bar{\mathbf{A}}$ band by band */
- 7 **for** $l = 1$ **to** p **do**
 /* Calculate the l th band */
 8 $\bar{a}_l \leftarrow \lambda_l^{-1} (\bar{\mathbf{C}}_3)_l - \lambda_l^{-1} (\bar{\mathbf{C}}_3)_l \bar{\mathbf{D}} \left(\lambda_l d \mathbf{I}_m + \sum_{t=1}^d \mathbf{D}_t^2 \right) \bar{\mathbf{D}}^H;$
 9 **end**
- 10 **Set** $\mathbf{A} = \mathbf{Q} \bar{\mathbf{A}} \mathbf{F}^H;$
Output: \mathbf{A}

summarized in Algorithm 4. Note that the above optimization is decoupled w.r.t. the columns of \mathbf{V} , denoted by $(\mathbf{V})_1, \dots, (\mathbf{V})_n$, which accelerates the projection dramatically.

Algorithm 4: Projection onto the Simplex \mathcal{A}

Input: $\mathbf{A}^{(t,k+1)} - \mathbf{G}^{(k)}$

- 1 **for** $i = 1$ **to** n **do**
- 2 $(\mathbf{A} - \mathbf{G})_i \triangleq i^{\text{th}}$ column of $\mathbf{A}^{(t,k+1)} - \mathbf{G}^{(k)};$
 /* Sorting the elements of $(\mathbf{A} - \mathbf{G})_i$ */
- 3 **Sort** $(\mathbf{A} - \mathbf{G})_i$ **into** \mathbf{y} : $y_1 \geq \dots \geq y_p$;
- 4 **Set** $K := \max_{1 \leq k \leq p} \{k | (\sum_{r=1}^k y_r - 1) / k < y_k\};$
- 5 **Set** $\tau := (\sum_{r=1}^K y_r - 1) / K;$
 /* The max operation is component-wise */
- 6 **Set** $(\hat{\mathbf{V}})_i := \max\{(\mathbf{A} - \mathbf{G})_i - \tau, 0\};$
- 7 **end**
- Output:** $\mathbf{V}^{(k+1)} = \hat{\mathbf{V}}$

In practice, the ASC constraint is sometimes criticized for not being able to account for every material in a pixel or due to endmember variability [26]. In this case, the sum-to-

one constraint can be simply removed. Thus, the Algorithm 4 will degenerate to projecting $(\mathbf{A} - \mathbf{G})_i$ onto the non-negative half-space, which simply consists of setting the negative values of $(\mathbf{A} - \mathbf{G})_i$ to zeros.

C. Optimization w.r.t. the Endmember Matrix \mathbf{M} (\mathbf{A} fixed)

The minimization of (10) w.r.t. the abundance matrix \mathbf{M} conditional on \mathbf{A} can be formulated as

$$\min_{\mathbf{M}} L_1(\mathbf{M}) + \iota_{\mathcal{M}}(\mathbf{M}) \quad (14)$$

where $L_1(\mathbf{M}) =$

$$\frac{1}{2} \|\Lambda_{\mathbf{H}}^{-\frac{1}{2}} (\mathbf{Y}_{\mathbf{H}} - \mathbf{M}\mathbf{A}_{\mathbf{H}})\|_F^2 + \frac{1}{2} \|\Lambda_{\mathbf{M}}^{-\frac{1}{2}} (\mathbf{Y}_{\mathbf{M}} - \mathbf{R}\mathbf{M}\mathbf{A})\|_F^2$$

and $\mathbf{A}_{\mathbf{H}} = \mathbf{A}\mathbf{B}\mathbf{S}$. By splitting the quadratic data fidelity term and the inequality constraints, the augmented Lagrangian for (15) can be expressed as

$$\mathcal{L}(\mathbf{M}, \mathbf{T}, \mathbf{G}) = L_1(\mathbf{M}) + \iota_{\mathcal{M}}(\Lambda_{\mathbf{H}}^{\frac{1}{2}}\mathbf{T}) + \frac{\mu}{2} \|\Lambda_{\mathbf{H}}^{-\frac{1}{2}}\mathbf{M} - \mathbf{T} - \mathbf{G}\|_F^2. \quad (15)$$

The optimization of $\mathcal{L}(\mathbf{M}, \mathbf{T}, \mathbf{G})$ consists of updating \mathbf{M} , \mathbf{T} and \mathbf{G} iteratively as summarized in Algorithm 5 and detailed below. As $L_1(\mathbf{M})$ and $\iota_{\mathcal{M}}(\Lambda_{\mathbf{H}}^{\frac{1}{2}}\mathbf{T})$ are closed, proper and convex functions and $\Lambda_{\mathbf{H}}^{\frac{1}{2}}$ has full column rank, the ADMM is guaranteed to converge to a solution of problem (14).

1) *Updating \mathbf{M}* : Forcing the derivative of (15) w.r.t. \mathbf{M} to be zero leads to the following Sylvester equation

$$\mathbf{H}_1\mathbf{M} + \mathbf{M}\mathbf{H}_2 = \mathbf{H}_3 \quad (16)$$

where

$$\mathbf{H}_1 = \Lambda_{\mathbf{H}}\mathbf{R}^T\Lambda_{\mathbf{M}}^{-1}\mathbf{R}$$

$$\mathbf{H}_2 = (\mathbf{A}_{\mathbf{H}}\mathbf{A}_{\mathbf{H}}^T + \mu\mathbf{I}_p)(\mathbf{A}\mathbf{A}^T)^{-1}$$

$$\mathbf{H}_3 =$$

$$\left[\mathbf{Y}_{\mathbf{H}}\mathbf{A}_{\mathbf{H}}^T + \Lambda_{\mathbf{H}}\mathbf{R}^T\Lambda_{\mathbf{M}}^{-1}\mathbf{Y}_{\mathbf{M}}\mathbf{A}^T + \mu\Lambda_{\mathbf{H}}^{\frac{1}{2}}(\mathbf{T} + \mathbf{G}) \right] (\mathbf{A}\mathbf{A}^T)^{-1}.$$

Algorithm 5: ADMM sub-iterations to estimate \mathbf{M}

Input: $\mathbf{Y}_M, \mathbf{Y}_H, \Lambda_M, \Lambda_H, \mathbf{R}, \mathbf{B}, \mathbf{S}, \mathbf{A}, \mu > 0$
1 Initialization: $\mathbf{T}^{(0)}, \mathbf{G}^{(0)}$;
2 for $k = 0$ **to stopping rule do**
 /* Optimize w.r.t \mathbf{M} */ * /
3 $\mathbf{M}^{(t,k+1)} \in \arg \min_{\mathbf{M}} \mathcal{L}(\mathbf{M}, \mathbf{T}^{(k)}, \mathbf{G}^{(k)})$;
 /* Optimize w.r.t \mathbf{T} */ * /
4 $\mathbf{T}^{(k+1)} \leftarrow \Pi_{\mathcal{T}}(\Lambda_H^{-\frac{1}{2}} \mathbf{M}^{(t,k+1)} - \mathbf{G}^{(k)})$;
 /* Update Dual Variable \mathbf{G} */ * /
5 $\mathbf{G}^{(k+1)} \leftarrow \mathbf{G}^{(k)} - \left(\Lambda_H^{-\frac{1}{2}} \mathbf{M}^{(k+1)} - \mathbf{T}^{(k+1)} \right)$;
6 end
7 Set $\mathbf{M}^{(t+1)} = \mathbf{M}^{(t,k+1)}$;
Output: $\mathbf{M}^{(t+1)}$

Note that $\text{vec}(\mathbf{AXB}) = (\mathbf{B}^T \otimes \mathbf{A}) \text{vec}(\mathbf{X})$, where $\text{vec}(\mathbf{X})$ denotes the vectorization of the matrix \mathbf{X} formed by stacking the columns of \mathbf{X} into a single column vector and \otimes denotes the Kronecker product [54]. Thus, vectorizing both sides of (16) leads to²

$$\mathbf{W} \text{vec}(\mathbf{M}) = \text{vec}(\mathbf{H}_3) \quad (17)$$

where $\mathbf{W} = (\mathbf{I}_p \otimes \mathbf{H}_1 + \mathbf{H}_2^T \otimes \mathbf{I}_{m_\lambda})$. Thus, $\text{vec}(\hat{\mathbf{M}}) = \mathbf{W}^{-1} \text{vec}(\mathbf{H}_3)$. Note that \mathbf{W}^{-1} can be computed and stored in advance instead of being computed in each iteration.

Alternatively, there exists a more efficient way to calculate the solution \mathbf{M} analytically (avoiding to compute the inverse of the matrix \mathbf{W}). Note that the matrices $\mathbf{H}_1 \in \mathbb{R}^{m_\lambda \times m_\lambda}$ and $\mathbf{H}_2 \in \mathbb{R}^{p \times p}$ are both the products of two symmetric positive definite matrices. According to the Lemma 1 in [55], \mathbf{H}_1 and \mathbf{H}_2 can be diagonalized by eigen-decomposition, i.e., $\mathbf{H}_1 = \mathbf{V}_1 \mathbf{O}_1 \mathbf{V}_1^{-1}$ and $\mathbf{H}_2 = \mathbf{V}_2 \mathbf{O}_2 \mathbf{V}_2^{-1}$, where \mathbf{O}_1 and \mathbf{O}_2 are diagonal matrices denoted as

$$\begin{aligned} \mathbf{O}_1 &= \text{diag}\{s_1, \dots, s_{m_\lambda}\} \\ \mathbf{O}_2 &= \text{diag}\{t_1, \dots, t_p\}. \end{aligned} \quad (18)$$

²The vectorization of the matrices \mathbf{M}, \mathbf{H}_1 and \mathbf{H}_2 is easy to do as the size of these matrices are small, which is not true for the matrices \mathbf{A}, \mathbf{C}_1 and \mathbf{C}_2 in (13).

Thus, (16) can be transformed to

$$\mathbf{O}_1 \tilde{\mathbf{M}} + \tilde{\mathbf{M}} \mathbf{O}_2 = \mathbf{V}_1^{-1} \mathbf{H}_3 \mathbf{V}_2. \quad (19)$$

where $\tilde{\mathbf{M}} = \mathbf{V}_1^{-1} \mathbf{M} \mathbf{V}_2$. Straightforward computations lead to

$$\tilde{\mathbf{H}} \circ \tilde{\mathbf{M}} = \mathbf{V}_1^{-1} \mathbf{H}_3 \mathbf{V}_2 \quad (20)$$

where

$$\tilde{\mathbf{H}} = \begin{bmatrix} s_1 + t_1 & s_1 + t_2 & \cdots & s_1 + t_p \\ s_2 + t_1 & s_2 + t_2 & \cdots & s_2 + t_p \\ \vdots & \vdots & \ddots & \vdots \\ s_{m_\lambda} + t_1 & s_{m_\lambda} + t_2 & \cdots & s_{m_\lambda} + t_p \end{bmatrix} \quad (21)$$

and \circ represents the Hadamard product, defined as the component-wise product of two matrices (having the same size). Then, $\tilde{\mathbf{M}}$ can be calculated by component-wise division of $\mathbf{V}_1^{-1} \mathbf{H}_3 \mathbf{V}_2$ and $\tilde{\mathbf{H}}$. Finally, \mathbf{M} can be estimated as $\hat{\mathbf{M}} = \mathbf{V}_1 \tilde{\mathbf{M}} \mathbf{V}_2^{-1}$. Note that the computational complexity of the latter strategy is of order $\mathcal{O}(\max(m_\lambda^3, p^3))$, which is lower than the complexity order $\mathcal{O}((m_\lambda p)^3)$ of solving (17).

2) *Updating \mathbf{T}* : The optimization w.r.t. \mathbf{T} can be transformed as

$$\arg \min_{\mathbf{T}} \frac{1}{2} \|\mathbf{T} - \Lambda_{\mathbf{H}}^{-\frac{1}{2}} \mathbf{M} + \mathbf{G}\| + \iota_{\mathcal{T}}(\mathbf{T}) \quad (22)$$

where $\iota_{\mathcal{T}}(\mathbf{T}) = \iota_{\mathcal{M}}(\Lambda_{\mathbf{H}}^{\frac{1}{2}} \mathbf{T})$. As $\Lambda_{\mathbf{H}}^{-\frac{1}{2}}$ is a diagonal matrix, the solution of (22) can be obtained easily by setting

$$\hat{\mathbf{T}} = \Lambda_{\mathbf{H}}^{-\frac{1}{2}} \min \left(\max \left(\mathbf{M} - \Lambda_{\mathbf{H}}^{\frac{1}{2}} \mathbf{G}, 0 \right), 1 \right) \quad (23)$$

where min and max are to be understood component-wise.

Remark. *If the endmember signatures are fixed a priori, i.e., \mathbf{M} is known, the unsupervised unmixing and fusion will degenerate to a supervised unmixing and fusion by simply not updating \mathbf{M} . In this case, the alternating scheme is not necessary, since Algorithm 1 reduces to Algorithm 2. Note that fixing \mathbf{M} a priori transforms the non-convex problem (10) into a convex one, which can be solved much more efficiently. The solution produced by the resulting*

algorithm is also guaranteed to be the global optimal point instead of a stationary point.

V. EXPERIMENTAL RESULTS

This section applies the proposed unmixing based fusion method to multi-band images associated with both synthetic and semi-real data. All the algorithms have been implemented using MATLAB R2014A on a computer with Intel(R) Core(TM) i7-2600 CPU@3.40GHz and 8GB RAM.

A. Quality metrics

1) *Fusion quality*: To evaluate the quality of the proposed fusion strategy, five image quality measures have been investigated. Referring to [11], [19], we propose to use the restored signal to noise ratio (RSNR), the averaged spectral angle mapper (SAM), the universal image quality index (UIQI), the relative dimensionless global error in synthesis (ERGAS) and the degree of distortion (DD) as quantitative measures. The larger RSNR and UIQI, the better the fusion. The smaller SAM, ERGAS and DD, the better the fusion.

2) *Unmixing quality*: In order to analyze the quality of the unmixing results, we consider the normalized mean square error (NMSE) for both endmember and abundance matrices

$$\text{NMSE}_{\mathbf{M}} = \frac{\|\widehat{\mathbf{M}} - \mathbf{M}\|_F^2}{\|\mathbf{M}\|_F^2}$$

$$\text{NMSE}_{\mathbf{A}} = \frac{\|\widehat{\mathbf{A}} - \mathbf{A}\|_F^2}{\|\mathbf{A}\|_F^2}.$$

The smaller NMSE, the better the quality of the unmixing. The SAM between the actual and estimated endmembers (different from SAM defined previously for pixel vectors) is a measure of spectral distortion defined as

$$\text{SAM}_{\mathbf{M}}(\mathbf{m}_n, \hat{\mathbf{m}}_n) = \arccos \left(\frac{\langle \mathbf{m}_n, \hat{\mathbf{m}}_n \rangle}{\|\mathbf{m}_n\|_2 \|\hat{\mathbf{m}}_n\|_2} \right).$$

The overall SAM is finally obtained by averaging the SAMs computed from all endmembers. Note that the value of SAM is expressed in degrees and thus belongs to $(-90, 90]$. The smaller the absolute value of SAM, the less important the spectral distortion.

B. Synthetic data

This section applies the proposed FUMI method to synthetic data and compares it with the joint unmixing and fusion methods investigated in [21] and [15]. Note that the method studied in [21] can be regarded as a one-step version of [15].

The reference endmembers are m reflectance spectra selected randomly from the United States Geological Survey (USGS) digital spectral library³. Each reflectance spectrum consists of $L = 224$ spectral bands from 383 nm to 2508 nm. In this simulation, the number of endmembers is fixed to $p = 5$. The abundances \mathbf{A} are generated according to a Dirichlet distribution over the simplex defined by the ANC and ASC constraints. There is one vector of abundance per pixel, i.e., $\mathbf{A} \in \mathbb{R}^{5 \times 100^2}$, for the considered image of size 100×100 pixels. The synthetic image is then generated by the product of endmembers and abundances, i.e., $\mathbf{X} = \mathbf{M}\mathbf{A}$.

- **Initialization:** As shown in Algorithm 1, the proposed algorithm only requires the initialization of the endmember matrix \mathbf{M} . Theoretically, any endmember extraction algorithm (EEA) can be used to initialize \mathbf{M} . In this work, we have used the *simplex identification via split augmented Lagrangian* (SISAL) method [56], which is a state-of-the-art method that does not require the presence of pure pixels in the image.
- **Subspace Identification:** For the endmember estimation, a popular strategy is to use a subspace transformation as a preprocessing step, such as in [39], [47]. In general, the subspace transformation is estimated *a priori* from the high-spectral resolution image, e.g., from the HS data. In this work, the projection matrix has been learned by computing the singular value decomposition (SVD) of \mathbf{Y}_H and retaining the left-singular vectors associated with the largest eigenvalues. Then the input HS data \mathbf{Y}_H , the HS noise covariance matrix $\mathbf{\Lambda}_H$ and the spectral response \mathbf{R} in Algorithm 1 are replaced with their projections onto the learned subspace as $\mathbf{Y}_H \leftarrow \mathbf{E}^T \mathbf{Y}_H$, $\mathbf{\Lambda}_H \leftarrow \mathbf{E}^T \mathbf{\Lambda}_H \mathbf{E}$ and $\mathbf{R} \leftarrow \mathbf{R}\mathbf{E}$, where $\mathbf{E} \in \mathbb{R}^{m_\lambda \times \tilde{m}_\lambda}$ is the estimated orthogonal basis using SVD and $\tilde{m}_\lambda \ll m_\lambda$. Given that the formulation using the transformed entities is equivalent to the original one but the matrix dimension is now much smaller, the subspace transformation brings huge

³<http://speclab.cr.usgs.gov/spectral.lib06/>

numerical advantage.

- **Parameters in ADMM:** The value of μ adopted in all the experiments is fixed to the average of the noise power of HS and MS images, which is motivated by balancing the data term and regularization term. As ADMM is used to solve sub-problems, it is not necessary to use complicated stopping rule to run ADMM exhaustively. Thus, the number of ADMM iterations has been fixed to 30. Experiments have demonstrated that varying these parameters do not affect much the convergence of the whole algorithm.
- **Stopping rule:** The stopping rule for Algorithm 1 is that the relative difference for the successive updates of the objective $L(\mathbf{M}, \mathbf{A})$ is less than 10^{-4} , i.e.,

$$\frac{|L(\mathbf{M}^{(t+1)}, \mathbf{A}^{(t+1)}) - L(\mathbf{M}^{(t)}, \mathbf{A}^{(t)})|}{|L(\mathbf{M}^{(t)}, \mathbf{A}^{(t)})|} \leq 10^{-4}.$$

1) *HS and MS image fusion:* In this section, we consider the fusion of HS and MS images. The HS image \mathbf{Y}_H has been generated by applying a 7×7 Gaussian filter (with zero mean and standard deviation $\sigma_B = 1.7$) and then by down-sampling every 4 pixels in both vertical and horizontal directions for each band of the reference image. A 7-band MS image \mathbf{Y}_M has been obtained by filtering \mathbf{X} with the LANDSAT-like reflectance spectral responses. The HS and MS images are both contaminated by zero-mean additive Gaussian noises. Our simulations have been conducted with $\text{SNR}_{H,i} = 50\text{dB}$ for all the HS bands with $\text{SNR}_{H,i} = 10 \log \left(\frac{\|(\mathbf{XBS})_i\|_F^2}{s_{H,i}^2} \right)$. For the MS image $\text{SNR}_{M,j} = 10 \log \left(\frac{\|(\mathbf{RX})_j\|_F^2}{s_{M,j}^2} \right) = 50\text{dB}$ for all spectral bands.

As the endmembers are selected randomly from the USGS library, 30 Monte Carlo simulations have been implemented and all the results have been obtained by averaging these 30 Monte Carlo runs. The fusion and unmixing results using different methods are reported in Tables II and III, respectively. For fusion performance, the proposed FUMI method outperforms the other two methods, with a competitive time complexity. Regarding unmixing, Berne's method and FUMI perform similarly for endmember estimation, both much better than Yokoya's. In terms of abundance estimation, FUMI outperforms the other methods.

2) *HS and PAN image fusion:* When the number of MS bands degrade to one, the fusion of HS and MS degenerates to HS pansharpening, which is a more challenging problem. In

TABLE II: Fusion Performance for Synthetic HS+MS dataset: RSNR (in dB), UIQI, SAM (in degree), ERGAS, DD (in 10^{-3}) and time (in second).

Methods	RSNR	UIQI	SAM	ERGAS	DD	Time
Berne2010	48.871	0.9995	0.169	0.1011	1.404	8.13
Yokoya2012	48.278	0.9995	0.188	0.1077	1.513	29.95
Proposed FUMI	50.100	0.9996	0.146	0.0877	1.235	8.50

TABLE III: Unmixing Performance for Synthetic HS+MS dataset: SAM_M (in degree), $NMSE_M$ (in dB) and $NMSE_A$ (in dB).

Methods	SAM_M	$NMSE_M$	$NMSE_A$
Berne2010	0.549	-39.44	-18.22
Yokoya2012	1.443	-31.91	-13.97
Proposed FUMI	0.690	-39.71	-22.44

this experiment, the PAN image is obtained by averaging the first 50 bands of the reference image. The quantitative results obtained after averaging 30 Monte Carlo runs for fusion and unmixing are summarized in Tables IV and V, respectively. In terms of fusion performance, the proposed FUMI method performs the best for all the quality measures, with the least CPU time. Regarding the unmixing performance, Berne's method gives the best estimation for endmembers whereas FUMI gives best abundance estimations.

TABLE IV: Fusion Performance for Synthetic HS+PAN dataset: RSNR (in dB), UIQI, SAM (in degree), ERGAS, DD (in 10^{-3}) and time (in second).

Methods	RSNR	UIQI	SAM	ERGAS	DD	Time
Berne2010	32.34	0.9887	0.669	0.682	6.776	6.74
Yokoya2012	33.00	0.9901	0.592	0.633	6.072	11.65
Proposed FUMI	36.16	0.9960	0.399	0.458	3.899	6.36

TABLE V: Unmixing Performance for Synthetic HS+PAN dataset: SAM_M (in degree), $NMSE_M$ (in dB) and $NMSE_A$ (in dB).

Methods	SAM_M	$NMSE_M$	$NMSE_A$
Berne2010	0.566	-39.03	-16.38
Yokoya2012	1.543	-29.31	-14.09
Proposed FUMI	0.716	-38.07	-18.49

C. Semi-real data

In this section, we test the proposed FUMI algorithm on semi-real datasets, for which we have the real HS image as the reference image and have simulated the degraded images from the reference image.

1) *Moffett dataset*: In this experiment, the reference image is an HS image of size $100 \times 100 \times 176$ acquired over Moffett field, CA, in 1994 by the JPL/NASA airborne visible/infrared imaging spectrometer (AVIRIS) [57]. This image was initially composed of 224 bands that have been reduced to 176 bands after removing the water vapor absorption bands. A composite color image of the scene of interest is shown in the top right of Fig. 1 and its scattered data have been displayed as the red points in Fig. 2. As there is no ground truth for endmembers and abundances for the reference image, we have first unmixed this image (with any unsupervised unmixing method) and then reconstructed the reference image \mathbf{X} with the estimated endmembers and abundances (after appropriate normalization). The number of endmembers has been fixed to $p = 3$ empirically as in [39].

The reference image \mathbf{X} is reconstructed from one HS and one coregistered PAN images. The observed HS image has been generated by applying a 7×7 Gaussian filter with zero mean and standard deviation $\sigma_B = 1.7$ and by down-sampling every 4 pixels in both vertical and horizontal directions for each band of \mathbf{X} , as done in Section V-B1. In a second step, the PAN image has been obtained by averaging the first 50 HS bands. The HS and PAN images are both contaminated by additive Gaussian noises, whose SNRs are 50dB for all the bands. The scattered data are displayed in Fig. 2, showing that there is no pure pixel in the degraded HS image.

To analyze the impact of endmember estimation, the proposed FUMI method has been implemented in two scenarios: estimating \mathbf{A} with fixed \mathbf{M} , referred to as *supervised FUMI* (S-FUMI) and estimating \mathbf{A} and \mathbf{M} jointly, referred to as *unsupervised FUMI* (UnS-FUMI). In this work, the S-FUMI algorithm has been run with a matrix \mathbf{M} obtained using SISAL.

The proposed FUMI algorithm (including both S-FUMI and UnS-FUMI) and other state-of-the-art methods have been implemented to fuse the two observed images and to unmix the HS image. The fusion results and RMSE maps (averaged over all the bands) are shown in

Figs. 1. Visually, S-FUMI and UnS-FUMI give better fused images than the other methods. This result is confirmed by the RMSE maps, where the two FUMI methods offer much smaller errors than the other two methods. Furthermore, the quantitative fusion results reported in Table VI are consistent with this conclusion as S-FUMI and UnS-FUMI outperform the other methods for all the fusion metrics. Regarding the computation time, S-FUMI and UnS-FUMI cost more than the other two methods, mainly due to the alternating update of the endmembers and abundances and also the ADMM updates within the alternating updates.

The unmixed endmembers and abundance maps are displayed in Figs. 3 and 4 whereas quantitative unmixing results are reported in Table VII. FUMI offers competitive endmember estimation and much better abundance estimation compared with Berne’s and Yokoya’s methods. It is interesting to note that S-FUMI and UnS-FUMI share very similar fusion results. However, the endmember estimation of UnS-FUMI is much better compared with S-FUMI, which only exploits the HS image to estimate the endmembers. This demonstrates that the estimation of endmembers benefits from being updated jointly with abundances, thanks to the complementary spectral and spatial information contained in the HS and high resolution PAN images.

TABLE VI: Fusion Performance for Moffett HS+PAN dataset: RSNR (in dB), UIQI, SAM (in degree), ERGAS, DD (in 10^{-2}) and time (in second).

Methods	RSNR	UIQI	SAM	ERGAS	DD	Time
Berne2010	16.95	0.8923	4.446	3.777	3.158	0.3
Yokoya2012	17.04	0.9002	4.391	3.734	3.132	1.1
S-FUMI	22.57	0.9799	2.184	2.184	1.488	21.1
UnS-FUMI	22.15	0.9778	2.346	2.292	1.577	32.2

TABLE VII: Unmixing Performance for Moffett HS+PAN dataset: SAM_M (in degree), $NMSE_M$ (in dB) and $NMSE_A$ (in dB).

Methods	SAM_M	$NMSE_M$	$NMSE_A$
Berne2010	7.568	-16.425	-11.167
Yokoya2012	6.772	-17.405	-11.167
S-FUMI	7.579	-16.419	-14.172
UnS-FUMI	7.028	-16.685	-14.695

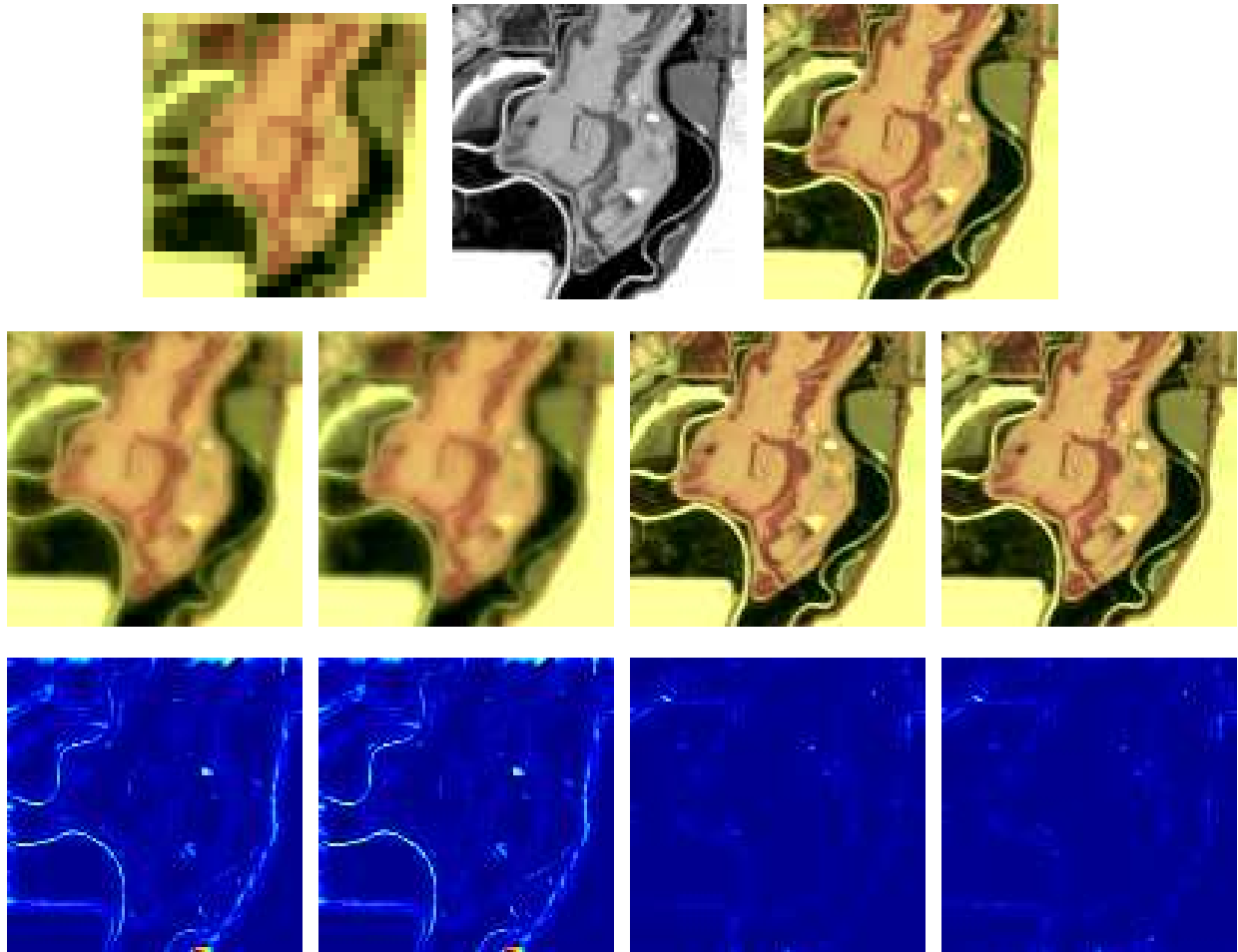


Fig. 1: Hyperspectral pansharpening results (Moffett dataset): (Top 1) HS image. (Top 2) MS image. (Top 3) Reference image. (Middle 1) Berne's method. (Middle 2) Yokoya's method. (Middle 3) S-FUMI (Middle 4) UnS-FUMI. (Bottom 1-4) The corresponding RMSE maps.

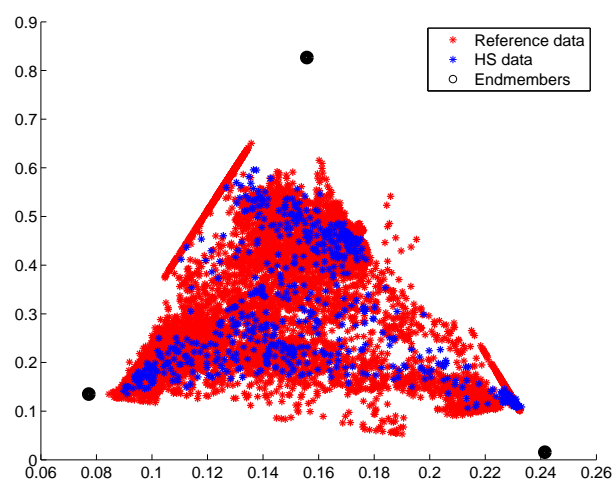


Fig. 2: Scattered Moffett data: The 1st and the 100th bands are selected as the coordinates.

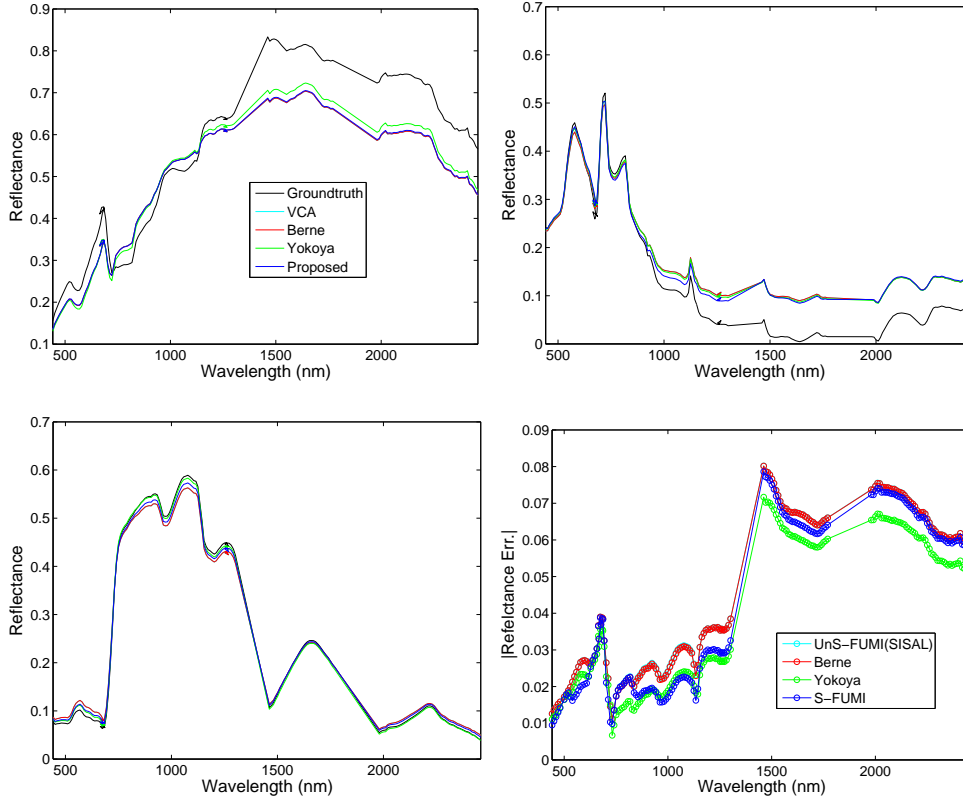


Fig. 3: Unmixed endmembers for Moffett HS+PAN dataset: (Top and bottom left) Estimated three endmembers and ground truth. (Bottom right) Sum of absolute value of all endmember errors as a function of wavelength.

2) *Pavia dataset*: In this section, we test the proposed algorithm on another dataset, in which the reference image is a $100 \times 100 \times 93$ HS image acquired over Pavia, Italy, by the reflective optics system imaging spectrometer (ROSIS). This image was initially composed of 115 bands that have been reduced to 93 bands after removing the water vapor absorption bands. A composite color image of the scene of interest is shown in the top right of Figs. 5. The observed HS and co-registered PAN images are simulated similarly to the Moffett dataset and are shown in the top left and middle of Figs. 5. The scattered reference and HS data are displayed in Fig. 6, showing the high mixture of endmembers in the HS image. The fusion results are displayed in Figs. 5 whereas the unmixed endmembers and abundance maps are shown in Figs. 7 and 8. The corresponding quantitative fusion and unmixing results are reported in Tables VIII and IX. These results are consistent with the analysis associated with the Moffett dataset. Both visually and quantitatively, S-FUMI and UnS-FUMI give competitive

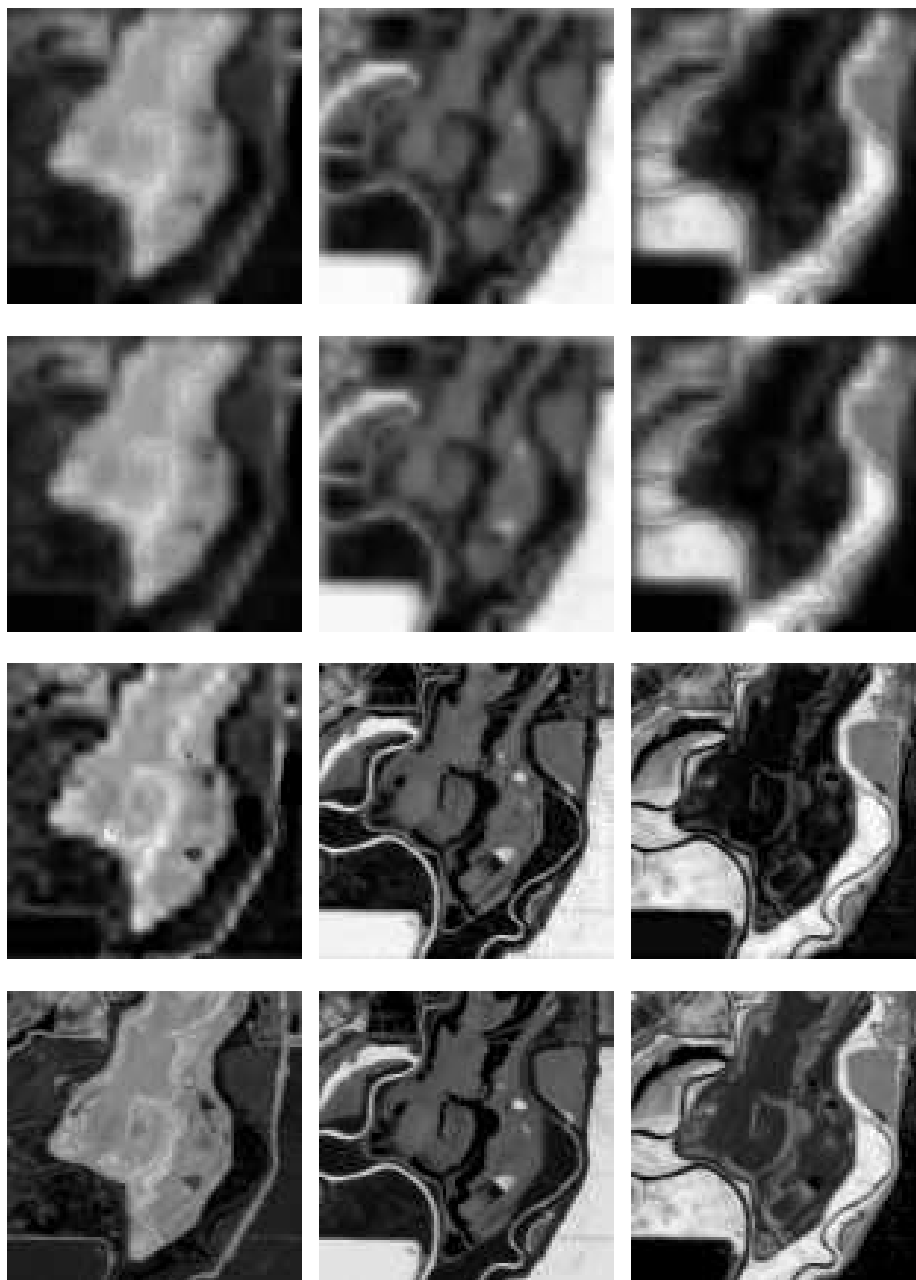


Fig. 4: Unmixed abundance maps for Moffett HS+PAN dataset: Estimated abundance maps using (Row 1) Berne's method, (Row 2) Yokoya's method, and (Row 3) UnS-FUMI. (Row 4) Reference abundance maps.

results, which are much better than the other methods. In terms of unmixing, UnS-FUMI outperforms S-FUMI for both endmember and abundance estimations, due to the alternating update of endmembers and abundances.

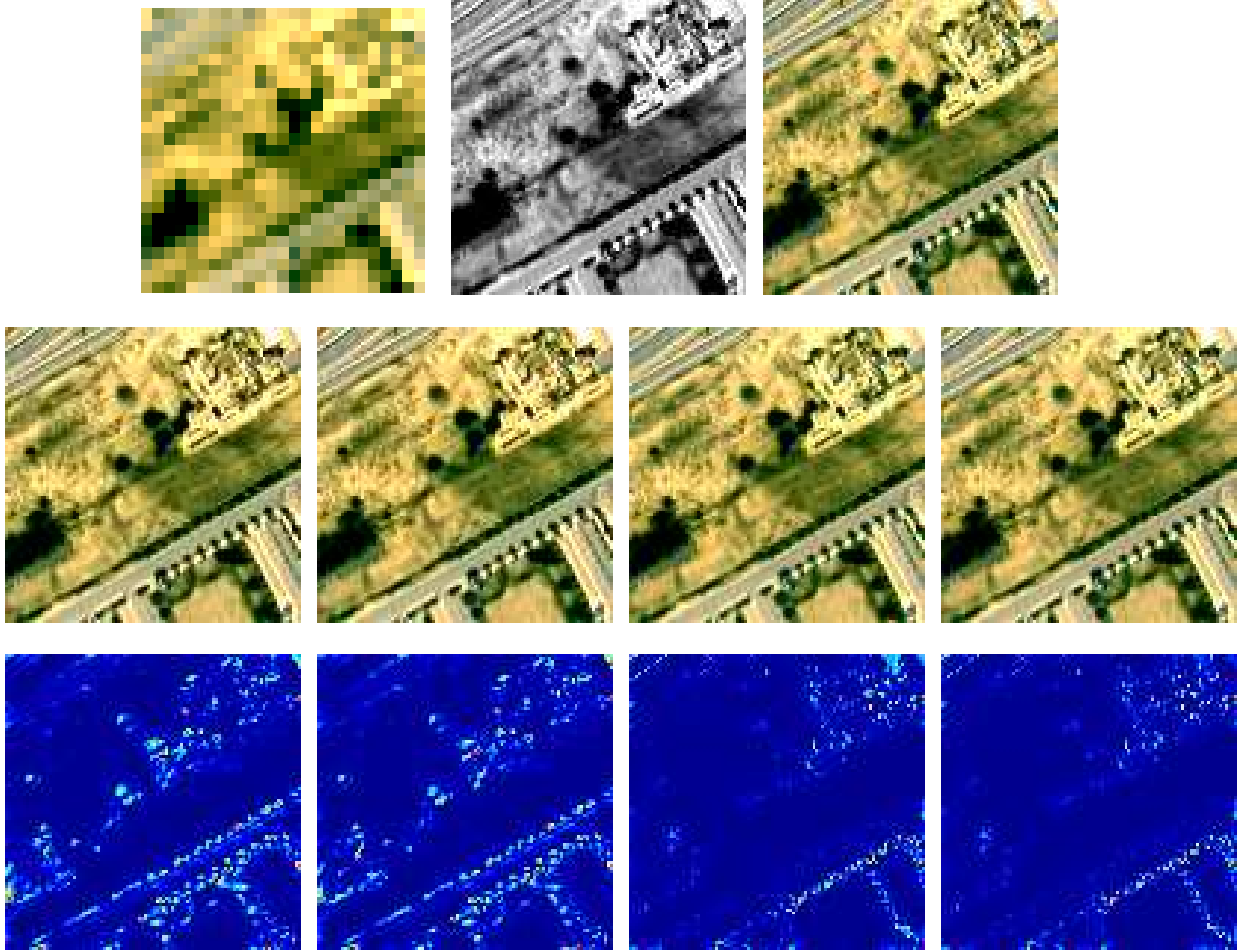


Fig. 5: Hyperspectral pansharpening results (Pavia dataset): (Top 1) HS image. (Top 2) PAN image. (Top 3) Reference image. (Middle 1) Berne's method. (Middle 2) Yokoya's method. (Middle 3) S-FUMI method. (Middle 4) UnS-FUMI method. (Bottom 1-4) The corresponding RMSE maps.

TABLE VIII: Fusion Performance for Pavia HS+PAN dataset: RSNR (in dB), UIQI, SAM (in degree), ERGAS, DD (in 10^{-2}) and time (in second).

Methods	RSNR	UIQI	SAM	ERGAS	DD	Time
Berne2010	21.53	0.9023	2.499	1.692	1.425	0.6
Yokoya2012	21.73	0.9119	2.416	1.655	1.388	3.3
S-FUMI	24.13	0.9456	1.504	1.261	0.948	4.9
UnS-FUMI	24.26	0.9504	1.541	1.215	0.925	34.3

VI. CONCLUSION

This paper proposed a new algorithm based on spectral unmixing for fusing multi-band images. In this algorithm, the endmembers and abundances were updated alternatively, both

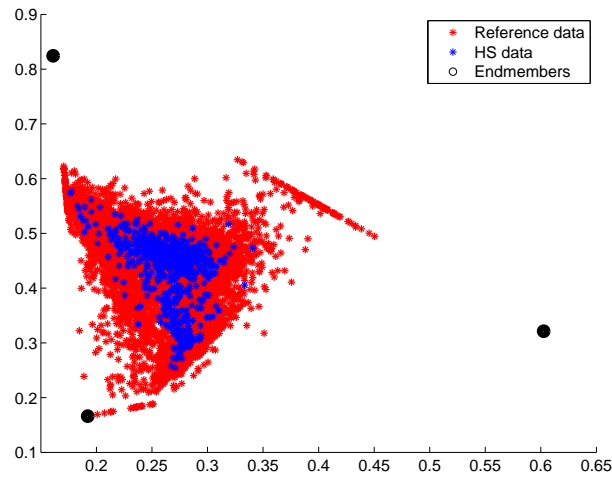


Fig. 6: Scattered Pavia data: The 30th and the 80th bands are selected as the coordinates.

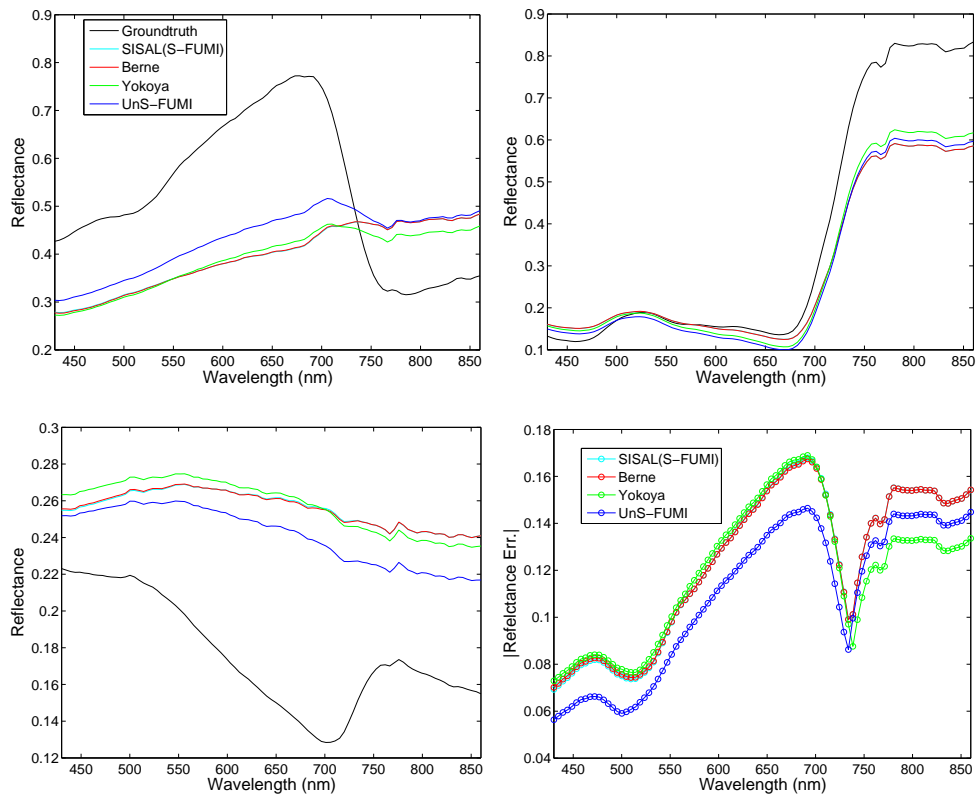


Fig. 7: Unmixed endmembers for Pavia HS+PAN dataset: (Top and bottom left) Estimated three endmembers and ground truth. (Bottom right) Sum of absolute value of all endmember errors as a function of wavelength.

using an alternating direction method of multipliers. The updates for abundances consisted of solving a Sylvester matrix equation and projecting onto a simplex. Thanks to the recently developed R-FUSE algorithm, this Sylvester equation was solved analytically thus efficiently,

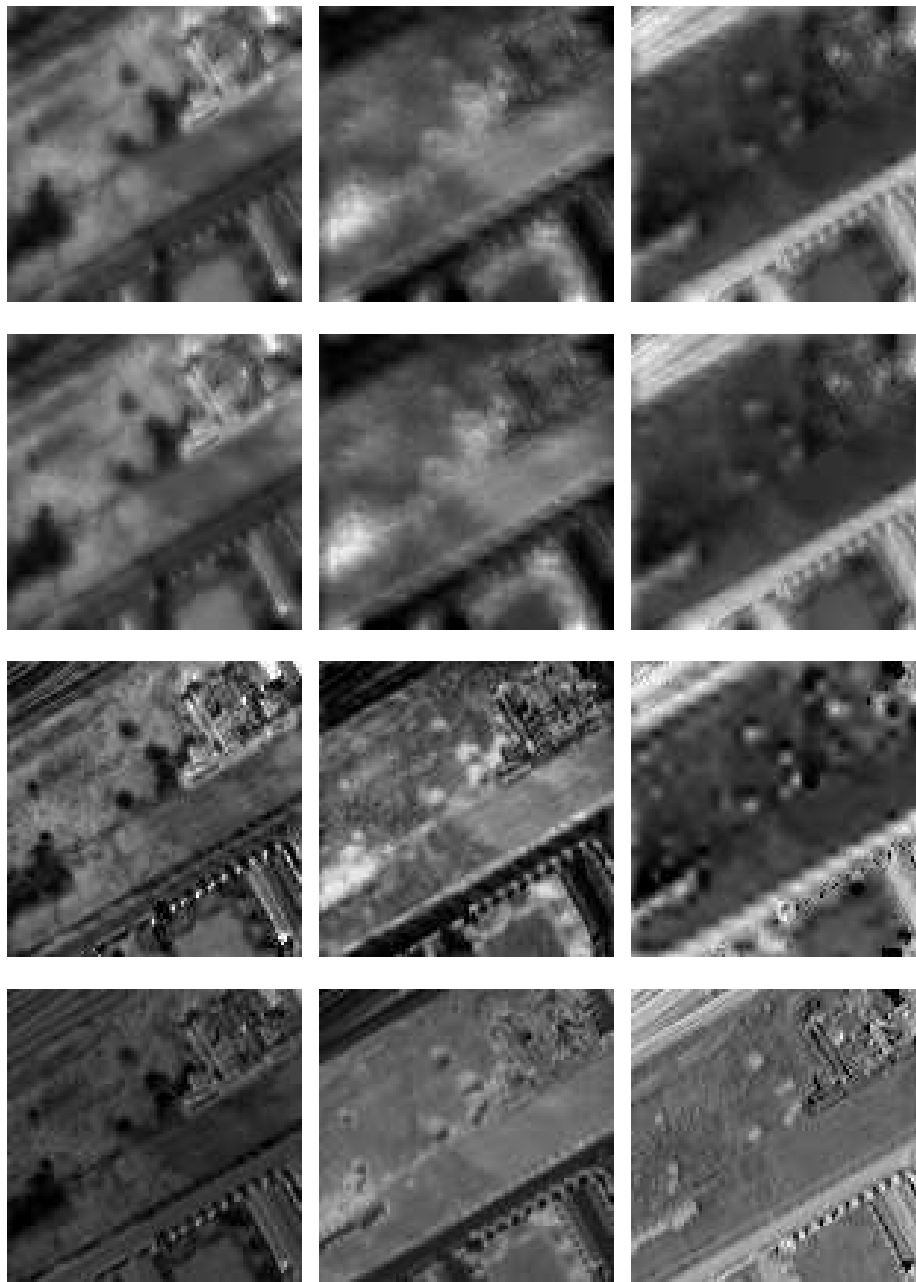


Fig. 8: Unmixed abundance maps for Pavia HS+PAN dataset: Estimated abundance maps using (Row 1) Berne's method, (Row 2) Yokoya's method, and (Row 3) UnS-FUMI. (Row 4) Reference abundance maps.

requiring no iterative update. The endmember updating was divided into two steps: a least square regression and a thresholding, that are both not computationally intensive. Numerical experiments showed that the proposed joint fusion and unmixing algorithm compared competitively with two state-of-the-art methods, with the advantage of improving the performance for

TABLE IX: Unmixing Performance for Pavia HS+PAN dataset: SAM_M (in degree), $NMSE_M$ (in dB) and $NMSE_A$ (in dB).

Methods	SAM_M	$NMSE_M$	$NMSE_A$
Berne2010	11.77	-8.78	-7.21
Yokoya2012	10.43	-9.21	-7.26
S-FUMI	11.80	-8.78	-6.19
UnS-FUMI	9.71	-10.04	-8.06

both fusion and unmixing. Future work will consist of incorporating the spatial and spectral degradation into the estimation framework.

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