MODIFIED NONNEGATIVE MATRIX FACTORIZATION FOR ENDMEMBER SPECTRA EXTRACTION FROM HIGHLY MIXED HYPERSPECTRAL IMAGES COMBINED WITH MULTISPECTRAL DATA

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ABSTRACT

In this paper, a new approach is proposed for linear endmember spectra extraction from a highly mixed hyperspectral image combined with high spatial resolution multispectral data containing pure pixels. This new approach, which is applied to unmix the considered hyperspectral image, is based on a modified version of nonnegative matrix factorization (NMF) coupled with nonnegative least squares (NLS). The multispectral data are used to initialize the hyperspectral NMF algorithm and to constrain it during matrix updates. Experiments based on synthetic and real data are performed to evaluate the performance of the proposed approach and to compare it with five methods from the literature only applied to the hyperspectral data. The obtained performance shows the superiority of the proposed approach as compared with all other methods. Also, the impact, on the proposed method, of spectral variability between hyperspectral and multispectral data is evaluated, and the obtained results show the robustness of the proposed method to this variability.

Index Terms— Hyper/multispectral imagery, mixed/pure pixels, endmember spectra extraction, nonnegative matrix factorization, nonnegative least squares

1. INTRODUCTION

Due to the limited spatial resolution of most hyperspectral sensors, the spectral vector measured in each pixel of a hyperspectral image is usually a mixture of contributions from several spectral signatures of elementary pure materials (usually called endmembers) that are present in the acquired data. In the simplest and most popular configuration, the mixture is supposed to be linear [1] and linear spectral unmixing (LSU) techniques are used to linearly decompose the spectral vector associated with each pixel into a collection of endmember spectra, and a set of corresponding abundance fractions. Mathematically, LSU is equivalent to the linear blind source separation (BSS) problem [4], [6], where the observed pixels, endmember spectra and corresponding abundance fractions can respectively be considered as the observations, mixing matrix and sources.

Most endmember spectra extraction approaches are based on a geometric formulation. Most of these approaches use minimum-volume-based techniques in order to retrieve the minimum-volume simplex among all possible simplices that circumscribe the hyperspectral data scatter space. The vertices of the retrieved simplex correspond to the endmembers. The first reported of these approaches assume that hyperspectral data contain at least one pure pixel per endmember. In this case, there is at least one observed spectral vector on each vertex of the data simplex. This pure pixel assumption is not valid in many hyperspectral datasets. Therefore, other geometry-based techniques have been designed in order to cope with the pure pixel assumption issue [12]. These techniques retrieve a simplex whose vertices, which correspond to the desired endmembers, are not belonging to the hyperspectral data scatter space.

In some applications, when unmixing a hyperspectral image, a multispectral image of the same scene or of another scene containing the same pure materials as the hyperspectral image may be available. Unlike hyperspectral images that may have hundreds of narrower and contiguous spectral bands, multispectral images contain three to ten large and discontinuous spectral bands. Also, multispectral images generally have a high spatial resolution so that the pure pixel assumption is quite realistic for them. Existing endmember spectra extraction techniques applied to hyperspectral data do not take into account the information available in such multispectral images.

In this paper, a new approach is proposed for linear endmember spectra extraction from a highly mixed (i.e. no pure pixels required) hyperspectral image, combined with high spatial resolution multispectral data containing pure pixels. This approach, which is applied to unmix the considered hyperspectral image, is based on a modified version of nonnegative matrix factorization (NMF) [2]. Standard iterative NMF algorithms are not guaranteed to converge to the same solution if they are initialized with different starting points [2]. Thus, unlike classical BSS methods, the NMF-based methods do not provide a unique solution to the considered linear unmixing problem. To avoid these limitations in the proposed approach, the multispectral image is used to initialize a hyperspectral NMF algorithm and to constrain it during matrix updates.

The remainder of this paper is structured as follows. In Section 2, the mathematical data model used in the LSU analysis is introduced. In Section 3, the proposed overall methodology is presented. Section 4 consists of test results with synthetic and real data. In that section, results obtained by the proposed method are compared with those obtained by some classical methods, which do not make use of the information available from the multispectral image. Also, the impact, on the proposed method, of spectral variability between hyperspectral and multispectral data is evaluated in that section. Finally, Section 5 concludes this paper.

2. MATHEMATICAL DATA MODEL

As explained above, each spectral vector associated with a pixel in a hyperspectral image is assumed to be a linear combination of the endmember spectra within the pixel. Mathematically, the nonnegative reflectance $x_i(p)$ at wavelength λ_i from pixel p of the hyperspectral image is given by:

$$x_i(p) = \sum_{j=1}^{L} a_{ij} s_j(p), \quad \forall\, i = 1 \ldots N \text{ and } \forall\, p = 1 \ldots K, \tag{1}$$

where a_{ij} denotes the nonnegative reflectance of endmember j at wavelength λ_i, $s_j(p)$ denotes the nonnegative abundance fraction of endmember j at pixel p, and L is the (known or estimated) number of endmembers. N and K are respectively the numbers of spectral bands and pixels of the hyperspectral image. The above equation can be written in matrix form as:

$$X = A\,S, \tag{2}$$

where X is a nonnegative $N\times K$ matrix, in which each row corresponds to one spectral band of the hyperspectral image (the K pixels are here rearranged as a one-dimensional array). Each column of the nonnegative $N\times L$ matrix A corresponds to one hyperspectral endmember spectrum. The nonnegative $L\times K$ matrix S contains abundance fractions: each row corresponds to all abundance fractions of one endmember in all pixels. The abundance fractions are subject to the abundance sum-to-one constraint:

$$\sum_{j=1}^{L} s_j(p) = 1, \forall\, p = 1 \ldots K. \tag{3}$$

3. PROPOSED APPROACH

The proposed approach is based on the NMF technique [2]. Given a nonnegative $N\times K$ matrix X, NMF aims at finding a nonnegative $N\times L$ matrix $\hat{A}$ and a nonnegative $L\times K$ matrix $\hat{S}$, such that

$$X \approx \hat{A}\,\hat{S}. \tag{4}$$

Basic NMF algorithms are very easy to use and implement. For instance, in [11], a fast algorithm is proposed, wherein the following cost function:

$$D = \frac{1}{2}\left\|X - \hat{A}\,\hat{S}\right\|^2_{\text{Frobenius}}, \tag{5}$$

is minimized using iterative alternating update rules, based on a projected gradient method defined by:

$$\hat{A} \leftarrow \max\{\varepsilon, \hat{A} - \alpha[(\hat{A}\,\hat{S} - X)\hat{S}^{\mathrm{T}}]\}, \tag{6}$$

$$\hat{S} \leftarrow \max\{\varepsilon, \hat{S} - \beta[\hat{A}^{\mathrm{T}}(\hat{A}\,\hat{S} - X)]\}, \tag{7}$$

where α and β are small positive and adaptive learning rates, and ε is a very small positive value. These alternating update rules, used with their adaptation procedure defined in Algorithm 4 of [11] for α and β, and their default value for ε, provide a solution to (5) under the nonnegativity constraints.

As stated in Section 1, NMF algorithms converge to different solutions given different initializations, and a key issue of these algorithms is how to initialize them. To solve this problem, multispectral data are here used for initializing a hyperspectral NMF algorithm and constraining it during iterations. The proposed approach is described hereafter.

Suppose the availability of a highly mixed low spatial resolution hyperspectral image and a high spatial resolution multispectral image containing the same pure materials as the hyperspectral image. In the proposed approach, these two images must be radiometrically corrected in order to obtain approximately the same pure material reflectances (but with highly different spectral resolutions) in the hyperspectral and multispectral images.

The multispectral image is supposed to contain some pure-pixel zones for each endmember, due to its high spatial resolution. These zones are detected and multispectral endmember spectra are extracted from them. This task may be fulfilled manually or automatically by applying to the multispectral image the approaches described in [8], [9]. These approaches are designed for unmixing remote sensing data containing pure-pixel zones, which is not the case for

the highly mixed hyperspectral image to be processed in this paper.

As mentioned in Section 2, the observed hyperspectral spectra are available at the narrow bands centered on the N wavelengths λ_1, λ_2,..., λ_N. The number of spectral bands in the multispectral image is denoted by M (naturally $M << N$). Thus, the observed multispectral spectra are available at the spectral bands centered on the M wavelengths $\lambda_{c(m)}$ with $m = 1\ldots M$. Considering slow variations of endmember spectra in a multispectral band, and first assuming, in the simplest configuration, that each multispectral wavelength $\lambda_{c(m)}$ is equal to one hyperspectral wavelength λ_i with $i = 1\ldots N$ (i.e., c(m) becomes an integer index i belonging to $\{1\ldots N\}$), the m^{th} point of the multispectral spectrum is a relevant approximation of the value of the hyperspectral spectrum at $\lambda_{c(m)}$. Now, if one multispectral wavelength $\lambda_{c(m)}$ is not equal to any hyperspectral wavelength λ_i with $i = 1\ldots N$, this multispectral wavelength $\lambda_{c(m)}$ can be replaced by the nearest hyperspectral wavelength λ_i, whereas the corresponding multispectral reflectance value is not changed. This slight multispectral wavelength change is not a major issue since the resulting multispectral wavelength is still included in the spectral band centered on the considered m^{th} point.

In the following, after assuming that the (unknown) endmember hyperspectral spectra at each wavelength $\lambda_{c(m)}$, with $m = 1\ldots M$, are approximately equal to the m^{th} point of the (known) endmember multispectral spectra, the endmember hyperspectral spectra are estimated at the other wavelengths.

Starting from each M-point endmember multispectral spectrum, an inter/extrapolation is performed by using cubic spline approximation [5], in order to obtain a first rough approximation of each hyperspectral endmember spectrum (with N samples). In order to satisfy the nonnegativity constraint of the NMF algorithm, negative inter/extrapolated values are set to a very small positive value γ. Then, a nonnegative $N \times L$ matrix $B = [b_{ij}]$ is formed. Each column of this matrix corresponds to one nonnegative inter/extrapolated hyperspectral endmember spectrum. The Matrix B is used as an initialization of matrix $\hat{A}$ (i.e. $\hat{A}^{(0)} = B$) in the hyperspectral NMF algorithm. To avoid random initialization of matrix $\hat{S}$, the NLS method [10] is used to derive an initial value $\hat{S}^{(0)}$ of $\hat{S}$. At this step, the NLS method is applied separately to each pixel position of the hyperspectral image.

Before running NMF iterative update rules based on the projected gradient method, two new constant $N \times L$ matrices $F = [f_{ij}]$ and $G = [g_{ij}]$ are formed. These two matrices do not evolve during NMF adaptation and their entries are defined as follows (in the simplest configuration)

$$f_{ij} = \begin{cases} 1 & \text{if } i = \mathrm{c}(1), \ldots, \mathrm{c}(M) \\ 0 & \text{otherwise} \end{cases}, \forall\, j = 1, \ldots, L, \qquad (8)$$

$$g_{ij} = \begin{cases} 0 & \text{if } i = \mathrm{c}(1), \ldots, \mathrm{c}(M) \\ 1 & \text{otherwise} \end{cases}, \forall\, j = 1, \ldots, L. \qquad (9)$$

These two matrices are used at each iteration of the modified NMF algorithm in order to adjust $\hat{A}$ after updating it by the standard NMF rules (6)-(7). This adjustment is performed as follows

$$\hat{A} \leftarrow F \odot \hat{A}^{(0)} + G \odot \hat{A}, \qquad (10)$$

where $A \odot B$ denotes element-wise multiplication.

The above adjustment constrains desired hyperspectral endmember spectra to get the corresponding multispectral endmember spectra values at wavelengths $\lambda_{c(m)}$, $m = 1\ldots M$. Since the spectra at these wavelengths are accurately estimated thanks to the pure pixels of the multispectral image, this constraint is likely to provide a better approximation of final desired hyperspectral endmember spectra.

Another constraint to be taken into account is the abundance sum-to-one natural property (3). In the proposed implementation of the NLS and NMF methods, this constraint is applied by using the technique described in [7].

The proposed algorithm is stopped when the number of iterations exceeds a predefined maximum number.

4. TEST RESULTS

4.1. Performance evaluation criterion

For real (thanks to ground truth) and synthetic data, the mean over all pure materials of the spectral angle mapper (SAM) [8] between the original and estimated hyperspectral endmember spectra is used to evaluate the performance of the proposed method.

4.2. Tested data

Experiments based on synthetic and real data are performed to evaluate the performance of the proposed method.

Synthetic data are generated as follows. Six hyperspectral endmember spectra are randomly selected from a spectral library compiled by the United States Geological Survey (USGS) [3]. Only 207 wavelengths from 0.4 to 2.5 µm are used in the selected hyperspectral endmember spectra. These spectra are then used to generate a 100×100 pixel synthetic hyperspectral image according to the linear mixing model. The six abundance fraction maps used to create these mixtures are derived from a real classification of land cover (by averaging pixel classification values on a sliding 5×5 pixel window). These abundance fraction maps are pre-processed so as to obtain highly mixed pixels (maximum abundance: 50%) while still satisfying the abundance sum-to-one constraint. Six multispectral endmember spectra are derived from the above hyperspectral endmember spectra by just averaging the samples of the latter spectra over the

wavelength regions corresponding to the Landsat Enhanced Thematic Mapper Plus (ETM+) bands 1-5 and 7. Thus, six multispectral endmember spectra with six wavelengths, corresponding to the centers of these bands, are obtained.
Real data are also used. These real multispectral and hyperspectral data (geometrically coregistered and radiometrically corrected), acquired on the same day (March 3, 2003) and at the same time (one minute interval), cover a part of Oran area, Algeria. The multispectral image, acquired by the Landsat ETM+ sensor, is characterized by 6 spectral bands and 30 m spatial resolution. The hyperspectral image is from the Earth observing-1 (EO-1) Hyperion sensor. This image, with 30 m spatial resolution, contains 125 spectral bands. To test the proposed approach with a hyperspectral image which does contain highly mixed pixels, the above original hyperspectral image is intentionally spatially downsampled by just averaging its pixel values, using a non-overlapping sliding 2×2 pixel window, which results in a downsampled hyperspectral image with 60 m spatial resolution. Using ground truth, four multispectral endmember spectra are manually extracted from the multispectral image. Also, using the same ground truth, the same four endmember spectra are manually extracted from the *original* hyperspectral image. These four *original* hyperspectral endmember spectra are used for comparison with the four *extracted* (from the downsampled hyperspectral image) hyperspectral endmember spectra.

4.3. Results and discussion

The proposed (modified NMF) and five classical methods are applied to the used data for comparison. These classical methods (described in [1]) are: sequential maximum angle convex cone (SMACC), vertex component analysis (VCA), minimum volume constrained nonnegative matrix factorization (MVC-NMF), minimum volume simplex analysis (MVSA), and simplex identification via split augmented Lagrangian (SISAL). These classical five methods do not make use of multispectral data and are only applied to the generated hyperspectral image. A standard NMF algorithm, which does not include adjustment rule (10), is also considered in the conducted experiments.
For each method, the values of the used performance criterion are reported in the following table.

Table I. Mean SAM values (°) for synthetic and real data.

Data / Method	Synthetic	Real
Modified NMF	**0.70**	**6.84**
NMF	9.87	11.10
SISAL	2.79	15.30
MVSA	3.43	18.62
MVC-NMF	6.85	10.23
VCA	14.11	28.99
SMACC	14.48	19.73

As stated in Section 3, the reflectance values at the multispectral wavelengths must be *approximately* the same for the hyperspectral and multispectral data. However, some spectral variability between the multispectral and hyperspectral images may occur. In order to evaluate the robustness of the proposed method to this spectral variability, two other tests are performed with the above synthetic data. In the first test, and in order to add a spectral variability between the hyperspectral and multispectral data, a random reflectance uniformly distributed between 0% and 5% of the original value is added to each sample of each derived multispectral endmember spectrum whereas the hyperspectral image is not modified. In the second test, and for the same reason, a random reflectance uniformly distributed between 5% and 10% of the original value is added to each sample of each derived multispectral endmember spectrum. The proposed method is applied to these modified synthetic data, and the mean values of the used performance criterion are given in the following table.

Table II. Mean SAM values (°) obtained by the proposed method with spectral variability on the synthetic data.

Spectral variability range	0% - 5%	5% - 10%
Mean of SAM	2.24	2.78

Globally, Table I shows that the proposed approach yields much better performance than all other used methods. For the synthetic data, the mean of SAM is 0.70° for the proposed approach, i.e. about 4 to 21 times lower than the means of SAM achieved by the other methods.
Moreover, Table II shows that the proposed method is robust to the spectral variability between the hyperspectral and multispectral data, with a limited loss of performance as compared to the performance obtained by the same method without spectral variability.

5. CONCLUSION

In this paper, a new approach, based on a modified version of nonnegative matrix factorization, was proposed for linear endmember spectra extraction from highly mixed remote sensing hyperspectral images combined with high spatial resolution multispectral data.
According to the obtained results, this new approach significantly outperforms some popular linear endmember spectra extraction methods which do not take into account multispectral data. Also, this new approach is robust to spectral variability which may exist between hyperspectral and multispectral data.
The combination of hyperspectral and multispectral data is therefore very attractive for linear hyperspectral endmember spectra extraction.

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