Endmember Extraction from Hyperspectral Imagery based on Probabilistic Tensor Moments

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Abstract

This letter presents a novel hyperspectral endmember extraction approach which integrates a tensor-based decomposition scheme with a probabilistic framework in order to take advantage of both technologies when uncovering the signatures of pure spectral constituents in the scene. On the one hand, statistical unmixing models are generally able to provide accurate endmember estimates by means of rather complex optimization algorithms. On the other hand, tensor decomposition techniques are very effective factorization tools which are often constrained by the lack of physical interpretation within the remote sensing field. In this context, this letter develops a new hybrid endmember extraction approach based on the decomposition of the probabilistic tensor moments of the hyperspectral data. Initially, the input image reflectance values are modelled as a collection of multinomial distributions provided by a family of Dirichlet generalized functions. Then, the unmixing process is effectively conducted by the tensor decomposition of the third-order probabilistic tensor moments of the multivariate data. Our experiments, conducted over four hyperspectral datasets, reveal that the proposed approach is able to provide efficient and competitive results when compared to different state-of-the-art endmember extraction methods.

Index Terms

Hyperspectral unmixing, endmember extraction, statistical models, tensor decomposition.

I. INTRODUCTION

Hyperspectral imaging (HSI) is one of the most important technologies to address many different applications within the remote sensing field [1]. In general, HSI sensors capture the Earth surface using hundreds of narrow and contiguous bands, providing valuable spectral and spatial information of the target scene [2]. Nonetheless, the higher the spectral precision of
the sensor, the smaller the spatial resolution of the recorded data, since the amount of photons captured at each band logically decreases [3]. In this context, Hyperspectral Unmixing (HU) plays a fundamental role to uncover sub-pixel information from the sensed spectra, because HU aims at decomposing HSI imagery into a collection of pure spectral signatures (endmembers) and a set of fractional abundances that represent pixel endmember proportions.

From geometrical techniques to statistical models, different paradigms have been successfully applied to unmix remotely sensed data [4]. Geometrical approaches exploit the HSI data geometry to estimate the spectral signatures and fractional abundances. The vertex component analysis (VCA) [5] is one of the most popular and effective geometrical methods. Specifically, VCA assumes that the endmembers of a given HSI scene define a simplex of minimum volume that encloses the data. In this way, spectral signatures can be efficiently estimated using convex set geometry. Another relevant approach is the minimum volume simplex analysis (MVSA) [6], which introduces some additional constraints on the abundance fractions to increase the model robustness to the absence of pure pixels, and also to the presence of noise. Statistical methods follow a probabilistic scheme to model endmembers and abundances as probability distributions, thus accounting for a higher data variability. For instance, in [7] Nascimento and Bioucas formulate fractional abundances as mixtures of Dirichlet densities. Similarly, other authors model the endmember variability using different distributions, such as the Gaussian distribution [8] or topic modeling [9].

Despite the remarkable performance achieved by these methods, alternative research work has been also conducted considering the data decomposition nature of the HU problem. In this sense, several papers in the literature adopt the non-negative matrix factorization (NMF) approach [10], which aims at decomposing the input HSI data into two multiplicative factors, i.e. endmembers and abundances. For instance, this is the case of the work presented in [11], where the authors introduce different regularization constrains over the elemental NMF scheme. Analogously, Li et al. propose in [12] a robust collaborative non-negative matrix factorization (CNMF) approach, which is able to work with an overestimated number of endmembers. As an alternative to the NMF scheme, some recent works show the advantages of considering a tensor-based decomposition framework, which allows preserving more spatial information, since the HSI data can be managed from a 3-D perspective. In this regard, Qian et al. present in [13] a matrix-vector non-negative tensor factorization (MVNTF) approach which is, to the best of our knowledge, the first method that employs a tensor-based scheme for HU. Other authors, such as
Feng et al. in [14], propose some additional constraints over the seminal approach that provide certain performance advantages.

With the recent emergence of multi-linear algebra to represent remotely sensed HSI data, HU methods no longer depend on traditional matrix decomposition techniques to uncover spectral signatures and fractional abundances. However, the lack of physical interpretation of the factorization process itself is often a conceptual limitation that still forces current decomposition-based HU approaches to impose additional restrictions, e.g. the sum-to-one and non-negativity abundance constraints [12], [13], [14]. In this sense, some recent statistical methods, such as [15], [16], [17], show the advantages of considering a probabilistic framework to deal with remotely sensed HSI imagery. In particular, assuming that the input data is sampled from a probability distribution makes the sum-to-one and non-negativity conditions inherent to the solution because the output result naturally belongs to the corresponding probability simplex [18], [9].

In this scenario, this letter proposes a new endmember extraction approach which aims at combining a tensor-based decomposition scheme with a probabilistic framework in order to take advantage of both technologies when unmixing remotely sensed HSI data. On the one hand, the latest research based on tensors [13], [14] reveals that this kind of factorization is able to provide very competitive and efficient results within the HU field. Nonetheless, the tensor decomposition approach does not show a literal meaning when estimating spectral signatures, which may eventually limit its physical interpretation while forcing some additional constraints. On the other hand, the probabilistic interpretation of the unmixing process [9] makes the probabilistic scheme very useful to represent the HSI data, since the image pixels are probabilistically distributed over the endmember space. In order to achieve this goal, we initially formulate the HU problem considering that the HSI data can be effectively modeled according to the multinomial distributions provided by a family of Dirichlet generalized functions. Then, the unmixing process is conducted using the third-order probabilistic tensor moments of the multivariate data. Our experiments, conducted over four HSI datasets, show the proposed approach exhibits competitive performance when compared to different state-of-the-art methods available in the literature.

II. METHODOLOGY

A. Endmember Extraction Formulation

Let $X \in \mathbb{R}^{B \times N}$ be a HSI image with $N$ pixels and $B$ bands. Let $K$ be the number of endmembers of $X$. The endmember extraction task consists of estimating the inherent set of
spectral signatures from $X$ as $S = \{s_1, ..., s_K\} \in \mathbb{R}^{B \times K}$. Considering the linear mixing model [4], it is possible to characterize each pixel $X^{(i)}$ as a mixture of $K$ endmembers:

$$X^{(i)} = \sum_{k=1}^{K} s_k a_k^{(i)}, \quad (1)$$

where $a_k^{(i)} \in \mathbb{R}$ denotes the fractional abundance of $s_k$ in $X^{(i)}$. In order to guarantee that fractional abundances lie on the corresponding $K$-dimensional probability simplex $\Delta^{K-1}$, let us assume that the abundance vectors $a = \{a^{(1)}, ..., a^{(N)}\} \in \mathbb{R}^{K \times N}$ are independently drawn from a Dirichlet distribution with a concentration parameter $\alpha = \{\alpha_1, ..., \alpha_K\}$, being $\alpha_0 = \sum_{k=1}^{K} \alpha_k$.

Consequently, the contribution of the endmembers to the image bands at the $i$-th pixel can be modeled using a multinomial distribution with parameters $a^{(i)}$, and the corresponding pixel reflectance values can be then derived from the endmember vectors $s_k \in \Delta^{B-1}$. The way we encode the HSI data is by expressing each $1/2^{16}$ reflectance fraction of each band as a binary vector [19]. Let $\{v_1, v_2, ..., v_B\} \in \mathbb{R}^{K \times B}$ be the standard coordinate basis for $\mathbb{R}^B$. Then, we characterize the $F$ reflectance fractions of $X$ as a set of column vectors $\{x_1, x_2, ..., x_F\} \in \mathbb{R}^{B \times F}$, which indicate the activation of the HSI bands. In other words, each reflectance fraction $x_f$ of $X$ is expressed by the standard coordinate basis vector $v_j$ corresponding to the band where the fraction $x_f$ was acquired. Note that this notation allows expressing the joint probabilities of the HSI reflectance fractions using the cross-moments of these vectors.

B. Probabilistic Tensor Cross-Moments

With the aforementioned problem formulation in mind, let us now define some properties of the hidden moments of the HSI data, following the general tensor decomposition theory for learning latent variable models [20]. Considering that the endmember mixture $a$ is drawn from a Dirichlet distribution, the expected value of the $k$-th element of this vector can be defined as follows:

$$E[a_k] = \frac{\alpha_k}{\alpha_0}. \quad (2)$$

According to the aforementioned notation, the expected value of a reflectance fraction $x_1 \in \mathbb{R}^B$ conditioned to the endmember mixture vector $a$ can be represented as:

$$E[x_1|a] = \sum_{k=1}^{K} s_k a_k. \quad (3)$$

Eq. (3) shows the relationship between the observed data $x_1$ and the spectral signatures $s_k$. However, it requires knowledge on the abundance vectors $a$, which are logically unknown. As a result, it can be considered the marginal expectation $E[x_1]$ to derive the following expression:
\[ E[x_1] = E[E[x_1 | a]] = \sum_{k=1}^{K} \frac{\alpha_k}{\alpha_0} s_k. \]  

(4)

This equation reveals that the moments of the observable data are useful to recover the endmember vectors \( s_k \). Nonetheless, the moments of a single reflectance fraction \( x_1 \) do not provide information to estimate spectral signatures that cover the complete HSI domain. For this reason, we consider the cross-moments of pairs of reflectance fractions as follows:

\[ E[x_1 \otimes x_2] = E[Sa \otimes Sa], \]  

(5)

where the symbol \( \otimes \) denotes the Kronecker product. Analogously, the third-order cross-moment of the data can be formulated as:

\[ E[x_1 \otimes x_2 \otimes x_3] = E[Sa \otimes Sa \otimes Sa]. \]  

(6)

Once the cross-moments of the input reflectance data are represented in terms of \( S \) and \( a \), it is also possible to derive a closed-form expression due to the assumption that the abundance vectors \( a \) are drawn from a Dirichlet distribution. According to the findings reported by Anandkumar et al. in [21], our observed reflectance data cross-moments could be explicitly written in terms of \( \alpha \) and \( S \) as follows:

\[ E[x_1 \otimes x_2] = \frac{1}{\alpha_0(\alpha_0 + 1)} \left( (S\alpha \otimes S\alpha) + \sum_{k=1}^{K} \alpha_k (s_k \otimes s_k) \right), \]  

(7)

\[ E[x_1 \otimes x_2 \otimes x_3] = \frac{1}{\alpha_0(\alpha_0 + 1)(\alpha_0 + 2)} \left( (S\alpha \otimes S\alpha \otimes S\alpha) + \sum_{k=1}^{K} \alpha_k (s_k \otimes s_k \otimes s_k) \right) + \sum_{k=1}^{K} 2\alpha_k (s_k \otimes s_k \otimes s_k). \]  

(8)

After isolating the last two terms in Eqs. (7)-(8) and applying Theorem 3.5 in [20], the probabilistic tensor moments can be expressed as a linear combination of \( s_k \):

\[ M_1 = \sum_{k=1}^{K} \frac{\alpha_k}{\alpha_0} s_k, \]  

(9)

\[ M_2 = \sum_{k=1}^{K} \frac{\alpha_k}{\alpha_0(\alpha_0 + 1)} (s_k \otimes s_k), \]  

(10)

\[ M_3 = \sum_{k=1}^{K} \frac{2\alpha_k}{\alpha_0(\alpha_0 + 1)(\alpha_0 + 2)} (s_k \otimes s_k \otimes s_k). \]  

(11)
C. Tensor Orthogonalization

In order to uncover the spectral signatures \( S \) from the defined probabilistic tensor cross-moments, it is necessary to express these moments as orthogonal matrices, to enable the use of regular tensor decomposition techniques [20]. Let us assume that there is a matrix \( W \) which orthogonalizes the second moment as follows:

\[
M_2(W, W) = W^T M_2 W = I,
\]

where \( I \) represents the identity matrix and \( T \) is the transpose operator. In this scenario, the second non-central moment can be defined by the following expression:

\[
M_2(W, W) = W^T \left( \sum_{k=1}^{K} \frac{\alpha_k}{\alpha_0(\alpha_0 + 1)} (s_k \otimes s_k) \right) W
\]

\[
= \sum_{k=1}^{K} W^T \left( \frac{\alpha_k}{\alpha_0(\alpha_0 + 1)} s_k \right) \otimes \left( \frac{\alpha_k}{\alpha_0(\alpha_0 + 1)} s_k \right)^T W
\]

\[
= \sum_{k=1}^{K} \phi_k \otimes \phi_k^T = I
\]  

As Eq. (12) shows, \( \phi_k = W^T \sqrt{\frac{\alpha_k}{\alpha_0(\alpha_0 + 1)}} s_k \) is a set of orthonormal vectors, since it orthogonalizes \( M_2 \). In addition, \( s_k \) can be recovered from \( \phi_k \), because it is a linear combination of \( s_k \) and \( W \) terms. Similarly, multiplying the third-order probabilistic moment by this orthogonalization matrix, we can obtain the following expression:

\[
M_3(W, W, W) = (W^T \otimes W^T \otimes W^T) M_3
\]

\[
= (W^T)^3 \left( \sum_{k=1}^{K} \frac{2\alpha_k}{\alpha_0(\alpha_0 + 1)(\alpha_0 + 2)} (s_k \otimes s_k \otimes s_k) \right)
\]

\[
= \sum_{k=1}^{K} \frac{2\sqrt{\alpha_0(\alpha_0 + 1)}}{(\alpha_0 + 2)\sqrt{\alpha_k}} \phi_k \otimes \phi_k \otimes \phi_k
\]  

In this letter, we efficiently compute the orthogonalization matrix by using the singular value decomposition (SVD) over the empirical second-order moments as \( \hat{M}_2 = A\Sigma A^T \), being \( W = A\Sigma^{-\frac{1}{2}} \). After the process, the dimensionality of this third-order tensor can be reduced from \( \mathbb{R}^{B \times B \times B} \) to \( \mathbb{R}^{K \times K \times K} \).

D. Tensor Power Method for Endmember Estimation

The so-called Tensor Power Method (TPM) decomposition approach [20] is used in this work to estimate the set of spectral signatures from the corresponding eigenvalues (\( \lambda \)) and eigenvectors (\( \theta \)). Initially, the aforementioned transformation for tensor orthogonalization and dimensionality reduction is conducted to enable the use of the TPM decomposition over the input HSI data. Being \( W \) the estimated orthogonalization matrix, we define the tensor \( T = M_3(W, W, W) \) to recover \( S \) by applying a power-deflation approach over \( T \). Specifically, TPM starts with \( \theta_0 \).
randomly sampled from the unit sphere. After several iterations, the power expression update shown in Eq. (14) reveals that the largest initialization component dominates the whole iterative process. Note that the $T(\cdot)$ operand generates a tensor by applying the Kronecker product to its arguments.

$$\theta_{t+1} = \frac{T(I, \theta_t, \theta_t)}{\|T(I, \theta_t, \theta_t)\|}. \tag{14}$$

Once the $\theta_k$ parameter is approximated, $\lambda_k$ can be recovered from $T(\theta_k, \theta_k, \theta_k) = \lambda_k$. That is, for each pair $(\theta_k, \lambda_k)$, it is possible to recursively compute the tensor $T - (\lambda_k \theta_k \otimes \theta_k \otimes \theta_k)$. Eventually, considering that the $s_k$ parameter is in the column space of $W$, the final endmember estimation can be conducted according to Eq. (15). Algorithm 1 shows a pseudo-code description of the considered TPM-based procedure.

$$s_k = \frac{\alpha_0 + 2}{2} \lambda_k W^T \theta_k. \tag{15}$$

III. EXPERIMENTS

A. Data sets

Four HSI datasets have been considered in this letter: Synthetic, Samson, Jasper and Urban. These images have been selected because they are used in multiple reference works in spectral unmixing, i.e. [5], [22], [23], [24], [25]. Besides, their corresponding ground-truth endmembers are publicly available from https://goo.gl/23ue7v.

- **Synthetic** [5] is a simulated HSI scene with $36 \times 36$ pixels and 224 spectral bands. This simulated data comprises three endmembers which have been selected from the U.S. Geological Survey (USGS) library: Actinolite, Ammonio and Erionite. This dataset has been generated considering an additive Gaussian noise level of 30dB (SNR), and without including any pure spectral pixels.

- **Samson** [23] is a real HSI scene with $95 \times 95$ pixels and 156 spectral bands, covering from 401 nm to 889 nm wavelengths. There are three materials in the Samson scene, i.e. soil, tree and water.

- **Jasper** [24] is another real dataset which contains $100 \times 100$ pixels and 198 spectral bands, ranging from 400 nm to 2500 nm. The Jasper scene contains a total of four endmembers, i.e. road, soil, tree and water.

- **Urban** [25] is a real image with $307 \times 307$ pixels and 162 bands. These data include four different materials, i.e. asphalt, grass, roof and tree.
Algorithm 1 TPM-based Endmember Extraction

**Input** $x$: Quantized HSI data (16-bit)

**Input** $K$: Number of endmembers

**Output** $S$: Estimated spectral signatures

1: Compute the empirical moments of $x$: $\hat{M}_*$
2: Estimate $\hat{W}$ using SVD over $\hat{M}_2$: $\hat{W} \leftarrow A\Sigma^{-\frac{1}{2}}$
3: Define the third-order tensor: $T \leftarrow M_3(\hat{W}, \hat{W}, \hat{W})$
4: Conduct the tensor decomposition: TPM($T$, $L$, $N$)
5: Recover the spectral signatures: $S \leftarrow$ Eq. (15)

6: procedure TPM($T$, $L = 100$, $N = 100$)
7:   for $\tau = 1$ to $L$ do
8:      $\theta_0 \leftarrow$ Random init. from the $\mathbb{R}^K$ unit sphere
9:   for $t = 1$ to $N$ do
10:      $\theta_t \leftarrow$ Compute the TPM update [Eq. (14)]
11:   end for
12:  end for
13:  Let $\tau^* = \arg \min_{\tau \in [L]}T(\theta_{\tau}, \theta_{\tau}, \theta_{\tau})$
14:  Carry out $N$ additional updates over $\theta_{\tau^*}$ [Eq. (14)]
15: end procedure

B. Experimental settings

The performance of our newly proposed approach in the task of uncovering pure spectral signatures from remotely sensed HSI data has been tested against different unmixing methods available in the literature. Specifically, the following endmember extraction algorithms have been considered: VCA [5], MVSA [6], NMF [11], CNMF [12], DEpLSA [9], SCM [26] and the proposed approach. All the tested methods have been used considering a given number of endmembers ($K$) and their corresponding default parameter configurations. Note that $K$ could be also estimated using any subspace identification method [4]. Since this letter is just focused on assessing the spectral signatures, null abundance sparsity constrains have been used in NMF and
DEpLSA methods. In the case of the proposed approach, a symmetric Dirichlet concentration parameter $\alpha_0 = 0.2$ has been adopted as a global setting. Regarding the evaluation protocol, the Spectral Angle Distance (SAD) has been employed as quantitative metric.

C. Results and Discussion

Table I presents the SAD quantitative assessment for the considered unmixing methods (in columns) and datasets (in rows). Note that the last row for each dataset contains the corresponding average results and the last row of the table provides the average computational time. Fig. 1 also provides a qualitative evaluation of the four best methods for the Samson collection. In this case, the corresponding ground-truth spectral signatures are visualized using dashed lines.

According to the reported results, it is possible to highlight some important observations. The first noteworthy point is related to the global quantitative performance obtained by the tested methods. As Table I shows, VCA, DEpLSA and SCM (together with the proposed approach) provide competitive unmixing results for the considered HSI collections. In the case of the Synthetic and Samson scenes, DEpLSA and VCA exhibit a remarkable spectral precision when
extracting spectral signatures. However, the proposed approach obtains the best reduction in terms of angular deviation between the estimated endmembers and the corresponding ground-truth ones, being 0.022 and 0.016 radians the improvement over VCA and DEpLSA, respectively.

When considering the Jasper dataset, DEpLSA, the proposed approach and SCM are the three best methods, obtaining 0.152, 0.194 and 0.235 average SAD values. Finally, the unmixing results in the Urban collection reveal that the proposed approach is the best method, followed by DEpLSA and SCM (for which the SAD is increased 0.027 and 0.039 radians, respectively).

Another relevant point arises when analyzing the quantitative endmember results in more detail. As it is possible to observe in Table I, CNMF, VCA, DEpLSA, SCM and the proposed approach are all able to produce some endmember estimates which are the most similar to the corresponding ground-truth spectral signatures in some cases. However, the proposed approach achieves the most consistent and robust results, since it frequently obtains the best endmember estimation across the all considered HSI images. The qualitative results displayed in Fig. 1 support this observation. More specifically, the proposed approach achieves the most accurate estimation for the water endmember while maintaining a competitive precision for the rest of the spectral signatures. Regarding the computational time, the presented endmember extraction method also exhibits a remarkable performance, being the second most efficient method and significantly better that regular statistical approaches.

In general, estimating the endmembers of a given HSI scene raises the challenge of uncovering the most spectrally pure components from mixed data, where the spectral properties of the materials can easily be masked. As a result, HU methods work for mitigating the ill-posed nature of the material dissociation problem by imposing some constraints and assumptions which
eventually relieve the uncertainty when uncovering pure spectral signatures. According to the conducted experiments, DEpLSA and SCM rank among the most effective methods. In this sense, the proposed approach considers an analogous statistical perspective, but using a rather different unmixing approach based on tensor moments, which allows us to estimate very competitive endmembers using an unconstrained tensor-based decomposition technique. As a result, the proposed approach allows us to avoid the use of (computationally demanding) optimization algorithms while achieving the benefits provided by a statistical basis.

IV. CONCLUSIONS AND FUTURE WORK

This letter introduces an approach to effectively uncover pure spectral signatures from HSI data using a new probabilistic tensor moment strategy. Whereas conventional statistical models generally provide remarkable unmixing performance using rather complex optimization algorithms, the latest research on tensors points out that this kind of technology is able to obtain competitive results using simpler factorization procedures. In this context, our newly proposed approach integrates a tensor-based decomposition scheme with a probabilistic unmixing framework to take advantage of both technologies when estimating endmembers. The conducted experiments reveal the proposed approach exhibits competitive performance when compared to different state-of-the-art methods available in the literature. Thus, the main conclusion that arises from this work is the potential of the considered third-order probabilistic tensor moments to effectively uncover pure spectral signatures from HSI data. In the future, we plan to extend this work to estimate both spectral signatures and fractional abundances from a probabilistic tensor-based perspective. We will also conduct a comparison with traditional tensor-based unmixing methods.

REFERENCES


