ON THE DETECTION OF LINEAR MIXTURES IN HYPERSPECTRAL IMAGES

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ABSTRACT

In order to provide reliable information on the instantaneous field-of-view considered in hyperspectral images through spectral unmixing, understanding the kind of mixture that occurs over each pixel plays a crucial role. In this paper, a new method for fast detection of linear mixtures is introduced. The proposed method does not need statistical information and performs an *a priori* test on the spectral linearity of each pixel. It uses standard least squares optimization to achieve estimates of the likelihood of occurrence of linear combinations of endmembers by taking advantage of geometrical properties of hyperspectral signatures. Experimental results on synthetic datasets show how the aforesaid algorithm is actually able to deliver a reliable and thorough assessment of the kind of mix on the scene.

1. INTRODUCTION

Spectral unmixing involves the estimation of pure spectral signatures (endmembers) and their corresponding abundances on each pixel of a hyperspectral scene. Nonlinear unmixing has become of great importance due to the complexity of the mixtures appearing in the scenes. As hyperspectral images can consist in heterogeneous reflectance schemes, unmixing algorithms should also be designed to be flexible and adaptive to properly fit and track the several interactions among materials [1], in order to achieve an efficient and reliable characterization of the physical-chemical composition of the hyperspectral scenes. Thus, the need of *a priori* tests for nonlinearity detection has become urgent in hyperspectral unmixing. Therefore, reliable detection of nonlinear reflectance behavior can play a key-role in enhancing hyperspectral unmixing performance. Recently, several papers have addressed the issue of nonlinearity detection under different assumptions on the models, environments and structures to be considered. Typically, they rely on statistical properties to be drawn out of the whole hyperspectral image [2], Markov random fields operating on spatial features [3], or Monte Carlo algorithms applied to the whole signatures' dataset [4]. Further, in [1], a framework for efficient p-linear unmixing that considers a pre-processing step to estimate the nonlinearity order of each pixel by artificial neural network (ANN) is introduced. Although the aforementioned methods might actually provide enhancement in understanding and quantifying the nonlinear reflectance interactions, computational complexity still represents an issue for actual implementation and development of those algorithms [1]. Indeed, those structures basically need to invert both linear and nonlinear mixture models, in order to obtain the error distribution. Then, the nonlinear effect detection strongly relies on statistical, stochastic and bayesian functions of the achieved variance. Therefore, the estimates proposed in [2], [3] and [4] represent *a posteriori* tests. Accordingly, these frameworks are computationally expensive, as they require to run at least two unmixing algorithms to detect nonlinearities. Further, the aforesaid architectures rely on several approximations in terms of modeling, statistics and nonlinear interactions. Hence, there is a need for novel methods able to perform computationally lighter *a priori* investigations of nonlinear effects in hyperspectral images to enhance understanding the physical phenomena occurring on the given scene. In this paper, instead of looking for nonlinear pixels, we develop a detector of linear mixtures. Specifically, taking advantage of the least squares optimization carried over linear and second-order combinations of endmembers, the proposed algorithm aims at delivering likelihood estimates of the occurrence of a linear mixing in each pixel. Experimental results on synthetic datasets show that the aforesaid algorithm can detect linear mixtures. The paper is organized as follows. Section 2 reports the description of the proposed method, while Section 3 delivers the experimental results. Finally, Section 4 provides the final remarks.

2. METHODS

Let $\underline{\underline{Y}} = \{\underline{y}_l\}_{l=1,\ldots,P}$ be a P-pixel image, where $\underline{y}_l = [y_{l_n}]_{n=1,\ldots,N}$ is the N-band spectral signature of the l-th pixel. Then, let $\mathcal{M} = \{\underline{m}_r\}_{r=1,\ldots,R}$ be the set of the endmembers that can be drawn over $\underline{\underline{Y}}$ according to an endmember extraction algorithm (EEA). Moreover, let us consider the fully constrained least squares (FCLS) [5] optimization algorithm in order to unmix the given image. Hence, when we run FCLS over the l-th pixel considering the endmembers' spectra in $\mathcal{M}$, we obtain

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$$\underline{y}_l = \underline{\hat{y}}_l^{(L)} + \underline{\hat{n}} = \sum_{r=1}^{R} \hat{a}_{lr}\underline{m}_r + \underline{\hat{n}}, \quad (1)$$

where $\underline{\hat{a}}_l = [\hat{a}_{lr}]_{r=1,\dots,R}$ are the coefficients that drive the linear mix as estimated by the FCLS, i.e., $\sum_{r=1}^{R} \hat{a}_{lr} = 1$ and $\hat{a}_{lr} \geq 0\, \forall r$. Moreover, $\underline{\hat{n}}$ is the noise residual that results from the FCLS linear unmixing. Hence, we can consider $\underline{\hat{y}}_l^{(L)}$ as the best linear approximation of $\underline{y}_l$ when we employ FCLS unmixing as driven by the endmembers' spectra. Let us now run FCLS according to the set delivered by the extracted endmembers and their second-order combinations, such that

$$\underline{y}_l = \underline{\hat{y'}}_l^{(L)} + \underline{\hat{y'}}_l^{(NL)} + \underline{\hat{n'}} = \sum_{r=1}^{R} \hat{a'}_{lr}\underline{m}_r + \sum_{r'=1}^{\binom{R}{2}+R} \hat{\beta'}_{lr'}\mathcal{M}_{r'}^{(2)} + \underline{\hat{n'}}, \quad (2)$$

where $\mathcal{M}_{r'}^{(2)}$ represents one of the second order combinations that can be drawn out of the endmembers' signatures in $\mathcal{M}$. Moreover, $\underline{\hat{a'}}_l = [\hat{a'}_{lr}]_{r=1,\dots,R}$ and $\underline{\hat{\beta'}}_l = [\hat{\beta'}_{lr'}]_{r=1,\dots,\binom{R}{2}+R}$ are the coefficients that drive the linear and bilinear mix as estimated by the FCLS, respectively. I.e., $\sum_{r=1}^{R} \hat{a'}_{lr} + \sum_{r'=1}^{\binom{R}{2}+R} \hat{\beta'}_{lr'} = 1$, $\hat{a'}_{lr} \geq 0\, \forall r$, $\hat{\beta'}_{lr'} \geq 0\, \forall r'$. Moreover, $\underline{\hat{n'}}$ is the noise residual that results when FCLS unmixing based on second order combinations of endmembers' spectra is used. Let us now assume that the l-th pixel results from a linear combination of the endmembers' spectra in $\mathcal{M}$, i.e., $\underline{y}_l = \sum_{r=1}^{R} a_{lr}\underline{m}_r + \underline{n}$, where $\underline{n}$ represents the noise delivered by acquisition system. In that case, the following equation holds: $\lim_{||\underline{n}||^2 \downarrow 0} ||\underline{\hat{y}}_l^{(L)} - \underline{\hat{y'}}_l^{(L)}||^2 = 0$. In other terms, when the l-th pixel represents a linear mixture of the R endmembers in the scene, the contribution provided by $\underline{\hat{y'}}_l^{(NL)}$ in (2) is negligible. Therefore, if we are interested in understanding whether the l-th pixel can be considered as a result of linear combinations of reflectances, in the ideal case (i.e., when the pixel noise is not relevant), we can just compute the Euclidean distance between $\underline{\hat{y}}_l^{(L)}$ and $\underline{\hat{y'}}_l^{(L)}$ and call for a linear mix on the l-th pixel if it is equal to zero. On the other hand, if the noise spectrum is such that $||\underline{n}||^2 \downarrow n^* > 0$, then the aforementioned property does not hold anymore. Indeed, it is true that $\lim_{||\underline{n}||^2 \downarrow n^*} ||\underline{\hat{y}}_l^{(L)} - \underline{\hat{y'}}_l^{(L)}||^2 = \delta^* \geq 0$. Thus, in order to estimate the correct thresehold value of δ^* that we could use in order to discriminate between the occurrence of linear or nonlinear combination of endmembers in the l-th pixel, we would need some more complex approach. Specifically, statistical approaches such as those delivered in [2], [3], [4], with all the benefits and flaws that have been previously discussed. Thus, in order to retrieve a reliable and efficient metric s.t. no *a posteriori* estimate of the kind of mixture the l-th pixel displays is drawn out, we can consider the displacement between $\underline{\hat{y}}_l^{(L)}$ and $\underline{\hat{y'}}_l^{(L)}$ from a geometrical point of view. Therefore, let us define $\underline{\hat{y}}_l^{(L)} - \underline{\hat{y'}}_l^{(L)} = \underline{\hat{\delta}} = \sum_{r=1}^{R} \hat{\delta}_r \underline{m}_r$, where $\hat{\delta}_r = \underline{\hat{a}}_{lr} - \underline{\hat{a'}}_{lr}$. Further, it is possible to notice $||\underline{\hat{\delta}}||^2 = \delta^*$. On the other hand, by considering (1) and (2), the following equation holds:

$$\underline{\hat{\delta}} = \underline{\hat{y'}}_l^{(NL)} + \underline{\delta}_n = \underline{\hat{y'}}_l^{(NL)} + (\underline{\hat{n'}} - \underline{\hat{n}}). \quad (3)$$

Therefore, we can assume that if the most of the $\underline{\hat{\delta}}$ displacement is collected by the nonlinear contributions in $\underline{\hat{y'}}_l^{(NL)}$, then the l-th pixel might represent a nonlinear combination of the endmembers in the scene. On the other hand, if the $\underline{\hat{\delta}}$ difference is mostly delivered by the noise residual difference in $\underline{\delta}_n = \underline{\hat{n'}} - \underline{\hat{n}}$, then we can assume that the nonlinear contributions as estimated by FCLS can be considered as negligible, s.t. the mixture provided by l-th pixel is carried by the linear combinations of the endmembers' spectra.

Hence, in order to retrieve a reliable overall metric of this effect, we must define a measure on which we could obtain coherent and thorough estimates and evaluations on the behavior of the displacements in (3). In that sense, volumetric measures and quantities can be effectively employed, as they accurately summarize the feature and properties of a given spectral signature [6], [1]. On the other hand, as volumes are to be computed on holomorphic hulls relying on coherent supports, the quantities in (3) must be referred to a mutual vectorial field, s.t. distance and difference definitions can be delivered according to Euclidean geometry [6]. Indeed, in order to retrieve consistent volume evaluations to be used for comparison and evaluation, it is important to provide a new metric space where each term in (3) can be projected. Thus, in order to deliver this new common environment for the signatures in (3), we might need to consider every quantity in (3) as an object in another space where likelihoods can be safely computed according to Euclidean distances geometry [6].

In that sense, considering the subspace induced by the endmembers' spectral signatures in $\mathcal{M}$ might help to achieve a thorough improvement in terms of reliability and accuracy of the investigation. Specifically, reducing the N-dimensional space to the $\mathcal{M}$ subspace induces a hull where the each endmember spectrum represents one of the basis. Therefore, as $|\underline{m}_r \cdot \underline{m}_s| \geq 0\ \forall \underline{m}_r, \underline{m}_s \in \mathcal{M}$, it is possible to achieve a close set where Euclidean geometry applies [6]. Indeed, as $\underline{\hat{\delta}}$ is defined as a weighted sum on the endmembers in $\mathcal{M}$, we can consider $\hat{\delta}_r$ as the projection of the displacement $\underline{\hat{a}}_l - \underline{\hat{a'}}_l$ onto the basis of the $\mathcal{M}$-induced subspace as determined by the r-th endmember. Thus, in order to obtain a coherent computation for volume comparison onto a consistent domain, it is necessary to evaluate the contribution provided by $\underline{\hat{y'}}_l^{(NL)}$ and $\underline{\delta}_n$ onto each endmember basis of the $\mathcal{M}$ vectorial field [6]. I.e., we aim at rewriting (3) as follows:

$$\underline{\hat{\delta}} = \sum_{r=1}^{R} \hat{\delta}_r \underline{m}_r = \sum_{r=1}^{R} \pi_r(\underline{\hat{y'}}_l^{(NL)})\underline{m}_r + \sum_{r=1}^{R} \pi_r(\underline{\delta}_n)\underline{m}_r, \quad (4)$$

where $\pi_r(\underline{z})$ identifies the nonorthogonal projection of $\underline{z}$ onto the direction imposed by the r-th endmember. Hence, (4) provides a coherent and consistent representation of each term in (3) onto the common domain delivered by the $\mathcal{M}$-induced subspace. Actually, as typically the endmembers in $\mathcal{M}$ are not perfectly orthogonal to each other, the computation of the π_r coefficients in (4) can not be performed according to orthogonal projection algorithms. Thus, in order to obtain the accurate estimation of each π_r, we can write a proper system of linear equations in order to take advantage of the properties of Clifford algebra [6]. Specifically, let us consider a N-element array $\underline{z}$ as defined as $\underline{z} = \sum_{r=1}^{R} \pi_r(\underline{z})\underline{m}_r$. Then, let us consider R linear equations obtained from the aforementioned representation of $\underline{z}$ by considering the inner product of every term onto an endmember. I.e., the i-th linear equation would be written as $\underline{z} \cdot \underline{m}_i = \sum_{r=1}^{R} \pi_r(\underline{z})\underline{m}_r \cdot \underline{m}_i$. Hence, we can write the whole system in matrix form as $\underline{\underline{A}}_{\mathcal{M}} \times \underline{\pi}(\underline{z})^T = \underline{b}^T$, where $\underline{\underline{A}}_{\mathcal{M}} = \{A_{\mathcal{M}_{jk}}\}_{(j,k)\in\{1,\ldots,R\}^2}$, $A_{\mathcal{M}_{jk}} = \underline{m}_j \cdot \underline{m}_k$, $\underline{\pi}(\underline{z}) = [\pi_i(\underline{z})]_{i=1,\ldots,R}$, $\underline{b} = [b_i]_{i=1,\ldots,R}$, $b_i = \underline{z} \cdot \underline{m}_i$. Then, we can use Cramer's rule in order to retrieve the elements in $\underline{\pi}(\underline{z})$ [6]. Specifically, let us consider $\underline{\underline{A}}_{\mathcal{M}} = [\underline{A}_{\mathcal{M}_1}|\cdots|\underline{A}_{\mathcal{M}_j}|\cdots|\underline{A}_{\mathcal{M}_R}]$, where $\underline{A}_{\mathcal{M}_j}$ identifies the j-th column of $\underline{\underline{A}}_{\mathcal{M}}$. Thus, let us define $\underline{\underline{A}}_{\mathcal{M}}^{(h)}$ as the matrix that we obtain by replacing the h-th column of $\underline{\underline{A}}_{\mathcal{M}}$ with $\underline{b}^T$. I.e., $\underline{\underline{A}}_{\mathcal{M}}^{(h)} = [\underline{A}_{\mathcal{M}_1}|\cdots|\underline{A}_{\mathcal{M}_{h-1}}|\underline{b}^T|\underline{A}_{\mathcal{M}_{h+1}}|\cdots|\underline{A}_{\mathcal{M}_R}]$. Hence, by Cramer's rule, it is possible to state as follows:

$$\pi_h(\underline{z}) = \det[\underline{\underline{A}}_{\mathcal{M}}^{(h)}] \cdot (\det[\underline{\underline{A}}_{\mathcal{M}}])^{-1} \tag{5}$$

Therefore, we can obtain the nonorthogonal projections in (4) by operating on matrices induced by inner products in the endmembers' space. Further, it is possible to obtain a quantitative measure of the ability of unmixing based on the given set of endmembers' spectra $\mathcal{M}$ to accurately track and recover the contributions on linear and nonlinear terms of the target spectral signature. In fact, each element of $\underline{\underline{A}}_{\mathcal{M}}$ is defined by the inner product of two endmembers' spectra. Thus, recalling the general crosscorrelation coefficient definition for two multidimensional signals $\underline{\theta}$ and $\underline{\zeta}$ over the same support as $\rho_{\underline{\theta}\underline{\zeta}} = (\underline{\theta} \cdot \underline{\zeta}) \cdot (|\underline{\theta}||\underline{\zeta}|)^{-1}$, it is possible to prove that the value of $\det[\underline{\underline{A}}_{\mathcal{M}}]$ can be computed as a function of the crosscorrelation coefficients that can be drawn over each pair of endmembers [6]. Further, since $\det[\underline{\underline{A}}_{\mathcal{M}}]$ is the rational of each nonorthogonal projection as in (5), it is possible to state that the ability of the unmixing architecture as delivered by considering the set of endmembers $\mathcal{M}$ improves as the spectral signatures in $\mathcal{M}$ get orthogonal to each other. Thus, it is possible to assume that the average crosscorrelation among endmembers' spectra can deliver a good estimate of the quality of the chosen endmembers' set for unmixing performance.

Once the $\underline{\pi}(\underline{z})$ coefficients are computed, the terms in (3) are mapped onto a coherent space. Thus, it is possible to compute the volume induced by the polytopes identified by $\hat{\underline{\delta}}$, $\hat{\underline{y}'}_l^{(NL)}$ and $\underline{\delta}_n$ according to the Cayley-Menger formula retrieved by distance geometry over the subspace delivered by the endmembers' set. Hence, it is possible to provide a likelihood for linear mixture occurrence over the l-th pixel as follows:

$$L_l = 1 - \frac{|V_{\hat{\underline{\delta}}} - V_{\underline{\pi}(\underline{\delta}_n)}|}{|V_{\hat{\underline{\delta}}} - V_{\underline{\pi}(\hat{\underline{y}'}_l^{(NL)})}| + |V_{\hat{\underline{\delta}}} - V_{\underline{\pi}(\underline{\delta}_n)}|} \tag{6}$$

where $V_{\underline{z}}$ identifies the volume of the polytope induced by $\underline{z}$ as computed according to the Cayley-Menger rule [6]. Hence, the likelihood in (6) aims at providing a measure of the linearity of the mixture that occurs over each pixel in the considered hyperspectral image. Further, the process that takes to the computation of L_l takes a small amount of operations and unmixing inversions. Therefore, the proposed framework actually delivers an efficient and effective estimation of the kind of spectral mixture that occurs onto the l-th pixel. The next Section reports the performance in detecting the pixels that result from linear mixtures on the given hyperspectral scene as achieved by the aforementioned method.

3. EXPERIMENTAL RESULTS

The architecture introduced in Section 2 has been tested over datasets that have been synthetically generated to deliver a reliable and solid evaluation of the detection capability of the proposed framework. We considered a data set of $P = 100 \times 100$ spectral signatures over $N = 100$ bands. Ten endmembers randomly chosen from USGS spectral library have been used to generate each pixel in the dataset. Specifically, each spectrum mixture has been drawn randomly from a p-linear mixing model representation: the order of the mix can be $p = 1$ or $p \in (1, p^+]$ with the same probability. Moreover, each mixture is affected by additive white Gaussian noise with a known signal-to-noise ratio (SNR). Finally, the endmembers that have been used to perform unmixing are characterized by the average crosscorrelation factor ρ, defined as $\rho = (\binom{R}{2})^{-1} \sum_{(i,j)\in\{1,\ldots,|\mathcal{M}|\}^2, i>j} \rho_{ij}$.

The results in detecting linear mixture are summarized in Table 1. Specifically, estimates for (6) have been thresholded according to Otsu algorithm [7] to discriminate the mixtures into linear and nonlinear. Further, outcomes are reported in terms of true positives, true negatives, false positives and false positives counts (TP, TN, FP, FN, respectively). Apparently, the proposed architecture delivers strong resilience to perturbations in spectral elements and noise signals. Moreover, the method we introduced is able to effectively detect the occurrence of linear mixtures also when higher order nonlinear effects have been applied to the dataset. Actually, when p^+ increases, the performance typically tends to degrade. However, when $p^+ = 6$ the provided detection seems to deliver slightly better estimates than the system set to $p^+ = \{4, 5\}$. This effect can arise from the way the datasets are generated. In

Table 1. Quantitative analysis of the detection of linear mixtures over synthetic datasets.

p^+	SNR	ρ	TP [%]	TN [%]	FP [%]	FN [%]	Accuracy (=TP+TN) [%]	Mismatch (=FP+FN) [%]
2	30	0.35	48.9	48.5	1.1	1.5	97.4	2.6
3			48.2	48.6	1.8	1.4	96.8	3.2
4			48	47.3	2	2.7	95.3	4.7
5			46.8	47.6	3.2	2.4	94.4	5.6
6			46.2	49.5	3.8	0.5	95.7	4.3
3	20	0.35	46.8	34.8	3.2	15.2	81.6	18.4
	25		45.9	42.4	4.1	7.6	88.3	11.7
	30		48.2	48.6	1.8	1.4	96.8	3.2
	35		48.6	49	1.4	1	97.6	2.4
3	30	0.25	48.8	49.1	1.2	0.9	97.9	2.1
		0.35	48.2	48.6	1.8	1.4	96.8	3.2
		0.45	45.3	43.5	4.7	7.5	88.8	11.2
		0.55	44.9	34.4	5.1	15.6	79.3	20.7

fact, the distribution of the nonlinear combinations is uniform over the interval of the nonlinearity orders $(1, p^+]$. Therefore, as the p^+ increases, the number of coefficients that drive the nonlinear mix increases while their absolute values tend to decrease overall. Thus, the volume of $\underline{\pi}(\hat{\underline{y}'}_l^{(NL)})$ gets lower as well, while the distance $|V_{\hat{\underline{\delta}}} - V_{\underline{\pi}(\hat{\underline{y}'}_l^{(NL)})}|$ drifts increasing, leading the performance to a slight degradation. Finally, the performance of the algorithm is affected by the choice of the endmembers' set, as previously mentioned in Section 2. Indeed, the proposed method can provide better and more reliable knowledge of the actual kind of the mixtures over the scene when the set of endmembers is chosen s.t. the endmembers' spectra tend to be orthogonal to each other. This feature provides a stronger ability to detect nonlinear effects while avoiding the saturation effect provided by linearly dependent endmembers, as previously mentioned. Thus, the endmember extraction algorithm is actually affecting the computation of the likelihoods as in (6), since it depends on $\det[\underline{\underline{A}}_{\mathcal{M}}]$ in (5). Hence, the endmembers should be carefully selected s.t. the nonlinear effects can be properly understood and quantified within the space induced by the endmembers.

4. CONCLUSIONS

A novel method for efficient detection of linear mixtures in hyperspectral datasets has been introduced. The proposed algorithm takes advantage of the geometrical features that least squares optimization provides, s.t. a priori estimates can be delivered. Specifically, by means of the nonorthogonal mapping onto the subspace induced by the endmembers, the proposed framework is able to accurately estimate the kind of the mixtures. Experimental results show how the aforesaid approach is able to deliver accurate performance in detecting linear mixture over the considered scenes by means of a framework with low computational costs. Finally, as no *a posteriori* tests are required, the proposed method efficiently implements a low complexity algorithm for *a priori* detection of the nature of the spectral mixtures. Future works will focus on improving endmembers' extraction and nonlinearity order evaluation.

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