

# NONNEGATIVE MATRIX FACTORIZATION WITH COLLABORATIVITY FOR HYPERSPECTRAL UNMIXING

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## ABSTRACT

Spectral unmixing is an important task for remotely sensed hyperspectral data exploitation. It expresses each (possibly mixed) pixel of the hyperspectral image as a combination of spectrally pure substances (called endmembers) weighted by their corresponding abundances. The spectral unmixing chain usually consists of three main steps: 1) estimation of the number of endmembers in a scene; 2) automatic identification of the spectral signatures of these endmembers; and 3) estimation of the endmember abundances in each pixel of the scene. Over the last years, several algorithms have been developed for each part of the chain. In this paper, we develop a new algorithm which can perform the three steps of the unmixing chain (at once) for hyperspectral images with significant amount of noise. The proposed algorithm, which does not require a previous subspace identification step to estimate the number of endmembers, starts with an overestimated number of endmember and then iteratively removes the less relevant endmember detected by a collaborative regularization prior. Our experimental results demonstrate that the proposed method exhibits very good performance when the number of endmember is not available *a priori*, a situation that is very common in practice.

**Index Terms**— Hyperspectral imaging, spectral unmixing, collaborativity, nonnegative matrix factorization

## 1. INTRODUCTION

Spectral unmixing is an important task for remotely sensed hyperspectral data exploitation [1]. It amounts at estimating the abundance of spectrally pure components (called *endmembers* in hyperspectral imaging literature). The spectral unmixing chain usually consists of three main steps: 1) estimation of the number of endmembers in a scene; 2) automatic

identification of the spectral signatures of these endmembers; and 3) estimation of the endmember abundances in each pixel of the scene. In the last few years, several techniques have been developed for addressing each part of the chain, with particular emphasis on the identification of endmembers (with and without assuming the presence of pure spectral signatures in the input hyperspectral data [2, 3]). However, there are very few spectral unmixing algorithms that can address all the stages involved in the hyperspectral unmixing process simultaneously. Further, the estimation of the number of endmembers by means of subspace identification algorithms is generally very effective when the hyperspectral images are noise free [4, 5], but this part of the chain is more challenging when the amount of noise increases. Let  $p$  denote the true number of endmembers in a hyperspectral image and let  $\hat{p}$  denote the number of endmembers estimated by a certain algorithm. When  $\hat{p} > p$ , the number of endmembers is overestimated and this is particularly critical for endmember identification algorithms designed without assuming that the true endmembers are present in the input hyperspectral data [6–11].

To address this relevant issue, in this paper we develop a new algorithm for hyperspectral unmixing which can provide the number of endmembers along with their signatures and their corresponding abundances at once. The proposed algorithm does not require a previous subspace identification step to estimate the number of endmembers, and is specifically designed to perform effectively in analysis scenarios dominated by noise. The proposed algorithm starts with an overestimated number of endmember and then iteratively removes the less relevant endmember detected by means of a collaborative regularization prior. Our experimental results demonstrate that the proposed method exhibits very good performance in noisy scenarios and without the need to know the number of endmember in advance.

The remainder of the paper is organized as follows. Section 2 describes the proposed approach, which is based on the concept of collaborative nonnegative matrix factorization (CoNMF). Section 3 describes the obtained experimental results. Section 4 concludes the paper with some remarks and hints at plausible future research.

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## 2. PROPOSED APPROACH

### 2.1. Collaborative Nonnegative Matrix Factorization (CoNMF)

Let  $\mathbf{Y} \equiv [\mathbf{y}_1, \dots, \mathbf{y}_n] \in \mathbb{R}^{d \times n}$  be a hyperspectral image with  $n$  spectral vectors and  $d$  spectral bands. The hyperspectral image is represented as a matrix, holding in its columns the spectral vectors  $\mathbf{y}_i \in \mathbb{R}^d$ , for  $i = 1, \dots, n$ . Under the linear mixing model [12], we have:

$$\begin{aligned} \mathbf{Y} &= \mathbf{M}\mathbf{S} + \mathbf{n} \\ \text{s.t. : } & \mathbf{S} \geq 0, \mathbf{1}_p^T \mathbf{S} = \mathbf{1}_n^T, \end{aligned} \quad (1)$$

where  $\mathbf{M} \equiv [\mathbf{m}_1, \dots, \mathbf{m}_p] \in \mathbb{R}^{d \times p}$  is a so-called mixing matrix containing  $p$  endmembers,  $\mathbf{m}_i$  denotes the  $i$ -th endmember signature, and  $\mathbf{S} = [\mathbf{s}_1, \dots, \mathbf{s}_p]^T \in \mathbb{R}^{p \times n}$  is the abundance matrix containing the endmember fractions for every pixel in the hyperspectral scene. Finally,  $\mathbf{n}$  collects the errors that affect the measurement process (e.g., noise). For each pixel, the abundance fractions should be no less than zero and sum to one, which are known as the non-negativity and sum-to-one constraints. These are represented in Eq. (1), where  $\mathbf{1}_p$  is a column vector containing  $p$  ones. In this work, we solve the optimization problem in Eq. (1) using non-negative matrix factorization (NMF) as follows:

$$\begin{aligned} (\widehat{\mathbf{M}}, \widehat{\mathbf{S}}) &= \arg \min_{\mathbf{M}, \mathbf{S}} \frac{1}{2} \|\mathbf{Y} - \mathbf{M}\mathbf{S}\|_2^2 \\ &+ \alpha \sum_{i=1}^{\widehat{p}} \|\mathbf{s}_i\|_2^q + \frac{\beta}{2} \sum_{i=1}^{\widehat{p}} \|\mathbf{m}_i - \bar{\mathbf{y}}\|_2^2 \\ \text{s.t. : } & \mathbf{S} \geq 0, \mathbf{1}_p^T \mathbf{S} = \mathbf{1}_n^T, \end{aligned} \quad (2)$$

where  $\alpha$  and  $\beta$  are regularization parameters and  $\bar{\mathbf{y}}$  is the mean value of the data. The regularization term on the abundance matrix is a collaborative prior which promotes complete lines of zeros, where  $0 < q \leq 1$  is a parameter controlling the degree of collaborativity. The other term on the mixing matrix constrains the distance between all the vertices of the simplex and the data [13, 14]. This term promotes minimum volume even if  $p$  is overestimated.

### 2.2. Proposed Approach

In this work we proposed a follow-up method to the CoNMF algorithm described in the previous subsection in order to determine the number of endmembers, the corresponding endmember signatures and their abundances, thus addressing the three steps in the standard hyperspectral unmixing chain by the same method. Let  $\zeta(i) = \|\mathbf{s}_i\|_2$ , for  $i = 1, \dots, \widehat{p}$ , denote the degree of collaborativity. With this notation in mind, the proposed approach can be described as follows:

- First, we run the CoNMF algorithm in an overestimated scenario, *i.e.*,  $\widehat{p} > p$ .

- Then, we compute  $\zeta(i)$ . The smaller  $\zeta(i)$ , the less relevant the  $\mathbf{m}_i$ . Therefore, it is likely that the minimum  $\zeta(i)$  corresponds to a “fake” endmember.
- We remove  $\mathbf{m}_i$  from the just obtained endmembers and use the remaining  $\widehat{p} - 1$  endmembers as the initial condition in order to run CoNMF again.
- The aforementioned steps are repeated until the reconstruction error diverges. If the reconstruction error is very large, meaning that we arrive at an underestimated scenario, the endmembers and abundances obtained in the previous step are the final output of the algorithm.

An important observation at this point is that the proposed method takes advantage from the results obtained in previous iterations and therefore, it adjusts itself. In this way, we do not need to optimize the related parameters for every number of endmembers. This is an important competitive advantage with regards to other techniques for spectral unmixing, which depend heavily on the number of endmembers used as an input to the chain. Furthermore, we have empirically observed that the proposed method is very stable regardless of the initial parameter settings. In other words, the algorithm automatically adapts to the analyzed data set and provides stable results by automatically identifying how many endmembers are present in the data, the spectral signatures of these endmembers, and the corresponding endmember abundances. Again, these are very important considerations in the unmixing literature, in which most available algorithms are parameter dependent and sensitive to noise. In the following section we will also show how the proposed approach can perform well under high noise conditions.

## 3. EXPERIMENTAL RESULTS

In our experiments we have considered linearly mixed simulated mixtures synthesized using the linear mixture model and a set of mineral spectral signatures from the United States Geological Survey (USGS) library available online<sup>1</sup>. Table 1 shows an evaluation of the performance of the proposed method in the unmixing of simulated hyperspectral data with signal to noise ratio (SNR) of  $\{10, 20, 30, 40\}$  dB, with a true number of endmembers of  $p = 4$ , and in which the initial estimated number of endmember is  $\widehat{p} = 7$ . In the table, several performance discriminators are reported, namely the root mean reconstruction error (RMSE), the spectral angle distance (SAD) [12] and two error metrics focused on the quality of the estimated endmembers,  $\|\widehat{\mathbf{M}} - \mathbf{M}\|_F$ , and on the quality of the estimated abundances,  $\frac{1}{n \times p} \|\widehat{\mathbf{S}} - \mathbf{S}\|_F$ , where  $F$  denotes the Frobenius norm of a given matrix  $\mathbf{X}$ , such that  $\|\mathbf{X}\|_F \equiv \sqrt{\text{trace}\{\mathbf{X}\mathbf{X}^T\}}$ .

<sup>1</sup><http://speclab.cr.usgs.gov/spectral-lib.html>

**Table 1.** Evaluation of the performance of the proposed method in the unmixing of simulated hyperspectral data with signal-to-noise ratio of  $\{10, 20, 30, 40\}$  dB. The true number of endmembers in this experiment is  $p = 4$  and the initial estimated number of endmember is  $\hat{p} = 7$ .

$\hat{p}$	SNR=10dB					SNR=20dB				
	RMSE	SAD	$\ \hat{\mathbf{M}} - \mathbf{M}\ _F$	$\frac{1}{n \times p} \ \hat{\mathbf{S}} - \mathbf{S}\ _F$	$\zeta(i): \min(\max)$	RMSE	SAD	$\ \hat{\mathbf{M}} - \mathbf{M}\ _F$	$\frac{1}{n \times p} \ \hat{\mathbf{S}} - \mathbf{S}\ _F$	$\zeta(i): \min(\max)$
7	0.0356	7.4389	2.0702	0.0478	5.4286(15.3470)	0.0043	3.3771	1.0669	0.0304	5.9593(16.4189)
6	0.0294	6.9041	1.8564	0.0386	5.8079(16.2086)	0.0034	1.7022	0.3843	0.0095	8.2185(17.3037)
5	0.0236	6.2244	1.5838	0.0292	6.6419(17.4830)	0.0024	1.5571	0.3638	0.0028	7.7122(18.5486)
4	0.0136	2.6051	0.5375	0.0048	16.6886(19.0613)	0.0015	1.4523	0.3428	0.0007	17.5498(19.2318)
3	0.0485	-	-	-	-	0.0214	-	-	-	-
$(\hat{p})$	SNR=30dB					SNR=40dB				
	RMSE	SAD	$\ \hat{\mathbf{M}} - \mathbf{M}\ _F$	$\frac{1}{n \times p} \ \hat{\mathbf{S}} - \mathbf{S}\ _F$	$\zeta(i): \min(\max)$	RMSE	SAD	$\ \hat{\mathbf{M}} - \mathbf{M}\ _F$	$\frac{1}{n \times p} \ \hat{\mathbf{S}} - \mathbf{S}\ _F$	$\zeta(i): \min(\max)$
7	0.0010	5.0920	1.1459	0.0467	4.2555(19.6217)	0.0006	3.8063	0.8540	0.0537	4.6899(18.3336)
6	0.0007	4.1628	1.2258	0.0476	7.1381(19.0932)	0.0003	2.8626	0.6083	0.0449	6.2983(17.7297)
5	0.0005	3.7760	1.1500	0.0391	12.2319(19.0773)	0.0002	2.3805	0.4969	0.0329	7.6539(17.6405)
4	0.0002	0.9819	0.2027	0.0003	18.0497(19.3300)	0.0001	0.7120	0.1352	0.0001	18.1826(19.0239)
3	0.0397	-	-	-	-	0.0260	-	-	-	-

From the results reported on Table 1 we can conclude that the proposed approach can successfully estimate the true number of endmembers in high noise conditions. For illustrative purpose, Fig. 1 demonstrates graphically the performance of the proposed method by projecting the simulated data on a two-dimensional subspace. In Fig. 1, we show the true endmembers in black color, the initial condition in cyan color (this corresponds to the endmembers provided by VCA which are used for initialization), and the iterative process: red color for  $\hat{p} = 7$ , green color  $\hat{p} = 6$ , blue color  $\hat{p} = 5$  and yellow color  $\hat{p} = 4$  from the initial to the final condition. We can observe that the proposed approach always converges to the true endmembers regardless of the initialization condition.

#### 4. CONCLUSIONS

In this paper, we have developed a new algorithm which can provide the three steps of the spectral unmixing chain: 1) estimation of the number of endmembers in a scene; 2) automatic identification of the spectral signatures of these endmembers; and 3) estimation of the endmember abundances in each pixel of the scene at once. The proposed approach is shown to be particularly effective in noisy analysis scenarios. In particular, the obtained experimental results demonstrate that the proposed method exhibits very good performance when the number of endmember is not available *a priori*. Although the obtained results are very encouraging, further experiments with real hyperspectral scenes are needed in order to fully substantiate the proposed approach.

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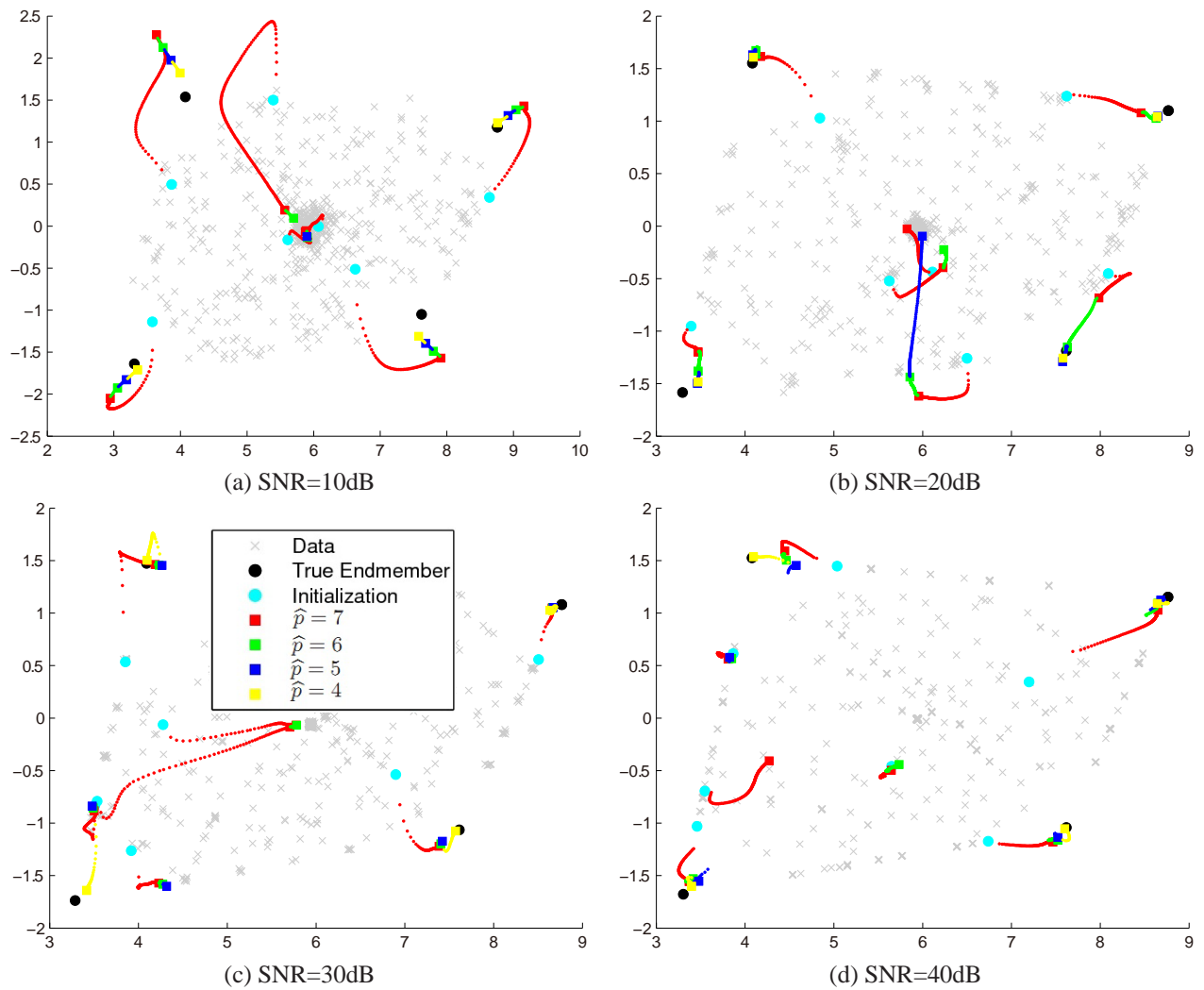
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**Fig. 1.** Graphical assessment of the performance of the proposed method in the unmixing of simulated hyperspectral data with signal-to-noise ration (SNR) of  $\{10, 20, 30, 40\}$  dB. The  $p = 4$  true endmembers are displayed in black color, the initial condition (endmembers produced by the VCA algorithm) is displayed in cyan color, and the iterative process: red color for  $\hat{p} = 7$ , green color  $\hat{p} = 6$ , blue color  $\hat{p} = 5$  and yellow color  $\hat{p} = 4$  from the initial to the final condition, is also represented in graphical form.