

2014

BioTechnology

An Indian Journal

FULL PAPER

BTAIJ, 10(21), 2014 [13583-13588]

Spectral unmixing based on nonnegative matrix factorization restrained by minimizing the sum of the maximum distances between endmembers

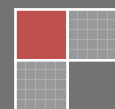
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ABSTRACT

The spectral signature of each hyperspectral image pixel commonly comprises the combined measured reflectance of components. These pixels are called mixed pixel. Spectral unmixing provides an efficient mechanism for the interpretation and classification of these mixed pixels. The algorithm of minimum volume constrained nonnegative matrix factorization (MVC-NMF) is a kind of algorithm which can extract endmembers from highly mixed hyperspectral images. It does not need to assume that pure pixels exist in hyperspectral images. Endmembers and its abundance can be obtained synchronously by this algorithm. However, the constraint condition of MVC-NMF algorithm need to calculate the volume of simplex, which cause the iterative process is complex and the amount of calculation is very large. This paper proposes a NMF algorithm under new constraint condition, which is restrained by minimizing the sum of all maximum distances between endmembers instead of minimizing simplex volume. Experimental results of spectral unmixing illustrate this new NMF algorithm has higher decomposition accuracy and efficiency than MVC-NMF algorithm.

KEYWORDS

Hyperspectral images; Spectral unmixing; Nonnegative matrix factorization (NMF); Endmember; Simplex.



INTRODUCTION

The main features of hyperspectral remote sensing is that the imaging spectrometer can obtain the information from the ultraviolet, visible light, near-infrared, mid-infrared region of the electromagnetic spectrum. Hyperspectral images have tens to hundreds of very narrow and continuous spectral bands. Therefore a continuous spectrum curve can be extracted from a pixel of hyperspectral image^[1]. Due to the limitation of spatial resolution of the imaging systems and the complex diversity of the earth surface, some pixels of hyperspectral images often contain a variety of ground object types. These pixels are called mixed pixels. How to extract the spectrum of typical ground objects (endmembers) and decompose the mixed pixels effectively become an important research topic in the quantitative analysis of hyperspectral remote sensing images. Under normal circumstances, the mutual influence between the endmembers can be neglected, therefore the formation mechanism of mixed pixel can be described by a linear mixture model^[2]. Facts have proved that the spectral unmixing method based on the linear mixture model can give a satisfactory decomposition results.

The decomposition algorithms of the mixed pixel based on the linear mixture model can be divided into two categories: the methods based on geometry and the methods based on statistics^[3]. Geometry methods assume that all the data points of hyperspectral image lie inside a simplex whose vertices correspond to the endmembers respectively. Thus extracting the endmembers is equivalent to finding simplex vertex. These methods include N-FINDR^[4], Vertex Component Analysis (VCA)^[5], Simplex Growing Algorithm^[6], Orthogonal Bases Algorithm (OBA)^[7] and so on. Because the geometry method is to find the vertex from the existing data set, therefore it is not suitable for the data set without "pure pixels". The statistics methods overcome the shortcomings of the geometry methods, which make full use of the statistical characteristics of the data set to solve out the endmember spectra. As a statistical method, nonnegative matrix factorization (NMF) proposed by Lee and Seung et al., in 1999 can guarantee non-negative and does not need to specify the iterative step^[8], therefore has been given more attention on hyperspectral unmixing in recent years. The objective function of NMF has significant non-convex characteristics, and therefore has a large number of local minima. In order to overcome this drawback, some constraint conditions was added to the algorithm according to the actual situation to prevent the results from falling into the irrational local minima.

A spectral unmixing algorithm based on minimum volume constrained NMF (MVC-NMF) was proposed in 2007 by Miao and Qi^[9], it make the simplex press near to the data cloud as far as possible by minimizing its volume, thereby obtain the real endmembers. In this algorithm, the simplex volume is calculated by matrix determinant, therefore the gradient calculation is complicated and uncontrollable in iterative process.

In this paper, we add an appropriate constraint to NMF algorithm according to the characteristics of hyperspectral data cloud, consequently propose a spectral unmixing algorithm based on non-negative matrix factorization constrained by minimizing the sum of the maximum distance between endmembers. Experiment shows that the computational complexity of this algorithm is smaller, and satisfactory spectral unmixing results are obtained.

LINEAR SPECTRAL MIXTURE MODEL

Linear spectral mixture model is the most commonly used data model in hyperspectral remote sensing images analysis. In the linear spectral mixture model, the grey values of the pixels on hyperspectral images are equal to the linear combination of the spectral vectors of all the endmembers according to their abundance. Here we use $R \in \mathbb{R}^{L \times N}$ represent hyperspectral remote sensing images with L bands and N pixels. Assuming it is mixed by the endmembers based linear spectral mixture model, R can be expressed as:

$$R = MS + E \quad (1)$$

$M = [m_1, m_2, \dots, m_p]^T \in \mathbb{R}^{L \times p}$ is referred to as the endmember matrix, in which m_j corresponds to the spectral vectors of the m_j -th endmember. $S = [s_1, s_2, \dots, s_p]^T \in \mathbb{R}^{p \times N}$ is abundance matrix, where $S_j = [S_{j1}, S_{j2}, \dots, S_{jN}]^T \in \mathbb{R}^{N \times 1}$ represents the abundance of the j -th endmember corresponding to all the pixels. E is the error matrix. According to the physical meaning of the abundance, in the spectral mixture model, the abundance must meet two conditions: abundance sum-to-one constraint (ASC) and abundance non-negative-constrain (ANC)^[2]:

$$\sum_{j=1}^p S_{jn} = 1, \quad S_{jn} > 0 \quad (2)$$

The Target of hyperspectral unmixing is to solve out M and S in the case of R being known. We can minimize the objective function based on Euclidean distance to obtain the optimal solution.

$$J(M, S) = \|R - MS\|^2 = \sum_{ij} (R_{ij} - (MS)_{ij})^2 \quad (3)$$

Since R, M and S are non-negative matrices, thus NMF algorithm can be used in hyperspectral unmixing^[8,9], the iterative formula in NMF algorithm is as follows:

$$M \cdot (RS)^T ./ (MSS^T) \rightarrow M \tag{4}$$

$$S \cdot (M^T R) ./ (M^T MS) \rightarrow S \tag{5}$$

In the above formula, "."* And "./" represent the multiplying and dividing of the elements in the matrix.

THE PRINCIPLE OF NONNEGATIVE MATRIX FACTORIZATION AND ITS SOLVING APPROACH

The mathematical model of NMF is very similar to the linear spectral mixture model based on the convex simplex, which makes it possible to apply NMF to spectral unmixing. The mission of NMF is to find the matrices $M \in R^{L \times P}$ and $S \in R^{P \times N}$ in which all elements are non-negative to satisfy $R=MS$. In the linear spectral mixture model R, M, S respectively correspond to the gray value of pixels, endmember matrix and abundance matrix. In recent years, a representative hyperspectral unmixing method based on NMF algorithm is the minimum volume constrained NMF (MVC-NMF) proposed by Miao and Qi in 2007.

MVC-NMF is a combination of statistical and geometric algorithms. From the perspective of geometry, the iterative process of NMF looks like several endmembers rotate around the data cloud and press close to it continuously. Here NMF can be seen as an "external force" to promote the endmembers to move away from data cloud. Minimum volume constraint is added to NMF, which will minimize the volume of the simplex surround the data cloud and make the endmembers move towards the data cloud to neutralize the effect of "external force". Therefore it can be seen as "internal force". When these two forces come into the balance, the algorithm converges and the obtained endmember will be very close to the true value.

Specifically, the objective function of MVC-NMF algorithm is as follows:

$$J(M, S) = \frac{1}{2} \|R - MS\|^2 + \lambda J(M) \tag{6}$$

Where R, M, S are pixel values, endmember matrix and abundances matrix respectively, and J (M) is the constraint of minimizing the simplex volume. In this algorithm, the volume of the simplex is obtained by computing determinant.

$$J(M) = \frac{1}{2(c-1)!} \det^2 \left(\begin{pmatrix} 1_c^T \\ \tilde{M} \end{pmatrix} \right) \tag{7}$$

Where c is the number of endmembers and \tilde{M} is obtained by reducing dimensions of M. Obviously, this kind of constraint by determinant will cause the algorithm diverge easily. In addition, this algorithm does not use an iterative multiplication, but use the projection gradient method^[10]. It forces all of the negative value set to 0 after each iteration to ensure nonnegative results, which will bring unpredictable effects to the convergence of this algorithm.

By constraining the size of the simplex in the process of NMF solution, we can make the simplex approximate the optimal one. However, the calculation formula of simplex volume is complex relatively and need dimension reduction by PCA algorithm, which reduces the efficiency and the decomposition accuracy of this algorithm.

According to the convex geometry theory, a point furthest from a known simplex vertex must be another vertex of the simplex, that is to say, a point furthest from a known endmember must be another endmember.

This paper proposes a kind of maximum endmember distance sum constrained NMF (MEDSC-NMF) to decompose mixed pixels, which control simplex size by minimizing the sum of all maximum distances between endmembers instead of minimizing simplex volume.

For an endmember in endmember matrix, we can find out the maximum distance between it and other endmember. Travelling all the endmembers and calculating out all the maximum distances, the sum of the maximum distances between endmembers can be written as:

$$MEDSC = \sum_{j=1}^P \sum_{i=1}^P \max(\|m_i - m_j\|) \tag{8}$$

The objective function can be constructed and written as:

$$\begin{cases} \min f(M, S) = \frac{1}{2} \|R - MS\|_F^2 + \lambda MEDSC \\ S_{i,j} \geq 0, M_{i,j} \geq 0, \sum_{i=1}^P S_{i,j} = 1 \\ MEDSC = \sum_{j=1}^P \sum_{i=1}^P \max(\|m_i - m_j\|) \end{cases} \quad (9)$$

In spectral unmixing algorithm based on NMF, the number of endmembers P can be estimated by some known algorithms and the endmember matrix A can be obtained by selecting P pixels randomly in hyperspectral images to initialize the algorithm. This paper uses Hysime algorithm to estimate the number of endmembers and choose spectral vectors of P pixels randomly to initialize the endmember matrix A .

The iterative solution of Equation (9) can be accelerated by using gradient projection algorithm. The specific iterative method for Equation (9) is decomposed into two sub problems to solve. In each sub problem A (or S) is fixed, but S (or A) is updated :

$$M^{k+1} = \min_M [f(M, S^k) \leq f(M^k, S^k)] \quad (10)$$

$$S^{k+1} = \min_S [f(M^{k+1}, S) \leq f(M^{k+1}, S^k)] \quad (11)$$

The iterative process can use maximum iterations number, error threshold, user interaction as termination conditions. In this paper, the iterative process is terminated by error threshold.

EXPERIMENT

The data set used in this experiment was acquired from Changzhou Xiaqiao area in China, a mixed agricultural area in China, using the PHI. the images (340×390 pixels) of 80 bands were tested, and their spectral ranges are from 0.417 to 0.854μm. Figure. 1 shows the experimental PHI image cube of Xiaqiao area. The ground truth spectral data were collected by field spectrometer FiledSpecRHandHeld. The field survey shows that ground coverage can be divided into 6 categories: road, corp, gravel, water, soil, vegetation.

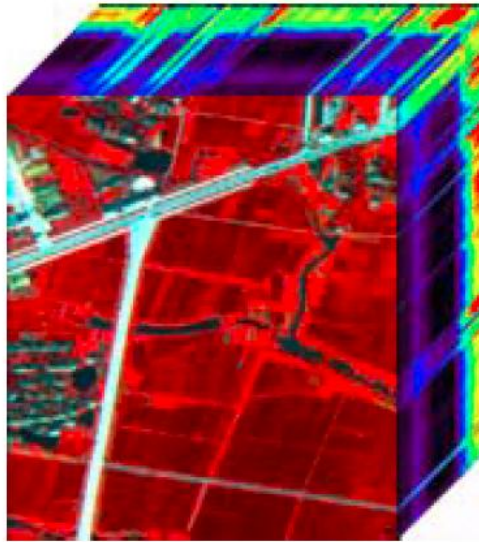


Figure 1: Experimental Xiaqiao PHI image cube

In experiment, we use error threshold as the iteration termination condition of MVC-NMF and MEDSC-NMF. If the ratio of the objective function value of two adjacent iterations is less than a threshold of 0.99, then the algorithm terminate automatically.

Figure.2 shows the enmembers extracted from the experimental data by MVC-NMF and MEDSC-NMF respectively and the reference spectra collected by field spectrometer FiledSpecRHandHeld.

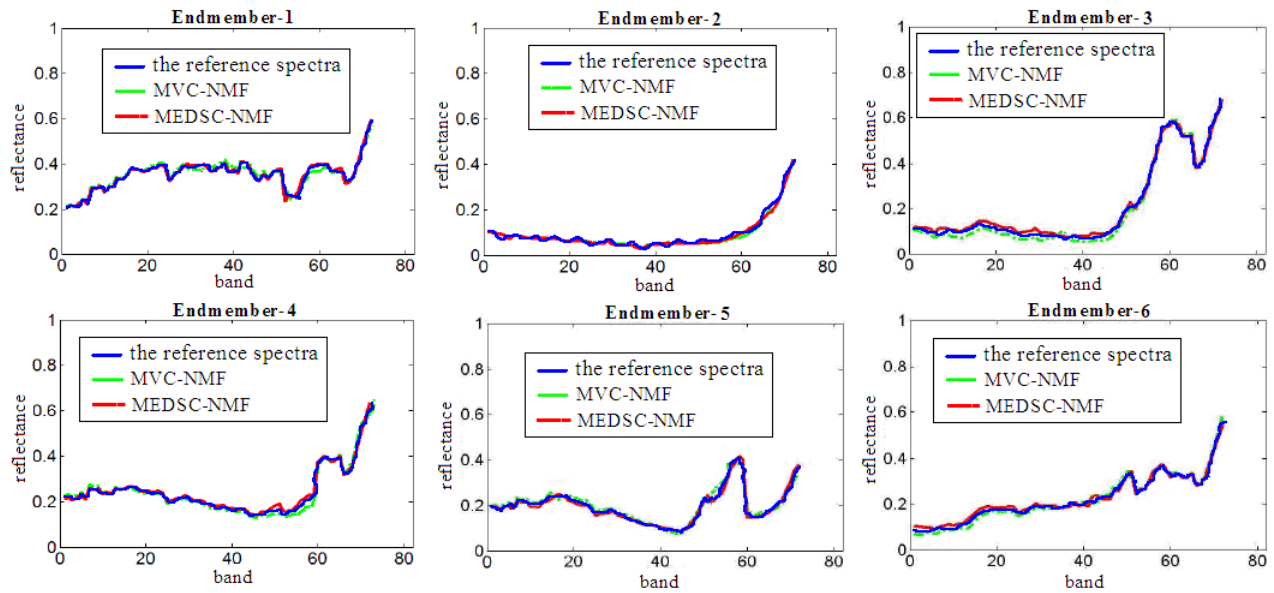


Figure 2: Comparison between the reference spectra and the extracted endmembers by MVC-NMF and MEDSC-NMF

TABLE 1 shows the running time and the root mean square error (RMSE) of spectral unmixing when MVC-NMF and MEDSC-NMF are applied to the experimental data respectively. Obviously, MEDSC-NMF has higher decomposition accuracy and efficiency than MVC-NMF.

TABLE 1: Experimental results of MVC-NMF and MEDSC-NMF

	MVC-NMF	MEDSC-NMF
running time	1213.2(s)	1008.8(s)
RMSE	0.0059	0.0056

CONCLUSION

MVC-NMF is conditioned by minimizing the simplex volume surrounding the data cloud, but the calculation of simplex volume needs a large number of iterative times, therefore the computational complexity of MVC-NMF is high. This paper proposes a kind of MEDSC-NMF algorithm, which restrains the simplex size by minimizing the sum of all maximum distances between endmembers instead of minimizing simplex volume. Experimental results show that MEDSC-NMF algorithm proposed in this paper has higher decomposition accuracy and efficiency than MVC-NMF algorithm.

ACKNOWLEDGMENT

This work was financially supported by Humanities and Social Science Foundation of the Ministry of Education of China (Grant No.14YJCZH172), National Natural Science Foundation of China (Grant No.11405041, 41301382), the Science and Technology Research Projects of Jiangxi Provincial Education Department of China (Grant No. GJJ14368).

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