SURVEY OF GEOMETRIC AND STATISTICAL UNMIXING ALGORITHMS FOR HYPERSPECTRAL IMAGES

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ABSTRACT

Spectral mixture analysis (also called *spectral unmixing*) has been an alluring exploitation goal since the earliest days of imaging spectroscopy. No matter the spatial resolution, the spectral signatures collected in natural environments are invariably a mixture of the signatures of the various materials found within the spatial extent of the ground instantaneous field view of the imaging instrument. In this paper, we give a comprehensive enumeration of the unmixing methods used in practice, because of their implementation in widely used software packages, and those published in the literature. We have structured the review according to the basic computational approach followed by the algorithms, with particular attention to those based on the computational geometry formulation, and statistical approaches with a probabilistic foundation. The quantitative assessment of some available techniques in both categories provides an opportunity to review recent advances and to anticipate future developments.

Index Terms— Spectral mixture analysis, hyperspectral imaging, statistical versus geometric unmixing.

1. INTRODUCTION

The availability of hyperspectral imagers with a number of spectral bands that exceeds the number of spectral mixture components [1] has allowed to cast the unmixing problem [2] in terms of an over-determined system of linear equations in which, given a set of pure spectral signatures (called *endmembers*) the actual unmixing to determine apparent pixel *abundance fractions* can be defined in terms of a linear numerical inversion process [3]. Mixed pixels can also result when distinct materials are combined into a homogeneous, intimate mixture [4]. Nonlinearities can also arise from multiple scattering in the atmosphere [5, 6] and instrument and calibration artifacts. Although the linear model has practical advantages such as ease of implementation and flexibility in different applications [7], *nonlinear* spectral unmixing may best characterize the resultant mixed spectra for certain endmember distributions [8, 9]. In practice, the nonlinear model requires *a priori* knowledge about the optical properties of the observed objects and is less computationally tractable.

In this paper, we provide an overview of existing techniques for endmember extraction and unmixing, as a follow-up to previous comparative efforts [10, 11, 12, 13, 14, 15], and with particular attention paid to the distinction between statistical and geometrical approaches for spectral unmixing. Section 2 describes the state-of-the-art in this research area. Section 3 briefly compares some statistical versus geometrical endmember extraction strategies via experiments. Section 4 concludes with some remarks.

2. GEOMETRIC VS STATISTICAL UNMIXING

2.1. Geometric algorithms

Geometric endmember determination techniques exploit the parallelism between mixing models and the geometric orientation of hyperspectral data in multidimensional spaces. *Linear* spectral unmixing [16, 11] assumes that the collected spectra at the spectrometer can be expressed in the form of a linear combination of endmembers weighted by their corresponding abundances. This definition fits well the geometrical selection endmembers from the vertices of a simplex, a polyhedron or a convex cone that minimally encloses or is maximally contained in the data in a scene. Within the linear algorithms, simplex-shrinking algorithms, starting from the seminal work of Craig (minimum volume transform or MVT [17]), try to find the minimum-volume simplex, i.e. the one that embraces the data cloud as tightly as possible. Simplex-growing algorithms try to figure out the endmembers through searching for a simplex growing from within the data cloud. The simplex identification via split augmented lagrangian (SISAL) [18] algorithm approximates the minimum volume simplex finding problem as a sequence of convex optimization problems. Other authors [19] use a simulated annealing procedure to obtain the minimum-volume simplex. The optical real-time adaptive spectral identification system (ORASIS) [20] is simplex-shrinking that finds endmembers from a scene autonomously. It uses a modified Gram-Schmidt (MGS) algorithm to factor the data matrix and then a shrink-

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wrapping technique to find an outer simplex that encloses the data. In all these cases, the extreme points of the outer simplex need not be data points.

N-FINDR [21] with its implementations, [22], is a simultaneous [23] simplex-growing code that runs autonomously and finds pure pixels that can be used to describe the mixed pixels in the scene. The algorithm finds an inner simplex within the data and selects the largest volume simplex. The pixel purity index (PPI) [24] is a simultaneous endmember extraction algorithm that works by projecting each pixel onto one vector from a set of random vectors spanning the reflectance space. A pixel receives a score when it represent an extremum of all the projections. Pixels with the highest scores are deemed to be spectrally pure. Iterative constrained endmembers (ICE) [25], with its sparsity-promoting version SPICE [26] fits a simplex to the data while penalizing the volume of such simplex. The ICE algorithm does need a dimension reduction step, performed by the minimum noise fraction (MNF) algorithm. Algorithms based on the nonnegative matrix factorization (NMF) try to find the cone or the convex polyhedron that best fits the data and identifies the vertices of such object as the endmember of the scene. Such methods do not require the presence of pure pixels.

The minimum volume constrained nonnegative matrix factorization (MVC-NMF) [27] introduces a volume regularization term in the MNF, much like the ICE. Robustness constraints, spatial correlation and conjugate gradient optimization have also been used [28]. The convex cone analysis (CCA) [29], is a simultaneous algorithms that builds a convex cone around the data starting from an orthogonal basis set obtained from a subset of the eigenvectors of the data correlation matrix. The number of basis vectors is a input to the algorithm. The simplex growing algorithm (SGA) [23] and the vertex component analysis algorithm (VCA) [30] are two sequential [23] algorithms. SGA and VCA both grow simplexes gradually vertex by vertex to find desired endmembers. However, there are two distinct features between the VCA and the SGA. The VCA repeatedly performs orthogonal subspace projections resulting from a sequence of gradual growing simplexes vertex by vertex to find new vertices. By contrast, the SGA finds maximum volumes for a sequence of gradual growing simplexes vertex by vertex. Similar to VCA is the maximum distance (MaxD) algorithm. The orthogonal bases algorithm (OBA), first introduced in [31] and named in [32], is a simplex-growing method which extracts endmembers sequentially using computations of largest simplex volumes like SGA. At each step, the algorithm substitutes searching for the simplex with the largest volume by calculating a determinant with searching for a new orthogonal basis which has the largest norm and which is taken to be the next endmember. sequential maximum angle convex cone (SMACC) [33] is a sequential algorithm that grows a convex cone instead of a simplex. A new endmember is identified based on the angle it makes with the existing convex cone. The data vector making the maximum angle with the existing convex cone is chosen as the next endmember to add to enlarge the endmember set. Abundance maps are simultaneously generated and updated at each step. Iterative error analysis (IEA) [34] is a sequential method which relies on the existence of relatively pure pixels. In this method, a series of linear, constrained unmixings is performed, each time choosing as endmembers those pixels which minimize the remaining error in the unmixed image.

Finally, although research on geometrical endmember extraction in *nonlinear* unmixing has been less active, a successful approach is to use nonlinear kernel functions to model the nonlinearity and another entails manifold learning techniques. The kernel methods approach the unmixing problem by mapping the data into a high dimensional feature space, where nonlinear relations in the original data-space can be transformed to become linear in a suitably chosen feature space [35]. The manifold learning approach employs nonlinear dimensionality techniques to capture the nonlinear structure of the data cloud (e.g. [5, 6]).

2.2. Statistical algorithms

If a spectral unmixing algorithm processes a mixed pixel by using statistical representations, then the algorithm is statistical. The representations can be analytical expressions that represent probability density function (parametric). An example of this family is the stochastic mixing model [36], in which each endmember distribution has Gaussian form. The work in [37] explores an algorithm for joint endmember extraction and abundance estimation for hyperspectral imagery. Each pixel of the hyperspectral image is decomposed as a linear combination of pure endmember spectra.The estimation is conducted by generating the posterior distribution of abundances and endmember parameters under a hierarchical Bayesian model. Another Bayesian model for unmixing is proposed in [38]. The method introduces Bayesian self-organizing maps (BSOM) and combines them with Gaussian mixture model (GMM) to model the spectral mixtures.

Some nonparametric statistical unmixing approaches propose variations on the independent component analysis (ICA) method. In [39] the algorithm, called ICA-based abundance quantication algorithm (ICA-AQA), is a high-order statistics-based technique, that can accomplish endmember extraction and abundance quantication simultaneously. The work in [40] analyzes the use of ICA and independent factor analysis (IFA) for unmixing tasks, showing that the statistically independent of the sources, assumed by ICA and IFA, is violated in the hyperspectral unmixing, compromising the performance of ICA/IFA algorithms for this purpose. As a result, a new unmixing method is introduced in [41] called dependent component analysis (DECA), which models the abundance fractions as mixtures of Dirichlet densities, thus enforcing the constraints on abundance fractions imposed by

Table 1. Spectral angles (degrees) between five USGS mineral spectra and their corresponding endmembers.

Algorithm	Alunite	Buddingt.	Calcite	Kaolinite	Muscovite	Mean
N-FINDR	9.96^{o}	7.71^{o}	12.08^{o}	13.27^{o}	5.24^{o}	9.65^{o}
OSP	4.81^{o}	4.16^{o}	9.62^{o}	11.14^{o}	5.41^{o}	7.03^{o}
VCA	10.73^{o}	9.04^{o}	6.36^{o}	14.05^{o}	5.41^{o}	9.12^{o}
AMEE	4.81^{o}	4.21^{o}	9.54^{o}	8.74^{o}	4.61^{o}	6.38^{o}
SSEE	4.81^{o}	4.16^{o}	8.48^{o}	11.14^{o}	4.62^{o}	6.64^{o}
SPP+N-FINDR	12.81^{o}	8.33^{o}	9.83^{o}	10.43^{o}	5.28^{o}	9.34^{o}
SPP+OSP	4.95^{o}	4.16^{o}	9.96^{o}	10.90^{o}	4.62^{o}	6.92^{o}
SPP+VCA	12.42^{o}	4.04^{o}	9.37^{o}	7.87^{o}	6.18^{o}	7.98^{o}

the acquisition process, namely non-negativity and constant sum. A kind of dependent component analysis approach for unmixing is also maximization of non-gaussianity (MaxNG) [42]. Support vector machines have also been recently used for unmixing [43, 44]. A novel method which integrates two-dimensional wavelet transform (2-DWT) and kernel independent component analysis (KICA) technique has also been used [45], as well as neural network models [46, 9, 47].

Finally, some methods have used spatial statistics to improve the (possibly geometrical) selection of endmembers. The automated morphological endmember extraction (AMEE) method [48] is a mathematical morphology inspired algorithm. The spatial-spectral endmember extraction algorithm (SSEE) in [49] is a projection based unmixing method that works by analyzing a scene in parts (subsets), such that it increases the spectral contrast of low contrast endmembers, thus improving the potential for these endmembers to be selected. A Markov random field (MRF) [50] has been used to define a partition of spectrally mixed pixels into spatially homogeneous regions. A spatial preprocessing (SPP) algorithm [51] can also be used in combination with an existing (geometrical or statistical) algorithm.

3. EXPERIMENTS

We briefly compare the performance of some statistical versus geometrical endmember extraction algorithms using the well-known Cuprite data set[1] obtained by NASA's airborne visible infra-red imaging spectrometer (AVIRIS) [1]. The Cuprite site is well understood mineralogically [52], and has several exposed minerals of interest included in a spectral library compiled by the U.S. Geological Survey (USGS)[2].

Table 1 tabulates the spectral angles (in degrees) obtained after comparing the USGS library spectra of five highly representative minerals in the Cuprite mining district with the corresponding endmembers extracted by different algorithms from the AVIRIS Cuprite scene (low values indicate high similarity). In all cases, the parameters of the different methods tested have been optimized so that the best performance for each method is reported. The number of endmembers to be extracted was set to 14 after using the Hysime method in [53]. Table 1 reveals that geometrical methods such as N-FINDR, VCA or OSP provide endmembers which are similar to the USGS reference signatures. However, statistical methods based on the incorporation of spatial information have the potential to improve the quality of the endmembers. In a separate experiment, the root mean square error (RMSE) after reconstructing the scene using the endmembers extracted by different methods was analyzed. We observed that geometrical methods can benefit from spatial preprocessing in terms of the quality of image reconstruction, while spatial-based methods such as AMEE and SSEE also have potential to provide lower reconstruction errors than geometrical methods.

[1] http://aviris.jpl.nasa.gov/html/aviris.freedata.html

[2] http://speclab.cr.usgs.gov/spectral-lib.htm

4. CONCLUSIONS AND FUTURE RESEARCH

In this paper, we have provided a survey of the state-of-the-art in statistical versus geometrical endmember extraction and unmixing. A few of the discussed approaches have been compared using real hyperspectral data. In future work, we will provide a much more exhaustive quantitative and comparative assessment of some of the most relevant approaches described in this survey, using additional hyperspectral scenes and evaluation metrics (including computational performance).

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