Abstract—Endmember extraction, which is an important technique for hyperspectral data interpretation, selects a collection of pure signature spectra of the different materials, called endmembers, which are present in a remotely sensed hyperspectral image scene. These pure signatures are then used in spectral unmixing algorithms to decompose the scene into abundance fractions, which indicate the proportion of each endmember’s presence in a mixed pixel. In other words, abundances can be obtained by the given endmembers. Correspondingly, endmembers can be extracted based on an abundance constraint. In this paper, we first propose an endmember extraction framework based on an abundance constraint whose efficiency is related to the abundance calculation. The mainstream existing spatial-spectral algorithms can have a very high complexity and are sensitive to outliers, or the spatial information is considered followed by the spectral information. We therefore propose a strategy to consider the spectral information followed by the spatial information, using an abundance-constrained framework. The spatial strategy is also assumed to be immune to outliers. Experiments on both synthetic and real hyperspectral data sets indicate that: 1) the abundance constraint is effective for endmember extraction; and 2) the proposed spatial processing method used in the abundance-constrained endmember extraction framework can effectively avoid outliers.

Index Terms—Abundance-constrained endmember extraction, endmember extraction, hyperspectral, spatial-spectral analysis, spectral unmixing.

I. INTRODUCTION

Due to the spatial resolution limitation of imaging sensors and the variability of the ground surface, the observation of one pixel may contain several different substances, which is called a “mixed pixel” [1]. Spectral unmixing is thus proposed, which aims at the decomposition of the mixed-pixel spectra into a collection of spectrally constituent and pure spectra, named endmembers, and the corresponding abundance fractions of each endmember. No matter what the spatial resolution is, the spectral signatures collected in natural environments are usually a mixture of the signatures of the various materials within the spatial extent of the ground instantaneous field view of the imaging instrument [2]. The appropriate extraction of endmembers from imagery is of great significance in hyperspectral image processing, providing prior information of the pure materials for spectral unmixing [3], [4], object classification [5], [6], and target detection [7], [8]. In fact, they act as the basic unit to quantitatively explore the fine spectral information from hyperspectral images. The practical applications include monitoring of the environment, urban design, risk prevention and response, and so on [9]–[11].

For simplicity, the mixing process for a pixel construction is often assumed to be linear, and the linear mixture model (LMM) has been widely used [12]–[16]. In practice, the LMM does obtain satisfactory results when the multiple scattering effects can be ignored [12]–[20].

Dimensionality reduction (DR), which can improve an algorithm’s performance and reduce its complexity and data storage, is one step in the hyperspectral unmixing chain [21]. A common DR approach is based on the projection of the hyperspectral data into the signal subspace [22], [23]. For example, principal component analysis (PCA) [24] and singular value decomposition (SVD) [25] are accomplished by selecting the principal components in accordance with the magnitude of their associated eigenvalues. Maximum noise fraction (MNF) [26] or noise-adjusted principal components (NAPC) transform [27] have been developed based on the signal-to-noise ratio (SNR). Another kind of DR method is nonlinear projections based on the preservation of the local topology; for example, curvilinear component analysis [28], curvilinear distance analysis [29], manifold learning [30], independent component analysis [31], projection pursuit [32], and wavelet decomposition [33].

During the past few decades, many endmember extraction algorithms have been proposed based on various different criteria [21]:

1) Geometrical-based approaches: The geometrical-based approaches are categorized into two main categories [21]: pure pixel (PP) based and minimum volume (MV) based. The former algorithms assume that at least one pure pixel per endmember exists in the data. They include: the pixel purity index (PPI) [22], N-FINDR [12], the simplex growing algorithm (SGA) [13], and vertex component analysis (VCA) [17], [34], [35]. MV approaches seek an endmember convex geometry with the minimum volume. They include minimum-volume simplex analysis (MVS) [36], the convex-analysis-based minimum-volume enclosing simplex (MVES) [37], minimum-volume constrained nonnegative matrix factorization (MVC-NMF) [38], and simplex identification.

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These points will now lie on an affine simplex or convex hull formed from the endmembers. Instead, the reconstructed data points no longer have to fall within a constraint set defined by the geometrical-based endmember extraction (ACEE). This kind of constraint, which may be more realistic, in practice, and this may seriously affect the analysis of the hyperspectral data. In fact, two definitions of outlier pixels have been presented in [11] and [54]. The first definition refers to the pixels that provide a constant readout or error readout, also called “dead” or “bad” pixels. Possible causes include sensor failure, errors during data transfer, and improper data correction. The second definition refers to the pixels that have rather different spectral signatures than the background representation. The former commonly occur in images, but are of no use for us, but the latter, which are actually small targets, may be useful. The outliers are thought of as the pixels that appear to deviate markedly from the rest of the data, so they may be easily considered to be endmembers if only their spectral information is used. By considering the abundances’ spatial distribution feature, an anomaly will present a sudden change in abundance from its neighbors, so our proposed method exploits this point to eliminate the effect.

Recent works have proposed an integrated framework in which both the spectral information and the spatial arrangement of pixel vectors are taken into account [50], [55]. Typical methods include automatic morphological endmember extraction (AMEE) [16], spatial-spectral endmember extraction (SSEE) [50], spatial preprocessing (SPP) using a sliding-window approach [19], and region-based spatial preprocessing (RBSSPP) [55]. However, these kinds of methods may consume a lot of processing time because of the large number of iterations or the preprocessing on the whole image before the endmember extraction algorithm. This paper introduces abundance-based spatial processing into the ACEE algorithm, which determines the final endmembers from the spatial neighboring candidate by the spectral information, resulting in a reduced computational burden.

Based on the above analysis, our paper focuses on proposing a novel abundance-constrained endmember extraction algorithm combining spatial and spectral information. Our contribution lies in: 1) an abundance-constrained endmember extraction framework is proposed; 2) a spatial processing method based on the abundance of a candidate endmember instead of spatial preprocessing for the whole image is introduced; and 3) minimizing the effects of outliers is also taken into consideration in the endmembers’ extraction framework.

The rest of this paper is organized as follows. Section II describes two classic spectral unmixing methods, which play an important role in the following abundance-constrained endmember extraction methods. Section III first presents some typical endmember extraction algorithms and then details the proposed methods, including abundance-constrained endmember extraction (ACEE) and spatial-spectral information based abundance-constrained endmember extraction.
II. HYPERSPECTRAL UNMIXING

In this section, we introduce two methods of spectral unmixing which are used in the subsequent endmember extraction.

A. Spectral Unmixing Based on the Least Squares Method

The linear unmixing of hyperspectral images is a popular approach used to determine and quantify materials in remotely sensed images. The linear mixing model assumes that the spectrum of each pixel within the scene is a linear combination of the material constituents within that pixel [56]:

\[ x_i = E a_i + n_i \]  

where \( x_i \) is a L-by-1 vector, representing a pixel of a hyperspectral image (L is the number of spectral bands); \( E \) is the L-by-M endmembers’ matrix (M is the number of endmembers, which is known already); \( a_i \) is an M-by-1 abundance column vector corresponding with the pixel \( x_i \); and \( n_i \) is a noise vector. To be physically meaningful, the abundances are generally subject to the abundance sum-to-one constraint (ASC) and the abundance non-negativity constraint (ANC):

\[ \text{ASC} : \sum_{j=1}^{M} a_j = 1, \quad j = 1, \ldots, M \]  
\[ \text{ANC} : a_j \geq 0, \quad j = 1, \ldots, M \]

Unmixing aims at figuring out abundances from the prior endmembers. If constraints (2) and (3) are not considered here, we can use the least squares (LS) method directly to find the solution. The unconstrained least squares (UCLS) solution for question (1) is obtained by:

\[ a_{\text{UCLS}}(x_i) = (E^T E)^{-1} E^T x_i \]  

The equality constraint is the simplest constraint to enforce, and can be incorporated by using Lagrangian multipliers, resulting in the optimal solution. The sum-to-one constrained least squares (SCLS) solution for (1) subject to (2) is obtained by:

\[ a_{\text{SCLS}}(x_i) = \left( I_M - \frac{(E^T E)^{-1} 1 1^T}{1^T (E^T E)^{-1} 1} \right) a_{\text{UCLS}}(x_i) + \frac{(E^T E)^{-1} 1}{1^T (E^T E)^{-1} 1} \]  

where \( I_M \) is the M-by-M unit matrix, and \( 1 = [1, 1, \ldots, 1]^T \) is the M-by-1 column vector.

Enforcing the nonnegative constraint is not as easy to handle as the equality constraint, since no closed-form solution exists [47]; however, it can be solved by using an iterative technique. The problem of estimating abundances subject to equality and nonnegative constraints, or the so-called FCLS, requires advanced iterative optimization methods [47].

B. Spectral Unmixing Based on the Volume of the Simplex

As a general rule, we accept here the assumption that the data fit a LMM. Therefore, we think that all the pixels in a hyperspectral image form a simplex, and the vertices of a convex simplex will be the endmembers of the image. In the two-dimensional space (as shown in Fig. 2), two bands and three endmembers, for example A, B, and C, represent the endmembers, and P is a mixed pixel. The abundances of A, B, and C in point P are then [57]:

\[ a_A = \frac{S_{PBC}}{S_{ABC}}, \quad a_B = \frac{S_{PAC}}{S_{ABC}}, \quad a_C = \frac{S_{PAB}}{S_{ABC}} \]

where \( S \) means the area in the two-dimensional space.

Similarly, in the high-dimensional space, the abundance of a given endmember \( e_j \) in each pixel \( x_i \) is closely related to the ratio of the volume of the endmembers, with \( e_j \) replaced with \( x_i \), and the volume of all the endmembers [57]. The abundance of in pixel is:

\[ a_{ij} = \frac{V_i}{V_0} \]

where:

\[ V_0 = \{e_1, e_2, \ldots, e_j, \ldots, e_M\}, \]
\[ V_i = \{e_1, e_2, \ldots, e_i, \ldots, e_M\}. \]

As with the N-FINDR algorithm, we can define the volume as [12]:

\[ V(E) = \frac{1}{(n-1)!} a_{bc}(|E|) \]

\[ F = \begin{bmatrix} 1 & 1 & \cdots & 1 \end{bmatrix} \]

III. METHODOLOGY

In this section, we first present some commonly used endmember extraction algorithms and discuss their shortcomings, and we then present the proposed abundance-constrained endmember extraction (ACEE) algorithm and the proposed spatial-spectral information based abundance-constrained endmember extraction (SSACEE) algorithm.

A. State-of-the-Art Algorithms for Endmember Extraction

1) VCA and IEA: Both VCA and IEA extract the endmembers based on convex geometry theory, under the assumption of the existence of pure pixels.
VCA models the data using a positive cone, whose projection onto a properly chosen hyperplane is a simplex, with vertices being the endmembers [17]. After projecting the data onto the selected hyperplane, VCA projects all the image pixels to a random direction and uses the pixel with the largest projection as the first endmember. The other endmembers are identified by iteratively projecting the data onto a direction orthogonal to the subspace spanned by the endmembers already determined. The new endmember is then selected as the pixel corresponding to the extreme projection.

In IEA, a series of linear, constrained unmixings are performed [45], and each time those pixels which minimize the remaining error in the unmixed image are chosen as endmembers. The algorithm stops when a termination condition is reached: typically either a certain predetermined number of endmembers are obtained, or a predetermined error tolerance is reached. The algorithm is executed directly on the spectral data. No dimension reduction is required. In the following experiments, we choose (5) for the unmixing, which consumes less time than the FCLS per iteration. What is more, in many cases, many pure pixels exist for every certain feature, and they form bundles (as shown in Fig. 9). In this condition, the abundances are subject to the ASC, but may not correspond to the ANC.

2) MVSA and SISAL: MVSA and SISAL belong to the minimum-volume class and are able to unmix hyperspectral data sets in which the pure-pixel assumption is violated. Fitting a simplex of minimum volume to hyperspectral data is a hard non-convex optimization problem, which may end up in local minima. To avoid poor-quality local minima, a good initialization is important. MVSA and SISAL solve the non-convex optimization problem with different techniques [36, 39].

3) AMEE (Automated Morphological Endmember Extraction): AMEE is a method integrating spatial information and spectral information to extract endmembers from an image. The algorithm begins by searching kernel neighborhoods around each pixel for the most spectrally pure and most highly mixed pixel, using the respective mathematical morphological operators of dilation and erosion. The MEI (morphological eccentricity index) is given by the following expression [16]:

\[
\text{MEI}(m, n) = \text{dist}(d(x, y), e(x, y))
\]

where \(d(x, y)\) is the most spectrally pure pixel, and \(e(x, y)\) is the most highly mixed pixel.

The previously described operation is repeated by using structuring elements of progressively increasing size in order to get better results. The final endmember set is obtained by applying a threshold to the MEI image.

B. The Abundance-Constrained Endmember Extraction Framework

According to [48], the ANC is not suitable for the least squares unmixing method when endmember bundles exist in the image, and taking only the sum-to-one constraint into account is preferred. The reconstructed data points using the endmembers and corresponding abundances, calculating abundance \(a_i\) by (5), will no longer necessarily fall within a simplex formed by all the endmembers. Instead, these points will now lie on a hyperplane constructed by the endmember set, some of which will be enclosed by the current endmember estimated simplex, and some will not (as shown in Fig. 1). All the points shown in the figure belong to the hyperspectral data set. The current endmember set is \(e_1, e_2, \ldots, e_M\). We can see that a smaller RE may not mean better results. As a result, the RE becomes a less useful measure of the fitness of the current estimated endmembers. Fortunately, this information is now contained within the abundances instead. A pixel with a higher abundance which is far away from the convex hull formed by the current endmember set is likely to be an endmember. Therefore, the abundance, instead of the RE, may be more appropriate for obtaining proper endmembers.

An important kind of endmember extraction algorithms are the geometric algorithms. These algorithms are based on the assumption that the data fit the LMM and form a simplex, with each endmember’s signature residing at a vertex [45].

Unmixing the image with endmember sets outputs the abundances of each land object per pixel. Pixels with abundances outside of the range of 0 to 1 will fall outside of the simplex (as shown in Fig. 1). Therefore, the larger the abundance, the more possible it is that the corresponding pixel is an endmember. After unmixing with the current endmember set, the pixel with the largest abundance value will replace the current one. The algorithm stops when the maximum abundance is less than a threshold.

Based on the above analysis, ACEE is summarized below:

\textbf{Given} noisy hyperspectral data, number of endmembers \(M\), threshold \(\epsilon_{\text{threshold}}\)

\textbf{step1.} dimension reduction, which is optional

\textbf{step2.} randomly select an initial endmember set \(E\)

\textbf{step3.} do

for \(j = 1:M\)

\begin{enumerate}
  \item calculate abundance \(c_{ij}\) for every pixel
  \item find the pixel \(t\) with the largest abundance, using \(t, j = \arg \max_{i,j} (|c_{ij}|)\) to replace the \(j\)th endmember with the spectra of pixel \(t\)
\end{enumerate}

end

\textbf{while} \(\max(|c_{ij}|) > 1 + \epsilon_{\text{threshold}}\)

\textbf{output the result}

where \(c_{ij}\) indicates the proportion of the \(j\)th endmember in the \(i\)th mixed pixel, and \(i\) means the location of the pixel.

Different algorithms have different ways of calculating the abundance \(c_{ij}\), so the appropriate values of \(\epsilon_{\text{threshold}}\) are also different. Essentially, the version of unmixing based on the simplex volume is very similar to an improved version of N-FINDR (iterative N-FINDR, using the endmembers extracted by the successive N-FINDR as the initial endmembers [58, 59]), except that the maximum abundance is used instead of the maximum volume. The threshold of the algorithms based on the
simplex volume can be set as 0, because the maximum abundance cannot be anything but 1 when we obtain endmember sets with the largest volume. However, for the least squares method, a smaller threshold may cause the algorithm’s convergence failure or take a lot of time for convergence, but a bigger threshold may lead to a bad result. Therefore, the threshold must balance these two aspects by subjective experience. For the version of least squares unmixing, 0.01–0.0001 is used empirically in our experiments.

C. The Spatial-Spectral Information Based Abundance-Constrained Endmember Extraction Framework

Most techniques available in the endmember extraction literature rely on exploiting the spectral properties of the data alone, and they are generally sensitive to outliers (mainly the noise) [12], [13], [45]–[47]. A possible strategy to address this problem is to incorporate spatial information into the traditional spectral-based endmember search process. For this purpose, a spatial processing method based on an abundance constraint is introduced to ACEE in order to avoid outlier points.

The purest signatures (endmembers) are usually distributed in spatially homogeneous areas, which is an important clue for distinguishing endmembers from outliers. As the abundance indicates the proportion of each endmember’s presence in the mixture, the abundances are intimately related to the spatial continuity between the pixel and its spatial neighbors. Therefore, it is reasonable to use abundances to calculate a scalar factor to spatially weight the spectral information associated with the pixel.

In order to define this procedure in mathematical terms, let us first consider a square-shaped spatial region with a size of \( w \times w \) pixels that is centered at pixel \( P(i, j) \) (as shown in Fig. 3). In this case, we assume that \( w \) is an odd number. A scalar factor \( \gamma(i, j) \) is defined as follows:

\[
\gamma(i, j) = (i+d) \sum_{r=i-d}^{i+d} \sum_{s=j-d}^{j+d} a(r-i, s-j) - a(i, j)
\]

where \( d = (w-1)/2 \); \( a(i, j) \) means the abundance in pixel \( (i, j) \) corresponding to the current endmember we are looking for; \( a(r-i, s-j) - a(i, j) \) is the spectral similarity metric between the central pixel and each pixel in the local neighborhood; and \( \beta(r-i, s-j) \) means the different weights for the pixels in the window, which is inversely proportional to the squared Euclidean distance between the central pixel and each neighbor. \( \beta(r-i, s-j) \) is given by [60]:

\[
\beta(r-i, s-j) = \begin{cases} 
\frac{1}{d(r, s)} & \text{while } d(r, s) = 0 \\
\frac{1}{d(r, s) \neq 0} & \text{while } d(r, s) \neq 0
\end{cases}
\]

(16)

(17)

where \( c_{t,j} \) indicates the proportion of the \( j \)th endmember in the \( t \)th mixture pixel, and \( \gamma_t \) is the scalar factor of the \( t \)th candidate endmember point.

The criteria for choosing the parameter \( \epsilon_{\text{threshold}} \) in the case of SSACEE are the same as with ACEE. The time complexity, convergence, and the quality of the results must be taken into consideration. \([0.01, 0.0001]\) is suitable in our experiments. \( \theta \) is used to control outliers and noise. Based on the spectral distance between adjacent pixels in a homogeneous area, 0.05 is used

Based on the above analysis, SSACEE is summarized as follows:

Given noisy hyperspectral data, endmember number \( M \), threshold \( \epsilon_{\text{threshold}} \) and \( \theta \)

step1. dimension reduction, which is optional

step2. randomly select an initial endmember set \( E \)

step3. do

for \( j = 1:M \)

calculate abundance \( c_{t,j} \) for every pixel \( t = 0 \);

do

\( c_{t,j} = 0 \)

find the pixel \( t \) from \( t, j = \arg \max_{i,j} \{ |c_{i,j}| \} \);

calculate \( \gamma_t \) with the abundance of the \( j \)th endmember

while \( (\gamma_t > \theta) \)

replace the \( j \)th endmember with the spectra of pixel \( t \)

end

while \( (\max|c_{i,j}| > 1 + \epsilon_{\text{threshold}}) \)

output the result
empirically in our experiments. When $\theta$ is equal to or greater than $\pi$, SSACEE is equal to ACEE.

It is worth noting that spatial processing is not the same as spatial preprocessing. Spatial preprocessing means analyzing each pixel’s spatial feature in the scene, while our proposed method only uses the spatial information to analyze the potential endmember pixels which were previously selected by the spectral information. It is obvious that spatial preprocessing is very time consuming, while the proposed spatial processing only results in a little more computational expense, but it can not only help in excluding the anomalous pixels, but also reduce the noise impact.

IV. Experiments and Analysis

This section describes the extensive experiments conducted on both simulated and real hyperspectral data, to allow a comprehensive analysis of the proposed methods when compared with the well-known endmember extraction algorithms. Because all the endmembers in a simulated image are known in advance, it is easy to manipulate the parameters precisely.

It is worth noting that the convergence of least squares unmixing based ACEE is related to the initial endmember set. For example, when randomly selecting the same signature twice from different spatial locations, unmixing is an ill-posed inverse problem, and the least squares unmixing based ACEE may not converge. In order to avoid this situation, it is necessary to impose a restriction on the initial endmember set. The spectral distance between the initial endmembers must be greater than a threshold, to increase the initial endmembers’ differences. Generally speaking, the differences are not necessarily too big, and, in our experiments, this threshold is equal to 0.01. Through experiments, we found that we could use this strategy to ensure the convergence of our algorithm.

In the experiments, we first prove that the abundance-constrained endmember extraction framework is effective with different abundance unmixing methods, and then prove that spatial processing based on abundance can avoid outlier points.

Additionally, we use the three methods introduced in Section II to calculate the abundances and get three different corresponding forms constructed from our proposed ACEE framework. For convenience, the notations are listed in Table I, for ease of later description.

In addition, for SSACEE, we choose unconstrained least squares (UCLS) to calculate the abundance, and choose a window size of $w = 5$. In fact, all three ACEE methods listed above can be expanded to SSACEE, and we choose only ACEE (UCLS) with the spatial information constraint in order to prove that the spatial information constraint based abundance estimation is effective for the ACEE framework and can avoid outlier pixels. The window size is determined by experiment.

We use the spectral angle distance (SAD) to evaluate the unmixing results, which is widely used in the study of hyperspectral unmixing. The SAD is widely used to compare the spectral similarity between each extracted endmember spectra and the library spectra. The well-known SAD metric between pixel $a$ and $b$ is given by:

$$SAD(a, b) = \cos^{-1}\left(\frac{x_a \cdot x_b}{\|x_a\| \cdot \|x_b\|}\right)$$

where $\|x_a\|$ and $\|x_b\|$ are the norms of $x_a$ and $x_b$, respectively.

Suppose $M = \{m_1, m_2, \ldots, m_p\}$ denote the set of $p$ endmembers extracted from a hyperspectral scene, and let $G = \{g_1, g_2, \ldots, g_q\}$ denote a set of ground-truth spectral signatures. With this in mind, the correspondence between ground-truth endmembers set $G$ and the endmembers obtained from the image data is established as follows: (1) All endmembers in set $G$ and endmembers in set $M$ have been labeled as ‘unmatched’. (2) For each unmatched endmember in set $G$, calculate the SAD between such endmember and all endmembers in the set $M$. The spectral curves’ shapes of a certain pair $\{m_i, g_j\}$ with minimum SAD value are compared with supervision. If they are proved not the same material (which means they are the incorrect pair), this process will go on with suboptimum pair until find the correct pair and label them as ‘matched’. (3) ‘Matched’ spectra are removed from set $M$ and $G$. Repeated from step 2 until all endmembers in set $M$ have been labeled as ‘matched’.

The experiments were implemented in Mathworks Matlab R2011b on a PC equipped with an Intel (R) Core Duo CPU T6600 @ 2.20 GHz and 2 Gb memory.

A. Synthetic Hyperspectral Image

In this experiment, we derive a subset of five endmembers from the USGS spectral library [58] and use them to generate a simulated hyperspectral image with $80 \times 100$ (five endmembers) pixels and a simulated hyperspectral image with $40 \times 60$ (three endmembers) pixels covering 224 bands. The data are generated using the LMM, and by imposing the ASC on each simulated pixel. The five signatures are chosen from the USGS library: Alunite AL706 (E1), Calcite CO2004 (E2), Kaolinite CM3 (E3), Montmorillonite CM20 (E4), and Muscovite GDS107 (E5). Taking five endmembers as an example, in the resulting image, illustrated in Fig. 4(a), there are pure-pixel regions as well as mixed-pixel regions, constructed by using mixtures ranging between two and five endmembers, spatially distributed in the form of distinct square regions. Figs. 4(b)–(e) respectively show the true fractional abundances for each of the five endmembers. The background pixels are made up of a mixture of all the endmembers.

1) Experiment 1: Simulated Image With No Outliers: Experiment 1 uses five endmembers to simulate the image, with the whole image containing the same noise (SNR = 30 dB) (as shown in Fig. 5(a)). The SAD values between the library reference spectra and the extracted spectra with VCA, IEA, MVSA, SISAL, AMEE, ACEE (V), ACEE (UCLS), ACEE (SCLS), and SSACEE are shown in Table II. The more the similarity, the
smaller the SAD value is. The numbers in bold correspond to the
best performances. For simulated data with no outliers, AMEE
achieves a slightly worse result than the others, and there is al-
most no difference between the results of VCA, IEA, and the
ACEEs. Table III shows the time consumption of each method.
The size of the spatial neighborhood, and the rule that only one
pixel could be selected in each spatial neighborhood, affect the
final result of the AMEE algorithm. What is more, AMEE takes
more time than the others (about 10 \( \leq 100 \) times), due to cal-
culating the cumulative distance \( D \), which needs two vector dot
product operations between two vectors. Although ACEE with
spatial processing spends more time than without spatial pro-
cessing, SSACEE still spends less time than VCA, MVSA, and
SISAL.

2) Experiment 2: With Outliers: Experiment 2 uses five end-
members to simulate the image, with half of the pure pixels
being implanted with strong noise \( (SNR = 10 \text{ dB}) \) as out-
liers, and the other simulated pixels contaminated with weak
noise \( (SNR = 30 \text{ dB}) \) (as shown in Fig. 5(b)). The SAD values
between the reference spectra and the extracted spectra with
VCA, IEA, MVSA, SISAL, AMEE, ACEE (V), ACEE (UCLS),
ACEE (SCLS), and SSACEE are shown in Table IV. The more
the similarity, the smaller the SAD value is. The numbers in
bold represent the best performances in each endmember’s esti-
mation. As we can see from Table IV, for the images containing
outliers, SSACEE clearly presents a better result than all the
other methods. The reason for this is that the VCA and IEA
methods, without taking the spatial abundance distribution into
consideration, will consider outliers as endmembers which de-
viate markedly from the rest of the data, and MVSA and SISAL
are sensitive to outliers or noise and perform better only in the
case of no pure pixels existing. Although the spatial information is considered in AMEE, spectral information has the leading role in endmember determination. Table V shows a time consumption comparison of the different methods. From Table V, it can be observed that AMEE takes more time than the others (about 10 ~ 100 times), and VCA, MVSA, SISAL, and ACEE (V) need much more time (about 10 times) than ACEE (UCLS), ACEE (SCLS), and SSACEE, because the many dot product operations contained in AMEE consume a lot of time.

3) Experiment 3: Different Numbers of Endmembers: Experiment 3 uses three endmembers to simulate the image, with the whole image containing the same noise. The SAD values of the three endmembers extracted by VCA, IEA, MVSA, SISAL, AMEE, ACEE (V), ACEE (UCLS), ACEE (SCLS), and SSACEE are shown in Table VI. It can be seen that there is almost no difference between the results of each algorithm.

4) Experiment 4: Different Noise Scenarios: Experiment 4 uses five endmembers to simulate the image, with SNR = 30 dB. The SAD values of the three endmembers extracted by VCA, IEA, MVSA, SISAL, AMEE, ACEE (V), ACEE (UCLS), ACEE (SCLS), and SSACEE are shown in Fig. 6. From the results, we can see that VCA and SISAL perform better than the others when the SNR is low. The differences between the results of each algorithm are very small when the SNR is high.

From the results of the above experiments we can conclude that: 1) For images with no outliers, all the algorithms have almost the same precision. 2) For the images containing outliers, SSACEE can best avoid the outlier points in the experiments. The existence of outliers is unavoidable in reality; therefore, SSACEE is both promising and practical. 3) Our methods, except for ACEE (V), have low time consumption. 4) VCA and SISAL are sensitive to outliers but robust with regard to noise.

B. Synthetic Hyperspectral Image

The real data set covering the Cuprite scene was captured by AVIRIS (Airborne Visible Infrared Imaging Spectrometer) in 1997, and is shown in Fig. 7. There are 50 bands in the data, with a size of 350 × 400, covering the wavelength range of 2.0–2.48 μm. The data set has become a popular benchmarking data set for algorithm evaluation, due to the extensive ground truth data...
The number of endmembers to be selected/generated in the experiment with Cuprite data set is estimated by HySime. The SAD values between the reference spectra and the extracted spectra with VCA, IEA, AMEE, ACEE (V), ACEE (UCLS), ACEE (SCLS), and SSACEE are shown in Table VII. The MVSA algorithm ran out of memory, even with another 8 Gb memory computer. In addition, in my experiments, parts of the SISAL algorithm’s results have no meaning (for example, some spectra with negative values). Only these spectra that can be found correct pairs from reference library are evaluated in our experiments, and those spectra with negative values are not taken into account. So Table VII only show SISAL’s valid results. The reason for this may be that the image data is very complex and the SISAL algorithm is sensitive to the outliers. We can see from Table VII that SSACEE obtains an obviously better result than the other methods that do not take the spatial abundance distribution into consideration. Furthermore, it can be observed from Table VII that the ACEE methods have almost the same precision as the well-known VCA and IEA algorithms if only spectral information is considered. Table VIII shows a time consumption comparison of the different methods. From the time consumption table, we can see that AMEE takes the most time, because a mass of dot product operations are done in AMEE, and ACEE (UCLS), ACEE (SCLS), and SSACEE. SSACEE consumes a little more time than ACEE (UCLS), because of the spatial information consideration, which increases the number of iterations when the candidate endmembers cannot meet the spatial information constraint, but SSACEE spends less time than SISAL. All the other methods, except SSACEE and VCA, consider outliers as endmembers (as shown in Fig. 8). Affected by the outliers and the initial direction, the results of VCA contain two strange spectra.

The ACEE algorithm is affected by $e_{\text{threshold}}$ and SSACEE is affected by $e_{\text{threshold}}$ and $\delta$. For ACEE (ACEE (UCLS), ACEE (SCLS)), the mean SAD is shown in Table IX with $e_{\text{threshold}}=\{1,0.1,0.01,0.001,0.0001,0.00001\}$. Since SSACEE is developed from ACEE, $e_{\text{threshold}}$ effects are the same with ACEE; only $\delta$ effects are discussed for SSACEE. For SSACEE, the mean SAD is shown in Table X with $\delta=[2,1,0.5,0.3,0.1,0.05]$ and $\delta=0.001$.

From the results of the above experiments we can conclude that: 1) abundance-constrained endmember extraction algorithms (ACEE) without spatial information are effective; and available for the scene from the USGS. Swayze and Clark have produced a report about the ground truth of the area [61].

<table>
<thead>
<tr>
<th>SAD/rad</th>
<th>VCA</th>
<th>IEA</th>
<th>SISAL</th>
<th>AMEE</th>
<th>ACEE(V)</th>
<th>ACEE(UCLS)</th>
<th>ACEE(SCLS)</th>
<th>SSACEE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alumite</td>
<td>0.0533</td>
<td>0.0978</td>
<td>0.1264</td>
<td>0.0860</td>
<td>0.0781</td>
<td>0.0596</td>
<td>0.0548</td>
<td>0.0527</td>
</tr>
<tr>
<td>Kaolinite</td>
<td><strong>0.0517</strong></td>
<td>0.0846</td>
<td>0.1136</td>
<td>$^\dagger$</td>
<td>0.0679</td>
<td>0.0663</td>
<td>0.0711</td>
<td>0.0651</td>
</tr>
<tr>
<td>Kaolinite</td>
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<td><strong>0.1128</strong></td>
<td>$^\dagger$</td>
<td>$^\dagger$</td>
<td>0.1327</td>
<td>0.1189</td>
<td>0.1148</td>
<td>0.1135</td>
</tr>
<tr>
<td>Halloysite</td>
<td>0.0959</td>
<td>$^\dagger$</td>
<td>$^\dagger$</td>
<td>$^\dagger$</td>
<td>0.0798</td>
<td>0.1074</td>
<td>0.0951</td>
<td>0.1095</td>
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<tr>
<td>Calcite</td>
<td><strong>0.0778</strong></td>
<td>0.0887</td>
<td>0.1396</td>
<td>0.0852</td>
<td>0.1124</td>
<td>0.1091</td>
<td>0.1095</td>
<td>0.1037</td>
</tr>
<tr>
<td>Buddingtonite</td>
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<td>0.1448</td>
<td><strong>0.1111</strong></td>
<td>$^\dagger$</td>
<td>0.1388</td>
<td>0.1484</td>
<td>0.1474</td>
<td>$^\dagger$</td>
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<tr>
<td>Clinoptilolite</td>
<td>0.1164</td>
<td>0.1157</td>
<td>$^\dagger$</td>
<td>$^\dagger$</td>
<td>0.1095</td>
<td><strong>0.1090</strong></td>
<td>0.1011</td>
<td>$^\dagger$</td>
</tr>
<tr>
<td>Chalcedony</td>
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<td>0.0912</td>
<td><strong>0.0058</strong></td>
<td>$^\dagger$</td>
<td>0.1086</td>
<td>0.0963</td>
<td>0.0929</td>
<td>0.0962</td>
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<tr>
<td>Illite</td>
<td>$^\dagger$</td>
<td><strong>0.0715</strong></td>
<td>$^\dagger$</td>
<td>$^\dagger$</td>
<td>0.0891</td>
<td>0.0759</td>
<td>0.0741</td>
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<tr>
<td>Muscovite</td>
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<td>0.1996</td>
<td>0.1127</td>
<td>0.1087</td>
<td>0.1036</td>
<td>0.1064</td>
<td>0.1047</td>
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<tr>
<td>Montmorillonite</td>
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<td>$^\dagger$</td>
<td>$^\dagger$</td>
<td>0.1075</td>
<td>$^\dagger$</td>
<td>$^\dagger$</td>
<td>$^\dagger$</td>
</tr>
<tr>
<td>Outlier</td>
<td>N</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>N</td>
</tr>
<tr>
<td>Mean</td>
<td>0.0923</td>
<td>0.0924</td>
<td>0.1160</td>
<td>0.1015</td>
<td>0.1021</td>
<td>0.0950</td>
<td>0.0945</td>
<td>0.0867</td>
</tr>
</tbody>
</table>

![Fig. 6. SAD values with different SNR.](image)

![Fig. 7. The AVIRIS Cuprite subscene (50 bands).](image)
TABLE VIII
TIME CONSUMPTION (* MEANS OUT OF MEMORY)

<table>
<thead>
<tr>
<th>Method</th>
<th>Time/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>VCA</td>
<td>1.754</td>
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<tr>
<td>IEA</td>
<td>1.876</td>
</tr>
<tr>
<td>MVSA</td>
<td>*</td>
</tr>
<tr>
<td>SISAL</td>
<td>58.893</td>
</tr>
<tr>
<td>AMEE</td>
<td>457.165</td>
</tr>
<tr>
<td>ACEE(V)</td>
<td>213.293</td>
</tr>
<tr>
<td>ACEE(UCLS)</td>
<td>1.607</td>
</tr>
<tr>
<td>ACEE(SCLS)</td>
<td>4.899</td>
</tr>
<tr>
<td>SSACEE</td>
<td>8.796</td>
</tr>
</tbody>
</table>

Fig. 8. Outlier spectra which are considered as endmembers.

TABLE IX
MEAN SAD FOR DIFFERENT \( \theta \)_threshold

<table>
<thead>
<tr>
<th>MSAD</th>
<th>1</th>
<th>0.1</th>
<th>0.01</th>
<th>0.001</th>
<th>0.0001</th>
<th>0.00001</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACEE(UCLS)</td>
<td>0.0717</td>
<td>0.0682</td>
<td>0.0713</td>
<td>0.0671</td>
<td>0.0664</td>
<td>0.0680</td>
</tr>
<tr>
<td>ACEE(SCLS)</td>
<td>0.0727</td>
<td>0.0712</td>
<td>0.0709</td>
<td>0.0709</td>
<td>0.0686</td>
<td>0.0674</td>
</tr>
</tbody>
</table>

TABLE X
MEAN SAD FOR DIFFERENT \( \theta \)

<table>
<thead>
<tr>
<th>MSAD</th>
<th>2</th>
<th>1</th>
<th>0.5</th>
<th>0.3</th>
<th>0.1</th>
<th>0.05</th>
</tr>
</thead>
<tbody>
<tr>
<td>SSACEE</td>
<td>0.0977</td>
<td>0.0951</td>
<td>0.0849</td>
<td>0.0798</td>
<td>0.0865</td>
<td>0.0843</td>
</tr>
</tbody>
</table>

2) SSACEE can eliminate outlier points more effectively (as shown in Fig. 8), but it may ignore the small-size targets.

C. Discussion of the Experiments

There were some problems in our experiments: 1) SSACEE considers a small target as an outlier, because of the small size and the fact that the spectral signature is different from the background representation. In our future work, we will investigate how to distinguish the first kind of outlier, which are harmful, and the second kind, which are useful. 2) The SISAL algorithm achieves part of poor results with no physical meaning. 3) Some materials cannot be extracted, and some may be extracted more than once.

The last two points can be explained by the effects of the endmember variability shown in Fig. 9. Points corresponding to the spectrally representative endmembers are contained within the labeled regions and not on the vertices. This may be because the number of vertices is more than the number of endmembers, under the situation shown in Fig. 9. For endmember extraction methods which assume that pure pixels exist, such as N-FINDR, VCA, and IEA, when the number of endmembers is estimated accurately, it may occur that some endmembers cannot be extracted and some are extracted more than once, because the number of vertices is more than number of endmembers. In other words, accurate estimation of the number of vertices can help us find all the endmembers, especially when noise and bundles exist in the image. This may lull us into a false sense that the number of endmembers has increased. For endmember extraction methods which assume that pure pixels do not exist [62], such as MVSA and SISAL, in order to encircle all the pixels, the resulting endmembers may be far away from the real endmember sets when noise, outliers, and endmember bundles exist. However, it is possible to provide a relatively straightforward example in which the algorithms will not produce the best pure data, and more research should be conducted on this issue in the future.

V. CONCLUSION AND FUTURE RESEARCH

This paper proposes a novel abundance-constrained endmember extraction algorithm combining spatial and spectral information. From extensive simulated and real data experiments, several conclusions can be drawn: 1) The abundance constraint can be considered to be successful for endmember extraction. 2) The SSACEE algorithm can effectively avoid outlier points and spend less time than the other methods with spatial processing. Thus, the consideration of the spatial structure around the pixels under observation is reasonable when distinguishing the improper spectral outliers. This is also a clue to the fact that the abundance constraint may be superior to an endmember constraint when the endmember number cannot be defined exactly beforehand. More research should be conducted in the future on how to exactly estimate the number of vertices, and the points mentioned in the last section.

REFERENCES


