Chapter 6

Iterative Bootstrapping: A Unified Framework for Complete Spectral Unmixing of Hyperspectral Data

In this chapter, we propose a novel approach for simultaneous estimation of number of endmembers, their signatures and corresponding abundances, by exploring the spatial, spectral as well as temporal characteristics of the hyperspectral data over the same area. A linear mixing model (LMM) with the additive white Gaussian noise is considered as the data model. Our work is based on following observations: 1) endmembers together with their abundances form the hyperspectral data, and 2) temporal change in the pixel reflectance is due to variations in abundances over the period of time [8, 9, 11]. A bootstrapping technique inspired from the linear electronics theory is employed to iteratively improve the estimates of all the three entities within a two-stage framework. A rough estimate obtained in the fist stage works as an effective input to the second stage that improves the estimation by incorporating the appropriate constraints and prior information on the solution. Given the data, in stage one we obtain a set of initial endmembers using orthogonal subspace projection (OSP) incorporating the number of endmembers as the lower bound set by the principal eigen-vectors of the data covariance matrix. Assuming them as noisy estimates they are used to find initial abundances using the total least squares - Tikhonov (TLS-Tikhonov) regularization approach that considers the error in data as well as in endmembers. Second stage involves refinement of both the endmembers
and abundances. Here, we first carry out band-wise endmember extraction using multi-temporal data (BEEM) using the initial abundances and obtain a constrained solution that gives improved endmembers. These are then incorporated in maximum a posteriori (MAP) with the data-dependent Huber - Markov random field (dHMRF) prior to further improve the abundances. Finally, the data reconstruction error (DRE) is used as a positive feedback to vary the number of endmembers. This feedback operation referred as bootstrapping is repeated on the two-stage operation until the DRE between the available and reconstructed reflectance is minimum. This process of iterative bootstrapping (IB) converges to an optimum solution (in the least-squares sense) for the complete spectral unmixing. We demonstrate the proposed work using multi-temporal datasets simulated using the real signatures of the USGS spectral library, and the results are compared with two standard hyperspectral unmixing processing chains. The proposed approach works as a self-regulatory mechanism for the complete spectral unmixing as well as serves as a basis to find the temporal changes in a hyperspectral scene based on changes in the abundances contributing to the scene reflectance over a period of time [10].

6.1 Introduction

Given the data, complete spectral unmixing solves for the three unknowns, i.e., it starts by identifying number of spectrally distinct materials in the data followed by extracting their spectral signatures called endmembers and finally estimating the corresponding ground cover fractions called abundances. The efficacy of the complete spectral unmixing can be assessed by checking the error between the available (or ground) reflectance and the reflectance reconstructed using the estimated unmixed components. Solving this inverse ill-posed problem using the mixing model poses major challenges due to the following factors: 1) variations in atmospheric conditions, sensor noise, material decomposition, location, and surrounding materials lead to inconsistent set of equations, 2) relatively larger IFOV and existence of mixed pixels due to altitude of the sensor makes the source separation difficult, and 3) the number of endmembers being significantly less than the available contiguous bands results in larger number of equations than the unknowns. Traditionally, the problem of linear spectral unmixing has been involved in estimating the three entities separately within a hyperspectral unmixing processing chain [5, 87, 86].
6.1 Introduction

Recently, attempts have been made by the researchers on joint estimation of the number of endmembers and abundances [159], the endmembers and abundances [160, 111, 161], and a study on the impact of initial endmembers in searching the number of endmembers and their signatures [162]. It is interesting to note that many of the approaches proposed for spectral unmixing make use of a single hyperspectral data cube of the scene captured at a time [5, 87, 86]. On the other hand, multi-temporal data in the remote sensing area is investigated mainly for detecting changes in an area over a period of time [219, 220, 221, 222, 18, 223] in order to better understand the scene. In the proposed work we show that one can obtain the complete solution for spectral unmixing by using the hyperspectral data captured over the same area at different times.

Generally the scene change is due to variations in its contents, illumination angles, weather conditions, time of a day and/or date including seasonal effects. The important changes observed in hyperspectral data correspond to materials reflectance of the scene [10]. Since endmembers together with the abundances constitute the pixel reflectance (intensities) in a hyperspectral imagery, such changes can be either due to variations in the both or due to scene abundances. Hence, it is a challenge to perform complete spectral unmixing using multitemporal data [8]. Researchers have recommended to explore statistical methods and Markov random field (MRF) based prior information to account for no-change in the data at different times [8, 10]. In this paper, we consider a case wherein endmembers remain same and the changes in the scene are due to their abundances. This is a practical scenario which is observed due to repetitive data acquisition within a season of a year [8, 9, 11]. Our work includes the statistical/MRF based methods in addition to the least-squares based minimization in order to better constrain the solution.

For complete spectral unmixing, the first step is to find the number of endmembers which often requires the knowledge of experts and/or ground survey. The task becomes difficult for physically inaccessible areas on the earth. Comparing the hyperspectral imaging with the pigeon-hole principle, the number of endmembers (pigeons) is found to be significantly less than the available bands (pigeon-holes). Hence, in general, it is difficult to estimate the number of endmembers exactly and a reasonable estimate can be obtained based on trial-and-error criterion [77, 224]. The researchers have tried to determine the same by using the concept of virtual dimensionality (VD) of the data [79], in which a binary hypothesis is formulated by the eigenvalues of data correlations and
covariance matrices. An eigen decomposition of estimated correlation matrices of the data and Gaussian noise for finding the number of endmembers is proposed in [80]. The method considers the noise covariance while estimating the number of spectrally distinct signatures. This method is well-known as HySime and it estimates the subspace of the data in the minimum mean-squared sense. In all the above approaches, the presence of noise in hyperspectral data affects the performance. In [159] a hierarchical Bayesian model is proposed in which the problem is formulated as constrained linear regression. Though the method simultaneously estimates the number of endmembers and abundances, it requires knowledge of endmembers. Recently, greedy algorithms have also been proposed using the sparse regression formulation [83, 84].

In many instances the signatures for the materials, i.e., endmember matrix elements, are available in a digital spectral library [85] or they can be extracted from the data using various algorithms [5, 86, 87, 109, 111]. The approaches for the endmember extraction are discussed in Chapter 5 that also introduced a new algorithm called BEEM. In most of these cases the number of endmembers is a priori known. Knowing the endmembers, unmixing can be done by estimating the corresponding abundances at each location. Since the abundances represent the fractions (weights) of the endmembers, they are required to satisfy nonnegativity constraint due to the passive remote sensing. Apart from this, the abundances must sum-to-one at each pixel location in the scene. Hence, it is difficult to solve this inverse problem and obtain a closed-form solution. Various algorithms for unmixing have been developed [117, 119, 74, 122, 126, 129, 130, 131, 132, 133, 134, 135, 157]. This is discussed in Chapter 3 that proposed TLS-Tikhonov approach [131], and the MAP-dHMRF approach [135, 157] proposed in Chapter 4 of this thesis.

In recent times, many researchers have started exploring multi-temporal unmixing of the hyperspectral data. An FCLS based unmixing is applied to multi-temporal hyperspectral data in [8] for the change detection. Their algorithm was tested on the data acquired using compact airborne spectrographic imager (CASI) in North Research Farm of Mississippi State University. An application of multi-temporal unmixing is shown in [9] for finding the vegetation index from the remotely sensed data. More recently, an unmixing analysis using nonnegativity constraint least-squares has been demonstrated in [11] for Hyperion images captured over Guanica dry forest in Puerto Rico. These approaches demonstrated results showing changes in the scene due to the variations in
6.1 Introduction

abundances over a period of time. But a limitation of these methods is that they require prior knowledge about the endmembers in a scene. An approach involving the spectral variability of the endmembers within the scenes while using the temporal data is proposed in [163]. However, no attempts have been made to use the multi-temporal data to solve for all the three entities in a single algorithm.

Few researchers have attempted the joint estimation of the endmembers and corresponding abundance maps. Such a joint estimation is formulated as a biconvex optimization problem in [160]. This is a heuristic algorithm based on alternatively updating endmember and abundance matrices via projected subgradients. To this end, fully Bayesian hierarchical algorithm is proposed in [161] which uses a computationally expensive generalized Gibbs sampler. The method illustrates the nonuniqueness of the solution while attempting the joint estimation.

In this chapter, by considering a linear data model for hyperspectral imagery we simultaneously solve for number of endmembers, their signatures and corresponding abundances. We consider a season of a year when the endmembers remain the same while changes in the scene reflectance are due to variations in their abundances. This is inspired from a real scenario recorded by the CASI over the North Research Farm of Mississippi State University from August to September in the year 2008 [8]. Our work uses an iterative bootstrapping approach as a positive feedback mechanism. Following are the salient features of the proposed IB approach, which distinguish it from the existing state-of-art algorithms, i) the method simultaneously estimates all the three unmixed components, ii) it considers the effects of noise by minimizing the data reconstruction error (DRE) iteratively in the least-squared sense for ensuring the correctness of the estimated number of endmembers, since the unmixing is carried out by satisfying both nonnegativity and sum-to-one constraints on the abundances [122, 99, 158], hence the reconstructed data points lie within the simplex form by the reconstructed data vectors, iii) the regularized TLS approach ensures a better initial estimate of abundances compared to the least-squares estimation when the endmembers are also perturbed along with the noise in the data, iv) band-wise endmember extraction performed using the temporal characteristics in addition to the spatial/spectral information over a set of data, acts as additional constraint on the endmembers, and v) the MAP-dHMRF method not only satisfy the fully constrained requirement but also incorporate appropriate prior on abundances in order
6.2 Overview of the proposed framework

In this section we briefly explain the proposed method for the complete spectral unmixing which is utilizing the temporal information of the data in addition to the spatial as well as spectral characteristics. We pose it as solving an inverse ill-posed problem involving overdetermined set of linear equations. For this purpose, we extend the linear mixing model (LMM) for the multi-temporal data, i.e., consider a set of spectrally distinct signatures (endmembers) undergo appropriate transformations represented by their abundances over a period of time. This process yields a set output vectors representing reflectance at different wavelengths over the scene. In our case, this transformation is equivalent to applying a linear operator on a vector to yield another vector in the same domain. Here, varying abundances at different locations represent the linear operators and the vector representing the endmembers is transformed to represent the resultant mixed reflectances within the IFOV of the sensor over the time.

In the LMM, the abundances are constrained by nonnegativity and sum-to-one at each pixel location. Hence, these can be conveniently represented by sample functions of Dirichlet process [136]. Further, generally the number of endmembers (e) present in a scene is significantly less than the total number of bands W. Therefore, the transformation matrix (linear operator at a pixel) representing the abundance fractions constitutes a sparse matrix $F_\alpha$ which has $W$ number of rows that correspond to shifted versions of one of the sample functions of the Dirichlet process. The transformation matrix $F_\alpha$ can
be represented as,

\[
F_{\alpha} = \begin{pmatrix}
\alpha_1 & \alpha_2 & \cdots & \alpha_e & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & 0 & \cdots & 0 & \alpha_1 & \alpha_2 & \cdots & \alpha_e & 0 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \\
0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \alpha_1 & \alpha_2 & \cdots & \alpha_e \\
\end{pmatrix}_{W \times We}
\]

\[\sum_{i=1}^{e} \alpha_i = 1 \text{ in each row, where } \alpha_i \in [0, 1].\]

Here, \(\alpha_1, \alpha_2, \ldots, \alpha_e\) represent the set of abundances corresponding to the column vectors \(m_1, m_2, \ldots, m_e\), of endmember matrix \(M\). Considering a hyperspectral data cube which has \(W\) number of spectral bands each of size \(l_1 \times l_2\) pixels, one may write a linear system of equations at every location as,

\[
r = F_{\alpha}m, \ F_{\alpha}: m^{R^+} \rightarrow r^{R^+}
\]

where, \(r\) represents the data vector of size \(W \times 1\), and \(F_{\alpha}\) is the \(W \times We\) sparse matrix. Here \(m\) is a vector of size \(We \times 1\) representing lexicographically ordered rows of the endmember matrix of size \(W \times e\). The input-output transformation given in equation (6.1) can be considered at every location to yield a reflectance data cube of size \(l_1 \times l_2 \times W\). The endmember vector \(m\) combined with \(F_{\alpha}\) at every pixel generate the corresponding output reflectance vectors forming a data cube. Let, \(F_{\alpha-i}\) represents the abundance matrix considering all the locations at a given time. Thus applying different transformations \(F_{\alpha-1}, F_{\alpha-2}, \ldots, F_{\alpha-K}\) on the endmembers \(m_1, m_2, \ldots, m_e\) we get \(l_1l_2W\) reflectance vectors for each of the \(N_1, N_2, \ldots, N_K\) data cubes. This indicates that appropriate transformations on the same endmembers corresponding to a scene lead to different valued data cubes. We make use of these data cubes of the same scene which are acquired at different times in order to better constrain the endmember values while solving for them.

Now the complete spectral unmixing problem can be formulated as follows: given the \(K\) data cubes, find the number of endmembers, their signatures (i.e., endmember values in each band) and corresponding abundances at every location. By considering additive white Gaussian noise at each pixel location in a data cube, one can represent the linear mixing model (LMM) [38] as,

\[
r = M\alpha + n,
\]

\[\text{(6.2)}\]
where the spectral measurement $r$ denotes a $W$-dimensional column vector same as in equation (6.1). Here, $M$ represents the endmember signature matrix which has a size of $W \times e$. The weights for endmembers, i.e., the abundances can be represented by $e$-dimensional vector $\alpha = [\alpha_1, \alpha_2, ..., \alpha_e]^T$, i.e. , $\alpha_i$ represents the fractional area covered by the $i^{th}$ endmember. In equation (6.2), $n$ corresponds to $W \times 1$ vector representing the white Gaussian noise of variance $\sigma^2$. Note that though equations (6.1) and (6.2) represent the same model, the endmember matrix $M$ multiplies vector $\alpha$ in (6.2) while in equation (6.1) an abundance matrix ($F_\alpha$) is multiplied with the vector representing endmember values.

In order to solve this inverse ill-posed problem, we incorporate the idea of bootstrapping from the field of electrical engineering. During the early days of research in linear electronics, a positive feedback process called bootstrapping technique was used for increasing the gain of an amplifier with a two-stage arrangement. It involves a feedback system in which a portion of an output from the second stage is feedback to the first stage (see Figure 6.2), that increases the input impedance of the circuit resulting in faithful amplification of the input signal. Thus, bootstrapping boosts the performance of the system without the need of external aids.

![Figure 6.1: Bootstrapping: portion of the output signal is fed back to Stage-1 increasing the gain of a two-stage amplifier.](image_url)

In our approach, all the three entities to be estimated are utilized in bootstrapping in order to improve their estimation. A feedback in the form of error between the given reflectance (data) and the reflectance reconstructed using the estimated unmixed com-
ponents is used to iteratively improve the solutions by changing the number of end-
members in every iteration. This feedback process repeats until the data reconstruction
error (DRE) is minimum making it an iterative bootstrapping (IB) approach. In or-
der to handle the severe ill-posedness in estimating the abundances, our approach uses
TLS-Tikhonov approach for obtaining the initial abundance values. In the second stage,
multi-temporal data are used to improve the estimation of endmember matrix using our
band-wise endmember extraction using multi-temporal data (BEEM) algorithm. The
improved endmembers are used to further enhance the abundances by using the MAP
framework taking care of the ill-posedness in the unmixing. In our approach the first
stage provides a rough estimate of the solution and works as an initial estimate for the
second stage that uses additional constraints and appropriate prior on the entities to be
estimated in order to enhance the accuracy of estimation.

In essence we use the multi-temporal data to estimate the endmembers, and the abun-
dances are estimated at every pixel location. Advantages of the proposed approach are,
1) performs the blind decomposition of the given data under the well accepted linear
mixing model, 2) carries out the complete spectral unmixing avoiding the necessity of
one or more entity estimated from other approaches, 3) identifies number of endmem-
bers without using \textit{a priori} knowledge of scene-dependent parameters, and 4) the entire
spectral unmixing process is carried out in a self-regulatory mechanism.

6.3 Proposed Method for Complete Spectral Unmixing

Figure 6.2 shows the complete block diagram of the proposed method. The input consists
of $K$ data cubes of the same scene acquired at different times. Using these, the proposed
approach first computes an initial estimate for number of endmembers and their signa-
tures. It is clear that since the data is contiguous in its spectral space, the column vectors
of $M$ may not be truly orthogonal, but one may assume linear independency of these vec-
tors as they represent pure spectra of the constituent materials. This motivates us to
use the principal component analysis (PCA) \cite{PCA} on the data, wherein eigen-directions
with significant eigen-values indicate the lower bound on the number of endmembers in
the data. So to begin with, we apply the PCA on each data cube and select the initial estimate for number of endmembers. Since the hyperspectral data is highly correlated in the spectral space, we choose the eigen-vectors that correspond to 95% of total energy to decide on the number of principal components. This represents the lower bound on the number of endmembers and treated as an initial estimate $\hat{e}$.

![Diagram](image)  

Figure 6.2: Block schematic of the proposed Iterative Bootstrapping (IB) method for complete spectral unmixing using multi-temporal hyperspectral data.

Once the initial number of endmembers is derived as $\hat{e}$, it is used in the OSP [96] algorithm to obtain an initial estimate of endmembers using the data cube having the smallest number of eigen-directions. It may be noted that one may use other state-of-art approaches like N-FINDR [98], AMEE [103] or VCA [102] to find the initial estimate for endmembers. Since OSP represents the pioneering approach among the existing state-of-art approaches, we resort to it for finding the initial endmembers. Using the available data and the number of endmembers, OSP proceeds by considering a pixel-vector having the largest norm as the first endmember from the data. The remaining endmembers are determined iteratively by exploiting orthogonality with respect to the available signatures within the data. However, this may result in poor estimate of endmembers under the noisy scenario [96]. Nevertheless, it gives us an initial set of signatures $M_{\text{init}}$ which
is then used in unmixing all the $K$ data cubes that gives us the initial estimates of corresponding abundance maps. To do this, we consider perturbations in both the data and endmembers. Our TLS-Tikhonov regularization [131] approach is then applied to obtain the initial estimate of abundances at every pixel location in each data cube as,

$$A_{\text{init}-i} = \left\{ \hat{\alpha}_{\text{init}} = \arg \min_{\alpha} \| [M; r] - [M_{\text{init}}; M_{\text{init}} \alpha] \|_F + \mu \| L \alpha_{(i,j)} \|_2, \forall i \times l_1 \times l_2 \right\}, \text{ and } i = 1, 2, ..., K \quad (6.3)$$

where, $\|.\|_F$ denotes the Frobenius norm of the matrix, $\mu$ is the regularization parameter, $L$ is the matrix representation of the derivative operator, and $l_1 \times l_2$ denotes the number of pixel locations in the data cube. The physical constraints on the abundances are taken care of while minimizing the objective function given in (6.3). Further details are available in the Chapter 3. It can be seen that the minimization of equation (6.3) over the $i^{th}$ data cube results in physically constrained abundances $A_{\text{init}-i}$ by considering the noise in data as well as endmember signatures in the $M_{\text{init}}$. We now have initial estimates for the endmembers ($M_{\text{init}}$) of the scene and the abundances for each of the multi-temporal data cubes, i.e., $K$ initial abundance cubes $A_{\text{init}-1}, A_{\text{init}-2}, ..., A_{\text{init}-K}$, each having a size of $l_1 \times l_2 \times e$. Note that these cubes have the same set of abundances as those in $F_{\alpha-1}, F_{\alpha-2}, ..., F_{\alpha-K}$ matrices as already discussed in Section 6.2. We form the $A_{\text{init}}$ matrix by first converting each of the $A_{\text{init}-i}$ into a matrix of size $l_1l_2 \times e$ and stacking all the resultant $K$ abundance maps to form a matrix of size $l_1l_2K \times e$. This initial abundance matrix $A_{\text{init}}$ which has the complete set of abundances of the multi-temporal data is utilized in obtaining an improved estimate of endmember matrix making use of the multi-temporal data. This approach to better estimate of endmembers is based on bandwise extraction.

Our algorithm of band-wise endmember extraction using multi-temporal data (BEEM) makes use of the entire $K$ data cubes so that the changes occurred in the scene over the time period can be taken into consideration in order to improve the solution. The process of endmember extraction is carried out by assuming a linear mixing model (LMM) on the multi-temporal data. This is discussed in Chapter 5 of this thesis. One may note that $e << W$, so the use of multi-temporal hyperspectral data better constrain the solution. This improves the estimates of endmembers even under the noisy conditions. The improved endmember matrix $\hat{M}$ is then used to further improve unmixing of all the
data cubes, i.e., \( \hat{A} \), using our MAP-dHMRF [157] approach at every pixel location in each data cube as,

\[
\hat{\alpha} = \begin{cases} 
\arg\min_{\alpha} \left\{ \frac{\| r - \hat{M}\alpha \|^2}{2\sigma^2} + \lambda \sum_{i=0}^{e-1} \left| \alpha_i - \alpha_{(i+1 \mod e)} \right|^2 \right\}, & \text{if } \alpha_d \leq \beta, \quad (6.4a) \\
\arg\min_{\alpha} \left\{ \frac{\| r - \hat{M}\alpha \|^2}{2\sigma^2} + \lambda \sum_{i=0}^{e-1} \left( 2\left| \alpha_i - \alpha_{(i+1 \mod e)} \right| - \beta^2 \right) \right\}, & \text{if } \alpha_d > \beta \end{cases}
\]

s.t.: \( \sum_{i=1}^{e} \hat{\alpha}_i = 1 \) and \( \hat{\alpha}_i \in [0, 1] \).

Here \( \alpha_d = |\alpha_i - \alpha_{(i+1 \mod e)}| \) and \( \beta \) is a suitable threshold and \( \lambda \) are derived from the available data as discussed in our earlier work [157]. Carrying out the minimization of equations (6.4a) and (6.4b) yields \( \hat{A}_1, \hat{A}_2, \ldots, \hat{A}_K \), corresponding to \( N_1, N_2, \ldots, N_K \), and collectively represented as \( \hat{A} \) representing the estimated abundances for all the data cubes. Once the abundances are found, they along with the \( \hat{M} \) are used to reconstruct the entire dataset, and the error \( (\epsilon) \) is calculated between the reconstructed and the available reflectance in the \( K \) data cubes as

\[
\epsilon = \frac{1}{K} \sum_{i=1}^{l_1 l_2 K} \left\| R_{Ni} - \tilde{R}_{Ni} \right\|_2 \quad (6.5)
\]

where, \( R_{Ni} \) and \( \tilde{R}_{Ni} \) represent the available and the reconstructed data vectors at \( i \)th location. It is clear that a low value of the \( \epsilon \) ensures the closeness of the \( \hat{M} \) and \( \hat{A} \), to their true ones, i.e., \( M \) and \( A \). A relatively high value of \( \epsilon \) indicates a miss-fit for the model we have chosen. In our approach, \( \hat{M} \) and \( \hat{A} \) are estimated using appropriate constraints and the relevant additional information, hence according to the LMM, the possible reconstruction error could be due to use of incorrect number of endmembers, i.e., \( \hat{e} \), [122, 99, 158]. Note that we have initialized the \( e \) with the least number of orthogonal directions, and hence this can be updated and the entire process of finding the endmembers and abundances can be repeated. This update is based on the data reconstruction error \( \epsilon \) as in equation (6.5). This process of updating the number of endmembers and recalculating \( \hat{M} \) and \( \hat{A} \) iteratively involves a feedback called the bootstrapping. The entire procedure is repeated with the updated value of the \( \hat{e} \) as \( \hat{e} + 1 \) till we obtain \( \epsilon << \)
threshold $\gamma$ ensuring the convergence in the least-squares sense [122]. This process is termed as iterative bootstrapping (IB). Since the minimization functions in the entire bootstrapping operation are quadratic, the convergence is guaranteed. We would like to mention here that since we employ regularization as well as additional constraints leading to a unique inverse mapping, the feedback mechanism used in the proposed IB technique works well avoiding the instability.

We now provide a geometric illustration for the working of the proposed IB approach using an exemplary data. For the sake of simplicity, we prefer to use a single data cube. Nevertheless, the explanation is equally applicable to the multi-temporal data. Figure 6.3 illustrates how the bootstrapping helps in gradually improving the solution.

![Figure 6.3](image)

Figure 6.3: Geometric illustration of the proposed Iterative Bootstrapping (IB) approach for complete spectral unmixing: (a) data vectors represented as points in the $W$-dimensional Euclidean space with 5 endmembers shown as vertices of a polygon, and (b-d) bootstrapping with increasing number of endmembers to improve the solution.

Figure 6.3 (a) shows the remotely acquired hyperspectral measurements over the $W$ contiguous bands and the data is represented as the points in the $W$-dimensional Euclidean space. We see that the use of linear mixing model (LMM) allows us to visualize the data in a convex cone formed by the endmembers. As shown in Figure 6.3 (a), there are 5 endmembers corresponding to spectrally distinct materials. Our algorithm is initialized by applying the PCA on this data and for the sake of illustration let us assume that there are 3 principal components. As discussed, the initial estimates of the endmembers and abundances are determined using the OSP and TLS-Tikhonov approach, respectively. This is followed by improved endmembers using the multi-temporal data (BEEM), and finally the abundances are recovered using the MAP-dHMRF. The entire data is reconstructed using these endmembers and abundances, and the data reconstruc-
tion error is calculated. This is depicted in Figure 6.3 (b) where it indicates that now the data has 3 endmembers with the corresponding improved estimates of abundances. It can be seen from the Figure 6.3 (b) that with the use of 3 endmembers, a significantly large error results in the data reconstruction. By using the iterative bootstrapping, the solution can be improved as illustrated in Figure 6.3 (c) and Figure 6.3 (d). Hence, the number of endmembers is increased by one, i.e., 4, and the entire process is repeated. Figure 6.3 (c) shows that the error is relatively reduced, but it is still significantly large. Once again \( \hat{e} \) is increased by one and the bootstrapping is repeated. As shown in Figure 6.3 (d), the error in this case is significantly reduced resulting in improved endmembers and abundances.

6.4 Iterative Bootstrapping (IB) Algorithm

Here we give algorithmic steps involved in our method. Given the multi-temporal data, the proposed algorithm performs blind decomposition as illustrated by using Algorithm 1. The symbols \( \hat{e}, \hat{M}, \) and \( \hat{A} \) are used to indicate estimated versions of number of end-members, endmember matrix and abundance matrix of the data cubes, respectively. The symbol \( \lambda_W \) is used to indicate a \( W \)-dimensional vector of eigenvalues for a data cube, and \( \tilde{R}_N \) denotes a reconstructed data vector.
Algorithm 1 Iterative Bootstrapping

INPUT: Hyperspectral data cubes $\mathbf{N}_1, \mathbf{N}_2, \ldots, \mathbf{N}_K$.
OUTPUT: Number of endmembers $e$, endmember matrix $\mathbf{M}$ and abundance maps $\mathbf{A}_1, \mathbf{A}_2, \ldots, \mathbf{A}_K$.

1: $\{\lambda_{w}\}_{i=1}^{K} = \text{PCA} \left( \{\mathbf{N}_i\}_{i=1}^{K} \right)$.
2: for $i = 1$ to $K$ do
3: set $\hat{e}_i = 0$.
4: for $j = 1$ to $W$ do
5: if $\lambda_j \geq 0.95 \left( \sum_{p=1}^{W} \lambda_p \right)$ then
6: $\hat{e}_i = \hat{e}_i + 1$.
7: end if
8: end for
9: $\hat{e} = \min(\hat{e}_1, \hat{e}_2, \ldots, \hat{e}_K)$, and corresponding data cube is $\mathbf{N}$.
10: $\mathbf{M}_{\text{init}} = \text{OSP} (\mathbf{N}, \hat{e})$.
11: $[\mathbf{A}_{\text{init}-1}, \mathbf{A}_{\text{init}-2}, \ldots, \mathbf{A}_{\text{init}-K}] = \text{TLS-Tikhonov} \left( \{\mathbf{N}_i\}_{i=1}^{K}, \mathbf{M}_{\text{init}} \right)$.
12: Set $x = 1$.
13: for $n = 1$ to $K$ do
14: for $i = 1$ to $l_1$ do
15: for $j = 1$ to $l_2$ do
16: $\mathbf{A}_{\text{init}}(x,:) = \mathbf{A}_{\text{init}-n}(i,j,:)$
17: $x = x + 1$
18: end for
19: end for
20: end for
21: for $j = 1$ to $W$ do
22: $\mathbf{R}_j(:,1) = \{\mathbf{N}_i(:,;j)\}_{i=1}^{K}$.
23: $\hat{m}_w = \arg\min_{\mathbf{m}_w} \| \mathbf{R}_j - \mathbf{A}_{\text{init}} \mathbf{m}_w \|_2$. s.t.: $\hat{m}_{i,j} \geq 0$, for $i = 1,2,...,W$, and $j = 1,2,...,e$.
24: $\hat{\mathbf{M}}(j,:) = \hat{\mathbf{m}}^T$.
25: end for
26: $[\hat{\mathbf{A}}_1, \hat{\mathbf{A}}_2, \ldots, \hat{\mathbf{A}}_K] = \text{MAP-dHMRF} \left( \{\mathbf{N}_i\}_{i=1}^{K}, \hat{\mathbf{M}} \right)$.
27: for $n = 1$ to $K$ do
28: for $i = 1$ to $l_1$ do
29: for $j = 1$ to $l_2$ do
30: $\hat{\mathbf{N}}_n(i,j,:) = \hat{\mathbf{M}} \hat{\mathbf{A}}_n(i,j,:)$
31: end for
32: end for
33: end for
34: for $i = 1$ to $l_1 l_2 K$ do
35: $\epsilon += \frac{1}{K} \| \mathbf{R}_{\hat{\mathbf{N}}_i} - \hat{\mathbf{R}}_{\hat{\mathbf{N}}_i} \|_2$
36: end for
37: if $\epsilon \ll \gamma$ then
38: $e = \hat{e}$, $\mathbf{M} = \hat{\mathbf{M}}$ and $\mathbf{A}_1 = \hat{\mathbf{A}}_1, \mathbf{A}_2 = \hat{\mathbf{A}}_2, \ldots, \mathbf{A}_K = \hat{\mathbf{A}}_K$.
39: else
40: $\hat{e} = \hat{e} + 1$ and go to step 10.
41: end if
42: STOP
6.5 Experimental Results

In this section we demonstrate the efficacy of our approach for simultaneous estimation of number of endmembers, their signatures and corresponding abundances. Due to unavailability of real data captured at different times, we experimented by simulating the dataset. The Hyperspectral Data Retrieval and Analysis (HYDRA) Synthesis tool package \cite{217} is used to generate the dataset for the experiments. All the algorithms are run on a Desktop PC with Intel\textregistered Core\textsuperscript{TM} i5-3210M CPU at 2.5 GHz with 4 GB of RAM.

Since the researchers have not attempted to solve for all the three entities using one algorithm, we compare our results with those spectral unmixing chains that combine the state-of-art algorithms for estimating the number of endmembers, their signatures and the corresponding abundances. These approaches include VD \cite{79}+VCA \cite{102}+FCLS \cite{122} and HySime \cite{80}+MVC-NMF \cite{111}. We use the MATLAB implementations of the VCA and HySime algorithms available online in \cite{218} and the VD implementation available in \cite{225}. The FCLS and MVC-NMF are implemented as per the descriptions of the algorithms with the recommended parameter settings in the literature.

Though we are simulating the data, many physical models for understanding the materials based on the reflected energy have been developed \cite{37}. The effects of the multi-temporal data acquisitions are modeled in \cite{226,10}. For our experiments, we considered seven endmembers namely Renyolds\_tunnel\_sludge, Green\_slime, Cyanide\_potassium\_ferro, Plastic\_grnhouse\_roof, Montmorillonite\_benzen, Cyanide\_zinc, and Ammonium\_chloride. These are contiguously spread over 480 bands in range of 400 – 2500 nm. The signatures for the endmembers are available at the USGS spectral library \cite{85} and the HYDRA has included them as a part of the package. Use of these seven spectral signatures gives us the endmember matrix $\mathbf{M}$ of size $480 \times 7$. By considering each band image of size $256 \times 175$ pixels, the abundance maps of the same size are generated using the spherical Gaussian field as available in the HYDRA package. The endmembers and the abundances are then combined using the LMM, i.e., $\mathbf{r} = \mathbf{M} \mathbf{a}$, to generate the hyperspectral data cube of size $256 \times 175 \times 480$ and this is denoted as Data-1. In order to generate the data cube for the same scene at a different time instant, we keep the $\mathbf{M}$ constant but vary their abundances, thus generating another cube of size $256 \times 175 \times 480$ that is denoted as Data-2. These two data cubes simulate the scenario of temporal variations in the
6.5 Experimental Results

scene occurred within a season of a year. This is similar to a practical scenario found in the CASI data during the months of August and September 2008 [8]. In this period of time, the endmembers remain the same while changes in the scene are observed due to variations in their abundances. The experiments are conducted for the complete spectral unmixing by adding different levels of noise in the simulated dataset. Note that the data digital numbers are in the range of 0 to 1. The mean images having average reflectance at each pixel location for the Data-1 and Data-2 are shown in Figure 6.4 (a) and (b), respectively, with the endmembers marked in the respective scenes. Looking at the two images, we observe that the scene has undergone changes because the distribution of the endmembers has been changed. Table - 6.1 lists the locations of the endmembers in the multitemporal data. The ground truth endmembers are shown in Figure 6.5 in which we show the plots of bands versus the endmember reflectance. The ground truth abundance maps of the dataset are displayed in Figure 6.6 and Figure 6.7 for the Data-1 and Data-2, respectively. Each abundance map is of size $256 \times 175$ pixels which satisfy the nonnegativity and sum-to-one constraint at every location in the respective scene data.

<table>
<thead>
<tr>
<th>Endmembers</th>
<th>Coordinates in Data - 1</th>
<th>Coordinates in Data - 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Renyolds_tunnel</td>
<td>(84, 49)</td>
<td>(5, 11)</td>
</tr>
<tr>
<td>Green_slime</td>
<td>(160, 29)</td>
<td>(164, 175)</td>
</tr>
<tr>
<td>Cyanide_potassium</td>
<td>(191, 17)</td>
<td>(2, 175)</td>
</tr>
<tr>
<td>Plastic_grnhouse</td>
<td>(128, 158)</td>
<td>(17, 17)</td>
</tr>
<tr>
<td>Montmorillonite_benzen</td>
<td>(240, 9)</td>
<td>(13, 31)</td>
</tr>
<tr>
<td>Cyanide_zinc</td>
<td>(26, 158)</td>
<td>(9, 63)</td>
</tr>
<tr>
<td>Ammonium_chloride</td>
<td>(225, 110)</td>
<td>(39, 125)</td>
</tr>
</tbody>
</table>

The result analysis and the performance comparisons are carried out as follows. We begin at gross-level analysis which includes finding data reconstruction error (DRE) maps for the data cubes, verification of number of endmembers in the scene, and time complexities of different algorithms. This is followed by a detailed performance comparison to assess the accuracy of extracted endmembers and abundances at different noise levels in the data. Finally an additional test is carried out to further validate the estimated unmixed components. This is done by adding both low variance ($\sigma^2 = 0.01$) and high variance ($\sigma^2 = 0.1$) noises to the data. In addition to this, noise sensitivity analysis is also carried out on different approaches by considering various noise levels.
6.5 Experimental Results

Figure 6.4: Mean images of multitemporal data: mean image of (a) Data-1, and (b) Data-2. Here the mean is taken at each location across the spectral bands. The dataset has seven endmembers and their locations in the scenes are labeled as R: Renyolds_tunnel_sludge_sm93-15.29328, G: Green_slime_sm93-14a.28199, Cp: Cyanide_potassium_ferro.28065, P: Plastic_grnhouse_roof_gga-54.28462, M: Montmorillonite_benzen.28220, Cz: Cyanide_zinc_k.28013, and A: Ammonium_chloride_gds77.27373.

We begin by calculating data reconstruction error for both the data cubes using the unmixed components as obtained from the standard chains of complete spectral unmixing, i.e., VD \cite{79}+VCA \cite{102}+FCLS \cite{122} and HySime \cite{80}+MVC-NMF \cite{111}, and compare the same with the proposed approach. In order to do this, the RMSE \cite{106} is calculated between the available and the reconstructed reflectance. Computing the RMSE at each pixel location gives us a DRE at that location. For an \(i^{th}\) location it is given as

\[
DRE_i = \left\| R_i - \tilde{R}_i \right\|^2, \forall i \in l_1l_2,
\]

where, \(R_i\) and \(\tilde{R}_i\) denote true and reconstructed data vectors at the \(i^{th}\) location. Therefore, \(\{DRE_i\}_{i=1}^{l_1l_2}\) gives us a DRE map which has the same size as the image representing in a band. Figure 6.8 and 6.9 show the DRE maps for the Data-1 and the Data-2, respectively, considering a noise variance of \(\sigma^2 = 0.1\) in the data. It can be observed from the figures that the DRE at each location as well as the average error and their standard deviation are drastically reduced using the proposed approach when compared...
Figure 6.5: Plots showing the spectral bands versus ground truth endmembers reflectance: (a) Renyolds_tunnel_sludge_sm93-15.29328, (b) Green_slime_sm93-14a.28199, (c) Cyanide_potassium_ferro.28065, (d) Plastic_grnhouse_roof_gga-54.28462, (e) Montmorillonite_benzen.28220, (f) Cyanide_zinc_k_1.28013, and (g) Ammonium_chloride_gds77.27373.
Figure 6.6: Ground truth abundances of Data-1. Abundance maps of (a) Renyolds_tunnel_sludge_sm93-15.29328, (b) Green_slime_sm93-14a.28199, (c) Cyanide_potassium_ferro.28065, (d) Plastic_grnhouse_roof_gga-54.28462, (e) Montmorillonite_benzen.28220, (f) Cyanide_zinc_k.1.28013, and (g) Ammonium_chloride_gds77.27373.
Figure 6.7: Ground truth abundances of Data-2. Abundance maps of (a) Renyolds_tunnel_sludge_sm93-15.29328, (b) Green_slime_sm93-14a.28199, (c) Cyanide_potassium_ferro.28065, (d) Plastic_grnhouse_roof_gga-54.28462, (e) Montmorillonite_benzen.28220, (f) Cyanide_zinc_k_1.28013, and (g) Ammonium_chloride_gds77.27373.
6.5 Experimental Results

to the state-of-art approaches. Here the average errors and their standard deviations are computed from the respective DRE maps. This shows that our unified framework for complete spectral unmixing performs significantly better. These DRE calculations use the estimated number of endmembers in the scene which in our case is verified by carrying out a sensitivity analysis. The total error computed by using the DRE map is utilized as the feedback mechanism in our iterative bootstrapping approach.

Figure 6.8: DRE maps for Data-1 at $\sigma^2 = 0.1$: (a) using VD [79] + VCA [102] + FCLS [122], (b) using HySime [80] + MVC-NMF [111], and (c) using the proposed IB approach. The average errors and standard deviations are mentioned on the top of each figure.

Figure 6.9: DRE maps for Data-2 at $\sigma^2 = 0.1$: (a) using VD [79] + VCA [102] + FCLS [122], (b) using HySime [80] + MVC-NMF [111], and (c) using the proposed IB approach. The average errors and standard deviations are mentioned on the top of each figure.

A crucial point in the spectral unmixing is to ensure the correct number of endmembers within the scene. Hence, to verify the performance of the proposed approach, we conducted the sensitivity analysis at different noise levels in the data and by increasing number of endmembers. This analysis tests the competence of our algorithm in obtaining accurate estimate of number of endmembers, i.e., $\hat{e}$. This is done by incrementing
the number of endmembers $e$ starting from a least number, i.e., 1, and measuring the mean-squared error between the true and reconstructed data using different approaches. In Figure 6.10 we display the plot of number of endmembers versus the average error for the two datasets at $\sigma^2 = 0.1$. Here the error is computed as mean of squared difference between the true and reconstructed data for each hyperspectral data cube and the two values are average out. It can be seen from the figure that for $e = 7$, the error has a minimum value of 0.0263 for the proposed method, and it remains constant there after indicating that there are seven spectrally distinct signatures present in the data. This number exactly matches with the ground truth validating the correctness of our approach in extracting the number of endmembers which is clearly evident from Figure 6.4. One may also observe that our approach has the least reconstruction error.

The execution time of an algorithm constitutes an important parameter in many of the remote sensing applications. Hence, the time complexity of the different algorithms are now compared in terms of the total processing time for the complete spectral unmixing. The individual execution times in the standard chains are added to compute their total
time for complete unmixing. For the proposed IB approach time taken till the convergence represents the total time. In Table 6.2 we give the processing time expressed as the averages over processing times for Data-1 and Data-2 for different approaches. We observe that the time complexity of the proposed approach is almost similar to the approaches based on the standard chains. However, the advantage of the proposed approach lies in blind decomposition of the data with a greater accuracy using only the hyperspectral data captured at different times. The proposed unified framework can easily be implemented on a GPU based hardware using the data-partitioning strategies [165] in order to speed-up the computations.

Table 6.2: Processing Time for Complete Spectral Unmixing of the Data-1 and Data-2 Averaged over different noise levels. Algorithms are run on a Desktop PC with Intel® Core™ i5-3210M CPU at 2.5 GHz with 4 GB of RAM.

<table>
<thead>
<tr>
<th>Algorithms</th>
<th>Time (in minutes)</th>
</tr>
</thead>
<tbody>
<tr>
<td>proposed IB</td>
<td>6.9142</td>
</tr>
</tbody>
</table>

After completing the coarse level analysis, we now turn to more refined analysis of results in terms of accuracy in estimating individual unmixed components which include endmembers and abundances. In order to do the same we again consider data with different noise levels. We first compare the performance of various methods on endmember extraction followed by their abundance estimation which is done by comparing them with their ground truths. Figure 6.11 shows the plots of the spectral bands versus ground truth as well as estimated endmember values using different approaches by considering a noise variance of 0.1 in the data. From the plots shown, it is clear that the estimated endmembers differ from their true values. However, a close examination reveals two important distinctions between the estimated endmembers of the proposed and other approaches. Firstly, one may notice that the plots of ground truth and that of estimated by using the MVC-NMF approach differ significantly. This is clearly visible in Figure 6.11 (a) for an endmember plot of Renyolds_tunnel. Secondly, even though the result due to VCA closely follows the ground truth, the plots of proposed approach are almost overlaid on the ground truth, indicating that the proposed approach outperforms other methods in estimating the endmembers. This is due to the fact that the proposed approach
restricts the solution space of the endmembers by making use of the same scene data captured at different times. This together with the better estimates of abundances by using bootstrapping results in better estimate of endmember values. Note that the results shown in Figure 6.11 are derived using the Data-1 for VCA as well as MVC-NMF, but, the proposed approach results are due to the usage of both Data-1 and Data-2. Similar results were obtained while using the Data-2 for the other methods which are not shown here.

Next we compare our results for the accuracy of estimated abundances. The abundance maps estimated using different approaches are shown in Figure 6.12 and 13 for the same noise variance of 0.1. Since the MVC-NMF approach uses the FCLS method to estimate the abundances, we display the same set of abundances for both these approaches for Data-1 in Figure 6.12 (a) to Figure 6.12 (g), and for Data-2 in Figure 6.13 (a) to Figure 6.13 (g). The abundances estimated using the proposed method are shown in Figure 6.12 (h) to Figure 6.12 (n), and Figure 6.13 (h) to Figure 6.13 (n) for the two datasets. The maps shown using our approach indicate that their spatial distribution is consistent and closer to the the respective ground truth abundance maps (see Figure 6.6 and Figure 6.7) when compared to the other approaches. This is because the proposed approach uses the MAP approach combined with IB that makes it to better handle the ill-posedness in the problem.

Our results on the endmember extraction and abundance estimation are now compared with the other approaches using different quantitative measures. For this the following quantitative measures: root mean squared error (RMSE) [106], spectral angle mapper (SAM) [107] and spectral information divergence (SID) [108] are used. The results on estimated number of endmembers \( \hat{e} \) are compared with VD [79] and HySime [80] methods. The comparison of the proposed approach for estimated endmembers \( \hat{\mathbf{M}} \) are shown with the VCA [102] and MVC-NMF [111] approaches while FCLS [122] and MVC-NMF [111] approaches are used in comparing the results of abundance estimation \( \hat{\mathbf{A}} \). Errors are computed between the ground truths and the estimated values using the different approaches. Lower values for all the measures indicate better performance. We would like to mention here that the quantitative comparisons are carried out separately for each data cube at increasing noise levels. Due to limited space the comparison is shown for only two noise levels. For a noise variance of \( \sigma^2 = 0.01 \), these measures are
Figure 6.11: Plots showing spectral bands versus estimated endmember reflectance for Data-1 with the noise variance of $\sigma^2 = 0.1$. Estimated endmember signature of (a) Renyolds_tunnel_sludge_sm93-15.29328, (b) Green_slime_sm93-14a.28199, (c) Cyanide_potassium_ferro.28065, (d) Plastic_grnhouse_roof_gga-54.28462, (e) Montmorillonite_benzen.28220, (f) Cyanide_zinc_k.1.28013, and (g) Ammonium_chloride.gds77.27373. Note that the results are derived using the Data-1 for VCA as well as for MVC-NMF. The figure also has the plots of ground truth signatures for the comparison purpose. One can see that plots of the proposed method almost coincide with the corresponding ground truth plots.

tabulated in Tables 6.3 and 6.4 for Data-1 and Data-2, respectively. Similarly for a noise variance of $\sigma^2 = 0.1$, they are listed in Tables 6.5 and 6.6 for the two datasets. Observe that the quantitative measures in Tables 6.3 and 6.4 for endmembers $\hat{M}$ are the same for the proposed approach. This is because our approach uses both the datasets for estimating the endmembers. This is equally applicable to Tables 6.5 and 6.6 for the results on endmember extraction. Note that the scores are averaged over the pixel locations of
Figure 6.12: Abundance maps estimated using different approaches at a noise level of $\sigma^2 = 0.1$ in the Data-1: Abundance maps estimated using (a-g) FCLS [122]/MVC-NMF [111] approaches, and (h-n) proposed IB approach. These abundances correspond to the endmembers of Renyolds_tunnel_sludge_sm93-15.29328 (a,h), Green_slime_sm93-14a.28199 (b,i), Cyanide_potassium_ferro.28065 (c,j), Plastic_grnhouse_roof_gga-54.28462 (d,k), Montmorillonite_benzen.28220 (e,l), Cyanide_zinc_k.1.28013 (f,m), and Ammonium_chloride_gds77.27373 (g,n). Visual inspection of the maps indicate that the abundances estimated using the proposed approach are consistent and closer to the ground truth maps (see Figure 6.6) when compared to the other approaches.

the data, for the abundances corresponding to each endmember. For instance, for Renyolds_tunnel, the RMSE is calculated at each pixel location between its ground truth and the estimated abundances using different approaches, and the average value is obtained using these. From the tables one can see that the proposed approach improves the complete spectral unmixing of the data when compared to the other approaches. We see that
Figure 6.13: Abundance maps estimated using different approaches at a noise level of \( \sigma^2 = 0.1 \) in the Data-2: Abundance maps estimated using (a-g) FCLS [122]/MVC-NMF [111] approaches, and (h-n) proposed IB approach. These abundances correspond to the endmembers of Renyolds_tunnel_sludge_sm93-15.29328 (a,h), Green_slime_sm93-14a.28199 (b,i), Cyanide_potassium_ferro.28065 (c,j), Plastic_grhhouse_roof_gga-54.28462 (d,k), Montmorillonite_benzen.28220 (e,l), Cyanide_zinc_k.1.28013 (f,m), and Ammonium_chloride_gds77.27373 (g,n). Visual inspection of the maps indicate that the abundances estimated using the proposed approach are consistent and closer to the ground truth maps (see Figure 6.7) when compared to the other approaches.

The \( \mathbf{\hat{e}} \) is correct for all the approaches as shown in the tables. However, the performances of the different approaches differ for endmembers and abundances estimation. As far as the endmember extraction is concerned, the proposed iterative approach outperforms the existing algorithms in terms of RMSE, SAM as well as SID. The errors in the abundance estimation are also greatly reduced due to the improved estimation of endmembers in
our approach. The better $\hat{M}$ and $\hat{A}$ result in significant error reduction in RMSE as seen from the tables.

In our approach of endmember extraction, we use the entire dataset while the other approaches in the literature extract endmember matrix separately for each data cube. Hence, we now show the comparison when the entire dataset is used in these methods for extracting endmembers. We carry out an experiment wherein both the data cubes are combined and are used to estimate the endmembers in other approaches. Table 6.7 shows the comparison in terms of average error scores where the endmembers are estimated from a combined data, i.e., combining the Data-1 and Data-2. Our proposed algorithm better restricts the solution space by utilizing the temporal characteristics along with the spatial and spectral information.

Finally, an additional cross-check is done on the accuracy of estimated unmixed components. For this purpose, we compute relative power of the components which are orthogonal to the identified endmembers [80]. The calculations are carried out using the obtained value of $e = 7$. To do this, we evaluate $\left\| \hat{M}_e \tilde{r} \right\|^2 / \| \tilde{r} \|^2$, $\forall \tilde{r}$, where, $\hat{M}_e$ has the columns orthogonal to the $\hat{M}$, and $\tilde{r}$ is the reconstructed data vector from the entities estimated using different approaches. For a noise variance of $\sigma^2 = 0.1$ in Data-1, the relative power maps for VCA [102]+FCLS [122], MVC-NMF [111] and for the proposed approach are shown in Figure 6.14 (a), (b) and (c), respectively, and the same are displayed in Figure 6.15 for the Data-2. Since the power is computed at each pixel, the size of these maps are same as size of each band-image, i.e., 256 × 175 pixels. Since the relative powers in this case indicate incoherence between $\hat{M}$ and $\tilde{r}$, we expect the resultant maps differ significantly from the scene data. It can be seen from the Figure 6.14 and Figure 6.15 that the maps do not show the scene details ensuring the correctness of the identified endmember matrices by our approach as well as by the other approaches.

6.6 Conclusions

We presented a novel algorithm for simultaneously solving for the three mixing components of a hyperspectral data. The number of endmembers is found by initializing it with a lower bound provided by the orthogonal decomposition of data covariance matrix, and increasing it until to satisfy the least-squared error criterion. The data reconstruction
Table 6.3: Quantitative measures for the estimated endmembers and abundances of Data-1 with an additive Gaussian noise $\sigma^2 = 0.01$.

<table>
<thead>
<tr>
<th>Measure</th>
<th>Algorithm</th>
<th>#</th>
<th>Endmembers $\hat{\mathbf{M}}$</th>
<th>Abundances $\hat{\mathbf{A}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Reynolds</td>
<td>Green</td>
</tr>
<tr>
<td>RMSE [106]</td>
<td>VD+VCA+FCLS</td>
<td>7</td>
<td>0.0126</td>
<td>0.0134</td>
</tr>
<tr>
<td></td>
<td>HySime+MVC-NMF</td>
<td>7</td>
<td>0.0075</td>
<td>0.0082</td>
</tr>
<tr>
<td></td>
<td>proposed IB</td>
<td>7</td>
<td>0.0021</td>
<td>0.0005</td>
</tr>
<tr>
<td></td>
<td>proposed IB</td>
<td>7</td>
<td>1.8214</td>
<td>1.8105</td>
</tr>
<tr>
<td>SID [108]</td>
<td>VD+VCA+FCLS</td>
<td>7</td>
<td>0.1125</td>
<td>0.6357</td>
</tr>
</tbody>
</table>

Table 6.4: Quantitative measures for the estimated endmembers and abundances of Data-2 with an additive Gaussian noise $\sigma^2 = 0.01$.

<table>
<thead>
<tr>
<th>Measure</th>
<th>Algorithm</th>
<th>#</th>
<th>Endmembers $\hat{\mathbf{M}}$</th>
<th>Abundances $\hat{\mathbf{A}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Reynolds</td>
<td>Green</td>
</tr>
<tr>
<td>RMSE [106]</td>
<td>VD+VCA+FCLS</td>
<td>7</td>
<td>0.0146</td>
<td>0.0182</td>
</tr>
<tr>
<td></td>
<td>HySime+MVC-NMF</td>
<td>7</td>
<td>0.1102</td>
<td>0.0324</td>
</tr>
<tr>
<td></td>
<td>proposed IB</td>
<td>7</td>
<td>0.0021</td>
<td>0.0005</td>
</tr>
<tr>
<td></td>
<td>proposed IB</td>
<td>7</td>
<td>1.8214</td>
<td>1.8105</td>
</tr>
<tr>
<td></td>
<td>HySime+MVC-NMF</td>
<td>7</td>
<td>0.1276</td>
<td>0.5673</td>
</tr>
</tbody>
</table>

$\#$ is the estimated number of endmembers while the $\hat{\mathbf{M}}$ and $\hat{\mathbf{A}}$ are the estimated endmember matrix and abundance maps, respectively. The scores are calculated between the ground truth and the estimated values using different approaches. The scores for $\hat{\mathbf{A}}$ are averaged for each abundance map corresponding to an endmember. Note that the endmembers $\hat{\mathbf{M}}$ in the Table 6.3 and 6.4 are the same for the proposed approach.
### Table 6.5: Quantitative measures for the estimated endmembers and abundances of Data-1 with an additive Gaussian noise $\sigma^2 = 0.1$.

<table>
<thead>
<tr>
<th>Measure</th>
<th>Algorithm</th>
<th>$#\hat{e}$</th>
<th>Endmembers $\hat{M}$</th>
<th>Abundances $\hat{A}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>RMSE $[10^6]$</td>
<td>VD+VCA+FCLS</td>
<td>7</td>
<td>0.0240 0.0288 0.0146 0.0118 0.0268 0.0116 0.0118</td>
<td>0.0489 0.0684 0.0687 0.0010 0.0243 0.0648 0.0221</td>
</tr>
<tr>
<td>HySime+MVC-NMF</td>
<td>7</td>
<td>0.1369 0.1420 0.1198 0.1036 0.2025 0.1008 0.1027</td>
<td>0.0351 0.3998 0.2691 0.2558 0.2196 0.2277 0.1398</td>
<td></td>
</tr>
<tr>
<td>proposed IB</td>
<td>7</td>
<td>0.0118 0.0093 0.0087 0.0086 0.0162 0.0056 0.0071</td>
<td>0.0079 0.0586 0.0322 0.0474 0.0233 0.0496 0.0206</td>
<td></td>
</tr>
<tr>
<td>SAM $[10^7]$</td>
<td>VD+VCA+FCLS</td>
<td>7</td>
<td>11.9056 4.9679 1.8154 1.4414 3.1583 1.2269 1.0788</td>
<td>0.1369 0.1420 0.1198 0.1036 0.2025 0.1008 0.1027</td>
</tr>
<tr>
<td>HySime+MVC-NMF</td>
<td>7</td>
<td>3.2712 $\rightarrow$ 2.1849 $\rightarrow$ 2.1740 $\rightarrow$ 2.3740 $\rightarrow$ 5.7875 $\rightarrow$ 2.7688 $\rightarrow$ 2.1945 $\rightarrow$</td>
<td>4.8490 $\rightarrow$ 2.1648 $\rightarrow$ 1.2125 $\rightarrow$ 1.1886 $\rightarrow$ 5.2822 $\rightarrow$ 7.8532 $\rightarrow$ 3.6191 $\rightarrow$</td>
<td></td>
</tr>
<tr>
<td>proposed IB</td>
<td>7</td>
<td>4.8490 $\rightarrow$ 2.1648 $\rightarrow$ 1.2125 $\rightarrow$ 1.1886 $\rightarrow$ 5.2822 $\rightarrow$ 7.8532 $\rightarrow$ 3.6191 $\rightarrow$</td>
<td>2.6534 $\rightarrow$ 2.4610 1.6424 $\rightarrow$ 7.8040 $\rightarrow$ 5.0630 $\rightarrow$ 2.4594 $\rightarrow$</td>
<td></td>
</tr>
</tbody>
</table>

$\#\hat{e}$ is the estimated number of endmembers while the $\hat{M}$ and $\hat{A}$ are the estimated endmember matrix and abundance maps, respectively. The scores are calculated between the ground truth and the estimated values using different approaches. The scores for $\hat{A}$ are averaged for each abundance map corresponding to an endmember. Note that the endmembers $\hat{M}$ in the Table 6.5 and 6.6 are the same for the proposed approach.

### Table 6.6: Quantitative measures for the estimated endmembers and abundances of Data-2 with an additive Gaussian noise $\sigma^2 = 0.1$.

<table>
<thead>
<tr>
<th>Measure</th>
<th>Algorithm</th>
<th>$#\hat{e}$</th>
<th>Endmembers $\hat{M}$</th>
<th>Abundances $\hat{A}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>RMSE $[10^6]$</td>
<td>VD+VCA+FCLS</td>
<td>7</td>
<td>0.0247 0.0260 0.0199 0.0131 0.0317 0.0195 0.0314</td>
<td>0.0478 0.0485 0.0759 0.0426 0.0273 0.0351 0.0276</td>
</tr>
<tr>
<td>HySime+MVC-NMF</td>
<td>7</td>
<td>0.1269 0.1365 0.1029 0.1157 0.1935 0.2131 0.1355</td>
<td>0.2673 0.3167 0.2566 0.2362 0.1534 0.2067 0.1086</td>
<td></td>
</tr>
<tr>
<td>proposed IB</td>
<td>7</td>
<td>0.0118 0.0093 0.0097 0.0086 0.0162 0.0056 0.0071</td>
<td>0.0093 0.0375 0.0293 0.0377 0.0229 0.0275 0.0193</td>
<td></td>
</tr>
<tr>
<td>proposed IB</td>
<td>7</td>
<td>5.9822 1.8200 1.3004 1.2745 1.8016 0.6345 0.6411</td>
<td>7.9055 14.0120 6.8797 6.2877 6.4141 5.2099</td>
<td></td>
</tr>
</tbody>
</table>

$\#\hat{e}$ is the estimated number of endmembers while the $\hat{M}$ and $\hat{A}$ are the estimated endmember matrix and abundance maps, respectively. The scores are calculated between the ground truth and the estimated values using different approaches. The scores for $\hat{A}$ are averaged for each abundance map corresponding to an endmember. Note that the endmembers $\hat{M}$ in the Table 6.5 and 6.6 are the same for the proposed approach.
Table 6.7: Average error scores for endmember extraction on the combined data with additive Gaussian noise $\sigma^2 = 0.1$.

<table>
<thead>
<tr>
<th>Endmembers M</th>
<th>Algorithm</th>
<th>Renyolds tunnel</th>
<th>Green slime</th>
<th>Cyanide potassium</th>
<th>Plastic greenhouse</th>
<th>Montmorillonite</th>
<th>Cyanide</th>
<th>Ammonium chloride</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>VCA [102]</td>
<td>0.9451</td>
<td>1.4144</td>
<td>1.5470</td>
<td>1.4013</td>
<td>1.4948</td>
<td>1.5328</td>
<td>1.8532</td>
</tr>
<tr>
<td></td>
<td>MVC-NMF [111]</td>
<td>1.8432</td>
<td>2.4324</td>
<td>2.4324</td>
<td>2.6553</td>
<td>3.4347</td>
<td>2.7058</td>
<td>2.5649</td>
</tr>
<tr>
<td></td>
<td>proposed</td>
<td>0.0118</td>
<td>0.0093</td>
<td>0.0097</td>
<td>0.0086</td>
<td>0.0162</td>
<td>0.0058</td>
<td>0.0071</td>
</tr>
<tr>
<td></td>
<td>SAM [107]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>proposed</td>
<td>5.9822</td>
<td>1.8220</td>
<td>1.3004</td>
<td>1.2745</td>
<td>1.8016</td>
<td>0.6345</td>
<td>0.6441</td>
</tr>
<tr>
<td></td>
<td>SID [108]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>VCA [102]</td>
<td>3.1244$e^{-05}$</td>
<td>2.2324$e^{-05}$</td>
<td>2.3535$e^{-05}$</td>
<td>2.4561$e^{-05}$</td>
<td>5.2356$e^{-05}$</td>
<td>2.5961$e^{-05}$</td>
<td>2.3539$e^{-05}$</td>
</tr>
<tr>
<td></td>
<td>MVC-NMF [111]</td>
<td>4.2201$e^{-05}$</td>
<td>4.0942$e^{-05}$</td>
<td>4.2234$e^{-05}$</td>
<td>4.2234$e^{-05}$</td>
<td>6.3434$e^{-05}$</td>
<td>4.5932$e^{-05}$</td>
<td>4.1692$e^{-05}$</td>
</tr>
<tr>
<td></td>
<td>proposed</td>
<td>3.2612$e^{-06}$</td>
<td>2.1849$e^{-06}$</td>
<td>2.1749$e^{-06}$</td>
<td>2.1749$e^{-06}$</td>
<td>5.7873$e^{-06}$</td>
<td>2.7688$e^{-06}$</td>
<td>2.1945$e^{-06}$</td>
</tr>
</tbody>
</table>

Figure 6.14: Relative power maps for Data-1 at $\sigma^2 = 0.1$ using (a) VCA [102]+FCLS [122], (b) MVC-NMF [111], and (c) proposed IB.

Figure 6.15: Relative power maps for Data-2 at $\sigma^2 = 0.1$ using (a) VCA [102]+FCLS [122], (b) MVC-NMF [111], and (c) proposed IB.

error is used in iterative bootstrapping framework resulting in optimal spectral unmixing of the given dataset. Simulation results conducted on synthetic dataset constructed using the real hyperspectral signatures and using different levels of additive white Gaussian
noise in the dataset demonstrate the effectiveness of the proposed algorithm when compared to the standard processing chain incorporating the state-of-art approaches. The proposed methodology has an additional advantage of performing the spectral unmixing of multi-temporal data in a single chain of processing as well as serves as a basis for change detection in a hyperspectral scene based on the variations in the estimated abundances over a period of time. Future work involves further testing the proposed algorithm on real multitemporal hyperspectral datasets as well as implementing on the graphical processing unit (GPU) for real-time applications.