Spectral Variability Augmented Sparse Unmixing of Hyperspectral Images

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Abstract—Spectral unmixing expresses the mixed pixels existing in hyperspectral images as the product of endmembers and their corresponding fractional abundances, which has been widely used in hyperspectral imagery analysis. However, the endmember spectra even for pixels from the same material of an image may include variability due to the influence of lighting conditions and inherent properties of materials within different pixels. Though the in situ spectral library has been used to accommodate such variability by using multiple in situ spectra to represent each kind of material, the performance improvement may be restricted due to the limited number of endmembers for each material. Therefore, in this article, spectral variability is directly extracted from an in situ endmember library and considered to be transferable among different endmembers for the first time. Furthermore, such a spectral variability is further used to augment sparse unmixing by synchronously performing endmember-based reconstruction and spectral variability-augmented reconstruction in the sparse unmixing model. By, respectively, imposing sparse and smoothness regularization over abundances and variability coefficients, a convex optimization-based spectral variability augmented sparse unmixing (SVASU) is finally proposed, and its convergence performance is also analyzed. Experiments conducted over synthetic and real-world datasets demonstrate that the proposed SVASU method not only significantly improves the unmixing performance of conventional spectral library-based unmixing but also outperforms several state-of-the-art sparse unmixing algorithms.

Index Terms—Convex optimization, hyperspectral images (HSIs), sparse unmixing, spectral library, spectral variability.

I. INTRODUCTION

WITH the rapid development of imaging spectroscopy, hyperspectral images (HSIs) containing rich spectral information over tens or hundreds of contiguous and narrow bands have been widely applied to various fields, such as agricultural remote sensing, geological exploration, and military investigation [1]–[3]. However, the phenomenon of mixed pixels is commonly present due to relatively low spatial resolution of HSIs, changeable atmospheric environment, and complex distribution of ground objects, which may cause severe problems for the quantitative analysis and interpretation of HSIs [4], [5]. To address such mixed-pixel problems, spectral unmixing (SU) has been developed as the decomposition of a mixed pixel into spectral signatures (endmembers) with corresponding proportions (abundances).

The linear mixing model (LMM) [6] has been widely adopted for SU due to its physical interpretability, computational tractability, and simplicity. It assumes that there is no mutual interference among distinct endmembers, and thus, the spectra of mixed pixels are a linear combination of several endmembers weighted by their associated fractional abundances. In general, an endmember extraction step is applied, and then, the abundance vector for each pixel is estimated. There are many algorithms for endmember extraction, such as N-FINDR [7], the pixel purity index (PPI) [8], and the vertex component analysis (VCA) [9]. However, the pure-pixel assumption of these algorithms is not always true in the case of limited spatial resolution. Therefore, virtual endmembers are also extracted for HSIs [10], [11]. Subsequently, abundance estimation algorithms are carried out to express each pixel in terms of a linear combination of endmembers, e.g., the fully constrained least-squares (FCLS) method [12] and the multichannel Hopfield neural network (MHNN) [13].

However, the spectral signatures of the materials contained in HSIs are generally affected by spectral variability due to different atmospheric effects, illumination, topographic changes, and the intrinsic variation of the spectral signatures of the materials (i.e., physicochemical differences), especially in HSIs with a higher spatial resolution [14]–[16]. Therefore, the spectral signatures for a given material cannot be well expressed by a single signature, while such ubiquitous errors seriously destroy the unmixing results under LMM assumption [17]. To address this problem, the existing methods can be generally categorized into two classes: 1) dictionary or bundle-based methods [18], [19] that intend to select several instances for each kind of material to address the variability

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and 2) model-based methods that describe endmember variability by a specific statistical distribution [20]–[22] or by incorporating the variability in the mixing model based on physically motivated concepts [23]–[25].

The dictionary or bundle-based approaches identify several instances for each endmember to form a spectral library, which offers multiple spectral representations per material [26], [27]. This category of methods selects appropriate spectra for each endmember class from spectral libraries according to the previously set criteria to alleviate the influence of spectral variability, which can be further classified into four types: multiple endmember spectral mixture analysis (MESMA), sparse unmixing, spectral transformations, and machine learning methods. The basic principle of MESMA is to search for the best reconstruction model within the linear combinations of endmember signatures in the spectral dictionary [28]–[30]. The MESMA algorithm and its variants formulate SU as a computationally demanding optimization problem and achieve good quality through a block sparse algorithm [31], incorporating spatial information by using segmentation algorithms [32], or imposing spatial-spectral constraints to search for an endmember subset per pixel [33]. Compared to MESMA, sparse unmixing models use mathematical relaxations that are computationally easier to be solved. In the spectral transformations group, transformed spectral information, which can greatly alleviate the effect of variability, is used as input to SU rather than the original reflectance data, such as derivative spectra or wavelet transformed spectra [34], [35]. However, such algorithms are empirically oriented techniques and require significant expert knowledge about the underlying applications. In addition, most machine learning-oriented methods formulate SU as a supervised regression problem, where the spectral variability is addressed by considering multiple spectral signatures for each endmember when training. Their objective is to learn transformations that map the observed (mixed) pixel to the abundance fractions using a supervised training procedure [36]–[38]. Others employ complex deep architectures to address the endmember variability in an unsupervised manner by learning the latent distribution of endmembers [39], [40]. Nevertheless, most of these methods require colossal computing resources and generally have no apparent physical motivation.

Owing to the availability of spectral libraries obtained by laboratory or in situ measurements, the sparse unmixing model has been widely developed, which is a kind of semisupervised method, and only needs to estimate the abundances [41], [42]. Recently, several new perspectives introducing spatial correlation, spectral similarity, and low rankness have fostered advanced developments in this field [43]–[47]. To enforce the sparsity of abundance matrices, the sparse unmixing algorithm via variable splitting and augmented Lagrangian (SUnSAL) [41] adopted the $l_1$ sparsity regularizer, while the collaborative SUnSAL (CLSUnSAL) [48] introduced the $l_{2,1}$ regularizer to impose joint sparsity. Exploiting spatial information also plays a crucial role in enhancing sparse unmixing as such a problem is usually simplified on a local scale [49]. Spatial information is generally introduced by total variation (TV) regularization [50]–[52], weights in spectral and spatial domains [53], or superpixel-based segmentation [54]. However, these techniques may yield oversmooth results and blurred boundaries in some regions. Due to adjacent pixels sharing not only the same endmembers with high probability but also approximated fractional abundances, the local spectral similarity of HSIs is also considered to replace the proximity in location [55]. Meanwhile, the low-rank constraint has attracted broad attention for its ability to maintain the local low-dimensional structure of abundance matrices [56], [57]. The alternating direction sparse and low-rank unmixing (ADSpLRLU) algorithm simultaneously enforced the sparsity and low-rank characteristics of abundance fractions [58]. The joint-sparse-blocks and low-rank unmixing (JSpBLRU) algorithm further imposed a block sparsity structure for abundances per pixel within the same window [59]. The recent superpixel-based reweighted low-rank and TV (SUSR-L-TV) sparse unmixing method applied reweighted low-rank regularization to superpixels in the homogeneous regions to remain more detailed features [60]. Though the above library-based sparse unmixing methods have been widely developed, existing libraries used in those models, e.g., the U.S. Geological Survey (USGS) digital spectral library, may be acquired in conditions that do not reflect the situation when the image acquired, resulting in significant unmixing errors. Therefore, libraries extracted directly from observed HSIs are much better to be used in these models [61], [62], and thus, the in situ spectral library is considered in this article.

Though recent library-based sparse unmixing methods have alleviated the influence of the spectral variability to some extent by using multiple spectra of each material, the limited representation ability of spectral variability restricts the performance improvement of SU. Therefore, for the first time, the spectral variability within each endmember spectrum is directly extracted, by which the in situ endmember library is divided into intrinsic spectra library and spectral variability library. By incorporating such a spectral variability library into the linear mixture assumption, a spectral variability augmented sparse unmixing (SVASU) model is proposed to improve the performance of conventional sparse unmixing. Furthermore, a convex optimization strategy is designed, and its corresponding convergence analysis is conducted. Finally, a series of experiments over synthetic and real hyperspectral datasets are conducted to assess the effectiveness and rationality of the proposed SVASU method for hyperspectral sparse unmixing. To sum up, the proposed SVASU model includes three main contributions.

1) Spectral variability is first explicitly extracted from the in situ endmember library using eigenvalue analysis. Such spectral variability is used to model microimaging conditions of each endmember spectra in the library and can be transferred to different pixels.

2) All the spectral variability within an image is considered as the linear combination of known spectral variability extracted from the in situ endmember library. As a result, the microimaging conditions of different pixels in the image can be well modeled using the extracted spectral variability library.

3) A novel SVASU model is proposed for sparse unmixing to address spectral variability, which enforces sparsity and smoothness over abundances and variability...
coefficients, significantly improving the unmixing performance.

The rest of this article is organized as follows. Section II briefly introduces the basic knowledge of the LMM and sparse unmixing model. The proposed SVASU model is presented in detail in Section III. Section IV portrays the experimental results conducted over both synthetic and real-world datasets. Finally, the conclusions are drawn in Section V, and the Appendix gives the convergence analysis of the update rules for the proposed SVASU.

II. SPARSE UNMIXING MODEL

A. Linear Mixture Model

Let $R \in \mathbb{R}^{b \times n}$ denote an observed HSI matrix, where $b$ and $n$ are the numbers of spectral bands and pixels in the image, respectively. By assuming that the observed HSI can be represented as a linear combination of several endmembers weighted by the corresponding fractional abundances, LMM is formulated as

$$R = EA + N$$

in which $E \in \mathbb{R}^{b \times p}$ denotes the matrix of spectral signatures containing $p$ endmembers, $A \in \mathbb{R}^{p \times n}$ is the abundances of the endmembers, and $N \in \mathbb{R}^{b \times n}$ represents the additive noise matrix.

Two constraints are usually imposed for fulfilling physically meaning, i.e., the abundance sum-to-one constraint (ASC) and the abundance nonnegative constraint (ANC), which are given by

$$\text{ASC: } 1^T_A = 1^T, \quad \text{ANC: } A \geq 0$$

where $1$ is a vector of all ones. It should be noted that the ASC constraint is usually enforced by adding a pseudoband to the data matrix and the endmember matrix [13].

B. Sparse Unmixing

A considerable number of sparse unmixing methods have been proposed to not only enhance the sparsity of solutions but also partly attempt to alleviate the effect of spectral variability, further study on how to model the spectral variability is still needed to eliminate the influence of nonuniform imaging conditions. Therefore, in this article, spectral variability with each endmember is explicitly extracted or separated from the $in situ$ spectral library. Such spectral variability reflects their microimaging conditions in the scene and can be transferred to other pixels. Then, all the spectral variability contained in an image, i.e., more microimaging conditions inside different pixels, can be well modeled by a linear combination of extracted spectral variability. As shown in Fig. 1, an SVASU method is further proposed to model the spectral variability under the assumption of the linear mixture. Eventually, a convex-optimization-based solving strategy is designed, along with the convergence analysis present in the Appendix.

A. Separation of Spectral Variability Library

Although existing sparse unmixing methods are broadly developed based on known libraries, the inconsistent absorption and scattering effects between the existing spectral library (e.g., the USGS spectral library) and the target image (e.g., the Cuprite dataset) may lead to significant unmixing errors. Therefore, extracting $in situ$ spectral libraries directly from observed HSIs is of crucial importance. In this article, the $in situ$ spectral library is adopted and simply composed of endmember candidates extracted from the observed image using spatial purity-based endmember extraction (SPEE) algorithm [63]. By searching for the representative spectral signatures in the detected pure spatial neighborhoods and further refining with spectral similarity, the final endmember candidates, also the $in situ$ spectral library used in this article, are composed of spatially independent and spectral representative spectral signatures. Let $X \in \mathbb{R}^{b \times l}$ be the $in situ$ spectral library containing $l$ spectra of $p$ materials known in advance. It can be denoted as

$$X = [X^{(1)}, X^{(2)}, \ldots, X^{(p)}]$$

$$X^{(i)} = [e^{(i)}_1, e^{(i)}_2, \ldots, e^{(i)}_l], \quad i = 1, 2, \ldots, p$$

$$l = l_1 + l_2 + \cdots + l_p$$

where $\|A\|_1, 1 = \sum_{j=1}^{n} \|A_j\|$ with $A_j$ being the $j$th column of $A$. Furthermore, to ensure that the same active set of endmembers are shared among all the pixels, the CLSU algorithm [48] introduced an $l_2, 1$ mixed norm to globally impose the row sparsity of abundances, which is formulated as

$$\min_A \frac{1}{2} \|R - MA\|^2_F + \lambda \|A\|_{2, 1} \quad \text{s.t. } A \geq 0$$

where $\|A\|_{2, 1} = \sum_{i=1}^{m} \|A_i\|_2$ with $A_i$ indicating the $i$th row of $A$. Note that, compared to SUnSAL, the main contribution of CLSU is to enforce joint sparsity in the whole images rather than employ pixelwise independent regressions.
in which $X_i(i = 1, 2, \ldots, p)$ represents the library subset corresponding to the $i$th possible material and is composed of $l_i$ spectral signatures of the $i$th material.

To separate the intrinsic endmember spectra and spectral variability from the $in$ $situ$ spectral library, the classical principal component analysis (PCA) is adopted. Generally, the main information of the original data can be retained by keeping the first $k$ principal components corresponding to the larger eigenvalue, and the remaining components correspond to noise, random error, and/or outliers. Let $\bar{X} = (1/l) \sum_{i=1}^l X_i$ be the average spectrum of $in$ $situ$ spectral library and $C$ denote the covariance matrix after standardization as

$$C = \frac{1}{l} \sum_{i=1}^l (X_i - \bar{X})(X_i - \bar{X})^T.$$  

(7)

PCA transform is performed on the covariance matrix of the $in$ $situ$ spectral library to compute eigenvectors and eigenvalues as

$$[W, Q] = \text{PCA}(C)$$  

(8)

where $\text{PCA}(\cdot)$ represents the PCA transform, $W = [w_1, w_2, \ldots, w_n]$ is composed of eigenvectors, and $Q = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ is the corresponding eigenvalue matrix with $\lambda_1 > \lambda_2 > \cdots > \lambda_n$. Among all the principal components, the first $k$ components correspond to the main information of the $in$ $situ$ spectral library, i.e., the intrinsic endmember spectra, while the rest of the components are related to the spectral variability.

Generally, $k$ can be determined by manually setting or introducing a certain threshold. Let $\zeta$ be the threshold defined in advance, and then, the first $k$ eigenvectors are separated until the ratio of their cumulative eigenvalues to the sum of all the eigenvalues reaches the threshold

$$\sum_{i=1}^k \lambda_i / \sum_{i=1}^n \lambda_i \geq \zeta.$$  

(9)

By considering endmember spectra make up most of the information in an HSI, the value of $k$ is consequently set to the number of endmembers in this article. Thus, the $k$ principal components, referred to as $F_1$, can be calculated as

$$F_1 = W_k^T (X - \bar{X})$$  

(10)

in which $W_k = [w_1, w_2, \ldots, w_k](k \leq n)$ involves the first $k$ eigenvectors. Then, the reconstructed spectral library by dominant characteristic components is termed as intrinsic endmember library $M \in \mathbb{R}^{l \times l}$

$$M = W_k F_1 + \bar{X} = W_k W_k^T (X - \bar{X}) + \bar{X}.$$  

(11)

The remaining $n-k$ components referred to as $F_2$ are calculated similarly as

$$F_2 = W_{n-k}^T (X - \bar{X})$$  

(12)

in which $W_{n-k} = [w_{k+1}, w_{k+2}, \ldots, w_n]$ consists of the rest of eigenvectors. To model the spectral variability existing in each endmember spectra of the $in$ $situ$ spectral library, such
components $F_2$ are adopted to construct the spectral variability library $V \in \mathbb{R}^{k \times l}$ as

$$V = W_{n-k}F_2 + \bar{X} = W_{n-k}W_{n-k}^T(X - \bar{X}) + \bar{X}. \quad (13)$$

Furthermore, assuming that such spectral variability can be transferred among different endmembers, all the spectral variability contained in an HSI, denoted as $V_1$, can be further modeled by a linear combination of extracted spectral variability, which can be expressed as

$$V_1 = VB \quad (14)$$

where $B \in \mathbb{R}^{l \times n}$ denotes the variability coefficients corresponding to spectral variability library $V$. Note that such variability $V_1$ actually reflects the microimaging conditions within all the pixels in the scene.

Consequently, by encountering such spectral variability, HSIs immune to spectral variability can be well modeled by intrinsic endmembers and corresponding abundances, which is expressed as

$$R - V_1 = MA. \quad (15)$$

Here, $A \in \mathbb{R}^{l \times n}$ denotes the abundances corresponding to the intrinsic endmember library $M$.

B. Spectral Variability Augmented Sparse Unmixing

Fig. 1 illustrates a schematic of the proposed SVASU model, where the image cube and spectral libraries of the well-known Jasper dataset are taken as an example. The spectral variability library is introduced and modeled under linear mixture assumption to augment sparse unmixing by synchronously performing endmember-based reconstruction and spectral variability-augmented reconstruction. Moreover, the sparsity and smoothness constraints are further imposed over abundances and variability coefficients to enhance the joint sparsity in rows and the moderate variability, respectively.

Based on the objective function in (5), the proposed SVSAU model consists of four parts: an intrinsic endmember library-based data fitting term, a spectral variability-based data fitting term, an $l_2,1$-norm-based sparsity constraint over abundances, and a smoothness constraint over variability coefficients, which is expressed as

$$\Theta = \min_{A, B} \|R - MA\|_F^2 + \alpha \|R - MA - VB\|_F^2$$

$$+ \beta \|A\|_{2,1} + \gamma \|B\|_F^2 \quad \text{s.t.} \quad A \geq 0 \quad (16)$$

where $\alpha$ balances the contribution of data fitting from both spectral spectra and spectral variability, and $\beta$ and $\gamma$ control the sparsity of abundances and the smoothness of spectral variability coefficients, respectively.

Following [64], we relax the term $\|A\|_{2,1}$ as $\text{Tr}(A^\top DA)$. Thus, the objective function in (16) can be rewritten as

$$\Theta = \min_{A, B} \|R - MA\|_F^2 + \alpha \|R - MA - VB\|_F^2$$

$$+ \beta \text{Tr}(A^\top DA) + \gamma \|B\|_F^2 \quad \text{s.t.} \quad A \geq 0 \quad (17)$$

where $D \in \mathbb{R}^{m \times m}$ is a diagonal matrix with the $i$th diagonal element formulated as

$$D_{ii} = \frac{1}{2\sqrt{A_i^\top A_i} + \epsilon} \quad (18)$$

in which $\epsilon > 0$ is a stabilization parameter. In order to integrate nonnegative constraint conditions into the objective function $\Theta$, we introduce a Lagrangian multiplier $\delta \in \mathbb{R}^{m \times n}_+$ to restrict $A \geq 0$. Therefore, the objective function (17) is equivalent to the following formula:

$$\Theta = \min_{A, B} \|R - MA\|_F^2 + \alpha \|R - MA - VB\|_F^2$$

$$+ \beta \text{Tr}(A^\top DA) + \gamma \|B\|_F^2 - \text{Tr}(\delta A^\top). \quad (19)$$

When $D$ is fixed, this problem can be turned into a general convex optimization problem. To find the optimal solution to such a convex optimization problem, an alternating projected gradient method is designed to update all matrices of the objective function iteratively. By taking the partial derivatives with respect to variables $A$ and $B$, respectively, we obtain the following formulations:

$$\frac{\partial \Theta}{\partial A} = 2((1 + \alpha)M^\top MA - (1 + \alpha)M^\top R$$

$$+ \alpha M^\top VB + \beta DA) - \delta \quad (20)$$

$$\frac{\partial \Theta}{\partial B} = 2(A^\top MA - a^\top R + a^\top VB + \gamma B).$$

With the KKT conditions, the following conditions should be satisfied:

$$2((1 + \alpha)M^\top MA - (1 + \alpha)M^\top R$$

$$+ \alpha M^\top VB + \beta (D + D^\top)A)_{ik} \cdot A_{ik} = 0 \quad (21)$$

$$2(a^\top MA - a^\top R + a^\top VB + \gamma B)_{ij} \cdot B_{ij} = 0.$$

Thus, the update rules of the alternating method for SVASU are summarized as

$$A^{t+1}_{ik} = A^t_{ik} \left(\frac{(M^\top R + \alpha M^\top VB - \alpha M^\top R^2)_{ik}}{((1 + \alpha)M^\top MA + \beta DA + \epsilon)_{ik}}\right)^{\frac{1}{2}} \quad (22)$$

$$B^{t+1}_{ij} = B^t_{ij} \left(\frac{a^\top R - a^\top VB + \gamma (A^\top A + \epsilon)_{ij}}{a^\top VB + \gamma B^t_{ij}}\right)^{\frac{1}{2}}.$$

Note that the convergence of the two update rules is analyzed in the Appendix. In the $(t + 1)$th iteration, $A$ is calculated with the $t$th update of $B$, and then, $B$ and $D$ are updated based on the calculated $A$. The iterative procedure is repeated until the algorithm converges. The pseudocode of the proposed SVASU proposed is summarized in Algorithm 1.

IV. EXPERIMENTS

In this section, a series of experiments over both simulated dataset and two real-world datasets (i.e., Jasper and Cuprite datasets) are designed to comprehensively evaluate the unmixing ability of the proposed SVASU algorithm.

Several well-known sparse unmixing algorithms are adopted for comparison, including UnSAL [41], CLSUnSAL [48], ADSpLRU [58], JSpBLRU [59], and MUA SLIC [54]. For all these methods, the selections of parameters refer to the reported optimal values. The in situ spectral library obtained by SPEE is adopted for all compared algorithms as the input.
A. Evaluation Metrics

For quantitative performance evaluation, two kinds of evaluation metrics related to reconstruction error are employed in the experiments. First, the root mean square error (RMSE) is used to measure the distance between the actual vector and its estimated version, by which a lower value of RMSE means more similar to the original vector. Thus, RMSER is defined to describe the reconstruction error of observed image R and its reconstructed version \( \hat{R} \), and RMSER_A depicts that of referenced abundance fractions A and its estimated version \( \hat{A} \), which are, respectively, defined as

\[
RMSE_R = \sqrt{\frac{1}{n} \sum_{j=1}^{n} ||R_j - \hat{R}_j||^2} \tag{23}
\]

\[
RMSE_A = \sqrt{\frac{1}{n} \sum_{j=1}^{n} ||A_j - \hat{A}_j||^2} . \tag{24}
\]

Furthermore, the signal-to-reconstruction-error (SRE) computing the power of the error related to that of the signal is also embraced to evaluate the quality of the reconstructed vectors obtained by different algorithms. The higher value of SRE (dB) implies much better performance. Similarly, we define SRE_R and SRE_A as

\[
SRE_R = 10 \log_{10} \left( \frac{\frac{1}{n} \sum_{j=1}^{n} ||R_j||^2}{\frac{1}{n} \sum_{j=1}^{n} ||R_j - \hat{R}_j||^2} \right) \tag{25}
\]

\[
SRE_A = 10 \log_{10} \left( \frac{\frac{1}{n} \sum_{j=1}^{n} ||A_j||^2}{\frac{1}{n} \sum_{j=1}^{n} ||A_j - \hat{A}_j||^2} \right). \tag{26}
\]

B. Experiments Over Synthetic Dataset

A simulated dataset is generated following [65] and [66] based on LMM defined by (1), which is made up of \( n = 10000 \) pixels. Five spectral signatures (Ammonialunate NMNH145596, Ammonium Chloride GDS77, Ammonio-llite/Semc GDS87, Ammonio-jaroite, and Andesine HS142.3B) are selected from the USGS spectral library, containing 420 bands with wavelengths from 400 to 2500 nm. Then, 10-dB Gaussian noise is added to each signature to simulate spectral variability. In each pixel, the abundance vectors of endmembers are generated according to a mixture of Dirichlet distributions [67]. Finally, 40-dB Gaussian noise is added to the whole image to simulate microimaging conditions within pixels. In this experiment, the in situ spectral library is simply composed of the selected five spectra from USGS and their corresponding spectra owning spectral variability. After the library segmentation by PCA according to (11) and (13), we acquire: 1) intrinsic endmember library and 2) spectral variability library, as shown in Fig. 2.

The influence of the regularization parameters over the unmixing performance, including \( \alpha, \beta, \) and \( \gamma \), is primitively discussed to determine their optimal values. All four evaluation metrics are adopted here for evaluation, which are the SRE and RMSE for both abundances and pixels, calculated by (23)–(26). Fig. 3 depicts the average SRE and RMSE results for estimated abundances and reconstructed pixels obtained by the proposed SVASU. Note that \( \alpha \) is varied in \([1, 5, 10]\); \( \beta \) and \( \gamma \) are ranged in \([1e0, 1e1, 1e2, 1e3] \) and \([1e2, 1e3, 1e4, 1e5]\), respectively. It is observed that, with the increase in \( \alpha \), the performance of constructing abundances and pixels encounters a degraded trend; thus, we set \( \alpha = 1 \).

In addition, as can be seen from the figures, the performance of pixel reconstruction remains steady, while abundance performance fluctuates gradually with changing \( \beta \) and \( \gamma \). Therefore, \( \beta \) and \( \gamma \) are set to \( 1e3 \) and \( 1e4 \), which acquires the lowest RMSE value and the highest SRE value.

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**Algorithm 1 Proposed SVASU Algorithm**

**Input:** Hyperspectral data matrix \( R \in \mathbb{R}^{b \times n} \); Intrinsic end-member library \( M \in \mathbb{R}^{b \times m} \); Spectral variability library \( V \in \mathbb{R}^{b \times l} \); Parameters \( \alpha, \beta, \) and \( \gamma \).

**Output:** Abundance fractions \( A \).

1. Initialize \( A \in \mathbb{R}^{m \times n} \) and \( B \in \mathbb{R}^{l \times n} \) randomly; \( t = 0 \);
2. Repeat:
   3. Calculate the diagonal matrix \( D \) of which the \( i \)-th diagonal element is \( \frac{1}{\sqrt{A_i \cdot A_i}} \);
   4. Update \( A_{t+1} \leftarrow A_t \odot (M^T R + \alpha M^T M - \alpha V^T V)^T ; \)
   5. Update \( B_{t+1} \leftarrow B_t \odot (\alpha V^T V \cdot \alpha V^T V + \gamma R)^T ; \)
   6. Calculate the objective function value \( \Theta_{t+1} \);
   7. \( t \leftarrow t + 1 \);
8. Until Convergence: \( \frac{||\Theta_{t+1} - \Theta_t||}{||\Theta_t||} < 10^{-5} \);
9. Return \( A \) and \( B \);
Table I lists a quantitative comparison of the proposed SVASU method and other considered algorithms with respect to SRE and RMSE results over the synthetic dataset. As observed from Table I, the proposed SVASU model outperforms the other five comparison algorithms. Specifically, compared with MUA\textsubscript{SLIC} producing suboptimal performance, the proposed SVASU algorithm promotes the SRE of abundance reconstruction by nearly 15 dB and that of pixel reconstruction by more than 1.5 dB. The vast performance difference between the classical sparse unmixing models and the proposed SVASU demonstrates that introducing the spectral variability library can significantly improve the performance of sparse unmixing for better abundance estimation and more accurate pixel representation.

C. Experiments Over Jasper Dataset

The Jasper dataset was captured by the airborne visible/infrared imaging spectrometer (AVIRIS) sensor\textsuperscript{1}, which covers 224 bands and a wavelength range of 380–2500 nm. In this experiment, a cropped image of 100 × 100 pixels is selected. Several bands are seriously distorted due to the influence of water-vapor absorption and atmosphere, including the bands 1–3, 108–112, 154–166, and 220–224. After removing these bands, 198 reflectance bands remain to be used. Four main endmembers are identified as tree, water, road, and soil.

Fig. 4 concretely displays the intrinsic endmember library and spectral variability library obtained from the Jasper dataset.

Table II shows the average SRE and RMSE values between the reference and estimated matrices (containing reconstructed images and abundances) acquired by different algorithms over the Jasper dataset. Depending on the augment of spectral variability-based reconstruction, the performance of pixel reconstruction by the proposed SVASU method is obviously much better than other advanced sparse unmixing algorithms. Meanwhile, the tradeoff between the intrinsic endmember-based data fitting and the spectral variability-augmented data fitting in the proposed objective function can also guarantee the excellent performance of abundance estimation. Fig. 6 shows the estimated abundances by the proposed SVASU method and the ground-truth abundances, which verifies the high consistence with the reference abundances.

To analyze the effect of the two data fitting terms, Fig. 7 depicts the visual results of the essential items owning to the proposed SVASU. Each visual result is averaged over each band, including the image data $\mathbf{R}$, the endmember library-based reconstruction item $\mathbf{MA}$, the spectral variability library-based reconstruction item $\mathbf{VB}$, the endmember library-based reconstruction error item $\mathbf{R} - \mathbf{MA}$, and the spectral variability-augmented reconstruction error item $\mathbf{R} - \mathbf{MA} - \mathbf{VB}$. It can be observed that the amount of information represented by $\mathbf{MA}$ is much larger than that by $\mathbf{VB}$.

\textsuperscript{1}Data available online at https://rslab.ut.ac.ir/data
Moreover, through the establishment of the spectral variability extended representation, the image reconstruction error of $R - MA - VB$ reduces to one-tenth of that by $R - MA$, which validates the proposed SVASU algorithm.

### D. Experiments Over Cuprite Dataset

The Cuprite dataset, acquired by AVIRIS, is also adopted in the experiments. The cropped image corresponds to a $350 \times 350$ pixels subset, and only 186 reflectance bands remain to be used after removing the low SNR bands (i.e., 1–4, 105–115, 150–170, and 223–224). For the number of endmembers, the HySime [68] provided an estimation of 16 under the input false-alarm probability $P_F = 10^{-5}$. Similarly, we obtain an intrinsic endmember library and a spectral variability library from the Cuprite dataset, as shown in Fig. 8. The optimal values of parameters in the proposed SVASU method are similarly discussed and determined to be $\alpha = 5$ and $\beta = \gamma = 1e4$.

Given that there is no available ground-truth data in terms of abundances of the Cuprite dataset, only the pixel reconstruction results are listed in Table III for quantitative evaluation. The mean SRE and RMSE results in Table III confirm the superior performance of our proposed SVASU algorithm over the Cuprite dataset that owns a relatively more complex distribution of ground objects. Especially, the proposed SVASU algorithm improves the performance of pixel reconstruction by at least 5 dB in terms of SRE compared to the suboptimal performance gained by JSpBLRU. In addition, Fig. 9 shows the visual abundance assessment for only a few available minerals, where the reference classification maps are produced by Tricorder software. It can be found that the estimated abundance maps by the proposed SVASU method are mostly similar to the distribution of the five materials in the classification maps.

Meanwhile, the visual results of each reconstruction term in SVASU are shown in Fig. 10. Similarly, each visual result is averaged over each band, including the two library-based reconstruction items $MA$ and $VB$, and their corresponding two data fitting error items $R - MA$ and $R - MA - VB$. As can be seen from Fig. 10, the amount of information of the image represented by intrinsic endmembers is much more than that by spectral variability. Moreover, introducing spectral variability library-augmented representation dramatically reduces the
image reconstruction error to less than one-tenth exactly. This also confirms that, in PCA processing, the main components are constructed by intrinsic endmembers, while the rest are related to spectral variability. In addition, through modeling the spectral variability within the image, the influence of microimaging conditions within all the pixels can be well modeled. Consequently, the effectiveness and advancement of the proposed SV ASU method are confirmed.

**E. Ablation Analysis**

The ablation study is also conducted to verify the necessity of each component in the objective function. Specifically, two other variants of the proposed SV ASU are considered, including $L_{\text{endmember}}$ without taking spectral variability into account and $L_{\text{variability}}$ removing the intrinsic endmember-based data fitting term, which is defined as

$$L_{\text{endmember}} = \min_A \| R - MA \|^2_F + \beta \text{Tr}(\delta^T DA)$$

$$L_{\text{variability}} = \min_{A,B} \| R - MA - VB \|^2_F + \beta \text{Tr}(\delta^T DA) + \gamma \| B \|^2_F - \text{Tr}(\delta^T A)$$

The ablation experiments are conducted over both synthetic and real-world datasets. As reported in Table IV, the sole use of the endmember-based data fitting term in the objective function $L_{\text{endmember}}$ ensures the completion of the unmixing task but with limited accuracy. Through adopting the spectral variability-based data fitting term, the performance of the objective function $L_{\text{variability}}$ improves a lot, in which the smoothness constraint further guarantees a moderate variation of the spectral variability. Moreover, the tradeoff of data fitting by the endmember library and both libraries ensure that the most information of the input image is reconstructed by the endmember library, further fitting the real situation and enhancing the unmixing performance. Hence, the proposed objective function of SVASU achieves optimal performance over all the cases.

**V. Conclusion**

This article proposes a convex optimization-based SVASU model, which explicitly extracts the spectral variability for the first time. Specifically, spectral variability is separated from the in situ spectral library by the eigenvalue analysis, i.e., PCA. Then, the microimaging conditions of all the pixels are modeled by a linear combination of extracted spectral variability of each endmember class, which are further used to augment the sparse unmixing. The proposed SVASU algorithm achieves a tradeoff between the endmember-based reconstruction and spectral variability augmented reconstruction, simultaneously enforcing the joint sparsity of abundances and the smoothness of variability. Experimental results over both synthetic and real-world datasets demonstrate that the proposed SVASU model can significantly enhance the performance of sparse unmixing, and through the introduction of the spectral variability library, the ability of the proposed framework to model the spectral variability is improved. Extracting in situ spectral variability is an interesting topic to improve the performance of HSI processing. We are working on this topic and the new-emerging in situ spectral variability will also be used in the proposed SVASU algorithm to improve the performance of mixed pixel unmixing.

**Appendix**

**Proof of Convergence of SVASU**

The problem in (17) contains two unknown matrices, and we design different rules to alternately update one by fixing the other. Following [69], [70], the auxiliary function approach is used to prove the convergence of the proposed update rules in (22). Function $Q(X, \hat{X})$ is an auxiliary function for $L(X)$ if the conditions

$$Q(X, \hat{X}) \geq L(X), \quad Q(X, X) = L(X)$$

are satisfied for any $X$ and $\hat{X}$. Then, if

$$X^{(t+1)} = \arg \min_X Q(X, X^{(t)})$$

TABLE IV

| Objective Function | Synthetic Data Set | Jasper Data Set | Cuprite Data Set |
|--------------------|--------------------|----------------|-----------------|
| $L_{\text{endmember}}$ | SRE$_R$ 8.0026 | SRE$_R$ 16.9934 | SRE$_R$ 16.3972 |
| $L_{\text{variability}}$ | RMSE$_R$ 32.7314 | RMSE$_R$ 18.8412 | RMSE$_R$ 26.2238 |
| $L_{\text{SVASU}}$ | RMSE$_A$ 1.2241 | SRE$_A$ 6.4242 | SRE$_A$ 0.0793 |
| $L_{\text{SVASU}}$ | $\beta$ 0.0682 | $\gamma$ 0.0777 | $\gamma$ 0.0260 |
| $L_{\text{SVASU}}$ | $\theta$ 0.0567 | $\theta$ 0.0749 | $\theta$ 0.0209 |
it has been proven that the following inequalities hold:
\[ L(X^{(r+1)}) \leq Q(X^{(r+1)}, X^{(t)}) \leq Q(X^{(t)}, X^{(t)}) = L(X^{(t)}). \] (31)
Thus, the function \( L(X) \) is monotonically decreasing.

A. Fixing \( B \), Minimizing \( A \)

First, when \( B \) is fixed, the minimization problem in (17) can be written as
\[
\min_A \|R - MA\|_F^2 + \alpha\|T - MA\|_F^2 + \beta\text{Tr}(A^TDA)
\] (32)
in which \( T = R - VB \). For the first two terms in (32), the following inequality holds [71]:
\[
\begin{align*}
L_1(A) &= \|R - MA\|_F^2 \\
&= \text{Tr}(R^T R) - 2\text{Tr}(R^T MA) + \text{Tr}(A^T M^T M A) \\
&\leq \text{Tr}(R^T R) - 2\text{Tr}(R^T M A) - 2\text{Tr}(R^T M Z) \\
&\quad + \frac{1}{2}\text{Tr}(P^T M^T M A) + \frac{1}{2}\text{Tr}(A^T M^T M A) \\
&= Q_1(A, \tilde{A})
\end{align*}
\] (33)
\[
\begin{align*}
L_2(A) &= \|T - MA\|_F^2 \\
&= \text{Tr}(T^T T) - 2\text{Tr}(T^T MA) + \text{Tr}(A^T M^T MA) \\
&\leq \text{Tr}(T^T T) - 2\text{Tr}(T^T M A) - 2\text{Tr}(T^T M Z) \\
&\quad + \frac{1}{2}\text{Tr}(P^T M^T M A) + \frac{1}{2}\text{Tr}(A^T M^T M A) \\
&= Q_2(A, \tilde{A})
\end{align*}
\] (34)
where \( P_{ik} = (A_{ik})^4 / (\tilde{A}_{ik})^3 \), and \( Z_{ik} = \tilde{A}_{ik} \ln(A_{ik} / \tilde{A}_{ik}) \). It is obvious that \( Q_1(A, A) = L_1(A), Q_2(A, A) = L_2(A) \). Taking \( Q_1(A, \tilde{A}) \) as an example, \( Q_1(A, \tilde{A}) \geq L_1(A) \) can be proved in detail as
\[
Q_1(A, \tilde{A}) - L_1(A) = 2\text{Tr}(R^T MA) - 2\text{Tr}(R^T M A) - 2\text{Tr}(R^T M Z) \\
+ \frac{1}{2}\text{Tr}(P^T M^T M A) + \frac{1}{2}\text{Tr}(A^T M^T M A) \\
- \text{Tr}(A^T M^T MA) \\
= \sum_{ik} 2R_{ik} M_{ik} \left( A_{ik} - \tilde{A}_{ik} - \tilde{A}_{ik} \ln \frac{A_{ik}}{\tilde{A}_{ik}} \right) \\
+ \sum_{ik} \frac{1}{2}(M_{ik})^2 \left( \frac{(A_{ik})^2}{\tilde{A}_{ik}} - \tilde{A}_{ik} \right)^2 \geq 0.
\] (35)
Thus, \( Q_1(A, \tilde{A}) \) and \( Q_2(A, \tilde{A}) \) can be selected as the auxiliary functions of \( L_1(A) \) and \( L_2(A) \) correspondingly.

Then, for the last term \( L_3(A) = \text{Tr}(A^T DA) \), the following auxiliary function \( Q_3(A, \tilde{A}) \) is constructed as:
\[
Q_3(A, \tilde{A}) = \frac{1}{2}\text{Tr}(P^T D \tilde{A}) + \frac{1}{2}\text{Tr}(A^T D \tilde{A}).
\] (36)
It is straightforward to verify that \( Q_3(A, A) = L_3(A) \). To show that \( Q_3(A, \tilde{A}) \geq L_3(A) \), we have the following calculation:
\[
Q_3(A, \tilde{A}) - L_3(A) = \sum_{ik} \frac{D_{ij} A_{ik}}{2(\tilde{A}_{ik})^3} + \sum_{ik} \frac{D_{ij} A_{ik}}{2(\tilde{A}_{ik})^2} - \sum_{ik} D_{ij} (A_{ik})^2
\] (37)
Thus, \( Q_3(A, \tilde{A}) \) can be an auxiliary function of \( L_3(A) \).

Finally, \( Q(A, \tilde{A}) = Q_1(A, \tilde{A}) + \alpha Q_2(A, \tilde{A}) + \beta Q_3(A, \tilde{A}) \) is an auxiliary function of \( L(A) = L_1(A) + \alpha L_2(A) + \beta L_3(A) \) in (17). Currently, according to (30), we find the minimum of \( Q(A, \tilde{A}) \) by fixing \( \tilde{A} \), which is given by
\[
0 = \frac{\partial Q(A, \tilde{A})}{\partial \tilde{A}_{ik}} = \frac{\partial Q_1(A, \tilde{A})}{\partial \tilde{A}_{ik}} + \alpha \frac{\partial Q_2(A, \tilde{A})}{\partial \tilde{A}_{ik}} + \beta \frac{\partial Q_3(A, \tilde{A})}{\partial \tilde{A}_{ik}}.
\] (38)
Then, we can get
\[
\tilde{A}_{ik} = \frac{\left( \frac{(M^T R + aM^T V - aM^T VB)_{ik}}{((1 + a)M^T MA + \beta D)_{ik}} \right)^2}{2 + \beta D_{ik}}.
\] (39)

B. Fixing \( A \) and Minimizing \( B \)

When \( A \) is fixed, the minimization problem in (17) can be written as
\[
\min_B \alpha\|T - VB\|_F^2 + \gamma \|B\|_F^2.
\] (40)
in which \( T' = R - MA \).

Similarly, the following two inequalities hold:
\[
\begin{align*}
L_1(B) &= \|T' - VB\|_F^2 \\
&= \text{Tr}(T'^T T') - 2\text{Tr}(T'^T VB) + \text{Tr}(B^T V^T VB) \\
&\leq \text{Tr}(T'^T T') - 2\text{Tr}(T'^T V B) - 2\text{Tr}(T'^T V Z') \\
&\quad + \frac{1}{2}\text{Tr}(P^T V^T V B) + \frac{1}{2}\text{Tr}(B^T V^T V B) \\
&= Q_1(B, \tilde{B})
\end{align*}
\] (41)
\[
\begin{align*}
L_2(B) &= \|B\|_F^2 \\
&= \text{Tr}(B^T B) \\
&\leq \frac{1}{2}\text{Tr}(P^T B) + \frac{1}{2}\text{Tr}(B^T B) = Q_2(B, \tilde{B})
\end{align*}
\] (42)
in which \( P'_{ij} = (B_{ij})^4 / (\tilde{B}_{ij})^3 \) and \( Z'_{ij} = \tilde{B}_{ij} \ln(B_{ij} / \tilde{B}_{ij}) \).

Thus, \( Q(B, \tilde{B}) = \alpha Q_1(B, \tilde{B}) + \gamma Q_2(B, \tilde{B}) \) is an auxiliary function of \( L(B) = L_1(B) + \gamma L_2(B) \) in (40). Currently, according to (30), we find the minimum of \( Q(B, \tilde{B}) \) by fixing \( \tilde{B} \), which is given by
\[
0 = \frac{\partial Q(B, \tilde{B})}{\partial \tilde{B}_{ij}} = \frac{\partial Q_1(B, \tilde{B})}{\partial \tilde{B}_{ij}} + \gamma \frac{\partial Q_2(B, \tilde{B})}{\partial \tilde{B}_{ij}}.
\]
Solving for $B_{ij}$, the minimum is

$$B_{ij} = B_{ij} \left( \frac{(\alpha^T V - \alpha^T V M A)_{ij}}{(\alpha^T V B + \gamma B)_{ij}} \right)^{\frac{1}{2}}.$$

Thus, updating A and B alternatively by using the rules in (39) and (44) can guarantee that the value of objective function in (17) is monotonically decreasing.

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