Hyperspectral Unmixing via Semantic Spectral Representations

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Abstract—We propose a new spectral unmixing method using a semantic spectral representation, which is produced via non-homogeneous hidden Markov chain (NHMC) models applied to wavelet transforms of the spectra. Previous studies have shown that the representation is robust to spectral variability in the same materials because it can automatically detect the diagnostic spectral features in the training data. Therefore, our method can successfully detect materials while automatically extracting diagnostic features, showing high resilience to spectral variability. Simulations indicate that our unmixing method could be effectively used on Hapke mixtures.

I. INTRODUCTION
Spectral unmixing aims at estimating the fractional abundances of pure spectral signatures (also called as endmembers) in each mixed pixel collected by an imaging spectrometer. Both linear [1] and nonlinear approaches [2] to unmixing have been proposed. In many situations, the identification of the endmember signatures in the original data set may be challenging due to insufficient spatial resolution, mixtures happening at different scales, and unavailability of completely pure spectral signatures in the scene. However, the unmixing problem can also be approached by assuming that the observed image spectra can be expressed in the form of combinations of a number of pure spectral signatures known in advance (e.g., spectra collected on the ground by a field spectroradiometer or in the laboratory from field samples). Unmixing then amounts to finding the optimal subset of signatures in a (potentially very large) spectral library that can best model each mixed pixel in the scene. In particular, approaches based on sparse regression have received attention in the literature [3–5].

At their core, hyperspectral unmixing methods based on sparsity assume a linear mixing model. However, several aspects of the physical measurement introduce nonlinearities in the mixing process. While detailed nonlinear mixing models have been proposed for specific scenarios (e.g. the ones introduced by Hapke that describes the scattering behavior of intimate particulate mixtures Hapke [6]), in many practical scenarios, it is difficult to assess the specific nonlinear parametric shape of mixed hyperspectral data clouds and a method for detecting endmembers that does not rely on a particular mixing model would be desirable.

Mixed spectra retain most of the diagnostic spectral information present in the endmember spectra, and this information can be leveraged in unmixing by identifying the endmember only through a set of diagnostic features. Diagnostic features are routinely manually defined by practitioners to discriminate spectral families (e.g. the Tetracorder algorithm [7]). It would be desirable to automate the process of extraction of diagnostic representations of the endmembers directly from the data.

It has been recently shown that training data in the form of material spectra can be used to automatically identify relevant diagnostic features [8, 9]. Specifically, a non-homogeneous hidden Markov chain (NHMC) model can be applied to the wavelet-domain representation of hyperspectral signatures, which automatically detects diagnostic features of each spectra in the training data set while suppressing uninformative information. Therefore, the NHMC representation enables us to identify materials independently of the mixtures observed, while automatically detecting a set of characteristic features of each material in the mixtures.

In this paper, we develop a new unmixing method using spectral representations obtained from the NHMC model. The model provides binary labels marking significant portions of the spectrum, some of which are shown to be preserved by the mixture process. We design an unmixing algorithm that searches for such discriminating labels, and is constituted by a set of endmember detectors. The algorithm makes therefore no assumptions on the mixing model that generated the data.

II. NHMC-BASED SPECTRAL UNMIXING
Assuming that we have a large spectral library, we consider the problem of detecting materials (endmembers) that are present in each observed mixture from its spectral signature. In our method, one detector is designed for each endmember, making the method independent from the pre-defined number of endmembers undergoing testing.

Our method is composed of three steps, described below, with the last two steps being illustrated in Fig. 1.

A. NHMC Model Labeling
We begin by training NHMC models using Daubechies-1 wavelet representations of a training set of mixture spectra [8–10]. Using the learned NHMC model, we obtain binary labels [8–10] for a set of pure and attenuated spectra of the endmembers. Each binary label matrix has size $S \times N$, where $S$ is the number of wavelet scales and $N$ is the length of the spectrum, and marks significant portions of the spectrum using “large” labels (illustrated in red) for the wavelet coefficients at the corresponding bands and scales, while assigning “small” labels (illustrated in blue) to wavelet coefficients that correspond to non-informative regions of the spectrum.

B. Learning Endmember Features
In the second stage, we identify dominant features that persist in the NHMC binary labels for an endmember even as it is attenuated. For that purpose, we build a dataset for each endmember consisting of attenuated versions of its spectra. The attenuations are multiplicative and range between 0.1 and 1, and so the dataset includes all of the original features. This work was supported by the National Science Foundation under grant number IIS-1319585.
Fig. 1. Schematic of our algorithm. (A) illustrates the stage where learning features and (B) describes how to detect materials from observations.

(A) Learning features in each material

- Spectra in the library
  - Pure and scaled
- NHMC labels
- (a) Spectra in the library
- (b) NHMC labels
- (c) Probability of high states
- (d) Thresholding
- NHMC parameters: $A$ and $\sigma$, obtained in the 1st step

(B) Rejection and detecting each material

- Observed Spectra
- Mapping to a feature space
- Clustering
- NHMC labels
- NHMC parameters: $A$ and $\sigma$, obtained in the 1st step

endmember spectra (cf. Fig. 1(A)(a)). We then use the NHMC model to obtain binary labels $\mathbf{H}_j^i$ for each one of the spectra $i = 1, 2, \ldots$ in the attenuated dataset for the $j$th endmember (cf. Fig. 1(A)(b)). The obtained labels are then aggregated through averaging, which effectively provides the percentage of samples among the attenuated spectra for which each label is marked as “large”, i.e., $\mathbf{P}_j^i = \frac{1}{M} \sum_{i=1}^{M} \mathbf{H}_j^i$, where $M$ is the number of samples in the attenuated endmember dataset. After that, we normalize each matrix $\mathbf{P}_j^i$ by dividing its entries by the value of the largest entry in the matrix. Thus, we can treat $\mathbf{P}_j^i$ as a normalized probability matrix that provides the likelihood of the “large” state for each wavelet coefficient among the $j$th endmember dataset (cf. Fig. 1(A)(c)).

In order to focus on the prevalent discriminant features in the endmember spectra, we consider only the labels for those band and scale combinations whose probability of a “large” state in $\mathbf{P}_j^i$ are larger than the specified threshold value $\tau$, which are then considered as the diagnostic features for the endmember binary labels (cf. Fig. 1(A)(d)). All other labels with probability of “large” state lower than the threshold are eliminated, i.e., we obtain the feature matrix $\hat{\mathbf{P}}_j^i = I(\mathbf{P}_j^i \geq \tau)$, where $I(\cdot)$ is an indicator function. In words, $\hat{\mathbf{P}}_j^i \in \{0, 1\}^{N \times N}$ is a binary matrix that encodes the set of diagnostic features in the NHMC binary labels for an endmember.

After this thresholding, the selected labels in $\hat{\mathbf{P}}_j^i$ are grouped into column clusters. Since spectral absorption features span at least several channels (wavelengths), we assume that labels close enough to each other represent a single spectral feature and we concatenate them together. Similarly, selected labels with less width than the narrowest absorption feature observed in the database should be considered spurious and be removed.

The grouping is performed by first constructing a vector of length equal to the number of wavelengths. The $i$-th element of such vector is one if the $i$-th column of the matrix $\hat{\mathbf{P}}_j^i$ has at least one “large” label, zero otherwise. Afterward, agglomerative hierarchical clustering with single linkage [11] is applied to this vector. The clusters are obtained by cutting the tree so that the maximum distance in any cluster is smaller than a threshold $\rho_d$. Additionally, clusters exhibiting widths smaller than a threshold $\rho_w$ are discarded. Fig. 1(A)(e) shows the groups (clusters) of features resulting from this stage with different colors.

Independently, we remove features likely to be present in any other material class, which would cause false alarms. To this end, we set another threshold value $\tau_R$ that represents the maximum allowance of the high probability state for each selected label in all other classes. If the probability of a “large” state is larger than $\tau_R$ for a given band and scale combination in any other class, the corresponding label is eliminated from
the feature under consideration. The outcome of this false-
alarm pruning step is a smaller set of features, as illustrated in Fig. 1(A)(f).

Finally, the features that survive the previous step are
segmented according to the labels assigned in the grouping
step, resulting in \( F_j \) discriminative features of one material
\( \{F_1^j, \ldots, F_N^j\} \) (cf. Fig. 1(A)(g)), where \( F_j \) represents the
number of clusters and \( F_j^j \) refers to a binary vector indicating
the \( j^{th} \) cluster obtained from \( \mathbf{P} \).

C. Detection of Endmembers

The NHMC labels for a mixture spectra are assumed to
have high similarity to the material’s features we introduce
because the features learned from each pure and scaled spectra
are diagnostic and preserved across many levels of concentra-
tion of the material. Based on similarity scores between these
binary arrays, we can determine the existence of each material
in the observed mixture sample.

To begin, we apply the NHMC model to the observed
spectra and obtain their binary label matrix representations
\( \{X_n\}_{n=1}^N \). Next, for each material, similarity scores
between the observed spectra and that material’s features are
computed by taking the matrix inner product between them (cf.
Fig. 1(B)(b)): \( \sigma^j_n(X_n) = \langle F_j^j, X_n \rangle \). We collect the similarity
scores for a label matrix \( X_n \) with the \( j^{th} \) endmember as a vector
\( y_n = [\sigma^j_n(X_n), \ldots, \sigma^j_{N}(X_n)] \).

The process described in this section may be considered
altogether as a mapping of the observed spectra into \( J \) feature
spaces, each of dimension \( F_j \), that measure similarity with
the \( J \) given endmembers. In these mapped spaces, we apply
\( k \)-means clustering with \( k = 2 \) clusters in order to separate
observed mixtures involving the endmember from those that
do not. After the two clusters are obtained, the cluster whose
centroid has larger norm has its samples labeled as “material
present”, while the samples of the other cluster are labeled
“material absent”.

III. EXPERIMENTS

To evaluate the performance of our algorithm, we generate
several synthetic spectral mixtures according to a simple ver-
sion of the Hapke model called the isotropic multiple scattering
approximation (IMSA) [6] and we attempt at detecting the end-
member using a library of pure mineral spectra. We compare the
performance of our algorithm with that of the SUnSAL
algorithm [12] applied to the same dataset. We have identified
SUnSAL as a direct competitor due to its use of a dictionary
of spectra for unmixing and to the fact that, although it uses
a linear mixing model, it is robust to small nonlinearities [3].
Data clouds generated by the IMSA model have been shown to
exhibit only very moderate nonlinearities [13].

A. Performance Metrics

To evaluate the performance of the unmixing algorithms,
we use two different measures: recall and false alarm rate
(FAR), defined as \( R = \frac{TP}{TP + FP} \), \( FA = \frac{FP}{TP + TN} \) where \( TP \)
and \( FP \) are the number of true and false positives, respectively,
and \( TN \) and \( FN \) are the number of true and false negatives,
respectively. These metrics are computed for the detectors of
materials present in the scene and their average is used as a
performance metric for the different unmixing schemes in our
experiments.

B. Nonlinear Mixtures with Hapke Model

Our experiment considers a synthetic dataset created by
Hapke mixtures model [6]. We extracted 599 spectral sig-
natures with 24 classes in total from the RELAB spectral
database\(^1\). We model our experiments under the assumption
that we have some discrepancy between endmembers in the
observations and in the library; usually, it is seldom the case
to observe the same instance of a spectrum for a material in the
endmember library and in the scene. Under such assumption,
we divide the available data into two sets (endmember and
scene) so that elements in the endmember library and the
observations for each mineral class are maximally different.
For this purpose, we apply \( k \)-means clustering with \( k = 2 \)
using cosine distance to each mineral class to maximize the
discrepancy. The resulting endmember set used for training has
357 samples, while the test set used for constructing mixtures
has 242 samples.

Once the test set is obtained, we construct three differ-
ent subsets by it containing three endmembers each, and
generate 2000 mixtures from each subset according to IMSA
model; we thus obtain 6000 synthetic IMSA mixtures without
any noise. To mimic the variability of endmembers in the
same mineral class, we constructed different endmembers by
IMSA mixtures of the samples in the same mineral classes
instead of selecting the endmembers from the library directly.
The abundances in each mixture are generated according to
a symmetric Dirichlet distribution of order \( K = 3 \) with
concentration parameter \( \alpha = 1 \). All the RELAB spectra in this
experiment were acquired incident \( i \) and emission \( e \) angles of
30° and 0° respectively. We set the same values for \( i \) and \( e \)
of the IMSA mixtures.

We apply the proposed NHMC-based endmember detection
method and the SUnSAL algorithm to each synthetic mixture.
We assume the exact mineral classes are obtained by an oracle
dictionary unmixing method before applying either unmixing
method.

In a first experiment, we investigate the performance of our
proposed method and SUnSAL and search for the best
parameter values over fixed ranges. For our method, \( \tau \) and \( \tau_R \)
are searched in \([0.1 : 0.1 : 1.0]\). Additionally, we set \( \rho_d = 4 \)
and \( \rho_w = 5 \). The SUnSAL trade-off parameter \( \lambda \), which
controls the sparsity of the result, is searched in the exponential
range \([0.5 : 1 : 2]\). Figures 2 and 3 show the performance for the
two unmixing approaches. Figure 2 demonstrates the
performance curve of SUnSAL as \( \lambda \) varies. Broadly, it can be
seen that \( R \) decreases and \( FA \) increases as \( \lambda \) increases, and
vice versa. When we define the optimal point as the closest
point to the upper left corner of the figure, the optimal value
obtained by SUnSAL is \( R = 0.80 \) and \( FA = 0.23 \), at \( \lambda = 0.1 \).
Similarly, Figure 3 presents the performance curves of the
proposed method for different values of \( \tau_R \), with \( \tau \) fixed for
each curve. The defined optimal point obtained by our method
is \( R = 0.83 \) and \( FA = 0.20 \) at \( \tau = 0.7 \) and \( \tau_R = 0.7 \), which
shows a slight improvement over that obtained from SUnSAL.

An important observation is that the proposed binary rep-
dresentation is robust with respect to the spectral variability
present in each mineral class. We calculate the separation
between the training and test subset clusters for all the mineral
classes in the original space and in the space of the NHMC

\(^1\)RELAB Spectral Database: Copyright 2008, Brown University, Provi-
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the physical characteristics of each material. Fig. 4 shows diagnostic features of alunite and olivine detected by our method that persist through the mixing process. Our method seems to succinctly detect discontinuities and slopes of each mineral. More specifically, it detects the same diagnostic features of alunite around 2.2 – 2.4µm regions as the ones defined by geologists in the Tetracorder.

V. CONCLUSION

We demonstrate a new spectral unmixing method using a new semantic representation. The simulation in which we mimic the real condition shows that our method yields slightly better detection performance compared to a state-of-the-art method. This fact indicates that the underlying model has a possibility to successfully determine discriminative features of the spectra and we could use them for unmixing problems. Further investigation is needed to improve the performance.

REFERENCES


