Unmixing urban hyperspectral imagery with a Gaussian mixture model on endmember variability

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Abstract—Spectral unmixing given a library of endmember spectra can be achieved by multiple endmember spectral mixture analysis (MESMA), which tries to find the optimal combination of endmember spectra for each pixel by iteratively examining each endmember combination. However, as library size grows, computational complexity increases which often necessitates a laborious and heuristic library reduction method. In this paper, we model a pixel as a linear combination of endmembers sampled from probability distributions of Gaussian mixture models (GMM). The parameters of the GMM distributions are estimated using spectral libraries. Abundances are estimated based on the distribution parameters. The advantage of this algorithm is that the model size grows very slowly as a function of the library size.

To validate this method, we used data collected by the AVIRIS sensor over the Santa Barbara region: two 16 m spatial resolution and two 4 m spatial resolution images. 64 validated regions of interest (ROI) (180 m by 180 m) were used to assess estimate accuracy. Ground truth was obtained using 1 m images leading to the following 6 classes: turfgrass, non-photosynthetic vegetation (NPV), paved, roof, soil, and tree. Spectral libraries were built by manually identifying and extracting pure spectra from both resolution images, resulting in 3,287 spectra at 16 m and 15,426 spectra at 4 m. We then unmixed ROIs of each resolution using the following unmixing algorithms: the set-based algorithms MESMA and AAM, and the distribution-based algorithms GMM, NCM, and BCM. The original libraries were used for the distribution-based algorithms whereas set-based methods required a sophisticated reduction method, resulting in reduced libraries of 61 spectra at 16 m and 95 spectra at 4 m. The results show that GMM performs best among the distribution-based methods, producing comparable accuracy to MESMA, and may be more robust across datasets.

Index Terms—spectral unmixing, endmember variability, Gaussian mixture model, MESMA, hyperspectral image analysis

I. INTRODUCTION

HYPERSPECTRAL images have important applications in astronomy, agriculture, geoscience, surveillance (such as object identification), material identification, and detecting processes [1]. Because limited photons enter the sensor when collecting narrow bandwidth channels from a high altitude, the spatial resolution of hyperspectral image is usually very coarse, i.e. a pixel may correspond to a region with a diameter of several meters. Hence, multiple materials may exist in this region and contribute to the measured pixel spectrum, also known as a mixed pixel [2]. One important problem in hyperspectral imagery is to decompose mixed pixels to identify the constituting materials (endmember) and their proportions (abundance) that form the pixel spectrum.

The most common model that relates endmembers and abundances to a pixel is the linear mixing model (LMM), which assumes that the reflectance measured within each pixel is a unique linear combination of the reflectances of each sub-pixel endmember, weighted by its abundance, plus some noise [3]. The intuition behind this model is that the fractional area of a material determines its representation in the measured signal. However, when unmixing a hyperspectral image with LMM, we usually encounter an additional problem that spectral reflectance for identical materials are often different. For example, asphalt spectra can vary significantly based on age, shadowing, and composite materials [4]. This is sometimes called endmember variability [5], [6].

Several factors can contribute to endmember variability, including both extrinsic factors and intrinsic factors. The most significant extrinsic factor is illumination. When solar incidence and emergence angles are different for a surface, the observed signal will be different [7]. Material angle matters as well, for example roofs can be present at a variety of angles relative to incoming solar radiation, producing different spectral signatures for one material. Atmospheric condition can be another extrinsic factor affecting reflectance, however this is usually corrected during image processing. Measurement scale represents an important intrinsic factor. Objects or materials that may be considered “pure” may in reality be composed of materials at smaller scales with varying reflectances [8]. For example, a tree canopy can be considered a single, pure endmember, however this ignores the spectral variety of tree leaves, bark, branches, and substrate that composes a single tree pixel [9]. Similarly, soils are composed of particles with different shapes, sizes, and chemical composition [6]. The larger scale we use to define an endmember, the larger intrinsic variability we may expect from its spectra. For example, trees and turfgrass can be defined as individual endmembers, however if we we wish to define a class of green vegetation comprised of both turfgrass and tree, its variability will not be less than the component endmember.

Considering endmember variability, we can generalize the LMM to the following equation:

\[
\begin{align*}
\text{Pixel} &= \sum_{i} \text{Endmember}_i \times \text{Abundance}_i + \text{Noise}
\end{align*}
\]
where $y_n \in \mathbb{R}^B$ is the spectrum of the $n$th pixel in the image, $B$ is the number of bands, $N$ is the number of pixels, $M$ is the number of endmembers, $m_{nj} \in \mathbb{R}^B$ is the $j$th endmember for the $n$th pixel, $\alpha_{nj} \in \mathbb{R}$ is the abundance that usually satisfies the positivity and sum-to-one constraints, i.e., $\alpha_{nj} \geq 0$, $\sum_j \alpha_{nj} = 1$. Finally, we have some additive noise $n_n$.

When it comes to unmixing in terms of $\{y\}$, we are referring to retrieving $\{m_{nj}, \alpha_{nj}\}$ from $\{y\}$, or $\{\alpha_{nj}\}$ from $\{y\}$ and a library of endmember spectra. The former is sometimes called unsupervised unmixing, and because it is undetermined this can be a difficult problem. Studies that have worked to solve unsupervised unmixing usually require several assumptions, such as spatial smoothness of the abundances and the existence of contiguous pure pixels [10], [11], [12]. The latter is called supervised unmixing and depends on a library of known endmember spectra. If the library is small enough to easily enumerate all possible spectral combinations, the task can be trivial. However, applying this scheme on larger libraries becomes computationally inefficient. This is the problem we are addressing in this study.

Previous studies that have worked to solve this problem have used methods that can be categorized as set-based or distribution-based [5]. Set-based methods treat the endmember library as an unordered set and try to pick the best combination of endmembers to model each pixel. A widely used set-based method is multiple endmember spectral mixture analysis (MESMA) [13]. The general idea of MESMA is to test every endmember combination and select the one with the smallest error within set thresholds that limit pixel complexity. There are many variations to MESMA. In multiple-endmember linear spectral unmixing model (MELSUM), the solution for abundances is obtained from directly solving the linear equations and discarding the negative values [14]. In automatic Monte Carlo unmixing (AutoMCU), pixels are unmixed using multiple sets of random combinations, with the mean fractional values assigned as abundances [15], [16]. In alternate angle minimization (AAM), projection is iteratively used to find the spectrum index of one endmember given the other endmembers fixed. Besides MESMA variants, there is sparse unmixing that used the full spectral library with a sparsity constraint on the abundances forcing them having only a few nonzero elements [17].

Contrary to set-based methods, distribution-based methods assume that the endmembers for each pixel are sampled from probability distributions, hence the linear combinations of these endmembers (pixels) also follow some distribution. It works by modeling the spectral library as statistical distributions, extracting parameters to describe these distributions, and unmixing the pixels based on the distribution parameters. The most widely used distribution is Gaussian, and its application for spectral unmixing is known as the normal compositional model (NCM) [18], [19], [10], [20], [21], [22]. The popularity of NCM comes from the fact that a linear combination of Gaussian random variables is also a Gaussian random variable whose mean and covariance matrix are linear combinations from the endmember means and covariance matrices. Hence, the resulting probability density function of the pixels has a simple analytical form. Fitting the actual pixel values to the pixel distribution, the abundances can be solved by several techniques, such as expectation maximization [20], sampling methods [18], [19], [10], and particle swarm optimization [22].

Following this philosophy, some have worked to extend the idea to distributions beyond Gaussian. In [23], the authors propose Beta distributions to model the spectral library. The benefit is that Beta distributions have a domain in the range 0 – 1, so are more suitable for the reflectance range, and the actual library may have a skewed mode in the distribution. In [24], the idea is further extended to use Gaussian mixture models (GMM) for distributions. The rationale comes from the observation that library endmembers may have multiple modes, whose shape cannot be represented by a simple Gaussian or Beta distribution. Since GMM is more flexible, it can approximate any distribution found in the library.

A. Our contribution

Many unmixing studies are not well evaluated in presence of ground truth. Commonly used hyperspectral datasets include Pavia University, Indian Pines, Cuprite, Mississippi Gulfport, etc., which are not validated with ground truth endmembers and abundances. Hence, the primary method for evaluating their results include:

1) Compare the estimated endmembers with spectra in the USGS spectra library (e.g. in Cuprite dataset) [25], [26].
2) Compare the estimated abundances with assumed segmentation maps of pure materials (e.g. in Indian Pines, Pavia University, Gulfport datasets) [21], [27].
3) Calculate the reconstruction error of estimated endmembers and abundances and assume that a lower reconstruction error implies a better result [10], [11].

Each of these methods can be problematic. First, different conditions (sensor, atmosphere, light source) during data collection will affect measured reflectances, making library comparison less ideal. Second, high spatial resolution hyperspectral images are primarily composed of pure pixels, and segmentation like abundance maps do not necessarily indicate good unmixing capability for mixed pixels. Third, reconstruction error is more related to model complexity than unmixing accuracy since small reconstruction error could be achieved by overfitting [28].

Moreover, these datasets are not comprehensive with respect to spatial scales, scene diversity and generalization. For example, the Pavia University and Gulfport datasets have about 1 m spatial resolution in which most are pure pixels. Also, they are focused on only a few urban sites, which contain mostly man-made materials with segmentation like abundance distribution. Developing unmixing algorithms on them will have a bias on forcing smooth and sparse abundance maps. Hence, it is unknown if the algorithms validated on these datasets can be applied to datasets with generalized scenarios.
In this work, we introduce a supervised unmixing algorithm based on modeling endmember variability by GMM distributions, and compare several set-based and distribution-based algorithms with a highly validated, comprehensive dataset of 128 images with different spatial scales. The algorithm was first introduced in [12], [23] and we modified it for this application. The dataset was developed in [29] but only used for evaluating MESMA. It contains two types of images, one with about 16 m pixel size, the other with about 4 m pixel size. It covers a wide range of landcover, including various kinds of road, roof, vegetation, and soil. Validation abundances were obtained by classifying high resolution images corresponding to the hyperspectral images. Unlike MESMA, which requires a small and well-curated spectral library, the GMM algorithm uses the original source library without modification to unmix fractions using inferred parameters from the library.

II. DATASET

We used two low-resolution images (16 m) and two high-resolution images (4 m) in this study. The low-resolution images were collected by the Airborne Visible/Infrared Imaging Spectrometer (AVIRIS) [1] over Santa Barbara, CA, on August 29, 2014. The spatial resolutions are 15.6 m/pixel and 15.8 m/pixel. The spectral range measures wavelengths from 380 – 2500 nm with 224 bands of approximately 10 nm bandwidth. High-resolution images were collected by AVIRIS-Next Generation with 3.9 m/pixel and 3.6 m/pixel spatial resolutions. The spectral resolution is also higher, recording 432 bands of about 5 - 6 nm bandwidth across a similar spectral range as the 16 m dataset. We spectrally resampled the AVIRIS-Next Generation imagery to 224 bands to produce an image with identical spectral parameters to the 16 m AVIRIS image. We also removed certain bands from analysis due to atmospheric interference, reducing the number of bands to 164. Initial image processing was conducted by the Jet Propulsion Laboratory, with additional processing in the lab to reduce the effects of elevation change on pixel location.

The study area includes the cities of Santa Barbara and Goleta as well as the land between them, near the California coast. Urban composition is typical of the southwestern United States, including man-made materials such as asphalt, concrete, metal, gravel, and brick, as well as vegetation in the forms of turfgrass, various tree species, and large areas of undeveloped land covered in senesced vegetation [30].

A. Validation Polygons

We produced 64 polygons that represented the variety of landcover within the study area. Each polygon was 180 m by 180 m in size, or 11-12 pixels wide in the 16 m images (46 or 50 pixels wide in the 4 m images). Validation polygons were randomly distributed across the area with a minimum distance 400 m. If a polygon contained large areas of open water or an undetermined material, it was discarded and a new polygon randomly generated. Cover was determined within each polygon using a 1 m NAIP high-resolution image. We used a combination of image segmentation, using ECognition, and manual adjustments to classify the cover within each polygon as turf, tree, paved, roof, soil, or non-photosynthetic vegetation (NPV). Cover was further confirmed by visually inspecting August 2014 Google Earth imagery. Fig 1 displays all polygons as they appear in the 16 m images.

Fig. 2 shows a scatter plot of the 64 ground truth abundances when the 6 endmember classes are merged to 3 categories of vegetation, impervious, and non-vegetated pervious. Most polygons are dominated by a mixture of impervious and vegetation materials. To improve the representation of less common mixtures in the scene, we added 5 polygons with high proportions of soil.

B. Library Building

We produced 240 polygons across the 4 m scene to extract pure spectra and build the full spectral libraries. The polygons were intended to capture class material variability as much as possible, and so included multiple roof types, asphalt, concrete, trees, turfgrass, soil, and NPV, as well as less common materials like rubber, solar panels, tennis courts, and plastic tarps. These materials were then grouped into one of our 6 endmember classes: turfgrass, NPV, paved, roof, soil, and tree.

The same polygons were used to extract spectra from the 16 m imagery, with necessary modifications as described in [29]. Together, we produced a library of 16 m spectra and a library of 4 m spectra. After removing duplicate spectra, the final 16 m library was comprised of 3,287 spectra and the 4 m library contained 15,426 spectra.

These full spectral libraries were used to train the parameters of distribution-based algorithms. However, they were too large to be used by MESMA, and required reduction. We performed reduction in two steps. First, iterative endmember selection (IES) [31] was used to automatically select a subset of spectra that represented the larger library. This is achieved iteratively, by gradually selecting the most representative spectra and evaluating their representativeness using a kappa coefficient. IES reduced the 16 m and 4 m library sizes to 226 and 187, respectively. Libraries were further reduced using iterative classification reduction (ICR), which uses MESMA as a classifier to quickly identify and remove spectra that tend to map materials incorrectly [29]. This reduced the libraries to a final size of 61 for 16 m images and 95 for 4 m images. The spectra for each endmember class for all the cases are plotted in Fig 3 and their numbers are shown in Table I.

| Endmember | 16 m | 4 m |
|-----------|------|-----|
| Turfgrass | 557  | 10  |
| NPV       | 884  | 14  |
| Paved     | 299  | 6   |
| Roof      | 435  | 17  |
| Soil      | 262  | 3   |
| Tree      | 870  | 11  |
| Total     | 3287 | 61  |

Table I: Number of Spectra for Each Endmember Class in the Libraries
Figure 1. Validation polygons on the site (a) and all 4 m ROI images (b). The two 16 m images are mosaicicked by geographic coordinates.

Figure 2. Scatter plot of ground truth total abundances in terms of 3 categories, green vegetation (turfgrass and tree), pervious (NPV and soil), and impervious (paved and roof). Most of them lie on the plane, which corresponds with the selection of ROIs where almost all the pixels fall into the 6 endmember classes.

III. METHOD

A. The Gaussian Mixture Model for Unmixing

Here we briefly introduce the GMM based unmixing [12], which is a generative model that models a distribution on the input space [32]. Suppose we have $M$ endmember classes, each has numerous spectra in the library. A pixel can be assumed to be generated by randomly picking one spectrum for each endmember, and linearly mixing them based on some abundances. In this way, if we use a probability density function to represent the spectral distribution, the actual endmembers can be assumed to be sampled from this distribution. Suppose the $j$th endmember for the $n$th pixel is sampled from a distribution modeled by GMM

$$p(\mathbf{m}_{nj} | \Theta) = \sum_{k=1}^{K_j} \pi_{jk} \mathcal{N}(\mathbf{m}_{nj} | \mu_{jk}, \Sigma_{jk}),$$

where $\Theta := \{\pi_{jk}, \mu_{jk}, \Sigma_{jk} : j = 1, \ldots, M, k = 1, \ldots, K_j\}$ are the GMM parameters. Allowing GMM to represent the library, we can get multiple Gaussian components for each endmember. Take the dataset in Section II as an example, which can be viewed from two perspectives. Fig. 4 shows the pixels from all the validation ROIs, library endmembers, and corresponding Gaussian components when projected to 2 dimensions. The method for estimating GMM parameters will be discussed later, however we can see that the ellipses formed by these parameters surround validation pixels at multiple positions on the edge of the pixel cloud. The pixels can be viewed as picking points within ellipses and combining these points linearly. Fig. 5 shows the Gaussian components from
Figure 3. Original and reduced spectral libraries. The numbers of spectra in each category are shown in Table I.

the wavelength-reflectance perspective, where the centers of Gaussian components and their variation patterns are shown as curves. Compared to MESMA, which evaluates every spectrum in the library, GMM tries to combine every center of Gaussian components, but allows the center to move according to its corresponding variation pattern.

Following the distribution assumption, if \( \{m_{nj} : j = 1, \ldots, M\} \) are independent and the noise is also sampled from a Gaussian \( p(n_n) = N(n_n|0, D) \), then \( y_n = \sum_j m_{nj} \alpha_{nj} + n_n \) implies that the pixel follows a distribution

\[
p(y_n|\alpha_n, \Theta, D) = \sum_{k \in K} \pi_k N(y_n|\mu_{nk}, \Sigma_{nk}),
\]

where \( K := \{1, \ldots, K_1\} \times \{1, \ldots, K_2\} \times \cdots \times \{1, \ldots, K_M\} \) is the Cartesian product of the M index sets, \( k = (k_1, \ldots, k_M) \in K, \pi_k \in \mathbb{R}, \mu_{nk} \in \mathbb{R}^B, \Sigma_{nk} \in \mathbb{R}^{B \times B} \) are defined by

\[
\pi_k = \prod_{j=1}^M \pi_{jk_j}, \quad \mu_{nk} = \sum_{j=1}^M \alpha_{nj} \mu_{jk_j}, \quad \Sigma_{nk} = \sum_{j=1}^M \alpha_{nj}^2 \Sigma_{jk_j} + D.
\]

If we assume each pixel is independently sampled, the probability density function of all the pixels is the product as

\[
p(Y|A, \Theta, D) = \prod_{n=1}^N p(y_n|\alpha_n, \Theta, D),
\]

where \( A := [\alpha_1, \ldots, \alpha_N]^T \in \mathbb{R}^{N \times M} \). Given \( Y, \Theta, D \), the abundances \( A \) can be estimated by maximum likelihood estimation (MLE). Specifically, we want to maximize \( p(Y|A, \Theta, D) \), or minimize \( -\log p(Y|A, \Theta, D) \), which becomes the following optimization problem by combining the above equations

\[
\mathcal{E}(A) = -\sum_{n=1}^N \log \sum_{k \in K} \pi_k N(y_n|\mu_{nk}, \Sigma_{nk}),
\]

s.t. \( \alpha_{nj} \geq 0, \sum_{j=1}^M \alpha_{nj} = 1, \forall n \).

The objective function can be minimized by a generalized expectation maximization (EM) algorithm, which alternates
Figure 4. Scatter plot of GMM components on the pixels and library spectra. The projection is determined by performing PCA on all the spectra in the library. The pixels of 64 images for each scale are combined and denoted by gray dots. The colored dots show the spectra in the library for each endmember class. The ellipses denote the Gaussian components.

Figure 5. Wavelength-reflectance plot of GMM components on the library spectra. The spectra are put into 2-dimensional bins of wavelength-reflectance to form a histogram shown as gray scale background images. The center of each Gaussian component is shown as solid curve. The center plus (minus) twice the square root of the largest eigenvalue with its corresponding eigenvector is shown as a dashed curve, which indicates the major variation pattern of a Gaussian component. The prior probabilities are shown in the legends.
between an E step and an M step [33]. The E step calculates the posterior probability of the latent variable given the observed data and old parameters. The M step increases the expected value of the complete data log-likelihood. In our case, the E step calculates
\[ \gamma_{nk} = \frac{\pi_k \mathcal{N}(y_n | \mu_{nk}, \Sigma_{nk})}{\sum_{k \in K} \pi_k \mathcal{N}(y_n | \mu_{nk}, \Sigma_{nk})} \] (2)
The M step tries to minimize
\[ \mathcal{E}_M = -\sum_{n=1}^{N} \sum_{k \in K} \gamma_{nk} \left\{ \log \pi_k + \log \mathcal{N}(y_n | \mu_{nk}, \Sigma_{nk}) \right\} \]
It does not have a closed form solution for \( \pi_k \). But we can use gradient descent to minimize \( \mathcal{E}_M \), where the derivative can be calculated by
\[ \frac{\partial \mathcal{E}_M}{\partial \pi_k} = -\sum_{k \in K} \Lambda_k \mathbf{R}_k^T - 2 \mathbf{A} \circ \sum_{k \in K} \Psi_k \mathbf{S}_k^T \] (3)
where \( \mathbf{R}_k \in \mathbb{R}^{M \times B}, \mathbf{S}_k \in \mathbb{R}^{M \times B^2} \) are defined by
\[ \mathbf{R}_k = [\mu_{1k}, \mu_{2k}, \ldots, \mu_{MK}]^T, \]
\[ \mathbf{S}_k = [\mathrm{vec}(\Sigma_{1k}), \mathrm{vec}(\Sigma_{2k}), \ldots, \mathrm{vec}(\Sigma_{MK})]^T, \]
and \( \Lambda_k \in \mathbb{R}^{N \times B}, \Psi_k \in \mathbb{R}^{N \times B^2} \) denote
\[ \Lambda_k = [\lambda_{1k}, \lambda_{2k}, \ldots, \lambda_{NK}]^T, \]
\[ \Psi_k = [\mathrm{vec}(\Psi_{1k}), \mathrm{vec}(\Psi_{2k}), \ldots, \mathrm{vec}(\Psi_{NK})]^T, \]
where \( \lambda_{nk} \in \mathbb{R}^{B \times 1} \) and \( \Psi_{nk} \in \mathbb{R}^{B \times B} \) are
\[ \lambda_{nk} = \gamma_{nk} \Sigma_{nk}^{-1} (y_n - \mu_{nk}), \]
\[ \Psi_{nk} = \frac{1}{2} \gamma_{nk} \Sigma_{nk}^{-T} (y_n - \mu_{nk}) (y_n - \mu_{nk})^T \Sigma_{nk}^{-T} \Sigma_{nk}^{-T} - \frac{1}{2} \gamma_{nk} \Sigma_{nk}^{-T} \]
Given an initial \( \pi_k \), we can update \( \gamma_{nk} \) and \( \pi_k \) alternately until convergence, which leads to a local minimum of the objective function. This algorithm requires several clarifications and we will explain them in the following subsections.

B. Determining the GMM Parameters
Suppose we have a library of endmember spectra \( \{Y_j \in \mathbb{R}^{N_j \times B} : j = 1, \ldots, M\} \), with which we can estimate the GMM parameters \( \Theta \). The difficulty comes from estimating the number of components \( K_j \) for each endmember, as once we know \( K_j \), \( \{\pi_{jk}, \mu_{jk}, \Sigma_{jk}\} \) can be estimated by the standard EM algorithm. Estimating this \( K_j \) is sometimes called model selection and has several approaches [34]. We will use cross-validation-based information criterion (CVIC) [35] as our metric to select \( K_j \).

Given a candidate \( K_j \), we can evaluate CVIC in the following way. Let \( Y^v_j \) be the spectra for the \( j \)th endmember in the library, we can divide them into \( V = 5 \) subsets with equal size. For each subset \( Y^v_j \), the remaining spectra are input to a MLE with \( K_j \) Gaussian components, and the trained parameters are used to evaluate the log-likelihood of \( Y^v_j \). Then the sum of all these log-likelihood values is calculated as \( \mathcal{L}_{K_j} \), which is our CVIC. Finally, the optimal \( K_j \) is the one that maximizes \( \mathcal{L}_{K_j} \) out of all the candidates. To avoid many components, we tried \( K_j = 1, 2, 3, 4 \).

This approach can serve as an ideal model selection. However, the number of combinations \( |K| = \prod_j K_j \) can still be very large, especially in real datasets where the libraries contain many spectra. Hence, we use a threshold \( T_{CVIC} \) to further reduce \( K_j \) manually. Let \( \mathcal{L}_j^c \) be the maximum CVIC for the \( j \)th endmember; we pick the smallest \( K_j \) such that \( \mathcal{L}_{K_j} < \mathcal{L}_j^c \). Hence when \( T_{CVIC} = 0 \), we have the ideal CVIC-based model selection. As \( T_{CVIC} \) increases, we can have a reduced number of components.

C. Projection
Analyzing the computation in Section III-A we see that the time complexity is \( O(|K| NB^3) \) [12]. In addition to the number of combinations, the number of bands is also crucial to execution time. We can reduce the time cost by reducing the dimensionality of the data.

We use PCA to reduce the dimensionality, which gives a center \( c \in \mathbb{R}^B \) and a projection matrix \( \mathbf{E} \in \mathbb{R}^{B \times d} \) such that all the spectra are processed as \( \mathbf{E}^T (y - c) \). Note that (1) still holds if both the pixel spectra and endmember spectra are projected in this way. Hence the estimated abundances for the projected spectra are the original abundances for the data. Also note that if an endmember follows a GMM distribution, the projected endmember also follows a GMM distribution. So we can directly estimate the GMM parameters from the projected library spectra.

As for the data input to find this projection, there are two possibilities. One is to use all the pixel data. This works if the image is big enough, such that all the endmembers have sufficient presence. However, if the image contains fewer pixels (e.g. in the 16 m dataset) with limited endmembers, the directions determined by PCA will present the variation within the image, which may not distinguish different endmembers. The other method is to use the spectral library, i.e. combine all the spectra in the library and perform PCA on them. We adopted this method for our dataset. Specifically, we selected an equal number of spectra for each endmember class in the library and concatenated them. This ensures that the relative sizes of endmember classes do not affect the direction, and also ensures that the mean lies in the center.

D. The Algorithm
The implementation of the algorithm is described in Algorithm [1]. In step 1, the spectra in the library are concatenated to form an input to PCA. We project the data to 10 dimensions in step 2. Step 3 is elaborated in Section III-B. Step 4 involves initialization of \( \mathbf{A} \), which utilizes the information of multiple means from the Gaussian components. To be specific, we set \( \alpha_{nk} \leftarrow (\mathbf{R}_k \mathbf{R}_k^T + c I_M)^{-1} \mathbf{R}_k \mathbf{y}_n \), project \( \alpha_{nk} \) onto the simplex space, and initialize \( \alpha_{nk} \leftarrow \alpha_{nk} \) where \( k = \text{arg min}_k \| y_n - \mathbf{R}_k \alpha_{nk} \|^2 \). Step 5 is the main body, in which the M step is the most complicated part. Because of the constraints on \( \alpha_{nk} \), we use projected gradient descent here. The projection function can be found in [36], [37]. The step size \( \tau \) can be set adaptively by using a small initial value.
Algorithm 1 Spectral unmixing with GMM

Input: $Y = \{y_1, \ldots, y_N\}^T$, $\{I_j : j = 1, \ldots, M\}$, $T_{CVIC}$.

1) Determine the projection matrix by PCA.
2) Project the pixels and the spectra in the library to a low dimensional subspace.
3) Estimate the numbers of components $\{K_1\}$ using CVIC and estimate the GMM parameters $\Theta$ using standard EM.
4) Initialize $A$ by choosing the $\alpha_{nk}$ that minimizes the reconstruction error.
5) Alternately update the E step and M step until convergence.
   - E step: update $\gamma_{nk}$ by (2).
   - M step: update $A$ by $\phi(A - \tau \frac{\partial L}{\partial A})$ where $\frac{\partial L}{\partial A}$ is defined in (3), $\tau$ is some step size, $\phi$ is the projection function to the simplex space.

Output: A.

and gradually increasing it by a multiplier of 10 as long as the objective function keeps decreasing. Since the covariance matrix from endmember variability is usually much larger than the noise covariance, the latter can be negligible in the computation and we use $D = 0.001^2 I_B$.

IV. RESULTS

A. Setup

We ran GMM on the 16 m and 4 m images after training it using the same resolution spectral libraries. Since GMM takes spectral libraries to estimate the Gaussian components, we used the same components on all 64 images. For reproducibility, we ran model selection of GMM 15 times, selected the most frequent combination, and applied it to the dataset. For comparison, we ran 2 set-based methods and 4 distribution-based methods:

1) MESMA [13]. It was implemented in IDL by the original authors and provided as an extension Viper Tool to ENVI. We used the same parameters as in [29], i.e. maximum RMSE 2.5%, threshold RMSE 0.7%, abundances constrained between 0 and 1, maximum shade threshold 80%, and a maximum of three endmembers plus shade for each pixel. Also, it will not allow multiple spectra from one endmember class in the mixture. The obtained fractions were normalized to give the final abundances.

2) Alternate angle minimization (AAM) [38]. Its code was implemented in Matlab and downloaded from Rob Heylen’s website. It tries every subset of endmembers, iteratively updates the spectrum index of each endmember such that the reconstruction error is minimized given the rest selected spectra, and hence finds the best combination and abundances. Since it uses projection to find the combination, theoretically it should work faster. It is different from MESMA in several ways. First, it may not find the global minimum because of its alternate optimization. Second, it may find a pixel mixed by many endmembers instead of maximum three. Finally, it does not include a shade endmember to adjust for brightness differences between endmember and measured spectra.

3) Gaussian mixture model (GMM). We used $T_{CVIC} = 0.05$ for the 16 m dataset, which produced 216 combinations from the library. Because the 4 m dataset was about 20 times larger, and the number of spectra in the library was 3 times larger, we used a larger $T_{CVIC} = 0.2$ (18 combinations) such that the whole process could still run in a few hours.

4) GMM-1. We set the number of combinations to be 1, i.e. one component for each endmember, which makes it to be NCM theoretically. However, it has the same implementation of GMM hence reflects the difference introduced by bringing multiple components.

5) Normal compositional model with sampling optimization (NCM Sampling). There are many variations of NCM, with different optimization approaches [18], [19], [10], [20], [21], [22]. We chose the sampling strategy in [39] which does not assume statistical independence between different bands.

6) Beta compositional model (BCM) [23]. It is available from Alina Zare’s website. Assuming the independence of bands, it uses Beta distribution to model each band and unmixes the pixels.

Excluding MESMA, which was implemented in IDL, all methods were implemented in Matlab. MESMA was run on a PC with Intel Core i7-2760QM CPU and 8 GB memory. The other methods were run on a PC with Intel Core i7-3820 CPU and 64 GB memory. For distribution-based methods, the original libraries were input to train the parameters for unmixing while set-based methods used the reduced libraries. We used two metrics to measure the differences between the estimated and ground truth fractions: mean absolute difference (MAD) and correlation coefficient ($R$). They were calculated for each endmember class based on the 64 pairs of values. To visualize the values, we used a variation of the Bland-Altman plot where the x-axis is the ground truth value and the y-axis is the estimated minus the ground truth value [40]. When comparing different algorithms for unmixing quality, we will mainly resort to MAD as correlation coefficient itself is not sufficient (slope and intercept are needed to accompany $R$).

B. Accuracy and Efficiency

16 m Case. Table II shows the MAD and correlation coefficient for the 16 m images. Original errors for 6 classes implies that GMM and AAM have the best accuracy, followed by MESMA. The difference comes from the paved, roof and tree classes, where GMM outperformed MESMA. In general, MESMA, AAM, GMM and GMM-1 had similar accuracy. Comparing all the distribution-based methods with same input, GMM has the best performance overall, with fewest errors for NPV, paved and roof.

Merged errors show that GMM and AAM retain their higher accuracy, with MESMA falling further behind due to poor impervious accuracy. Since merged errors are differences between summed up quantities of similar materials, such as paved and roof, if the errors are enlarged compared to
individual errors, it means that both of the similar materials are overestimated or underestimated, i.e. the algorithm tends for confuse even dissimilar materials, such as pervious and impervious.

Fig. 6 compares the estimated total abundances to validated abundances for each material. We can see that NCM Sampling and BCM tend to ignore paved or roof when they have presence. The difference statistics between the estimated and the ground truth are plotted in the Bland-Altman plots in Fig. 7 where the set-based methods and GMM appear to be better than the others.

4 m Case. The error statistics of 4 m data are shown in Table III. MESMA and GMM are the most accurate, with AAM is not as good as MESMA. One possible reason for the high accuracy of MESMA is that MESMA inherently takes shade into account while AAM only combines input library spectra. Hence, the slightly better performance of GMM over AAM is more significant since they both ignore shade.

Fig. 8 and Fig. 9 show the scatter plots and Bland-Altman plots for this data. Similar to the statistics in Table III, GMM has an advantage over the other distribution-based methods on paved and roof. Compared to AAM, GMM presents stable results to some extremely bad outliers for soil in AAM.

Efficiency. Since they were run on different machines with different implementation (MESMA and NCM Sampling have multiple threads), the time costs are not for comparison, but for reference. In general, all the algorithms run in a few hours. The fastest algorithm is GMM-1, which is our implemented GMM with only one combination. NCM Sampling turns out to be the slowest algorithm. It is expected since sampling algorithms are usually slower than deterministic algorithms. The times costs on the 4 m dataset are usually more than 10 times slower than those on the 16 m dataset. This is because the image size of the former is 16-19 times larger than the latter and the library size is also larger. The least gap comes from GMM because of a changed $T_{CV/IC}$ leading to a significantly less number of combinations. In [38], the authors show that with the same implementation AAM is much faster than MESMA, but here the result is converse. One reason is that the parameters of MESMA force it to pick at most 3 endmembers for a pixel instead of all the combinations. Also, multi-threading and implementation techniques impact the real world time costs significantly.

C. Extend to Semi-realistic Images

We extended the experiments to semi-realistic images to check if the algorithm implementation or library reduction was overfitted to this particular dataset. The method was to test the algorithms on another batch of synthetic images generated by the library spectra. Since all the algorithms assumed that a pixel was a linear combination of endmember spectra from the library, the creation of this synthetic dataset would use this assumption.

We created this dataset following the literature that emphasizes realistic simulation [41]. For each image in the original dataset, we randomly sampled spectra from the full library while the number of spectra for each endmember class is equal to the number in the reduced library. Then we used AAM to unmix the image with these sampled spectra. The obtained abundances were sorted to keep the largest three while the other were set to 0, and rescaled such that their summation was one. This is to conform with the assumption of MESMA. The endmembers and abundances were combined according to the LMM to generate pixels. In this way, we can have a dataset where the endmembers are randomly picked from the full library, and the spatial distribution of abundances looks similar to the original one. Fig. 10 shows all the 4 m synthetic images generated in this way. Comparing it with Fig. 1 we can see its similarity. But inherently, the synthetic images follow exactly the LMM with at most 3 endmembers for each pixel and they are randomly picked from the full library.

We ran all the algorithms on this simulated dataset. Table IV shows the unmixing results on this dataset. We can see that GMM and NCM Sampling turn out to be the best methods. The superior performance of NCM contrasts sharply to its worst result in Table III. Since we evaluate the difference between total abundances for a material, it is possible that the relatively large pixel abundance error is mitigated by averaging them. This is more possible for sampling algorithms because statistically they tend to sample values around the correct ones.

Compared to the negligible difference between GMM and set-based methods in Section IV-B, the advantage of GMM is more obvious. Since the endmembers were randomly sampled from the big library, set-based methods were less capable to unmix the pixels using a reduced library that was derived based on the another dataset. It is possible that a different reduced library based on this simulated dataset may lead to better results for set-based methods. However, that means, set-based methods may not be as robust as GMM across datasets.

V. Discussion and Conclusion

We have proposed an unmixing algorithm based on endmember variability modeled by GMM distributions. We validated the algorithm on a dataset consisting of 128 images across 2 scales, with ground truth abundances obtained by inspecting high resolution images. The results show that with large libraries, GMM achieves comparable accuracy to MESMA without the need for guided manual library reduction. We will discuss several issues regarding the dataset, algorithm and results in this Section.

The dataset was well developed with various scenes, but the ground truth has intrinsic errors coming from UTM coordinates. It happens when the universal coordinates are used in the hyperspectral images and the other high-resolution images for region correspondence. Because these airborne images are spatially calibrated from its unstable collection process, the coordinates derived from the map information may not accurately reflect the real coordinates. Therefore, the region for calculating the total abundances may have a small shift compared to the region in the hyperspectral image. This is more likely in the 16 m data, which may explain larger overall errors for all the algorithms, and could be mitigated by registering the two images to find exact correspondence in the future [43].
In applying GMM on the dataset, there are several implementation details that affected the results. First, the projection affected the results of GMM. Hence, we used a carefully determined projection in Algorithm [1]. Second, the number of combinations impacted the performance. If some training data affected the results of GMM. Hence, we used a carefully selected set of training data. Third, we didn’t use a spatial prior in BCM. We found that the prior made it work better on some images, while worse on some other images when applied to this dataset. In total, it didn’t improve the results much. This has two possible reasons: (i) the pixel size is big enough such that smoothness and sparsity are not obvious on the abundance maps; (ii) the dataset contains a variety of scenes in which some of them violate this property.

We also have some remarks on the results. For the real dataset, GMM is slightly better than MESMA for the 16 m data while slightly inferior for the 4 m data, so they are close in accuracy. However, MESMA used a library reduction
method that relied on manual guidance and user knowledge of the study area, while GMM used the original library without refinement. Hence, GMM may be more applicable to datasets without ground truth. Second, the results of MESMA were refinement. Hence, GMM may be more applicable to datasets in the study area, while GMM used the original library without standard deviation of these differences.

Figure 7. Bland-Altman plots of 64 abundance values in 16 m for ground truth and estimated. The x-axis is the ground truth. The y-axis is the difference between estimated and ground truth. The solid line in each plot is the mean of these differences while the dashed lines show the mean plus (minus) twice the standard deviation of these differences.

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Table III
COMPARISON OF ERROR AND CORRELATION COEFFICIENT FOR THE 4 M IMAGES

|                | Set-based | Distribution-based |
|----------------|-----------|--------------------|
|                | MAD / $R^2$ | MESMA | AAM | GMM | GMM-1 | NCM Sampling | BCM |
| Individual     |            |        |     |     |       |             |     |
| Turfgrass      | 0.028 / 0.740 | 0.033 / 0.712 | 0.036 / 0.811 | 0.027 / 0.811 | 0.033 / 0.754 | 0.049 / 0.710 |
| NPV            | 0.084 / 0.695 | 0.059 / 0.674 | 0.052 / 0.789 | 0.052 / 0.867 | 0.068 / 0.872 | 0.074 / 0.822 |
| Paved          | 0.034 / 0.829 | 0.070 / 0.782 | 0.082 / 0.556 | 0.075 / 0.794 | 0.070 / 0.597 | 0.030 / 0.509 |
| Soil           | 0.040 / 0.714 | 0.078 / 0.257 | 0.169 / 0.458 | 0.100 / 0.250 | 0.199 / 0.655 | 0.115 / 0.181 |
| Tree           | 0.045 / 0.794 | 0.065 / 0.793 | 0.038 / 0.904 | 0.038 / 0.839 | 0.065 / 0.667 | 0.094 / 0.759 |
| Average        | 0.046 / 0.918 | 0.065 / 0.735 | 0.086 / 0.903 | 0.063 / 0.759 | 0.098 / 0.820 | 0.086 / 0.623 |
| Merged         |            |        |     |     |       |             |     |
| Pervious       | 0.053 / 0.915 | 0.091 / 0.858 | 0.075 / 0.916 | 0.082 / 0.906 | 0.087 / 0.866 | 0.078 / 0.897 |
| Impervious     | 0.084 / 0.945 | 0.027 / 0.817 | 0.086 / 0.923 | 0.075 / 0.911 | 0.092 / 0.895 | 0.131 / 0.784 |
| Average        | 0.049 / 0.941 | 0.069 / 0.568 | 0.082 / 0.927 | 0.067 / 0.919 | 0.079 / 0.904 | 0.116 / 0.837 |

* the entries in red fonts denote the best two results in each category.

Figure 8. Scatter plots of 64 abundance values in 4 m for ground truth (x-axis) and estimated (y-axis).

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Figure 9. Bland-Altman plots of 64 abundance values in 4 m for ground truth and estimated.

Figure 10. Simulated 4 m ROI images. They are very similar to the real images in Fig. 1.
Table IV
Comparison of error and correlation coefficient for the synthetic images

| Set-based | Distribution-based |
|-----------|-------------------|
|           | MAD / R² | MESMA | AAM | GMM | GMM-1 | NCM Sampling | BCM |
| Irisgrass | 0.092 / 0.797 | 0.043 / 0.837 | 0.021 / 0.913 | 0.025 / 0.916 | 0.016 / 0.954 | 0.042 / 0.827 |
| NPV       | 0.003 / 0.948 | 0.022 / 0.940 | 0.023 / 0.962 | 0.026 / 0.956 | 0.018 / 0.978 | 0.041 / 0.848 |
| Roof      | 0.063 / 0.771 | 0.038 / 0.780 | 0.017 / 0.745 | 0.016 / 0.739 | 0.010 / 0.760 |
| Soil      | 0.038 / 0.643 | 0.040 / 0.643 | 0.040 / 0.653 | 0.022 / 0.635 | 0.019 / 0.659 |
| Tree      | 0.050 / 0.779 | 0.050 / 0.779 | 0.040 / 0.757 | 0.035 / 0.729 | 0.027 / 0.752 |
| Average   | 0.046 / 0.779 | 0.047 / 0.782 | 0.038 / 0.780 | 0.049 / 0.767 | 0.030 / 0.787 | 0.054 / 0.718 |

* The entries in red fonts denote the best two results in each category.

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