Nonlinear spectral unmixing with a linear mixture of intimate mixtures model

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Abstract—We present a new model for nonlinear spectral mixing observed in hyperspectral imagery, and demonstrate how this model can be used for unmixing and obtaining abundance maps. The model is based on the idea that a single pixel can contain several spatially segregated areas containing different mineral mixtures, and fuses Hapke's radiative transfer model for intimate mineral mixtures with the traditional linear mixing model. The resulting model allows a great flexibility for generating spectra, provides abundances in terms of total relative ground cover for each endmember, and can be reduced to several other nonlinear mixing models by an appropriate choice of the parameters. Experiments on laboratory mineral mixtures and real hyperspectral imagery show reduced reconstruction errors and more accurate abundances compared to the linear mixing model or the recently introduced multi-mixture pixel model. Moreover, the reconstruction error improvement can be used as a per-pixel measure of the size of the intimate mixing component.

Index Terms—Hyperspectral imaging, Spectral analysis

I. INTRODUCTION

Due to the low spatial resolution of hyperspectral imaging systems, the spectra observed in each pixel often contain a mixture of several distinct components. In hyperspectral image unmixing [1], one decomposes each spectrum into a combination of endmember spectra with associated abundances. The simplest model is the linear mixing model (LMM), where the observed spectrum is simply a convex linear combination of endmember spectra. While this LMM is adequate for many applications or image scenes, severe deviations from this linear behavior can be often observed. Examples of such situations are shallow water areas, multiple reflections observed in tree canopies, or intimate mineral mixtures where multiple reflections between the grains play an important role.

Many nonlinear unmixing methods have recently been introduced [2], and often show significant improvements over the LMM. In [3] and [4], one introduces nonlinearities in the LMM by inclusion of bilinear terms as extra virtual endmembers. These bilinear terms can be interpreted as secondary reflections. In [5], this bilinear model is extended to the generalized bilinear model (GBM), where a large model flexibility is introduced by giving each bilinear interaction between two endmembers its own parameter, which allows to tune or fit each interaction separately. This model is shown to yield much better reconstruction errors, and mapping the magnitude of the bilinear interactions indeed shows strong nonlinear interactions on e.g. water interfaces.

A popular model for nonlinear spectral interactions in intimate mineral mixtures is the radiative transfer model derived by Hapke [6], [7]. the Hapke model results from a semi-empirical treatment of the radiative transfer of light through mineral mixtures. For that purpose several contributions to the reflected light intensity, which correspond to different physical phenomena, are distinguished: single and multiple volume scattering, the shadow hiding opposition effect, coherent backscattering, macroscopic roughness effects, and effects of compactness. Each contribution is treated with a specific resolution scheme. In particular, provided that the intrinsic radiative properties, i.e., single scattering albedo and phase function, are known for each particle, the volume scattering term can be calculated analytically. This simplicity is achieved at the cost of the mathematical and physical rigor when solving the classical problem of the radiative transfer [8]. The version of the Hapke model that is cited and used in this paper is the restricted to the volume scattering contribution with the additional hypothesis that all phase functions are isotropic.

The Hapke model is linear in the single-scattering albedo (SSA) of the composing particles, weighted by their relative surface area, and equations are provided to convert this SSA to the reflectance values, depending on the acquisition and viewing geometry. This allows one to use linear unmixing techniques in the SSA space instead of in reflectance space, and yields very good results on laboratory spectra [9], [10], [11]. This relation between SSA and reflectance has also been exploited in [12], to create a kernelized fully-constrained least-squares unmixing algorithm incorporating this nonlinear behavior.

However, the prevalent model in hyperspectral unmixing of areal scenery is still the LMM. If the hyperspectral scene contains mineral deposits or layered vegetation structures, the Hapke model for intimate mixtures might be more appropriate. Unfortunately, choosing one over the other can have drastic effects on the results: It is observed [9], [10] that linear unmixing of intimate mixtures can yield abundance errors of more than 30%, while on the other hand, several areal scenes can be accurately unmixed by the LMM, and applying intimate mixture techniques here would lead to deviating results.

Recently, a model has been proposed that combines the
LMM with the Hapke model for intimate mixing: the multi-
mixture pixel (MMP) model [13]. In this model one proposes
to add an additional endmember to the LMM consisting of a
mineral mixture described by the Hapke model. It is shown
that this model can yield better results than the LMM in
several scenarios involving mineral mixtures. In this paper,
we extend this unmixing method to more than one mineral
mixture by considering the spectrum in each pixel as a linear
combination of intimate mineral mixtures. We show how the
resulting linear mixture of intimate mixtures (LIM) model
can be used to obtain the abundances by using constrained
optimization and sequential quadratic programming, and how
the model can be reduced to either the LMM, the Hapke
model or the MMP model by an appropriate choice of the
model parameters. These models are compared on laboratory
data sets and real hyperspectral imagery, and we show that a
large improvement can be obtained on the level of abundance
accuracies. In real mineral data sets, such as the AVIRIS
Cuprite data set, contiguous areas of differing abundances and
improved reconstruction errors can be observed, corresponding
to regions with mixed mineral deposits.

The outline of this paper is as follows: In section II we
introduce the LIM model and its physical interpretation, and
how one can use the model to obtain abundances. In section
III we present results on laboratory data sets of mixtures of
minerals, and execute the algorithm on the Cuprite data set.
Section IV contains the conclusions and future work.

II. THE LIM MODEL

A. Linear mixing

In the LMM, one assumes that the $M$ endmembers
$\{e_m\}_{m=1}^M$ are located in spatially segregated regions in the
pixel’s field of view, also referred to as a checkerboard pattern.
The observed reflectance $x$ is hence a linear combination of the
weighted reflectances of the individual endmembers $\{e_m\}_{m=1}^M$, with abundances $\{a_m\}_{m=1}^M$ that are positive and
sum to one:

$$x = \sum_{m=1}^M a_m e_m \tag{1}$$

These abundances represent the areal percentage that each
endmember represents in that pixel. In the case of intimate
mineral mixtures however, the different mineral components
are present as a compact configuration of scatterers in close
proximity, leading to complex optical interactions between
these scatterers. Because in these cases, multiple reflections
and shadowing effects play an important optical role, the LMM
can no longer be applied.

B. Hapke’s model for intimate mixing

In [6], the relation between reflectance and the physical
parameters of the different mineral components was derived.
The type of reflectance one typically uses in hyperspectral
remote sensing is the bidirectional reflectance factor, where the
reflectance of each pixel is determined in direct sunlight, and
relative with respect to a perfectly white Lambertian surface.

With the assumption that the particles scatter isotropically, that
the medium is densely packed, and that we can ignore the
opposition surge effect, the relative reflectance can be written
approximately as [6], [7]:

$$x = R(w) = \frac{w}{(1 + 2\mu\sqrt{1-w})(1 + 2\mu_0\sqrt{1-w})} \tag{2}$$

where all operations should be interpreted on a per-band
basis. Here $\mu_0$ and $\mu$ are the cosines of the angles of the
incoming and outgoing radiation with respect to the normal to
the surface, and $w$ is the wavelength-dependent SSA of the
medium, defined as the probability that a photon incoming on a
unit volume of the medium is scattered in any direction divided
by the probability that this photon interacts with the same
volume either by scattering or absorption. The SSA varies
from 0 for a totally absorbing medium to 1 for a lossless
medium. The simplicity of Hapke’s mixture model rests in
the fact that the SSA $w$ of a mixture of minerals equals the
weighted sum of the individual SSA’s $\{w_i\}_{i=1}^M$ of the particles
[7]. The weights are the relative areas of each mineral in the
mixture:

$$w = \sum_{m=1}^M a_m w_m \tag{3}$$

If the reflectance of a pure mineral is known, we can obtain
the associated SSA vector by inversion of (2):

$$\sqrt{1-w} = \frac{[(\mu_0 + \mu)^2x^2 + (1 + 4\mu_0\mu)(1 - x)]^{\frac{1}{2}} - (\mu_0 + \mu)x}{1 + 4\mu_0\mu x} \tag{4}$$

C. Combining linear and intimate mixing

The mixing equation of the MMP model [13] is given by

$$x = \sum_{m=1}^M a_m e_m + a_{m+1} R \left( \sum_{k=1}^M f_{mk} w_k \right) \tag{5}$$

with $e_k = R(w_k)$, given by (2). The physical interpretation
is to add an intricate mixture endmember to the LMM.

The LIM model extends this idea, and considers each spatial
patch to be a possible intimate mixture. The interpretation
is that the spectrum observed in a pixel can be a spatially
segregated mixture, or checkerboard pattern, of different
mineral mixtures, each with its own particular composition. If we
assume that there are $M$ pure mineral components present in
the scene, we can express this as:

$$x = \sum_{m=1}^M a_m R \left( \sum_{k=1}^M f_{mk} w_k \right) \tag{6}$$

While technically only the second sum needs to run from
1 to $M$, and the first sum represents the number of spatial
regions in the pixel, choosing the two upper summation limits
the same allows us to have the LMM, the Hapke model and
the MMP model as special cases of (6), by a correct choice of the abundances \( \{ a_m \}_{m=1}^M \) and \( \{ f_{mk} \}_{m,k=1}^M \).

The abundance coefficients still have to obey positivity and sum-to-one constraints, for the linear mixture and for each intimate mixture separately:

\[
\sum_{m=1}^M a_m = 1 \quad \forall m \in \{1, \ldots, M\} : \sum_{k=1}^M f_{mk} = 1
\]

(7)

(8)

The LIM model has a total of \( M(M+1) \) abundances: \( M \) abundances describing the relative surface areas of the mixtures, and for each of these \( M \) areas, we have \( M \) abundances describing the mixture in this area. While this is a large number of free parameters for increasing \( M \), other nonlinear models with the same amount of free parameters have been used successfully in the literature, e.g., the GBM [5]. The total areal fraction \( A_k \) of mineral \( k \) is given by

\[
A_k = \sum_{m=1}^M a_m f_{mk}
\]

(9)

This leads us to the following unmixing procedure: Suppose that the endmembers \( \{ e_m \}_{m=1}^M \) are known as reflectance vectors, e.g. as expert knowledge, or extracted from the image data by an endmember extraction algorithm such as vertex component analysis (VCA) [14], and that also the acquisition geometry is known. We want to unmix a pixel \( x \):

- Unmix \( x \) with a linear unmixing algorithm, e.g. FCLSU. These abundances are the initial guess for the set \( \{ a_m \}_{m=1}^M \).
- Convert the endmember set \( \{ e_m \}_{m=1}^M \) to a set of SSA’s \( \{ w_m \}_{m=1}^M \) with equation (4).
- Set all the \( f_{mk} = 0 \) for \( m \neq k \), and set \( f_{mk} = 1 \) for \( m = k \). Equation (6) reduces to the LMM with these initial settings.
- Use a nonlinear constrained optimization program to minimize the reconstruction error \( \| y - x \|_2 \), with \( y \) the spectrum modeled by (6). The positivity and sum-to-one constraints have to be included in the optimizer.
- If after optimization, the resulting error is larger than what we started the optimization with, the optimizer failed to find a better solution, and we replace the found solution by the linear unmixing result found in the first step.
- The final total abundances of each mineral in the spectrum are given by (9).

In practice, we used the FMINCON function of Matlab as optimizer, which allows the inclusion of the positivity and sum-to-one constraints (7) and (8) via matrix identities, and can optimize any target function with respect to a set of parameters. Internally, the optimizer uses sequential quadratic programming, and the convergence can be sped up by providing the Jacobian of the reconstruction error \( \| y - x \|_2 \) with respect to the optimization variables \( \{ a_m \}_{m=1}^M \) and \( \{ f_{mk} \}_{m,k=1}^M \).

### III. Results

#### A. Laboratory mixtures

We have used the LIM model to unmix spectra of mixtures of minerals, obtained in a laboratory setup. The spectra used are mixtures of quartz and alunite from the RELAB spectral database [15]. These minerals are composed of particles that have approximately the same size, shape and density, and hence the weight and surface fractions can be considered equivalent. We created two data sets from these mixtures: one data set simply contained the intimate mixtures themselves, and a second data set was created by linearly mixing two intimate mixture spectra with known abundances. We unmixed these spectra with the LIM model, the LMM model by employing FCLSU, the Hapke model by linearly unmixing the SSA’s, and the MMP model. The spectra of the pure minerals were available in the database as well, and are used as endmembers. The angle of incidence was 30° from the normal, and the observation angle is 0°.

Two typical unmixing results are shown in Fig. 1. It is clear that the LIM, MMP and Hapke model obtain very similar reconstructions for intimate mixtures, but that the LIM and MMP models obtain better fits than the LMM or the Hapke model for the linear mix of intimate mixtures. Both the LIM and the MMP models show similar behavior in both cases.

In Table I, we have listed the abundances obtained by the LIM model for the pure intrinsic mineral mixtures. Several conclusions can be drawn: For the 100/0 and the 0/100 mixtures, only a single areal component is found, indicated by either \( a_1 = 1 \) or \( a_2 = 1 \). The corresponding nonlinear abundances indicate pure mineral components as well. In the case of the 50/50 mixture, also a single areal component is found, containing an intrinsic mixture with the correct proportions. This explains the similar results obtained by the LIM and the MMP model for these spectra, since both models can be reduced to pure linear of Hapke mixtures. For the 25/75 and 75/25 mixtures however, the best model fit is obtained by combining two different mineral mixtures. The resulting total abundances show a larger deviation from the true solution here.

**TABLE I:** The different percentual mixtures of quartz/alunite by weight fraction (qua/alu), the linear abundances indicating the sizes of the areal mixtures \( \{ a_m \}_{m=1}^2 \), the corresponding intimate mixture components \( \{ f_{mk} \}_{m,k=1}^2 \), and the resulting total areal abundance \( \{ A_m \}_{m=1}^2 \).

<table>
<thead>
<tr>
<th>qua/alu</th>
<th>( a_1 )</th>
<th>( f_{11} )</th>
<th>( f_{12} )</th>
<th>( a_2 )</th>
<th>( f_{21} )</th>
<th>( f_{22} )</th>
<th>( A_1 )</th>
<th>( A_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>100/0</td>
<td>1.00</td>
<td>1.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>0.00</td>
</tr>
<tr>
<td>75/25</td>
<td>0.20</td>
<td>0.99</td>
<td>0.01</td>
<td>0.80</td>
<td>0.48</td>
<td>0.52</td>
<td>0.58</td>
<td>0.42</td>
</tr>
<tr>
<td>50/50</td>
<td>0.00</td>
<td>0.98</td>
<td>0.02</td>
<td>1.00</td>
<td>0.51</td>
<td>0.49</td>
<td>0.51</td>
<td>0.49</td>
</tr>
<tr>
<td>25/75</td>
<td>0.12</td>
<td>0.91</td>
<td>0.09</td>
<td>0.88</td>
<td>0.00</td>
<td>1.00</td>
<td>0.11</td>
<td>0.89</td>
</tr>
<tr>
<td>0/100</td>
<td>0.00</td>
<td>1.00</td>
<td>0.00</td>
<td>1.00</td>
<td>0.00</td>
<td>1.00</td>
<td>0.00</td>
<td>1.00</td>
</tr>
</tbody>
</table>

**TABLE II:** The composition of the mixtures, and their resulting total areal fractions \( \{ B_m \}_{m=1}^2 \).

<table>
<thead>
<tr>
<th>name</th>
<th>comp1</th>
<th>%</th>
<th>comp2</th>
<th>%</th>
<th>( B_1 )</th>
<th>( B_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>mix1</td>
<td>75/25</td>
<td>50</td>
<td>25/75</td>
<td>50</td>
<td>0.3</td>
<td>0.7</td>
</tr>
<tr>
<td>mix2</td>
<td>75/25</td>
<td>10</td>
<td>25/75</td>
<td>90</td>
<td>0.75</td>
<td>0.25</td>
</tr>
<tr>
<td>mix3</td>
<td>100/0</td>
<td>50</td>
<td>50/50</td>
<td>50</td>
<td>0.75</td>
<td>0.25</td>
</tr>
<tr>
<td>mix4</td>
<td>25/75</td>
<td>25</td>
<td>100/0</td>
<td>75</td>
<td>0.81</td>
<td>0.19</td>
</tr>
</tbody>
</table>
This is known to not be fully true in these mixtures [15].

All these techniques significantly outperform the LMM. We can conclude that overall the Hapke model yields the best abundance estimations, and that the MMP and the LIM model often yield the same abundances, although the LIM model can show smaller deviations with the true solution.

We tested the different models on a 100 × 80 pixel section of the well-known AVIRIS Cuprite data set (See Fig. 2 (a)). This data set contains an area in the Cuprite mining region in Nevada, USA, and contains mostly minerals, and little artificial structures or vegetation. It can be expected that some intimate mineral mixing might be present in this data set.

First, we extracted \( M = 10 \) endmembers using the VCA algorithm. We then unmixed the data set using the LMM, Hapke, MMP and LIM models. The solar angle could be calculated from the metadata to be 10° from the normal, while we consider the camera to point straight down.

We have no ground truth available to assess this data set, so we will use the reconstruction error as a measure of performance, with the caveat that it is not guaranteed that better reconstructions also give rise to better abundance maps.

A histogram of the relative reconstruction error (RRE) is displayed in Fig. 3, relative to the errors obtained by the LMM. These histograms demonstrate that both the LIM and the MMP model will obtain reconstruction errors that are always better than those obtained with the LMM. The Hapke model has smaller reconstruction errors for some pixels, but performs worse than the LMM for most of the pixels, indicating that the Hapke model might not be ideal for unmixing the Cuprite data set. The LIM model will yield the largest reduction in

Next, we created several linear mixtures of intimate mixtures according to table II, and determined the abundances with the LIM model. These abundances are listed in table III. The final abundance of the quartz component obtained by all 4 unmixing methods is displayed in table IV. One can conclude that overall the Hapke model yields the best abundance estimations, and that the MMP and the LIM model often yield the same abundances, although the LIM model can show smaller deviations with the true solution. All these techniques significantly outperform the LMM. We must note that the conversion from areal abundances to weight abundances depends strongly on the physical properties of the particles, and we used the assumption here that the two mixture components possess identical physical parameters. This is known to not be fully true in these mixtures [15].

\[
\begin{array}{cccccc}
\text{name} & f_{11} & f_{12} & f_{21} & f_{22} & A_1 & A_2 \\
mix1 & 0.28 & 0.93 & 0.07 & 0.72 & 0.08 & 0.92 \\
mix2 & 0.16 & 0.91 & 0.09 & 0.84 & 0.00 & 1.00 \\
mix3 & 0.48 & 1.00 & 0.00 & 0.52 & 0.55 & 0.45 \\
mix4 & 0.77 & 1.00 & 0.00 & 0.23 & 0.00 & 1.00 \\
\end{array}
\]

\[
\begin{array}{cccccc}
\text{name} & \text{true} & \text{LMM} & \text{Hapke} & \text{MMP} & \text{LIM} \\
100/0 & 1.00 & 1.00 & 1.00 & 1.00 \\
75/25 & 0.75 & 0.34 & 0.72 & 0.55 & 0.58 \\
50/50 & 0.50 & 0.21 & 0.50 & 0.51 & 0.51 \\
25/75 & 0.25 & 0.08 & 0.25 & 0.11 & 0.11 \\
0/100 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
mix1 & 0.50 & 0.21 & 0.54 & 0.32 & 0.32 \\
mix2 & 0.30 & 0.10 & 0.32 & 0.15 & 0.15 \\
mix3 & 0.75 & 0.60 & 0.92 & 0.77 & 0.77 \\
mix4 & 0.81 & 0.77 & 0.97 & 0.77 & 0.77 \\
\end{array}
\]
The interpretation is that this LIM model allows for spatially
on linear combinations of intimate mixtures. The physical
however does find better solutions in most cases. The optimization strategy
obtained with mixing equation (6). The optimization strategy
improvements over the LMM in these types of data sets, by
improvements over the LMM
reconstruction error.
In Fig. 2, the relative error improvement (REI), defined as
(1–RRE), is shown for both the MMP and the LIM model. This figure indicates that the improvements over the LMM are similar for both techniques, although generally the LIM model will obtain larger improvements. We did not show the map resulting from the Hapke model since it does not show an overall improvement.
Three typical abundance maps corresponding to the alunite, beryl and opal mineral are displayed in Fig. 4. Subtle differences in these maps can be noticed in the area of improved error, while the rest of these maps are the same between the two methods. It can be concluded that the LIM model can yield improvements over the LMM in these types of data sets, by taking intimate mixing into account. Repeating this experiment with the MMP model yields similar improvements, although the abundance differences are less pronounced.
As a final comment, it must be stated that the optimization algorithm can get stuck in local minima, and hence it is not guaranteed that the found solutions are the best that can be obtained with mixing equation (6). The optimization strategy however does find better solutions in most cases.

IV. CONCLUSIONS
We have presented a new spectral mixing model, based on linear combinations of intimate mixtures. The physical interpretation is that this LIM model allows for spatially segregated regions of different intimate mineral mixtures, a situation that can be expected to exist in many real-world scenarios. The model can be reduced to the LMM, the Hapke mixture model, or the MMP model by appropriate selection of the parameters. The model parameters can be obtained with an optimization procedure, and can be converted to the traditional concept of areal abundances of each endmember. The technique is demonstrated on laboratory spectra and on the AVIRIS Cuprite image. These results demonstrate improved abundance estimation, evolution towards pure linear or Hapke mixtures in the case of pure mixtures, much better spectral fits, and lower reconstruction errors. Plotting the improvement in reconstruction error reveals maps that indicate where the addition of intimate mixing terms improves the model fit. The abundance maps also show small differences between the LMM and the LIM model. Future work concerns the development of similar models with less free parameters, development of an improved optimization strategy, experiments on the initialization of the algorithm, and benchmarking against data set where ground truth is available.

REFERENCES