NONLINEAR UNMIXING WITH A MULTILINEAR MIXING MODEL

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ABSTRACT
We introduce a new nonlinear hyperspectral mixing model which takes all orders of spectral interactions between endmembers into account. This model can be considered an extension of bilinear models to all orders, and is based on a Markov chain interpretation of the optical reflection process in a medium or scene. The resulting multilinear mixing (MLM) model is shown to be physically plausible, and an unmixing strategy based on this model is proposed. Furthermore, the model can also be used to assess the size of nonlinear effects in a hyperspectral scene.

1. INTRODUCTION
In hyperspectral unmixing applications, one typically assumes that several elementary materials, called endmembers, are present in a scene in different proportions. As the field of view of a single pixel is relatively large, spectral mixing effects will occur, and the observed reflectance is a function of the individual endmember spectra, their abundances, and possible additional parameters depending on the geometry or other physical parameters. Probably the most popular spectral mixing model is the linear mixing model (LMM), where one assumes that the observed reflectance is a convex linear combination of the endmember reflectances. The underlying reasoning is that every incoming light ray will interact with exactly one endmember, and the probability of interaction is proportional to each endmember’s abundance. This leads to the linear spectral mixing behavior with convexity constraints on the abundances: the abundance non-negativity constraint (ANC) and the abundance sum-to-one constraint (ASC) [1].

However, in several scenarios the results obtained with the LMM are not accurate, and nonlinear mixing models need to be applied [2, 3]. Two examples are scenes with significant three-dimensional structures, such as trees or buildings, where shadowing and mutual illumination start to play a large role, and intimate mineral mixtures, where a light ray will typically undergo several interactions with the individual mineral components before reaching the observer. While many approaches exist to deal with nonlinear mixing effects [2, 3], a popular class of such models are the bilinear models, where the LMM is augmented with additional bilinear interactions, representing light rays that interact with two endmembers instead of one. Typically, these models scale the bilinear interaction terms with their respective abundances, reasoning that the probability of interacting with two given endmembers should be proportional to their respective abundances. Examples are the Fan model [4], the generalized bilinear model (GBM) [5] and the polynomial post-nonlinear model (PPNM) [6, 7].

In this work, we aim to extend this type of bilinear models to an unlimited number of interactions. The resulting multilinear mixing (MLM) model has only a single additional free parameter for each pixel, and is based on clear physical assumptions about the reflection process. An unmixing methodology based on this model is presented as well, along with a technique to detect and assess the size of nonlinear effects in an image. Unmixing results are presented on the AVIRIS Cuprite data set.

2. THE MULTILINEAR MIXING MODEL
2.1. Derivation
Consider a data matrix $X = (x_1, \ldots, x_N)$ containing columnwise the $N$ data points $\{x_i\}_{i=1}^N$ in a $d$-dimensional spectral space, and $p$ endmembers listed columnwise in the endmember matrix $E = (e_1, \ldots, e_p)$. We use a ray-based approximation of light, and trace the path that a single light ray follows before reaching the observer. This path is modeled as a discrete Markov chain, subject to the following rules:

- A light ray incoming from the source will interact with at least one endmember.
- After each interaction with an endmember, the ray will have a probability $P$ of undergoing further interactions, and a probability $(1 - P)$ of escaping the scene and reaching the observer.
- The probability of interacting with endmember $e_i$ is proportional to its abundance $a_i$. 


their corresponding probability: these contributions over all possible paths, each weighted by $e_i$ in the diagram in Fig. 1, where a directed graph is used to represent the transition probabilities. The probability that a light ray will follow a sequence $(e_{i_1}, e_{i_2}, \ldots, e_{i_R})$ before reaching the observer is given by

\[
\text{Prob}(e_{i_1}, e_{i_2}, \ldots, e_{i_R}) = (1 - P)^{P-1} a_{i_1} a_{i_2} \ldots a_{i_R}
\]

The spectral contribution of such a path is $e_{i_1} \odot e_{i_2} \odot \ldots \odot e_{i_R}$, with $\odot$ the Hadamard product (component-wise vector multiplication). To obtain the total reflectance we have to sum these contributions over all possible paths, each weighted by their corresponding probability:

\[
x = \sum_{R=1}^{\infty} \left( \sum_{i_1=1}^{p} \ldots \sum_{i_R=1}^{p} \right) (1 - P)^{R-1} \sum_{k=1}^{R} (a_{i_k} e_{i_k})
\]

\[
= (1 - P) \sum_{i=1}^{p} a_i e_i + (1 - P) \sum_{i=1}^{p} \sum_{j=1}^{p} a_i a_j e_i \odot e_j + (1 - P)^2 \sum_{i=1}^{p} \sum_{j=1}^{p} \sum_{k=1}^{p} a_i a_j a_k e_i \odot e_j \odot e_k \ldots
\]

A closed-form equation can be obtained by first introducing the shorthand $y = \sum_i a_i e_i$, and employing self-identification:

\[
x = (1 - P)y + (1 - P)Py^2 + (1 - P)^2 y^3 \ldots
\]

\[
= (1 - P)y + Py \odot ((1 - P)y + P(1 - P)y^2 \ldots)
\]

\[
= (1 - P)y + Py \odot x
\]

The solution yields the mixing equation of the MLM model. We slightly abuse the notation by assuming multiplication, division and powers of vectors on a per-component basis:

\[
x = \frac{(1 - P)y}{1 - Py} = \frac{(1 - P)\sum_{i=1}^{p} a_i e_i}{1 - P\sum_{i=1}^{p} a_i e_i}
\]

We still assume the ANC and ASC on the abundances. The reflectance values allowed by (2) will always lie in the interval $[0, 1]$ for $P < 1$. Remark that we obtain the LMM for $P = 0$. There is a single parameter $P$ in addition to the set of abundances $\{a_i\}_{i=1}^{p}$, which is the probability of undergoing further interactions, and hence specifies the fraction of the nonlinear component in the model. This can be used for detecting where nonlinear effects are present in an image.

Furthermore, it must be noted that (2) is also well defined for $P < 0$, but the reasoning that led to (2) is no longer valid as such a situation would require negative probabilities. Such situations might occur in scenarios where light is received from objects outside of the IFOV of a pixel. Remark that the reflectance will still be constrained to $[0, 1]$, as the mixing equation (2) will become unity in the limit for $P \to -\infty$. An illustration of the data manifold generated by (2) is shown in Fig. 2 (left), and the values of $x$ as a function of $y$ given by (1) are shown in Fig. 2 (right). It can be seen from these figures that values of $P$ in $[0, 1]$ will cause a decrease of the reflectance with respect to the LMM, while $P < 0$ will cause an increase.

2.2. Unmixing with the MLM model

To unmix with the MLM model, we assume that the endmembers are known beforehand, or extracted from the data. The aim is to find the set of abundances $\{a_i\}_{i=1}^{p}$ and the value of $P$ that minimizes the reconstruction error with the data point $x$, according to the mixing equation (2):
argmin \{a_i\}_{i=1}^{n}, P \left\| \begin{bmatrix} x = \frac{(1 - P) \sum_{i=1}^{P} a_i e_i}{1 - P \sum_{i=1}^{P} a_i e_i} \right\| \right.

The abundances are subject to the ANC and ASC, while $P < 1$. This minimization problem can be solved by constrained minimization techniques, such as active set approaches or quadratic programming. In practice, we used sequential quadratic programming. The minimization is done with respect to the abundances and the $P$ variable, with the constraints on these variables implemented through the proper matrix identities. The function tolerance was set to $10^{-10}$, while the constraint tolerance was set to $10^{-8}$. For all the results in all experiments in this paper, the minimizer found a local minimum within the tolerance limits.

3. EXPERIMENTS

3.1. AVIRIS Cuprite image

We have unmixed the well-known AVIRIS Cuprite data set using the MLM model, and have used the several alternatives from the bilinear family for comparison. First of all, 10 endmembers were extracted by the VCA algorithm [8], and identified by locating the spectra of minimal spectral angle in the USGS spectral database. Next, the abundance maps were generated using the Fan model, the GBM, the PPNM, and the proposed MLM model.

The abundance maps for two well-known minerals are presented in Fig. 3 for all mixing models. Unfortunately, no ground truth exists for the Cuprite data set, hence we cannot perform a quantitative analysis of these abundance maps. However, it should be clear that the abundance maps obtained by the different methods show subtle differences. The MLM model abundance maps show a large overlap with the LMM maps, but also some significant differences in small areas of the image.

3.2. Nonlinearity detection

The $P$ values obtained by the MLM model have a clear physical meaning for $P \in [0, 1]$. They indicate the probability that a light ray will undergo further reflections after each interaction, and can thus be used to assess the size of the effects of nonlinearity in a pixel.

In Fig. 4, we have plotted the histograms of the $P$ values obtained in the Cuprite data set. It can be seen that $33\%$ of the pixels has $P < 0$, and that the $P$ values generally stay small. This is physically plausible, as one would not typically expect a very large fraction of light rays to undergo multiple interactions. For instance, ray tracing results present in the literature [9] show that a fraction of up to $20\%$ of light rays will undergo multiple interactions in a vegetation scenario, which would correspond with $P = 0.2$.

Fig. 4: Histogram of the values of $P$ obtained by the MLM model.

When we plot the values for $P$ as a color map, one can observe where the nonlinear effects will be the strongest. This map is displayed in Fig. 5, and shows several contiguous areas where relatively strong nonlinear effects seem to be present. These areas are also the areas where the abundance maps show the largest differences (see Fig. 3). Also the asphalt road crossing north-south, and the dirt road in the north, seem to show strong nonlinear effects.

Fig. 5: The values of $P$ for each pixel. Positive (negative) values are indicated as gray (red) values.

4. CONCLUSIONS

By using a ray-based approximation of light, and considering the reflection process as a simple Markov chain, we have derived a mixing equation which takes all possible higher-order reflections into account. This MLM model requires one additional parameter describing the probability of having further optical interactions, and can be fitted to data by using constrained minimization of the reconstruction error. Two applications based on this model are demonstrated: Nonlinearity detection, and unmixing.

Future work concerns further evaluation of the model on real hyperspectral images, artificial data, and laboratory spectra. We will perform further theoretical comparisons with more advanced models for optical interactions, such as layered models or models based on radiative transfer. Finally, to avoid reliance on inefficient off-the-shelf optimizers, a computationally efficient implementation of the unmixing proce-
procedure based on convex optimization theory will be developed.

5. REFERENCES


