Harmonic Mixture Modeling for Efficient Nonlinear Hyperspectral Unmixing

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Abstract—Higher order nonlinear material mixtures provide a good model to explain the effects of physical–chemical phenomena on hyperspectral remote sensing measurements. Therefore, inverting nonlinear effects starting from the measured spectral values is a very challenging yet fundamental task to provide a thorough and reliable characterization of the materials in a scene. In this paper, this task is achieved by inverting a new model for nonlinear hyperspectral mixtures. Specifically, we show that it is possible to effectively unmix hyperspectral data by assuming a harmonic description of the higher order nonlinear combination of the endmembers. The rationale for this model is that the harmonic analysis is able to understand and quantify effects that cannot be effectively described by classic polynomial combinations. Although the model is nonlinear, unmixing is performed by solving a linear system thanks to the recently proposed polytope decomposition (POD). Experimental results show that inverting this model leads to improved performances with respect to the state of the art in terms of endmember abundance estimation both over synthetic and real datasets.

Index Terms—Harmonic mixture model, nonlinear hyperspectral unmixing, polytope decomposition.

NOMENCLATURE

ATGP Automatic target generation procedure.
BMM Bilinear mixing model.
DEM Digital elevation model.
EEA Endmember extraction algorithm.
FCLS Fully constrained least squares.
GPMM General polynomial mixture model.
HEI Human–environment interaction.
HSU Hyperspectral unmixing.
IFOV Instantaneous field-of-view.
LMM Linear mixing model.
LQM Linear-quadratic mixture.
MFI Mineralogical fraction image.
NLMM Nonlinear mixing model.
pHMM p-harmonic mixing model.

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I. INTRODUCTION

UNMIXING can provide effective and reliable surveys of the physical elements in the IFOV of an hyperspectral sensor. Therefore, HSU plays a key-role in understanding and quantifying the HEIs occurring over a given spatio-temporal region [1], [2]. Generally speaking, HSU methods aim at separating the target pixel spectrum into a set of constituent spectral signatures (endmembers) and a set of fractional abundances. However, as the recorded scenes can be very complex both geometrically and spectrally, nonlinear interactions are crucial to assess the microscopic and/or macroscopic interactions among materials in the scene [3], [4]. Indeed, NLMMs may be helpful to describe as photonic interactions at a microscopic scale or multilayer mixtures [5], [6]. These models, however, result from theoretical analyses and aim to accurately trace the reflectance behavior when considering a scene having specific geomorphic, chemical, and physical properties. Hence, they require an almost perfect knowledge of the target and sensor geometries, which make those models quite difficult to use and exploit.

Similarly, several mixing models have been proposed in literature [3] to improve the description of the macroscopic-scale interactions among materials. Specifically, intimate mixture models have been introduced to characterize reflectance interactions occurring at microscopic scale [5]. On the other hand, macroscopic scale effects are typically faced by means of bilinear mixture models, such as those presented in [7]–[10]. Nonlinear models that aim at describing macroscopic and microscopic mixtures altogether have been proposed as well. In [11], a model that considers a linear mixture model and an additive function of the average single scattering albedo has been introduced. Further, in [12] a model that combines LMM with the Hapke model for intimate mixtures is proposed. Finally, in [6], the authors introduced a structure that aims at characterizing linear mixtures of intimate mixtures by properly combining LMM and microscopic scale mixing.

Typically, HSU algorithms that rely on the aforesaid NLMMs employ convex, piece-wise convex, or nonconvex optimization.
schemes to obtain the coefficients that drive the nonlinear mix for each pixel [3], [13]. Kernel-based methods have been used as well [14]–[17], such as SVMs [18], [19]. Further, manifold learning methods that aim at solving unsupervised nonlinear unmixing problems have been recently developed and proposed [20], [21].

Typically, these algorithms face a trade-off between computational complexity and unmixing accuracy. For this reason, LMMs and BMMs have been widely employed for their low computational complexity. However, LMMs do not consider nonlinear effects, whilst BMMs do not provide efficient reconstruction of scenes where reflectance interactions among more than two endmembers occur. Therefore, in order to provide more information on higher order nonlinearities with low computational complexity, a compact form for polynomial model that aims at representing order-$p$ macroscopic nonlinear multiple scatterings and interferences provided by $R$ endmembers over the $l$th pixel can be analytically written as follows:

$$
y_l = \sum_{r=1}^{R} a_{rl} m_r + \sum_{k=2}^{p} \left\{ \sum_{\tau_1=1}^{\tau_2=1} \sum_{j=\tau_2}^{R} \left[ \partial_{ijkl} m_i \circ \partial_{jkl} m_j \right]^k \right\} + \sum_{k=1}^{k-1} \left[ c_{ijkl} m_i \circ \zeta_{jkl} m_j \right]^k \right\} \right\} \quad (1)$$

where

- $y_l = \left[ y_{nl} \right]_{n=1, \ldots, N}$, $y_{nl} \in \mathbb{R}$ is the $N$-band spectral signature of the $l$th pixel;
- $a_{rl}$ is the contribution to the linear mixture over the $l$th pixel provided by the $r$th endmember, which is identified by the spectral signature $m_r = [m_{rn}]_{n=1, \ldots, N}$;
- $\nu_k = k - \xi_k$, $(\tau_1, \tau_2) \in \{(R-1, i+1), (R, i)\}$, $m_{ij}$ and $m_{ik}$ are the spectral signature of the $i$th and $k$th endmember, respectively.
- $c_{ijkl}$ and $\zeta_{jkl}$ quantifies the nonlinear effects provided by the $i$th endmember over the $l$th pixel within the $k$th order interactions.

Fig. 1 reports an example of a scene where higher order nonlinear combinations of the reflectances recorded by the sensor occur as a result of multiple scatterings, interactions, and interferences. It is worth to note that the interplay among elements arises also at a finer spatial resolution than the one provided by the sensor.

Note that, to achieve a thorough characterization of all the possible scatterings and interferences among the scene elements, $p$ in (1) should be set to $+\infty$. This setup would unfortunately lead to a spectral mixture modeling that is impossible to manage and invert.

In this paper, we introduce a new model for nonlinear HSU that aims at characterizing superlinear interactions and interferences. In this model, as described in the next section, the local reflectance spectrum is described by a combination of harmonics of the endmember spectra. Furthermore, we propose a method for sinusoidal HSU based on the so-called polytope decomposition [22], [23] (called siPOD) to provide with an excellent reconstruction and nonlinear HSU performance.

This paper is organized as follows. Section II describes the proposed NLMM and the siPOD method used to invert it and perform the unmixing. Section III presents a comprehensive experimental validation of the proposed approach using both simulated and real hyperspectral data. Section IV provides the reader with the final remarks and introduces some interesting future research lines.

II. METHODS

A. Background on Nonlinear HSU

As previously mentioned, several spectral mixture models have been proposed in the last decade, and Table I reports the formulation of the main HSU models. The same table delivers the proper setting of the parameters in (1), s.t. the analytical expressions of those HSU mixture models are equivalent to (1).

Among the HSU models in Table I, LMM definitely represents the scheme with the lowest computational cost. LMM is able to characterize scenes where elements in the IFOV contribute separately to the energy record delivered by the hyperspectral sensors [25]. However, if the constituent materials interact and interfere with each other, more complex models are needed.

A first way to implement the model is to use polynomial functions to model nonlinearities provided by geometrically complex scenes. Within this class of HSU methods, BMMs play an important role [7], [9]. By definition, BMMs fully express the interactions of pairs of endmembers and can thoroughly describe up to order-$2$ nonlinearities within the target spectral
strong and discontinuous fluctuations around local optima. It is worth to note that the aforementioned requirements are necessary to provide efficient and reliable characterization of the considered nonlinear mixture. Indeed, as the distribution and behavior of $f(\cdot)$ directly maps onto the coefficient search space, the trajectories of the optimization scheme must not fall into singularities induced by the nonlinear function. Therefore, the choice of $f(\cdot)$ must be carefully selected, as it can jeopardize the overall performance of the system.

According to these properties, we decided to consider $f(\cdot)$ in the GPMM as the result of a harmonic combination, i.e., $f(\cdot) = \cos(\cdot) + \sin(\cdot)$, as the sinusoidal functions are bounded, Lipschitz continuous, and order-$\infty$ differentiable. Furthermore, sine and cosine can be written as series of infinite polynomial terms as follows:

$$\sin x = \sum_{z=0}^{+\infty} \frac{(-1)^z x^{2z+1}}{(2z+1)!}$$

$$\cos x = \sum_{z=0}^{+\infty} \frac{(-1)^z x^{2z}}{(2z)!}. \tag{2}$$

Thus, trigonometric functions can be used to provide a harmonic model of the mutual effects among the spectral signatures which can be used to consider reflectance effects whose nonlinearity order is not constrained and could eventually tend up to order-$\infty$. Hence, replacing $f(\cdot)$ in the GPMM analytical expression would drive to a harmonic mixture modeling that can be effectively used to retrieve the coefficients that describe the linear and nonlinear reflectance combinations of endmember spectra. Further, given the representation in (2), sines and cosines deliver a reliable tracking of higher order nonlinear combinations as well as superlinear effects that might rise up in hyperspectral scenes, while avoiding high-computational complexity costs. Indeed, as the aforementioned harmonic function can be described as an infinite sum of polynomial terms according to (2), the resulting harmonic mixture model can be considered as an extension of pLMM when $p \uparrow +\infty$. Therefore, harmonic mix responds to the physical motivation of reliable and thorough understanding of spectrally and geometrically complex scenarios, where higher order nonlinear and superlinear combinations of endmembers may result in relevant contributions to the recorded energy at the acquiring sensors.

Thus, the proposed approach aims at providing a solid architecture for understanding and quantifying higher order nonlinear effects which might affect hyperspectral images.
Indeed, the use of harmonic functions within the GPMM representation helps in describing interactions among endmembers that may arise when in geometrically complex scenarios. Hence, the proposed harmonic mixture model can be used in order to retrieve a thorough and reliable characterization of the reflectance combinations that sum up into the target spectral signatures, carrying information about the physical–chemical composition of the considered IFOV at the same time. On the other hand, the proposed approach aims at avoiding high-computational costs, as harmonic functions summarize in a very compact form a sum of infinite polynomial terms. Therefore, the proposed HSU structure represents a valid alternative to other HSU architectures.

The following section outlines the harmonic mixing characterization and the nonlinear HSU method designed to efficiently recover the \( \hat{a} \) and \( \hat{\beta} \) distributions.

\subsection*{B. Proposed Approach}

As previously mentioned, harmonic combinations can be used to help in retrieving and characterizing nonlinear effects not modeled by pLMM. Although sine and cosine can describe polynomial combinations up to any possible order, their Taylor series shows that higher order contributions might suffer because of relevant compression. In order to counteract this effect, we use only the first \( \tilde{p} \) harmonics of the endmember signatures

\[
y_{l} = \sum_{r=1}^{\tilde{p}} \tilde{a}_{rl} (\cos m_{r} + \sin m_{r}) + \sum_{k=2}^{R} \sum_{r=1}^{\tilde{p}} \tilde{\beta}_{rk} (\cos m_{k} + \sin m_{k})
\]

(3)

where \( \cos m_{r} = [\cos m_{r}]_{n=1,...,N} \), \( \sin m_{r} = [\sin m_{r}]_{n=1,...,N} \), and \( n = 1, \ldots, N \). Moreover, \( \tilde{a} \) and \( \tilde{\beta} \) represent the coefficients that drive the linear and nonlinear contributions in the mixture, respectively. Hence, the system in (3) can be referred as a \( \tilde{p} \)-harmonic mixture model (\( \tilde{p} \)HMM).

The goal of nonlinear HSU is to evaluate each \( \hat{a} \) and \( \hat{\beta} \) terms. It can be proved that the coefficients driving the nonlinear combination in (3) can be obtained by means of a linear system involving the original hyperspectral data and the endmember spectra obtained by an EEA. Specifically, it is possible to exploit the definition of the \( \hat{a} \) and \( \hat{\beta} \) terms by taking into account a new system of linear equations properly tuned according to [22] and [23] w.r.t. the model in (3). The new method is a sinusoidal version of POD method, which is named sIPOD.

Specifically, the POD introduced in [22] and [23] relies on the overdetermination of the characterization of the parameters according to the H-representation of the polytope representing a spectral signature in the \( N \)-dimensional space. The process for efficient determination of the \( \hat{a} \) and \( \hat{\beta} \) terms relies on a linear programming scheme where the sum-to-one and non-negativity constraints apply. The POD approach relies on a system of linear equations written as follows:

\[
G \omega = b_{l}
\]

(4)

where \( \omega = [\omega_{l}^{(j)}]_{j=1,...,R} \), being \( \omega_{l}^{(j)} = [\psi_{l}^{(j)}]_{k=1,...,\tilde{p}} \), where \( \omega_{l}^{(j)} = \tilde{a}_{jl} \) when \( k = 1 \), whereas \( \omega_{l}^{(j)} = \tilde{\beta}_{jkl} \) when \( k > 1 \). \( G = [g_{l,s}] \) is a \( M \times \tilde{p}R \) matrix, where \( M = \binom{N}{2} \), \( \kappa \in \{1,...,M\} \) and \( \lambda \in \{1,...,\tilde{p}\} \).

Let us assume that \( \kappa = \rho_{t} + \eta_{t} \), where \( t \in \{1,\ldots,N-1\} \), \( \eta_{t} \in \{1,\ldots,N-t\} \), and \( \rho_{t} = \sum_{u=1}^{t-1} N-u \) if \( t > 1 \), whereas \( \rho_{t} = 0 \) if \( t = 1 \). Then, in order to invert the model in (3), each element \( g_{l,s} \) must be defined as follows:

\[
g_{l,s} = g_{l(\rho_{t}+\eta_{t}),s} = (\cos m_{s}^{\psi_{l}} + \sin m_{s}^{\psi_{l}}) + y_{l_{t},l_{t+\eta_{t}}} \cdot (\cos m_{s}^{\psi_{l_{t+\eta_{t}}}} + \sin m_{s}^{\psi_{l_{t+\eta_{t}}}})
\]

(5)

where \( \lambda = (z-1)\tilde{p} + \psi_{l_{t}} (z, \psi_{l_{t}}) \in \{1,\ldots,\tilde{p}\} \times \{1,\ldots,\tilde{p}\} \).

By this way, the nonlinear HSU based on the model in (3) results in a linear programming problem that involves the original hyperspectral data and the endmembers spectra [29], [28]. Moreover, all elements in \( \omega \) fulfill the sum-to-one and non-negativity constraints.

Once the linear and nonlinear coefficients have been extracted, in order to accurately evaluate the abundance set distribution, we propose to use an aggregate metric based on the polytope H-representation. Specifically, we consider the overall contribution of the \( r \)-th endmember to the reconstruction of the \( l \)-th pixel over the \( r \)-th band, represented by the term \( \varphi_{rl} = \sum_{k=1}^{\tilde{p}} \omega_{l}^{(k)} (\cos m_{r}^{k} + \sin m_{r}^{k})/(\cos m_{r} + \sin m_{r}) \). Furthermore, it is possible to think of \( \varphi_{rl} \) as the compression/expansion factor of the \( r \)-th endmember over the \( l \)-th direction in the \( N \)-dimensional space. As the relevance of the \( r \)-th endmember in contributing to the reconstruction of the \( l \)-th pixel increases, the amplitude of \( \varphi_{rl} \) gets larger as well.

Thus, in order to quantify the contribution of each endmember to the reconstruction of the \( l \)-th pixel, let us consider the polytope that is induced by the vertices identified by \( \varphi_{rl} \). Given our assumptions, such a polytope is a simplex [30] and we can define its volume \( V_{\varphi_{rl}} \) according to

\[
V_{\varphi} = \frac{1}{N!} \det(\Delta(\Gamma)) = \frac{1}{N!} \prod_{n=1}^{N} \Gamma_{n}
\]

(6)

because \( \Delta(\Gamma) = [\delta_{ij}^{(l)}(\Gamma)]_{(i,j)\in\{1,\ldots,N\}^{2}} \) is the diagonal matrix induced by the \( \Gamma = [\Gamma_{n}]_{n=1,...,N} \) spectral signature [30], i.e., \( \delta_{ij}^{(l)}(\Gamma) = \Gamma_{n} ^{t} \leftrightarrow i = j = n \), whereas \( \delta_{ij}^{(l)}(\Gamma) = 0 \) otherwise. Hence, \( V_{\varphi_{rl}} \) can be used to determine a valid and reliable characterization of \( r \)-th endmember aggregate abundance, as (6) involves all the spectral interactions provided by the aforesaid endmember. Thus, the \( r \)-th endmember abundance \( \hat{a}_{rl} \) can be defined as follows:

\[
\hat{a}_{rl} = \frac{V_{\varphi_{rl}}}{\sum_{l=1}^{R} V_{\varphi_{rl}}}
\]

(7)

The basic workflow of the proposed approach is summarized in Fig. 2.

The computational load of the proposed architecture is dominated by the thin QR factorization [23]. Being
\[ \sigma = \max \{ M, R \tilde{p} \} , \] it is possible to prove that the computational complexity of this factorization is upper bounded by \( O(\nu^2) + \frac{3}{2} \nu^3 \) [27]. In hyperspectral imagery \( N \propto 10^2 \rightarrow M = \left( \frac{N}{2} \right)^2 \propto 10^3 \). On the other hand, as in the examples that have been previously showed, the \( R \tilde{p} \) term is upper bounded by \((R\tilde{p})^+ \), where \((R\tilde{p})^+ \propto 100 \). Hence, it is safe to state that the computational complexity of the thin QR factorization is a function of \( M \).

Moreover, the setup of \( G_i \) matrix (i.e., the matrix that has to be QR factorized) has a computational complexity that can be written as \( O(M(R\tilde{p} + 1)) \). Thus, the overall computational complexity of the siPOD method results into

\[
C_{\text{siPOD}} = \frac{4}{3} M^3 + O(M^2) + O[M(R\tilde{p} + 1)]. \tag{8}
\]

III. EXPERIMENTAL RESULTS

To validate the proposed approach, it was tested on synthetic and real hyperspectral data and compared whenever possible with existing literature results. All the experiments and the corresponding results are reported in the following sections.

A. Synthetic Datasets

We first tested the performance of the proposed method for nonlinear spectral unmixing over a synthetic image having \( 100 \times 100 \) pixels and \( N = 100 \) bands. The number of endmembers \( R \) was set to 5. Five mixture models have been used to generate the synthetic datasets: the five selected endmembers were mixed according to an LMM, the LQM in [10], the \( p \)-linear model in Table I with \( p = 2, 4 \), and the new \( \tilde{p} \)-harmonic model with \( \tilde{p} = 4 \). Similarly, five unmixing methods have been considered: the LMM-based FCLS algorithm [25], the LQM-based bilinear model [10], the POD method with \( p = 2, 4 \), and the siPOD method with \( \tilde{p} = 4 \).

In order to test the resilience to spurious signals, we injected white and colored noise to the synthetic images according to the scheme in [31]. Specifically, we added to each image sample a \( N \)-dimensional array \( \eta_i \), whose correlation matrix is \( \mathbf{R}_{\eta_i} = \text{diag}(\sigma_i^2) \), with \( \sigma = [\sigma_i]_{i=1}^N \). Furthermore, each \( \sigma_i \) follows a Gaussian shaped distribution that is centered over the \( N/2 \) band, i.e., \( \sigma_i \) can be written as follows:

\[
\sigma_i = \frac{\exp \left( -\frac{(i-N/2)^2}{2\eta_G^2} \right)}{\sqrt{\sum_{j=1}^N \exp \left( -\frac{(j-N/2)^2}{2\eta_G^2} \right)}} \tag{9}
\]

where \( \sigma \) controls the overall noise power and the \( \eta_G \) parameter is the variance of the Gaussian shaped distribution (e.g., when \( \eta_G \to \infty \) the noise is white).

For this model, the signal-to-noise ratio (SNR) will be equivalent to

\[
SNR = 10 \log_{10} \frac{E[y_i^T \tilde{y}_i]}{E[\eta_i^T \eta_i]} \tag{10}
\]

where \( \tilde{y}_i \) is the \( N \)-dimensional spectral signature of the \( i \)-th pixel without the noise.

In our experiments, we set the SNR to 10, 15, and 20 dB. Table II reports the performances achieved in terms of abundance root mean square error (RMSE), defined as \( \sqrt{\frac{1}{P} \sum_{i=1}^P \left\| \hat{\mu}_i - \tilde{\mu}_i \right\|^2} \), where \( \hat{\mu}_i \) identifies the estimated endmember abundance distribution of the \( i \)-th pixel. Specifically, the \( \hat{\mu}_i \) terms are set according to (7) when the \( p \)-linear model and the \( \tilde{p} \)-harmonic model are used. Instead, the estimated abundances are set equal to the sole linear contributions when LMM-based and LQM-based algorithms are used. As a result of the comparison in this table, POD and siPOD show robust resilience to white and colored noise. As expected, siPOD performs better on harmonic synthetic data, and gives very similar results than POD on polynomial mixtures.

B. Simulated Crater Dataset

As a second test we used a more complex dataset, artificially generated in [32]. Specifically, the authors in [32] provide a simulation of a crater obtained by modifying a martian regolith. This target shows a complex photometric behavior because of its DEM and the Hapke’s model-based mixture of the composing minerals (i.e., basalt, palagonite, and tephra). The target scene is composed by \( 186 \times 174 \) pixels. 16 bands in a wavelength range from 400 to 1100 nm were considered. Fig. 3(a) shows the reflectance map of the aforementioned scene over the 16th band. Finally, the abundance maps of basalt, palagonite, and tephra are reported in Fig. 3(b)–(d), respectively.

In [32], the authors deliver several methods to unmix the aforementioned image by deconvoluting the mixing process. These algorithms differ in the available quantitative information of the target they use to perform the unmixing process. Specifically, given the bidirectional reflectance image, they can consider conversion in single scattering albedo, information on incidence and emergence angles, material properties and surface macroscopic roughness in a pixel. On the other hand, the \( p \)-linear mixture model and the \( \tilde{p} \)-harmonic mixture model are
TABLE II

| Mixture model | $\eta_G$ | SNR [dB] | LMM | LQM | POD, $p = 2$ | POD, $p = 4$ | $\tilde{\text{POD, } \tilde{p} = 4}$ |
|---------------|---------|---------|-----|-----|-------------|-------------|----------------|---------|
| LMM           | $\infty$ | 10      | 2.19| 3.76| 2.32        | 2.51        | 2.42           |         |
|               | 15      | 1.56    | 2.51| 1.92| 2.23        | 2.23        | 2.22           |         |
|               | 20      | 1.22    | 2.21| 1.73| 2.29        | 2.18        |                |         |
|               | 10      | 4.46    | 6.22| 4.57| 5.62        | 5.23        |                |         |
|               | 15      | 3.62    | 5.03| 4.36| 5.37        | 5.11        |                |         |
|               | 20      | 3.35    | 4.86| 3.91| 5.11        | 4.98        |                |         |
| LQM           | $\infty$ | 10      | 23.44| 3.31| 3.28        | 3.55        | 3.46           |         |
|               | 15      | 17.67   | 2.57| 2.62| 3.08        | 2.88        |                |         |
|               | 20      | 16.89   | 2.28| 2.34| 2.85        | 2.72        |                |         |
|               | 10      | 25.22   | 5.75| 5.14| 6.34        | 6.12        |                |         |
|               | 15      | 19.66   | 4.63| 4.26| 5.13        | 5.02        |                |         |
|               | 20      | 18.24   | 3.99| 4.02| 4.82        | 4.61        |                |         |
| $p$-linear, $p = 2$ | $\infty$ | 10      | 26.33| 4.22| 1.08        | 1.35        | 1.34           |         |
|               | 15      | 22.12   | 2.89| 0.51| 1.04        | 1           |                |         |
|               | 20      | 21.74   | 1.93| 0.34| 0.93        | 0.85        |                |         |
|               | 10      | 28.65   | 5.33| 2.87| 3.31        | 3.42        |                |         |
|               | 15      | 24.83   | 3.62| 1.68| 2.46        | 2.5         |                |         |
|               | 20      | 23.92   | 3.13| 1.14| 2.08        | 2.03        |                |         |
| $p$-linear, $p = 4$ | $\infty$ | 10      | 26.67| 6.86| 4.98        | 1.89        | 1.88           |         |
|               | 15      | 24.13   | 2.23| 1.18| 0.66        | 0.66        |                |         |
|               | 20      | 23.52   | 1.95| 1.02| 0.42        | 0.48        |                |         |
|               | 10      | 29.4    | 11.96| 7.3 | 3.73        | 3.71        |                |         |
|               | 15      | 26.81   | 6.09| 2.51| 1.23        | 1.36        |                |         |
|               | 20      | 25.96   | 4.88| 2.17| 1.07        | 1.16        |                |         |
| $\tilde{p}$-harmonic, $\tilde{p} = 4$ | $\infty$ | 10      | 37.12| 11.2| 7.7         | 4.68        | 1.21           |         |
|               | 15      | 36.3    | 9.3 | 6.16| 3.79        | 0.73        |                |         |
|               | 20      | 35.9    | 6.8 | 5.83| 3.22        | 0.52        |                |         |
|               | 10      | 36.66   | 15.37| 10.22| 5.37        | 1.36        |                |         |
|               | 15      | 36.01   | 14.4| 2.51| 9.87        | 0.99        |                |         |
|               | 20      | 35.71   | 12.5| 2.17| 9.11        | 0.87        |                |         |

used to unmix the bidirectional reflectance image by considering the endmembers’ reflectance spectra provided in [32] by means of POD and siPOD, respectively. It is worth noting that no other information but the target and the endmembers’ reflectance spectra are available both for POD and siPOD.

We compared the unmixing performance by computing the mean absolute difference of the MFIs [32] for each endmember. Then, we computed the percentage of mean absolute difference between calculated MFI and ideal MFI for each algorithm. Fig. 4 reports the aforesaid quantity for the methods used in [32] in addition to LMM and $\tilde{p}$HMM, where $p = \tilde{p} = 5$.

Apparently, POD delivers very poor performance in reconstructing the crater scene. On the other hand, the harmonic mixture model can effectively track nonlinearities. Hence, the harmonic approximation as delivered by the model in (3) can provide a good characterization of intimate as well as macroscopic mixtures. Therefore, HMM can deliver good performance in tracking nonlinear and superlinear effects without a specific knowledge of the geometrical and spectral features of the considered scenes.

Fig. 5 shows the distribution of the average MFI error for a $\tilde{p}$-harmonic mixture model with $\tilde{p} = 5$ ($5$HMM). The MFI error distribution is sparse over the whole crater scene. Indeed, the same spatial behavior is reported for $5$LMM. Hence, Fig. 5 shows that higher order nonlinear (both $p$LMM and $p$HMM) errors do not depend on geometrical and topological structures. Instead, errors are due to the mismatch between Hapke’s model, the $p$LMM and $p$HMM.

Actually, $p$HMM works better than $p$LMM (i.e., with lower errors) because the high flexibility provided by harmonic mixing allows the HMM-based unmixing to adapt to Hapke’s model. In fact, as sines and cosines represent polynomial contributions up to order-\(\infty\), HMM is able to somehow approximate the nonlinear effects provided by microscopic scale combinations as in Hapke’s model. Therefore, as the crater scene has been obtained from mixing the mineral spectra according to the Hapke’s model [32], HMM-based unmixing is affected only by the spectral noise fluctuation and error occurrences arise with no dependence on morphological or geometrical features. On the other hand, as $p$LMM clips the nonlinearity order of the contributions to a fixed value, $p$th order nonlinear unmixing has less degrees of freedom than $p$HMM, s.t. $p$LMM cannot track the superlinear effects delivered by microscopic scale combinations as effectively as $p$HMM.
C. Hyperion Datasets

To further prove the suitability of the new model and the siPOD unmixing technique, we tested the proposed method on two real hyperspectral images recorded by the Hyperion sensor on board of the EO-1 satellite. In both tests, we considered only 198 out of the original 223 bands of the Hyperion sensor, discarding the noisy ones, in a wavelength range spanning from 426.82 to 2395.5 nm.

The first image depicts an eastern portion of the Marmara Sea (Turkey) and was recorded in 2001. The scene [shown in Fig. 6(a)] is composed by $400 \times 400$ pixels. Before performing unmixing, five endmembers were extracted by means of the ATGP algorithm [33].

Fig. 6(b)–(j) reports the abundance maps of three endmembers (water, roof tile, and grass) over the eastern Marmara Sea scene [whose RGB composite is shown in (a)]. (b)–(d) $a_i$ have been estimated from the unmixing performance based on linear-quadratic model (LQM) [10], (e)–(g) $p$-linear mixture model when $p = 5$, and (h)–(j) $\tilde{p}$-harmonic mixing model when $\tilde{p} = 5$. The red box shows the area that is shared with Fig. 7.

More precise information on the physical–chemical composition of the scene can be retrieved by harmonic unmixing and, accordingly, we expect improvements in classification, segmentation, and characterization tasks. This effect is emphasized in Fig. 7, where the abundance maps for the red box area in Fig. 6 are reported. Since we do not have real abundance
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Fig. 7. Abundance map of three endmembers (water, roof tile, grass) over the red box in Fig. 6 [whose RGB composite is shown in (a)]. (b)–(d) \( \hat{a}_i \) have been estimated from the unmixing performance based on linear-quadratic model (LQM) [10], (e)–(g) \( p \)-linear mixing model when \( p = 5 \), and (h)–(j) \( \tilde{p} \)-harmonic mixing model when \( \tilde{p} = 5 \).

Fig. 8. Reconstruction error performance over the eastern Marmara site scene as delivered by linear-quadratic model (LQM) [10], \( p \)-linear mixing model when \( p = 5 \), and \( \tilde{p} \)-harmonic mixing model when \( \tilde{p} = 5 \).

values to compare with, Fig. 8 shows the RE performance of LQM, 5LMM, and 5HMM over the eastern Marmara Sea scene, where \( RE = \sqrt{\sum_{l=1}^{P} ||\hat{y}_l - \hat{\hat{y}}_l||^2} \) and \( \hat{\hat{y}}_l \) identifies the reconstructed spectral signature of the \( l \)th pixel. This result further highlights the ability of higher order nonlinear models to recover a better characterization of the hyperspectral images than LQM [10].

The second Hyperion image used for validation depicts the area around Fukushima (Japan) and was recorded in 2011. The scene [Fig. 9(a)] is composed by \( 1100 \times 600 \) pixels. In this case, the ATGP algorithm extracted ten endmembers, used as inputs to the unmixing procedure. Fig. 9(e) depicts the abundance distribution of urban material endmembers over the scene. Fig. 9(b)–(d) reports instead the results obtained by LMM, LQM, and POD with \( p = 5 \).

Apparently, the comments and observations drawn for the previous test can be considered valid for this dataset as well. Specifically, the substantial gain provided by the \( \tilde{p} \)-harmonic mixture model is clearly visible in the more accurate discrimination between urban and non-urban areas in the abundance maps of Fig. 9(e).

IV. CONCLUSION

In this paper, we introduced a new order-\( \infty \) nonlinear mixture model based on harmonic combinations which aims at providing a thorough characterization of the physical-chemical composition of spectrally and geometrically complex hyperspectral images. Indeed, the proposed architecture is designed to deliver a complete description of macroscopic scale reflectance scatterings and interferences of any order among the elements in the scene. Specifically,

1) a new harmonic mixture model has been introduced and discussed;
2) an approach to invert this model by considering the POD techniques has been developed and applied to multiple synthetic and natural data;
3) results prove qualitatively and quantitatively that the new model is more precise in estimating mixture parameters and has the same or superior performance than the polynomial model recently introduced by the same authors.

Future works will explore the possibility to further generalize the harmonic mixture model, and to parallelize its implementation for near-real-time performance.
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