IDENTIFICATION OF MAFIC MINERALS ON MARS BY NONLINEAR HYPERSPECTRAL UNMIXING

Andrea Marinoni[1] *and Harold Clenet*[2]

[1]Dip. di Ingegneria Industriale e dell'Informazione, Università degli Studi di Pavia, Pavia, Italy.
E-mail: andrea.marinoni@unipv.it
[2]SB-ICMP-EPSL, Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland.
E-mail: harold.clenet@epfl.ch

ABSTRACT

Typically, quantitative interpretation of Mars mineralogy from spectra can be retrieved by analyzing the overlaps of absorption features. It is possible to achieve a thorough description of the abundances of each mineral the considered scene is composed of by applying proper deconvolution techniques such as those based on modified Gaussian model (MGM). However, MGM-based methods are sensitive on initial parameters for statistical distribution definition, or they are very time consuming when fully automatized. In this paper, a new method for identification of minerals on Mars surface by means of higher order nonlinear hyperspectral unmixing framework is introduced. Abundance distribution of magmatic minerals (olivine and pyroxenes) compounds is retrieved according to polytope decomposition algorithm. Experimental results show how the proposed method is able to provide actual abundance maps which are highly correlated to those obtained by an automatized MGM-based technique.

Index Terms— Mars mineralogy, mafic minerals, nonlinear hyperspectral unmixing, modified Gaussian model, polytope decomposition.

1. INTRODUCTION

The geophysical and atmospheric conditions on Mars may have allowed primitive bacteria-like life to be harbored very early in its history [1]. Moreover, as Mars is a terrestrial differentiated planet such as Earth, a detailed description of Mars surface can help in further understanding physical-chemical processes occurring on Earth as well. The characterization of Mars surface is typically conducted according to modal and chemical studies of rocks[2]. Indeed, as the chemical composition of mafic minerals give insights on the igneous processes that have occurred on the planet, detecting and investigating compositions of olivine and pyroxenes is crucial to understand the magmatic evolution of Mars. Moreover, the quantitative interpretation of mineralogy from spectra can be retrieved by analyzing the overlaps of absorption features. Hence, it is possible to achieve a thorough description of the abundances of each mineral the considered scene is composed of by applying proper deconvolution techniques such as those based on modified Gaussian model (MGM) [2]. Although the outcomes of the aforementioned methods might be very accurate, it is also true that MGM results are affected by proper choice of initial parameters, and the fully automatized approach is very time consuming. Therefore, their application is constrained by the properties of the considered datasets.

Hyperspectral unmixing (HSU) can help in that sense [3], [4]. Specifically, HSU methods aim at separating the target pixel spectrum into a set of constituent spectral signatures (endmembers) and a set of fractional abundances. It has been proved how unmixing techniques are able to provide accurate description of the materials in instantaneous field-of-view by characterizing the interactions among elements. Moreover, since the inversion process carried out over the mixture models depends only on the endmember spectra, HSU methods are not sensitive on statistical distribution parameters. As absorption characteristics vary nonlinearly according to the abundance distribution, nonlinear HSU methods are appropriate for understanding and quantifying the physical-chemical composition of the materials on Mars surface. Further, Mars surface composition is strongly depending on intimate mixture features, such as grain size and illumination angles. Therefore, higher order nonlinear HSU algorithms can play a key-role in retrieving accurate characterization of Mars scenes, as it has been proved how actually they can provide solid and reliable description of spectrally and geometrically complex scenarios [5].

In this paper, we aim to use higher order nonlinear HSU methods to achieve accurate characterization of the mineralogical composition of Mars surface. Specifically, by employing higher order linear and harmonic mixture models, efficient description of the minerals' abundance distribution can be recovered. Moreover, the coefficients that drive the spectral mixture can be properly used in order to retrieve an estimate of the mineral which mainly composes every pixel. Experimental results are validated according to the outcomes obtained from accurate MGM-based techniques, showing that

the proposed approach is actually able to deliver important information on the Mars surface composition. The paper is organized as follows. Section 2 describes the proposed method. Section 3 describes the experimental results. Finally, Section 4 concludes with some final remarks.

2. METHODS

Higher order nonlinear mixture model for the l-th pixel in a given scene can be summarized as follows:

$$\underline{y}_l = \sum_{k=1}^{p} \sum_{r=1}^{R} \omega_{krl} \psi_k(\underline{m}_r) \tag{1}$$

where $\underline{y}_l = [y_{l_n}]_{n=1,\dots,N}$, $y_{l_n} \in \mathbb{R}$ is the N-band spectral signature of the l-th pixel. Moreover, R is the number of endmembers, $\underline{m}_r = [\underline{m}_{r_n}]_{n=1,\dots,N}$ is the N-band spectral signature of the r-th endmember. Then, $\psi_k(\cdot)$ represents a k-th order nonlinear function of the given endmember spectrum. Hence, when $\psi_k(\underline{m}_r) = \underline{m}_r^k$ (where $\underline{m}_r^k = [m_{r_n}^k]_{n=1,\dots,N}$), (1) identifies the p-linear mixture model (pLMM). On the other hand, if $\psi_k(\underline{m}_r) = \cos \underline{m}_r^k + \sin \underline{m}_r^k$ (where $\cos \underline{m}_r^k = [\cos m_{r_n}^k]$ and $\sin \underline{m}_r^k = [\sin m_{r_n}^k]$, $n = 1, \dots, N$), (1) represents the p-harmonic mixture model (pHMM).

The goal of nonlinear spectral unmixing is to evaluate each ω term, in order to understand the nature of the endmember combination that delivers the given target observation spectral signature. Further, the coefficients driving the nonlinear combination in (1) can be obtained by means of a linear system involving the original hyperspectral data and the endmembers' spectra delivered by an endmember extraction algorithm (EEA). Indeed, it is possible to explicit the contribution of the ω terms by taking into account a new system of linear equations properly tuned according to the aforesaid models. Indeed, it is possible to solve nonlinear mixture combinations by means of linear problems that can be derived according to a polytope decomposition scheme. Specifically, applying proper algebraic properties to each possible dimension pairs, we can write $\underline{\underline{G}}_l \underline{\omega}_l = \underline{b}_l$, where $\underline{\omega}_l = [\omega_l^{(r)}]_{r=1,\dots,R}$, being $\omega_l^{(r)} = [\omega_{krl}]_{k=1,\dots,p}$. $\underline{\underline{G}}_l = [g_{l_{\kappa\lambda}}]$ is a $M \times Rp$ matrix, where $M = \binom{N}{2}$, $\kappa \in \{1, \dots, M\}$ and $\lambda \in \{1, \dots, Rp\}$. Finally, $\underline{b}_l$ a vector of M elements. Indeed, let us assume $\kappa = \rho_t + \eta_t$, where $t \in \{1, \dots, N-1\}$, $\eta_t \in \{1, \dots, N-t\}$ 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 (1), each element $g_{l_{\kappa\lambda}}$ must be defined according to $g_{l_{\kappa\lambda}} = g_{l_{(\rho_t+\eta_t),\lambda}} = Z_{\tau_1} + y_{l_t}(y_{l_{t+\eta_t}})^{-1} Z_{\tau_2}$, where $\lambda = (z-1)\pi + \psi_\pi$, $z \in \{1, \dots, R\}$ and $\psi_\pi \in \{1, \dots, \pi\}$. Finally, $b_{l_\kappa} = b_{l_{(\rho_t+\eta_t)}} = 2y_{l_t}$. Z_{τ_1} and Z_{τ_2} have to be set according to the model that is used. Hence, (Z_{τ_1}, Z_{τ_2}) is set to $(m_{z_t}^{\psi_p}, m_{z_{t+\eta_t}}^{\psi_p})$ when pLMM is used. Moreover, if pHMM is considered, $Z_{\tau_1} = \cos m_{z_t}^{\psi_{\tilde{p}}} + \sin m_{z_t}^{\psi_{\tilde{p}}}$ and $Z_{\tau_2} = \cos m_{z_{t,t+\eta_t}}^{\psi_{\tilde{p}}} + \sin m_{z_{t,t+\eta_t}}^{\psi_{\tilde{p}}}$. Then, nonlinear HSU based on pLMM and pHMM results in an overdetermined linear programming problem that involves the original hyperspectral data and the endmembers' spectra [3], where constraints are induced according to $\underline{\underline{G}}_l \underline{\omega}_l = \underline{b}_l$, $\sum_{k,r} \omega_{krl} = 1 \forall l$, $\omega_{krl} \geq 0 \forall (r,k)$. Then, a proper combination of linear and nonlinear coefficients can provide a more accurate estimation of the endmember abundances. In order to accurately evaluate the abundance set distribution, a global metric based on the polytope representation the aforementioned unmixing process relies on can be used. Indeed, given $\underline{\omega}_l$ as extracted according to the overdetermined linear programming optimization, it is possible to derive the spectral representation of the reconstructed pixel $\underline{\hat{y}}_l$. In other terms, each element in $\underline{\hat{y}}_l$ can be represented as $\hat{y}_{l_n} = \sum_{r=1}^{R} \varphi_{rl_n} \psi_1(m_{r_n}) = \sum_{k=1}^{p} \sum_{r=1}^{R} \omega_{krl} \psi_k(m_{r_n})$, where φ_{rl_n} is the overall contribution of the r-th endmember to the reconstruction of the l-th pixel over the n-th band. Hence, it is possible to think to φ_{rl_n} as the compression/expansion factor of the r-th endmember over the n-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 $\underline{\varphi}_{rl} = [\varphi_{rl_n}]_{n=1,\dots,N}$ 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 $\underline{\varphi}_{rl}$. Given our assumptions such a polytope is a simplex [3]. Therefore, we can define its volume as $V_{\underline{\varphi}_{rl}} = (N!)^{-1} \det[\Delta(\underline{\varphi}_{rl})] = (N!)^{-1} \prod_{n=1}^{N} \varphi_{rl_n}$, where $\Delta(\underline{\varphi}_{rl}) = [\delta_{ij}(\underline{\varphi}_{rl})]_{(i,j) \in \{1,\dots,N\}^2}$ is the diagonal matrix induced by the $\underline{\varphi}_{rl}$ spectral signature. [3]. Hence, $V_{\underline{\varphi}_{rl}}$ can be used to determine a valid and reliable characterization of r-th endmember aggregate abundance, as $V_{\underline{\varphi}_{rl}}$ involves all the spectral interactions provided by the aforesaid endmember. Thus, the r-th endmember abundance $\hat{a}_{rl}$ can be defined as $\hat{a}_{rl} = V_{\underline{\varphi}_{rl}} / \sum_{i=1}^{R} V_{\underline{\varphi}_{il}}$. The abundance estimates $\hat{a}_{rl}$ fulfill the sum-to-one and the non-negativity constraints [6]. Furthermore, it is possible to consider $\hat{a}_{rl}$ as an aggregate metric to estimate the abundance of the r-th endmember in a pixel, where the contributions of each order is weighted by the endmember itself. This results in a more stable and reliable metric in order to get an evaluation of the presence of each endmember in the scene [6]. As previously mentioned, acquiring univocal and well defined spectral signatures of minerals over Mars surface can be cumbersome. Indeed, geomorphological and geophysical properties as well as illumination conditions can strongly affect the signals that are remotely sensed by spectrometers. Therefore, in order to give a thorough overview of the actual occurrence of each element in the considered scene, several spectral signatures which identify minerals with different geophysical features are used to shape the endmembers' library. Hence, several endmember spectra used to perform unmixing might refer to the same mineral element. Indeed, the overall endmember li-

brary $\mathcal{M} = \{\underline{m}_r\}_{r=1,\ldots,R}$ can be written as $\mathcal{M} = \bigcup_{s=1}^{S} \mathcal{M}_s$, where $\mathcal{M}_s$ identifies the set of spectral signatures which can be associated with the s-th specific mineral compound. Thus, let $\hat{\alpha}_{sl}$ be the estimate of the actual actual abundance of the s-th mineral over the l-th pixel. Then, it is possible to retrieve a thorough estimate of the each $\hat{\alpha}_{sl}$ as follows:

$$\hat{\alpha}_{sl} = \sum_{j:\underline{m}_j \in \mathcal{M}_s} \hat{a}_{jl} \cdot (\sum_{r=1}^{R} \hat{a}_{rl})^{-1} \quad (2)$$

Further, since MGM-based methods typically result in the distribution of the mineral elements which are more likely to occur over each pixel, the quantities in (2) are clipped s.t. a single compound can be associated with the l-th pixel $\forall l$. Indeed, a proper map of major abundance estimate can be retrieved by processing the parameters in (2) as follows:

$$\bar{\alpha}_l = \arg\max_s \hat{\alpha}_{sl} \quad (3)$$

Experimental results in the next Section are evaluated according to the $\bar{\alpha}$ map that can be derived by means of the aforementioned procedure.

3. EXPERIMENTAL RESULTS

In this study, we used data acquired by the Compact Reconnaissance Imaging Spectrometer for Mars (CRISM) onboard the Mars Reconnaissance Orbiter (MRO) spacecraft. CRISM observations provide visible and near-infrared (VNIR) spectral coverage (0.32 3.92) with a maximum spatial resolution of 18 m/pixel [7]. CRISM observations were processed as described in [8] to account for atmospheric and photometric contributions. If needed, noise was removed using the despiking and destriping algorithms available under CAT 6.7 for TRR3 datasets. Visible and near-infrared channels were also coregistred in order to use the entire available spectral domain. The 2387 $\times$ 2116 pixels mosaic of five CRISM images we produced is located in the Nili Patera caldera, ontop the Syrtis Major volcano [9]. The Syrtis Major volcanic complex is a type example of Hesperian-aged plains volcanism on Mars, and evidences of an ancient hydrothermal system (i.e. possible habitable environments) were found in the caldera [10]. A previous study used a fully automatized MGM approach to characterize the composition of magmatic rocks in this region using OMEGA/MEx hyperspectral images [2]. We choose to use it as a reference to test the results of our novel approach. The reference map was produced using MGM (originally developed by [11]) adapted by [12]. In this approach an automatic procedure involving different numbers of Gaussians, depending on the potential complexity of the mixture, has been implemented on the original MGM core. The resulting band parameters are used to interpret the spectrum in terms of modal abundances and chemical compositions [12]. Validation processes have been made on both laboratory and natural data [12, 2].

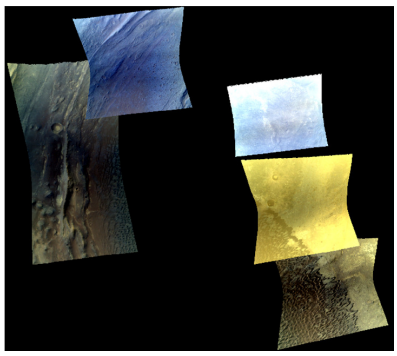

Fig. 1. False color composite of the Nili Patera region on Mars.

The nonlinear HSU schemes proposed in the previous Section have been used according to order-7 linear and harmonic mixture models [3], [4]. 72 435-bands spectral signatures in the 0.43-2.6 μm range of mafic elements collected from laboratory and experimental observations have been used as endmembers to feed the nonlinear HSU frameworks. Moreover, the endmembers have been pooled into nine groups of major mineral compounds, i.e., $S = 9$ in (2). These materials result from pure mafic elements [namely olivine (OL), plagioclase (PL), orthopyroxene (OPX) and clinopyroxene (CPX)] and mixtures of the aforesaid minerals [namely OL-OPX, OL-OPX-PL, OPX-CPX, OPX-CPX-OL, CPX-OL].

Fig. 2 shows the results that have been obtained when estimating the mineral composition of the scene in Fig. 1. Specifically, Fig. 2(a) reports the mineral composition expected according to the low resolution architecture relying on the OMEGA instrument [2]. Moreover, Fig. 2(b) and (c) show the mafic mineral distribution achieved according to the framework introduced in Section 2 based on 7LMM and 7HMM, respectively. Thus, it is possible to appreciate how the proposed scheme based on higher order nonlinear HSU is actually able to retrieve an accurate description of the mafic mineral display over the Nili Patera region according to the OMEGA results. Indeed, the correlation factor between Fig. 2(a) and Fig. 2(b) is 82.6%, whilst it results equal to 78.8% when Fig. 2(a) and Fig. 2(c) are considered.

Hence, the proposed framework can be definitely used to identify the mineral compound displacement over the Mars surface. Moreover, the aforesaid method can be employed in order to estimate the actual distribution of each mafic element over the considered region. For instance, Fig. 2(d) shows the abundance map of the CPX element. This allocation estimate has been achieved by considering the distribution of the $\hat{\alpha}$ coefficients as computed in (2) according to 7LMM. Thus, if we do not clip the parameters estimated in (2), we can achieve a soft metric to measure the actual occurrence of each mineral in every pixel. Further, from visual inspection of all the figures in Fig. 2, it is possible to state that the metric based on

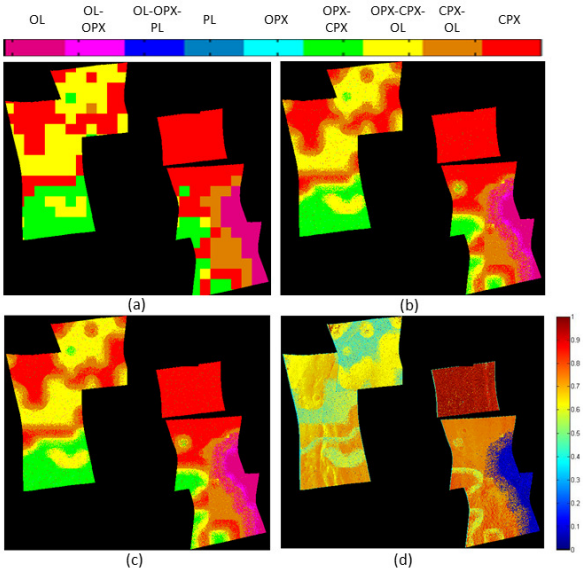

Fig. 2. (a): low resolution expected mineralogical composition of the Nili Patera region as estimated by OMEGA instrument [2]. (b),(c): mafic mineral compounds' distribution as estimated by the proposed framework based on nonlinear hyperspectral unmixing according to 7LMM and 7HMM, respectively. Mineral composition is reported in (a), (b) and (c) according to the colormap above the figures. (d): abundance map of clinopyroxene element (CPX).

the $\hat{\alpha}$ coefficients provide a reliable estimate of the mafic mineral distribution. Therefore, the proposed structure for higher order nonlinear HSU can be used to deliver a thorough detection, identification and estimation metric of mafic minerals over Mars surface.

4. CONCLUSION

In this paper, we introduce an architecture relying on higher order nonlinear HSU for identifying mafic minerals over Mars surface. The proposed method aims at identifying elements by properly pooling and processing results from unmixing based on p-linear and p-harmonic mixtures. Experimental results show how the proposed approach is actually able to provide mafic minerals' maps which are highly correlated to reference mineral distributions. Future works will focus on exploiting the results obtained from the proposed method to achieve high-resolution high-accuracy quantification of the mafic minerals.

5. REFERENCES

[1] J.-P. Bibring et al., "Global mineralogical and aqueous Mars history derived from OMEGA/Mars Express data," *Science*, vol. 312, pp. 400–404, 2006.

[2] H. Clenet et al., "A systematic mapping procedure based on the modified gaussian model to characterize magmatic units from olivine/pyroxenes mixtures: Application to the syrtis major volcanic shield on mars," *Journal of Geophysical Research: Planets*, vol. 118, pp. 1632–1655, Aug. 2013.

[3] A. Marinoni and P. Gamba, "A novel approach for efficient p-linear hyperspectral unmixing," *IEEE J. Sel. Top. Sign. Proc.*, vol. 9, no. 6, pp. 1156–1168, Sept. 2015.

[4] A. Marinoni, A. Plaza, and P. Gamba, "Harmonic mixture modeling for efficient nonlinear hyperspectral unmixing," *IEEE J. Sel. Top. App. Earth Obs. Rem. Sens.*, Jan. 2016.

[5] A. Marinoni, J. Plaza, A. Plaza, and P. Gamba, "Nonlinear hyperspectral unmixing using nonlinearity order estimation and polytope decomposition," *IEEE J. Sel. Top. App. Earth Obs. Rem. Sens.*, vol. 8, no. 6, pp. 2644–2654, June 2015.

[6] R. Heylen, M. Parente, and P. Gader, "A review of nonlinear hyperspectral unmixing methods," *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 7, no. 6, pp. 1844–1868, June 2014.

[7] S. L. Murchie et al., "Compact Reconnaissance Imaging Spectrometer for Mars (CRISM) on Mars Reconnaissance Orbiter (MRO)," *Journal of Geophysical Research*, vol. 112, pp. E05S03, 2007.

[8] B. L. Ehlmann et al., "Identification of hydrated silicate minerals on Mars using MRO-CRISM: geologic context near Nili Fossae and implications for aqueous alteration," *Journal of Geophysical Research*, vol. 114, pp. E00D08, 2009.

[9] G. G. Schaber, "Syrtis Major: A Low-Relief Volcanic Shield," *Journal of Geophysical Research*, vol. 87, no. B12, pp. 9852–9866, 1982.

[10] J.R. Skok et al., "Silica deposits in the Nili Patera caldera on the Syrtis Major volcanic complex on Mars," *Nature Geoscience*, vol. 3, pp. 838–841, 2010.

[11] J.M. Sunshine and C.M. Pieters, "Estimating modal abundances from the spectra of natural and laboratory pyroxene mixtures using the modified Gaussian model," *Journal of Geophysical Research*, vol. 98, pp. 9075–9087, 1993.

[12] H. Clenet et al., "A new systematic approach using the Modified Gaussian Model: Insight for the characterization of chemical composition of olivines, pyroxenes and olivinepyroxene mixtures," *Icarus*, vol. 213, pp. 404–422, 2011.