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Removal of atmospheric features in near infrared spectra by means of principal component analysis and target transformation for the study of hydrated minerals on Mars

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Abstract

The aim of this work is to extract the surface contribution in the Martian visible/near-infrared spectra removing the atmospheric components by means of Principal Component Analysis (PCA) and target transformation (TT). The developed technique is suitable for separating spectral components in a data set large enough to enable an effective usage of statistical methods, in support to the more common approaches to remove the gaseous component. In this context, a key role is played by the estimation, from the spectral population, of the covariance matrix that describes the statistical correlation of the signal among different points in the spectrum. As a general rule, the covariance matrix becomes more and more meaningful increasing the size of initial population, justifying therefore the importance of sizable datasets. Data collected by imaging spectrometers, such as the OMEGA (Observatoire pour la Minéralogie, l'Eau, les Glaces et l'Activité) instrument on board the ESA mission Mars Express (MEx), are particularly suitable for this purpose since it includes in the same session of observation a large number of spectra with different content of aerosols, gases and mineralogy. The methodology presented in this work has been first validated using a simulated dataset of spectra to evaluate its accuracy. Then, it has been applied to the analysis of OMEGA sessions over Nili Fossae and Mawrth Vallis regions, which have been already widely studied because of the presence of hydrated minerals. These minerals are key components of the surface to investigate the presence of liquid water flowing on the Martian surface in the Noachian period. Moreover, since a correction for the atmospheric aerosols (dust) component is

32 also applied to these observations, the present work is able to completely remove the atmospheric
33 contribution from the analysed spectra. Once the surface reflectance, free from atmospheric
34 contributions, has been obtained, the Modified Gaussian Model (MGM) has been applied to spectra
35 showing the hydrated phase. Silicates and iron-bearing hydrated minerals have been identified by
36 means of the electronic transitions of Fe^{2+} between 0.8-1.2 μm , while at longer wavelengths the
37 hydrated mineralogy is identified by overtones of the OH group. Surface reflectance spectra, as
38 derived through the method discussed in this paper, clearly show a lower level of the atmospheric
39 residuals in the 1.9 hydration band, thus resulting in a better match with the MGM deconvolution
40 parameters found for the laboratory spectra of Martian hydrated mineral analogues and allowing a
41 deeper investigation of this spectral range.

42
43 *Keywords:* Mars, atmosphere, surface reflectance, OMEGA, mineralogy

44 45 **1. Introduction**

46 The main purpose of this work is to apply the PCA and the target transformation (TT) method to
47 data acquired by imaging spectrometers on board space missions orbiting Mars, in order to remove
48 the atmospheric contribution. This will allow for the isolation of the surface spectra in order to
49 investigate hydrated mineral features. Imaging spectrometers measure a signal in the near-infrared
50 spectral range that contains information about the atmosphere as well as about the surface. The
51 measured spectra result in a combination of these different spectral contributions and a
52 methodology is necessary to separate the atmospheric component from the surface reflectance. The
53 high resolution spectral data provided between 0.4 and 2.5 μm by both the OMEGA (Observatoire
54 pour la Minéralogie, l'Eau, les Glaces et l'Activité) and CRISM (Compact Reconnaissance Imaging
55 Spectrometer for Mars) imaging spectrometers, on board the ESA/Mars Express and the
56 NASA/MRO respectively, allow for the identification and mapping of different minerals (e.g.,
57 Bibring et al., 2004; Murchie et al., 2007a). However, while the electronic absorption features
58 diagnostic of transitional elements bearing minerals (e.g., ferro-magnesian silicates) occur at
59 wavelengths not affected by Mars atmospheric composition, the vibrational overtone absorptions
60 bands due to water, OH, and $(\text{CO}_3)^{2-}$ in minerals overlap the absorption of water and CO_2 in the
61 atmosphere. Therefore, an accurate removal of the atmospheric components (aerosols and gaseous
62 species) is necessary to extract the actual surface contribution in the spectra. The standard
63 processing approach to remove the atmospheric contribution is to divide the spectra by a scaled
64 atmospheric spectrum measured across Olympus Mons (Langevin et al., 2005; McGuire et al.

65 2009). Then, the residual errors are suppressed by ratioing the target spectrum by a low spectral
66 contrast reference spectrum of the same **observational session (or cube)**, apparently without any
67 relevant features and characterized by a smoother continuum (e.g., Bibring et al., 2005). Bakker et
68 al. (2014) introduced a new method to obtain the surface reflectance deriving atmospheric
69 transmission models (ATM) from the OMEGA image itself. This method has the advantage to take
70 into account the seasonal and diurnal variability of the atmospheric gases (CO₂ and H₂O), but no
71 attempt was made to correct for aerosols effects.

72 Bandfield et al. (2000) and D'Amore et al. (2013) have already applied the multivariate analyses
73 techniques to the Thermal Emission Spectrometer (TES) on board the NASA Mars Global Surveyor
74 satellite and to the Planetary Fourier Spectrometer (PFS) instrument on board the ESA Mars
75 Express (MEx) spacecraft, respectively. The authors were able to properly recover the atmospheric
76 contribution (dust and water ice clouds) to the observed radiation in the thermal/far-infrared spectral
77 range. **Glotch and Bandfield (2006) found the surface spectral components and atmospheric spectral
78 shapes at Meridiani Planum applying the PCA and TT to the Miniature Thermal Emission
79 Spectrometer (Mini-TES). Glotch and Rogers (2013) used factor analysis and TT to search for
80 carbonate decompositions products on the surface of Mars. Smith et al. (2000) successfully
81 separated the contribution of atmospheric and surface components in TES data assuming that each
82 spectrum is a linear combination of its components. Thomas and Bandfield (2013) used the TT on
83 CRISM data to confirm the presence of Mg-rich carbonates near Nili Fossae region on Mars, while
84 Thomas et al. (2014) used the TT to identify diagnostic serpentine spectral features in the CRISM
85 near-infrared data on the same Martian region. Klassen (2009) found a set of spectral end-members
86 applying the PCA and TT to near infrared cube images of Mars acquired by the NASA Infrared
87 Telescope Facility. In our work, we apply the same technique, hereafter called Surface Atmosphere
88 Separation (SAS) method, to the OMEGA data in the near-infrared spectral range. In particular, we
89 focused on surface reflectance spectra that show the hydrated absorption bands, which occur in the
90 spectral range between 1.8 and 2.2 μm that is strongly influenced by the atmospheric absorption of
91 H₂O and CO₂.**

92 Section 2 gives a short description of the OMEGA instrument and the set of data used in the present
93 work. Section 3.1 summarizes the theoretical background of the PCA and target transformation
94 approach, while the application of the method to a test case is shown in Section 3.2. Section 4 is
95 devoted to the analysis of two OMEGA orbits passing through Nili Fossae (Section 4.2) and
96 Mawrth Vallis (Section 4.3), where different mineral assemblages and the presence of
97 phyllosilicates were already recognized (e.g., Poulet et al., 2005; Mustard, et al., 2007; Mangold et

98 al., 2007; Ehlmann et al., 2008; Poulet et al., 2008; Bishop et al., 2008; Noe Dobrea, et al., 2010).
99 The presence of these minerals on the Noachian crust of Mars implies likely the presence of liquid
100 water during the first billion year (e.g., Loizeau et al., 2007) and strong climate changes between
101 the present time and the epoch in which phyllosilicates formed. The application of the multivariate
102 analyses techniques to OMEGA spectra in order to remove the gaseous atmospheric components is
103 completed by the removal of atmospheric dust component as described in Section 4.4. The spectral
104 surface component classification and deconvolution are addressed in Section 5, **where it is shown**
105 **that the SAS method permits an improvement in the identification of the mineralogical phases by**
106 **means of MGM, in particular for the investigation of hydrated mineralogy.** Finally, the **discussion**
107 **and conclusions are in Section 6 and 7, respectively.**

108

109 **2. Instrument and dataset**

110 In each resolved pixel (1.2x1.2 mrad instantaneous field of view, IFOV) OMEGA acquires a
111 spectrum in 352 contiguous spectral elements (spectels) from 0.35 to 5.1 μm , with a spectral
112 sampling ranging from 7 nm (in the visible and near infrared (VNIR) channel, between 0.38 and
113 1.05 μm) to 14 nm (short wavelength range, SWIR-C, between 0.93 and 2.73 μm) and 20 nm
114 (SWIR-L, which covers the interval 2.55–5.1 μm). The signal-to-noise ratio (SNR) is > 100 over
115 the whole spectral range (Bibring et al., 2004) **for observations obtained in nadir mode and**
116 **considering low solar zenith angles.** The data products are organized in three-dimensional arrays (or
117 cubes), with one spectral and two spatial dimensions (x, y, λ). Due to the MEx spacecraft elliptic
118 orbit, the scan widths in each orbit are changed (16, 32, 64, 128 pixels) accordingly to the variation
119 of the observing distance, e.g., 16 pixels are used for the low-**elevation** (< 350 km, orbit peri-center)
120 and consequently for high-resolution (300 m/pixels) observations, whereas the 128 pixels mode is
121 adopted for **elevations** above 1500 km to provide wide images with **spatial sampling greater than 2**
122 **km/pixel.** Data and calibration software are publicly available through ESA's Planetary Science
123 Archive. The OMEGA VNIR and SWIR-C channels data are co-registered according to Carrozzo et
124 al. (2012). Together with CRISM, **OMEGA** allowed for the first time the clear detection of hydrated
125 minerals such as hydroxides, sulphates and in particular phyllosilicates (e.g., Poulet et al., 2005;
126 Gendrin et al., 2005; Arvidson et al., 2005; Milliken et al., 2008).

127 In order to investigate regions where hydrated minerals have been already found and to include a
128 variety of mineralogical units, in this work we focus on the two MEx orbits: 0422_4 and 0353_3.
129 Orbit 0422_4 includes the north of Syrtis Major Planum, passing through Nili Fossae and highlands

130 of Nili Fossae. This OMEGA observation contains 44,640 spectra and, besides the considerable
131 mineralogical diversity, it shows significant variability in gas absorption due to an altimetry
132 variation of 4.7 km. This observational session has been acquired on May 20th, 2004 during Martian
133 year 27 (the Martian years start on 1955, April 11 at solar longitude 0°, following the convention
134 used in Clancy et al, 2000), at solar longitude 36.1° (northern spring). The ground track goes from
135 south to north crossing a changing elevation from -2.97 km to 1.73 km. Orbit 0353_3 passes
136 through Mawrth Vallis, a region located at mid-low latitude in the west part of Arabia Terra, with
137 an elevation spanning from a minimum of -5 km to a maximum of -700 m. This observational
138 session has been acquired on April 30th, 2004 during Martian year 27, at solar longitude 26.8°
139 (northern spring) and contains 99,820 spectra.

140

141 3. Method and validation

142 3.1 Principal component analysis and target transformation

143 This Section follows closely the methodology given in Bandfield et al. (2000). In statistical
144 methods the covariance matrix is used, with different approaches, to derive the **eigenvectors**, a set
145 of N_e orthogonal spectral functions summarizing the variability of the sample. They can be
146 organized in a $m \times N_e$ matrix R (m being the number of spectral points), whose rows can be linearly
147 combined to reproduce every spectrum in the dataset. More specifically, being D the full set of
148 measured spectra ($n \times m$ matrix, gathering n sampled spectra in m spectral bands), it holds

$$149 \quad D=R \cdot C \quad (1)$$

150 where C is a $N_e \times n$ matrix whose columns give the contribution (weights) of each endmember to
151 the different spectra in the population. To derive the matrix R (composed by eigenvectors of D) we
152 use the PCA. However, there are many works that use instead the Factor Analysis (FA), such as
153 Bandfield et al. (2000, 2002), D'Amore et al. (2013), Glotch and Bandfield (2006), Glotch and
154 Rogers (2013), and Hamilton et al. (2012). PCA and FA have the same purpose: reduce the
155 dimensionality of the variables. However, they reach this goal in two different ways: PCA uses the
156 variance of the observed variables and finds the principal components, while FA accounts for
157 common variance in the data and finds a smaller set of latent variables or scores (the original
158 variables are defined as linear combinations of the factors). Both methods provide significant
159 components (or eigenvectors) to be transformed in physically meaningful end-members by means
160 the Target Transformation. In our opinion and for the goal of our work, both methods are useful in

161 the same way, and, we suppose, they could afford to achieve same or similar results. Therefore, we
162 proceed using the PCA approach.

163 The main purpose of the PCA is to reduce the number of variables and found the minimum set of
164 eigenvectors whose linear combinations are able to reconstruct the original measured spectra. The
165 original population of spectra can be represented in a space with dimensionality given by the
166 number of spectral channels. In the PCA approach, the diagonalization of the covariance matrix is
167 used to represent the original information in a rotated space of reduced dimensionality, but
168 preserving the most part of the original variance. Once the eigenvalues are sorted by decreasing
169 values, the first eigenvector (principal component 1) accounts for the maximal variance, the second
170 eigenvector (principal component 2), orthogonal to the previous one, accounts for the maximum
171 variability that has not been counted from the first one, and so on. Once all eigenvalues and
172 eigenvectors (their initial number is equal to the original dimension of data) have been found, the
173 dimensionality can be reduced by retaining the minimum N_e number of components that actually
174 influence the dataset. Even if ideally N_e should be strictly related to the number of spectral end-
175 members present in the dataset, actually secondary eigenvectors could still contain spectral
176 information. As explained in Section 3.2, we use a chi-square test to constrain the number of
177 eigenvectors. The eigenvectors associated to the N_e eigenvalues or principal components can thus
178 reproduce the measured signal, while the remaining eigenvectors are featureless and contain mostly
179 random noise.

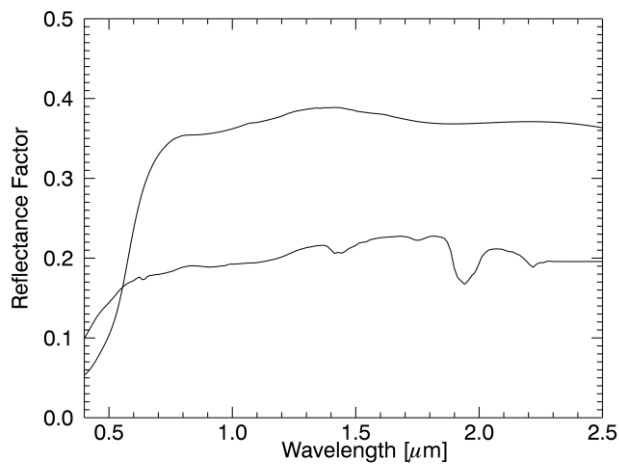
180 Since the eigenvectors do not necessarily have a physical meaning, target transformation (Hopke,
181 1989) is used to assign a physical significance to this abstract matrix by rotating the space defined
182 by the meaningful eigenvectors to be geometrically realigned to a set of predefined axes, called test
183 vectors, representing the possible physical contributions to the measured data. For this purpose, a
184 set of trial (or test) spectra have been computed by means of a radiative transfer (RT) code (Ignatiev
185 et al., 2005), each one representing the gaseous spectral end-members: carbon dioxide, carbon
186 monoxide and water vapour transmittances. The trial spectra describing the surface components can
187 be laboratory spectra or retrieved surface components obtained with existing methods, e.g., the so
188 called Mons Olympus' method (Langevin et al. 2005), hereafter MO method, which is also often
189 referred as "volcano scan" (e.g., McGuire et al., 2009). The spectral components (R matrix in
190 Formula 1) are then retrieved fitting the trial spectra with a linear combination of N_e eigenvectors.
191 Finally, the projection of the initial spectral population into the space defined by the retrieved
192 spectral components allows finding the weight matrix (Hopke, 1989). Considering the retrieved
193 end-members of the surface only, the gaseous components are removed from the spectra.

194 The assumption of linear combination of spectral end-members can be done only when the dust
195 content in the atmosphere is very low, otherwise their contribution is far from being linear.
196 Moreover, in the visible and near-infrared range of the spectrum it is difficult to disentangle the
197 effect of dust on the bright, dusty terrains from that in the atmosphere. For this reason we will adopt
198 a further step to remove the effect of atmospheric dust scattering, as described in Section 4.4.
199 Therefore, in our first analysis the aerosol component is not included, and the assumed contribution
200 to the spectra is only given by the gases transmittance and surface reflectance.

201

202 **3.2 Synthetic datasets used as a test**

203 To validate and check the accuracy of the described method we proceed with preliminary tests on
204 simulated data and make a direct comparison between final results and initial input (which we call
205 “true”). We consider a population of synthetic spectra computed by means of the RT algorithm and
206 convolved with a Gaussian kernel at the OMEGA spectral resolution. The synthetic population has
207 been constructed using the observational geometries of OMEGA orbit 0248_1 (16th pixel) that
208 includes 2848 scans and shows an altimetry variation from -3.53 km to 1.96 km.



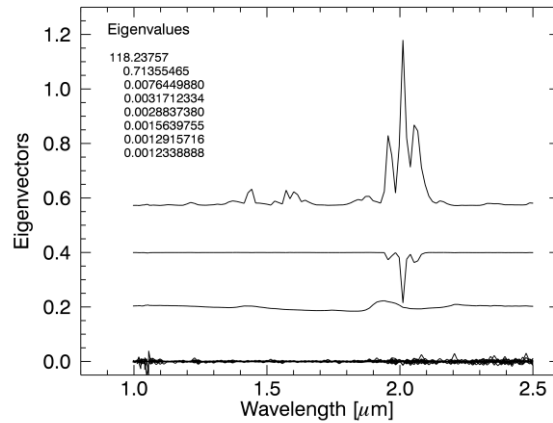
209

210 Figure 1. Reflectance of a bright surface (upper spectrum) and dark surface (lower spectrum) used as input for the
211 surface reflectance in the RT code.

212

213 In the simulated dataset we consider a bright surface reflectance (in Figure 1, the upper curve) and a
214 dark surface reflectance (the lower curve in Figure 1, taken from a spectrum of a hydrated mineral
215 measured in laboratory). The two reflectances (Figure 1) are mixed with uniform random weights in
216 each of the 2848 different spectra of the population and used as input for the surface reflectance in
217 the RT code. The gaseous components include CO₂, CO and H₂O. Realistic gases abundances and
218 pressure-temperature vertical profiles are extracted from the Mars Climate Database (MCD, Lewis

219 et al., 1999; Forget et al., 1999). Deep space measurements from OMEGA orbit 0285_0 have been
 220 used to derive the standard deviation of random instrumental radiometric noise. Series of normally
 221 distributed random numbers have eventually allowed us to simulate a realistic measurement error
 222 for each spectrum. Since the visible portion of the spectrum does not have gaseous absorption
 223 bands, this analysis involves the spectral range from 1 μm to 2.5 μm .

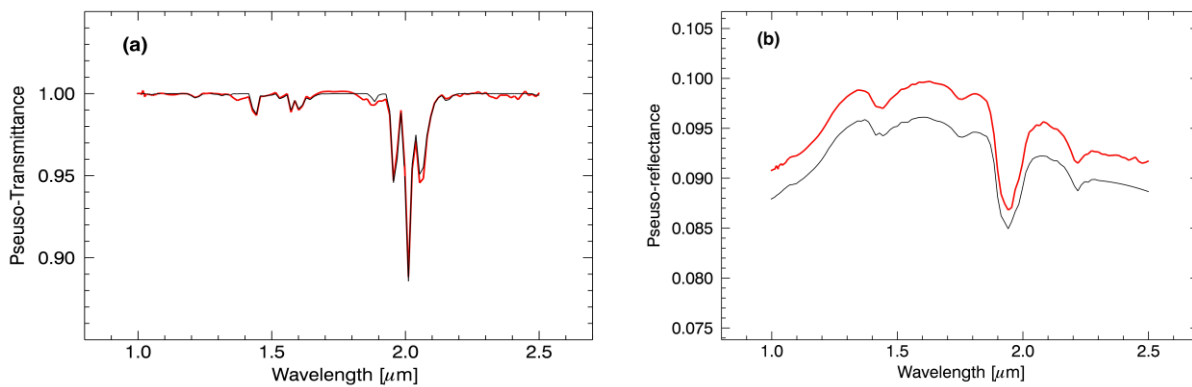


224
 225 Figure 2. Eigenvectors retrieved using PCA for the simulated dataset, shifted for clarity. Only the first eight eigenvalues
 226 are listed.

227
 228 The PCA applied to the synthetic population identifies a significant contribution of three principal
 229 components, which are found to be essentially the gases components (the first two eigenvectors)
 230 and the surface (the third eigenvector), as shown in Figure 2, whereas all the other eigenvectors
 231 contain mostly noise. However, the correct number of principal components, which represents the
 232 eigenvector space size, has been defined iteratively considering the best-fit value ($\chi^2 = [\sum_{ij} (x_{ij} -$
 233 $y_{ij})/\sigma_{ij}^2]/n_{\text{points}}$, where i is the index on the spectra and j is the index on the spectral points, σ is
 234 the noise, x is the reconstructed spectrum, y is the original spectrum and n_{points} is the number of
 235 spectral points considered) between the reconstructed spectra and the initial spectra (Hopke, 1989),
 236 considering a signal to noise ratio of 100. Before PCA is performed, we cast the problem in the
 237 logarithm space, therefore multiplicative contributions become additive: this step extend the validity
 238 of eq. 1 to the solar-dominated region of the spectrum. Then we remove the mean that obviously is
 239 equivalent to a ratio of each spectrum by the average. Then the mean is included as an additional
 240 component. However, it is not necessary to remove the mean before the analysis is performed.
 241 Indeed, the retrieved spectral components are quite the same in both cases.

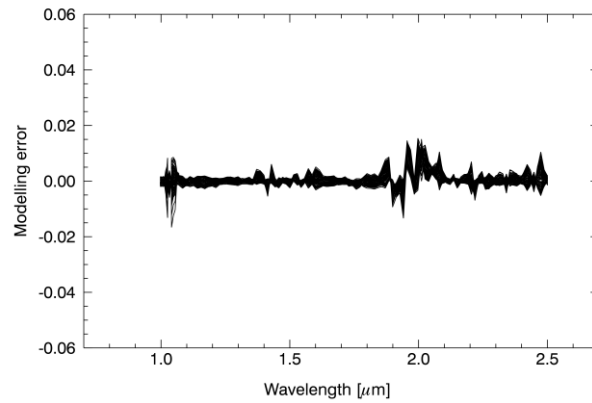
243 Based on the method described above, we compute the surface components for the simulated
244 population. Figures 3a and 3b show the result of target transformation applied to the gas and surface
245 components, respectively.

246 The **retrieved gas spectral end-member** (red line in Figure 3a), in addition to the strong CO₂
247 absorptions, shows the contribution of CO and H₂O (e.g., absorptions at about 1.35 μm and 1.9 μm
248 for H₂O and at about 2.3 μm for the CO) even if they have not been included in the trial spectrum,
249 showing the ability of the method to recognize spectral signatures even if not present in the trial
250 spectrum. **Figure 3b shows that the TT is able to infer the correct shape of the surface spectral end-**
251 **member (red line).**



252
253 Figure 3. (a) Gas spectral component (red line) retrieved by fitting the trial spectra (black line) with a linear
254 combination of significant eigenvectors. The gas trial spectrum (black line) is a simulated spectrum, which considers
255 the contribution of carbon dioxide only. (b) Surface spectral component (red line, shifted for clarity) defined as the best-
256 fit representation of trial spectrum (black line) with a linear combination of significant eigenvectors. The trial spectrum
257 for the surface component (black line) is the linear combination of the dark and bright surface reflectance shown in
258 Figure 1.

259
260 Once the weights of each spectral component have been computed for every spectrum of the
261 population, the surface reflectance is retrieved. The residuals (Figure 4) show the percentage error
262 of the method and it is computed as the difference between the true surface and the retrieved surface
263 normalized to the true surface. The error is less than 1% except in few spectral points where it
264 reaches values of about 2%.



265

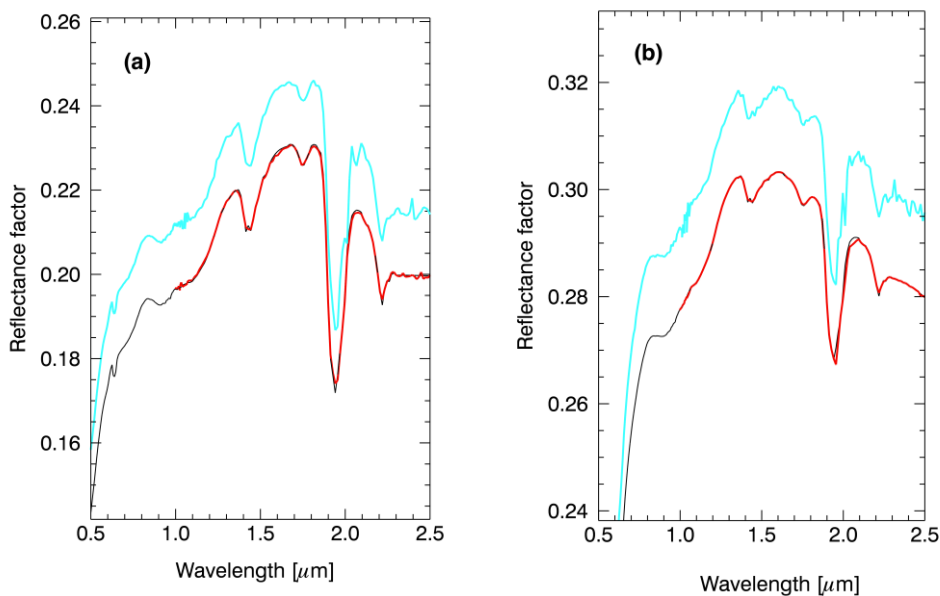
266

267 Figure 4. Modelling error computed as the difference between the true surface and the retrieved surface normalized to
 268 the true surface.

269

270 Figure 5 shows the retrieved surface components (red spectra) for two spectra of the population.
 271 The method, described in the present work, **permits** a successful reconstruction of the surface
 272 **reflectance** (being the residual errors less than 2%) and of the spectrum (Figure 6). **We check also if**
 273 **the elevation variability is necessary for the application of the method. Therefore, we consider a**
 274 **simulated population where the atmospheric path length is uniform and only the surface spectra are**
 275 **variable. The method works very well even in this case, showing almost the same residuals of**
 276 **Figure 4. Indeed, we still have a variability that makes the PCA working fine.**

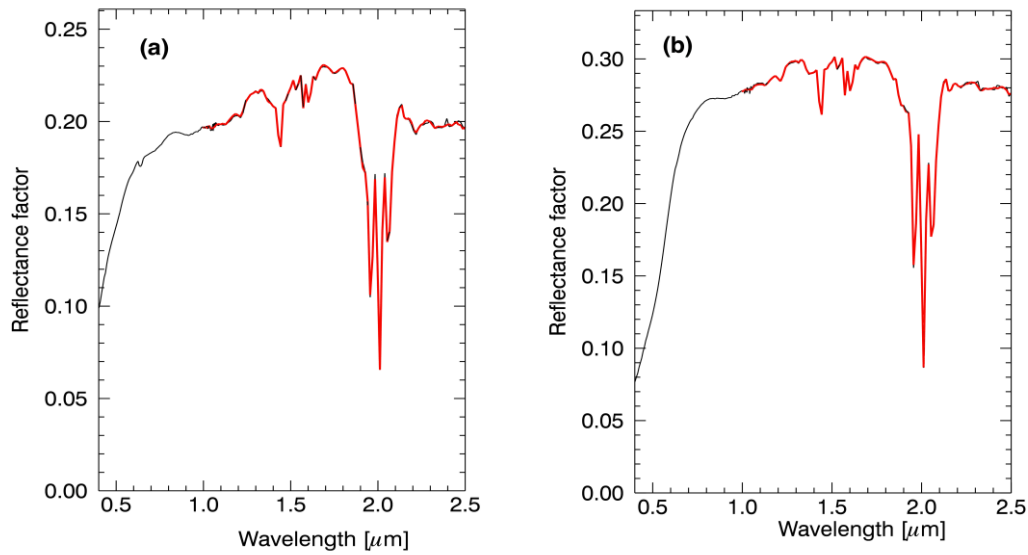
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278

279 Figure 5. (a) Spectrum whose surface reflectance is made by 1% of bright component and 99% of dark component. (b)
 280 Spectrum whose surface reflectance is made by 50% of dark component and 50% of bright component. The retrieved
 281 surface reflectances are the red line over imposed to the true surface reflectance (black line). Shifted for clarity the

282 surface reflectance obtained with the MO method (cyan line).



283

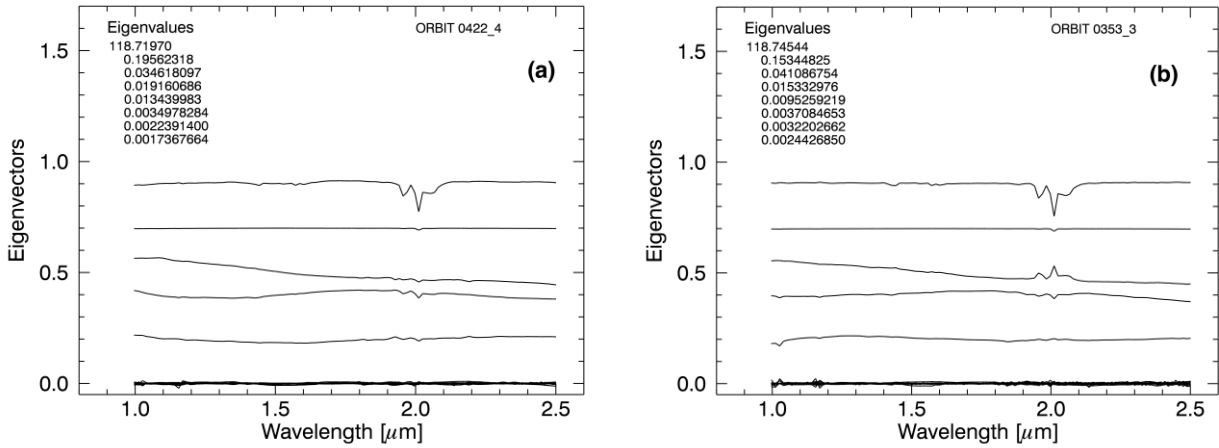
284 Figure 6. Reconstructed spectrum (red line) compared to the initial population (black line) for the same cases of Figure
285 5.

286

287 4. Application to the OMEGA data

288 4.1 Trials and first guess discussion

289 We have applied the procedure described in Section 3 to OMEGA cubes 0422_4 and 0353_3,
290 covering Nili Fossae and Mawrth Vallis, respectively. The application of the PCA to both datasets
291 reveals that five eigenvectors (Figure 7a and 7b, for cube 0422_4 and 0353_3, respectively) have a
292 spectral shape above the noise, meaning that at least five components mostly influence the dataset.
293 We apply the same procedure described in Section 3.2 and chose as trial spectra for the surface the
294 reflectance obtained using the MO method, while the gas components are the same used for the test
295 case with a correction at 2.039 μm because of a bad spectel (Forget et al, 2007). By using the
296 **already existing spectral shape for the surface end-member** as a first guess in the SAS analysis we
297 can reach meaningful solution for every spectrum in the analyzed dataset. In fact, the MO method
298 provides a surface reflectance that at first order well represent the mineralogical diversity as
299 reported in the OMEGA and CRISM data analysis literature and in the derived spectral indexes
300 used to map on a global scale the different class of minerals found on Mars (eg. Poulet et al., 2008;
301 Pelkey et al., 2007; Carrozzo et al., 2012; Ody et al., 2012).



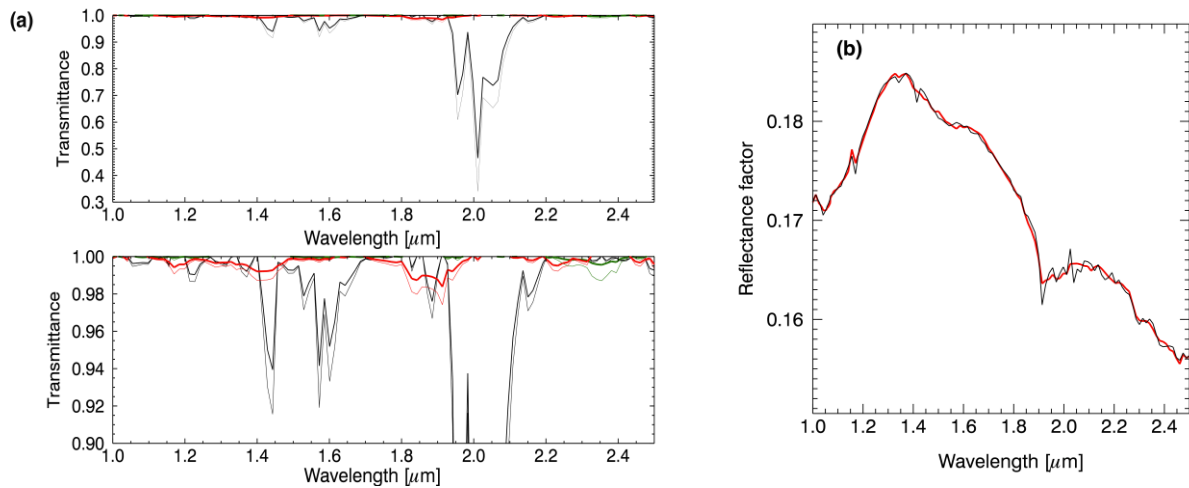
302

303 Figure 7. Eigenvectors (shifted for clarity) retrieved using PCA for the two considered orbits. Only the first eight
 304 eigenvalues are listed.

305

306 4.2 Nili Fossae, orbit 0422_4

307 The eigenvectors obtained after the PCA has been applied to the spectral population of orbit 0422_4
 308 clearly indicate that the principal components that influence this dataset are characterized by
 309 gaseous spectral features and surface spectral shape (Figures 7a). As described in the test case, we
 310 consider a number of eigenvectors that gives the best reconstruction of the spectra when compared
 311 (by means of the chi-square test) with the original spectra measured by OMEGA. This ensures that
 312 we are observing the best combination of the retrieved end-members. Figure 8a shows the retrieved
 313 gas spectral components and their amplitude in the dataset. This is possible using the retrieved
 314 weights (C matrix in Formula 1) obtained by projecting the spectral population in the space defined
 315 by the retrieved end-members. The weights of the gas spectral components multiplied to the gas
 316 end-member give the gases opacities, since we are working in the logarithm space. Target
 317 transformation projection of surface trials in the space defined by the eigenvectors and the resulting
 318 best fit of the linear combination of the selected eigenvectors with the trial component is plotted in
 319 Figure 8b for a spectrum where the hydrated band is present.



320

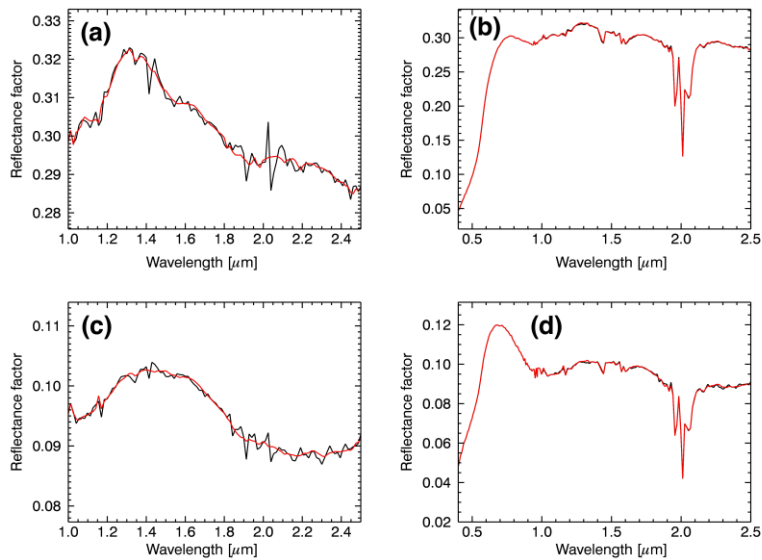
321 Figure 8. (a) Retrieved transmittances corresponding to the maximum (thick line) and minimum (thin line) weights. The
 322 CO₂ transmittances are the black lines, the H₂O transmittances are the red lines and the CO transmittances are the green
 323 lines. The lower panel is a widening of the upper panel to have a better viewing of the CO and H₂O transmittances.
 324 (b) Surface trial (black line) and retrieved surface end-member (red line) for a case where the hydrated band is present.

325

326

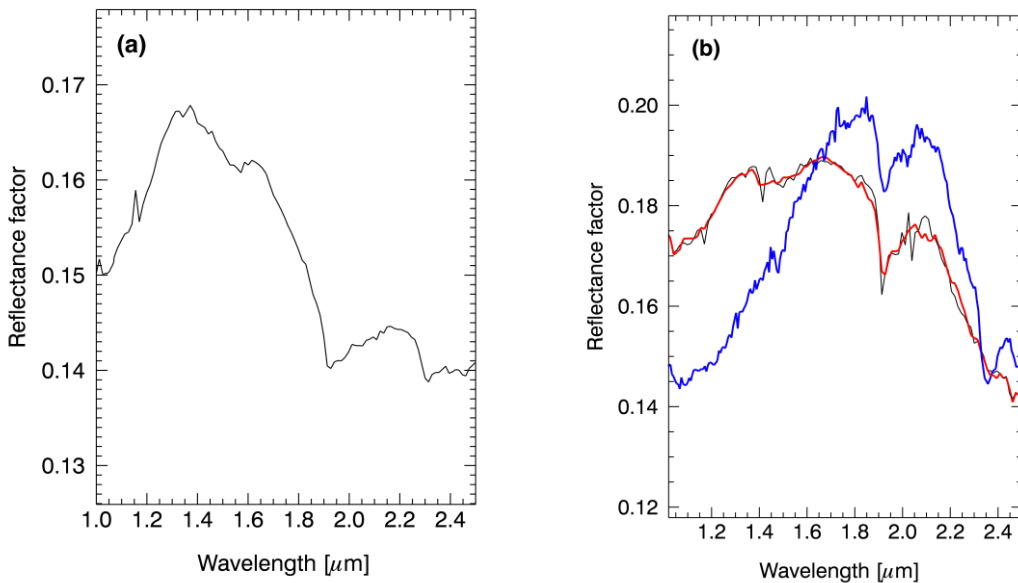
327 Figure 9 displays the retrieved surface reflectance for bright and dark surfaces from cube 0422_4.
 328 The surface reflectances obtained using SAS procedure are similar to the ones retrieved with MO
 329 method, but a reduced noise and a better evaluation of the spectral shape of the surface are obtained
 330 in the spectral region where the gaseous component is stronger, in particular around 2 μm.

331 In Nili Fossae region the 2.3 μm band has been detected (e.g., Poulet et al., 2005; Mangold et al.,
 332 2007; Mustard et al., 2007; Michalski et al., 2010) in association with the hydration band at 1.9 μm.
 333 This combination of absorptions was attributed to Fe/Mg-rich clays. Figure 10a shows one of these
 334 peculiar spectra as an example of the result obtained by the application of the SAS procedure to a
 335 surface spectrum characterized by phyllosilicates features. In some cases we also observe a shift in
 336 the minimum of the band at 1.9 μm (see one case in Figure 10b, red line). This shift consists of one
 337 spectral point compared with the spectra of surface obtained with MO method (black line). In order
 338 to make a deeper check on this result, we search for spectra of surface in the same region of Mars
 339 using the dataset of CRISM/MRO instrument. Figure 10b shows a spectrum (blue line) from
 340 CRISM instrument (on the same spatial region, even if CRISM spectrum is obtained at much higher
 341 spatial resolution than OMEGA spectrum) where the position of the 1.9 μm band coincides with
 342 that of our retrieved surface reflectance.



343

344 Figure 9. Spectra from orbit 0422_4 crossing bright and dark surfaces. (a and c) Surface reflectance factor retrieved
 345 using the methodology described in the paper (red spectra) overlying to surface reflectance obtained using MO method
 346 (black spectra). (b and d) Original OMEGA spectra (black line) underlying the retrieved spectra (red line) using the
 347 SAS procedure (red line).

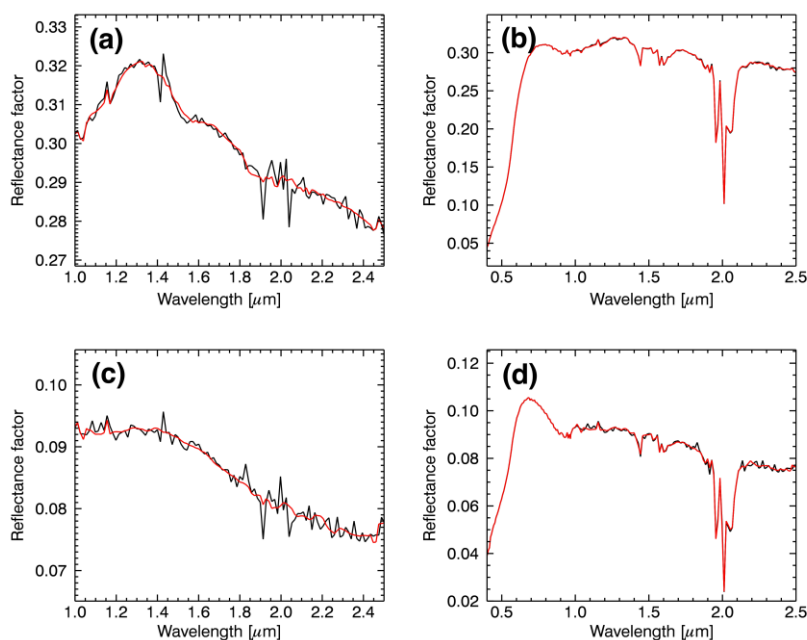


348

349 Figure 10. (a) Surface reflectance from orbit 0422_4 showing the absorption at 1.9 μm associated to 2.3 μm band
 350 indicating Fe/Mg-rich clays. (b) Surface reflectance factor showing the spectral feature of hydrated minerals at 1.9 μm ,
 351 2.3 μm and 1.4 μm in Nili Fossae region of Mars (MEX orbit 0422_4). The red line is the surface reflectance retrieved
 352 with the SAS procedure, the black line is the surface reflectance obtained with MO method, and the blue line is a
 353 CRISM observation of the same region but with a higher spatial resolution. The SAS method has not been applied to the
 354 CRISM spectrum in the figure, but the atmospheric features have been removed with “volcano scan” method (McGuire
 355 at al., 2009).

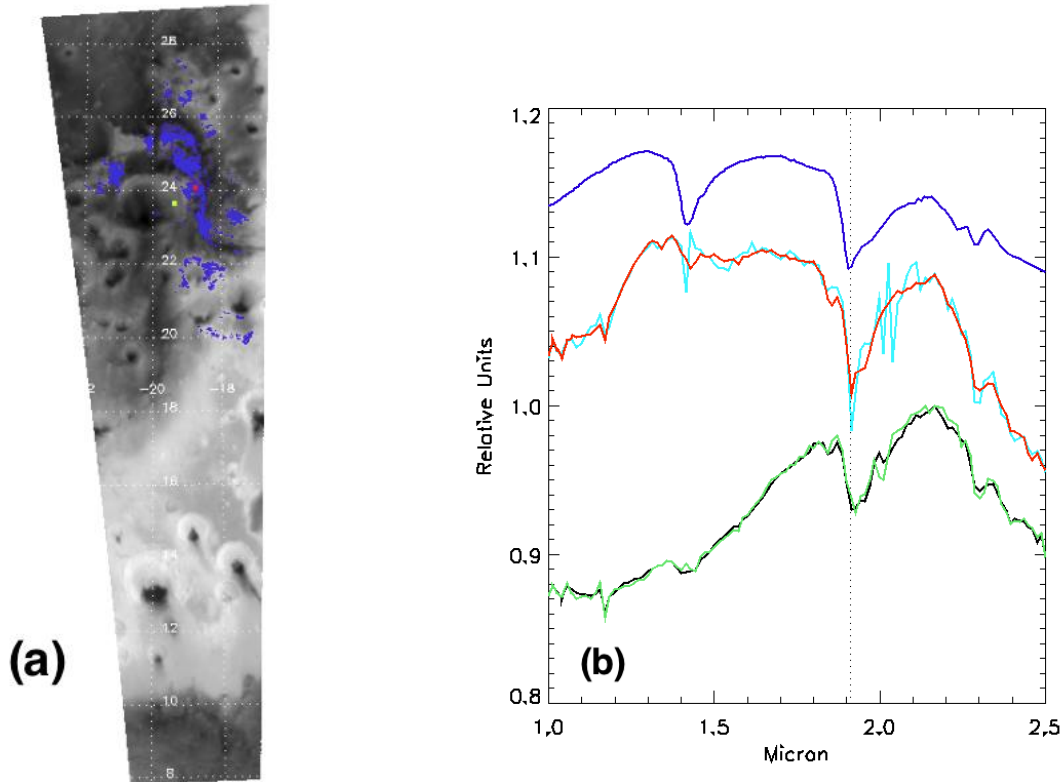
357 **4.3 – Mawrth Vallis, orbit 0353_3**

358 In this session we present and discuss the results of the SAS procedure to the OMEGA spectra from
 359 orbit 0353_3. Figure 7b shows that the principal components obtained with the PCA have the
 360 typical features of the gas and surface shape. The application of target transformation can be seen in
 361 Figure 11. The reconstructed spectra with the SAS method are indistinguishable from the original
 362 spectra except for the noise that is reduced after the application of SAS method. The absorption at
 363 1.9 μm is present in many regions of the area as shown in the map of Figure 12a, where the violet
 364 colour indicates spatial regions where the spectral index values of 1.9 μm band (as defined in
 365 Loizeau et al., 2007) derived from the retrieved surface, are higher than 2.5%. We consider an
 366 average of nine surface spectra (the average should remove random noise), from both the MO and
 367 SAS methods, located in the region of the map indicated with a red box. These spectra are all
 368 characterized by hydrated mineral features and their average is shown in Figure 12b with cyan and
 369 red colours for MO and SAS method, respectively. To remove residuals due to atmospheric gases,
 370 the ratio with a featureless surface reflectance measured in a region (yellow box in Figure 12a) very
 371 near to the selected area has been considered and shown as green and black coloured spectra in
 372 Figure 12b for MO and SAS method, respectively. The spectrum retrieved with our statistical
 373 analysis shows clearly the main hydrated features if compared with the spectrum of nontronite
 374 (violet line) taken from the USGS mineral spectral library (Clark et al., 1993) and does not differ
 375 substantially from the normalized spectra.



377 Figure 11. Spectra from orbit 0353_3 crossing bright and dark surfaces. (a and c) Surface reflectance factor retrieved
 378 using the methodology described in the paper (red spectra) overlying to surface reflectance obtained using MO method
 379 (black line). (b and d) Original OMEGA spectra (black line) underlying our retrieved spectra (red line).

380



381

382 Figure 12. (a) The violet area is characterized by a band depth at $1.9 \mu\text{m}$ higher than 2.5% (as derived from the retrieved
 383 surface) overlying the albedo map at $1 \mu\text{m}$ of orbit 0353_3. (b) The violet spectrum is a laboratory spectrum of
 384 nontronite, red and cyan spectra are surface reflectance (normalized at $1.4 \mu\text{m}$ and shifted for clarity) obtained with the
 385 SAS and MO analysis respectively and corresponding to the region indicated with a red box in the map. Green and
 386 black lines are surface reflectances measured around the pixel indicated with the red box and rationed with a featureless
 387 spectrum measured in the region indicated with a yellow box in the map, considering the MO and SAS method
 388 respectively.

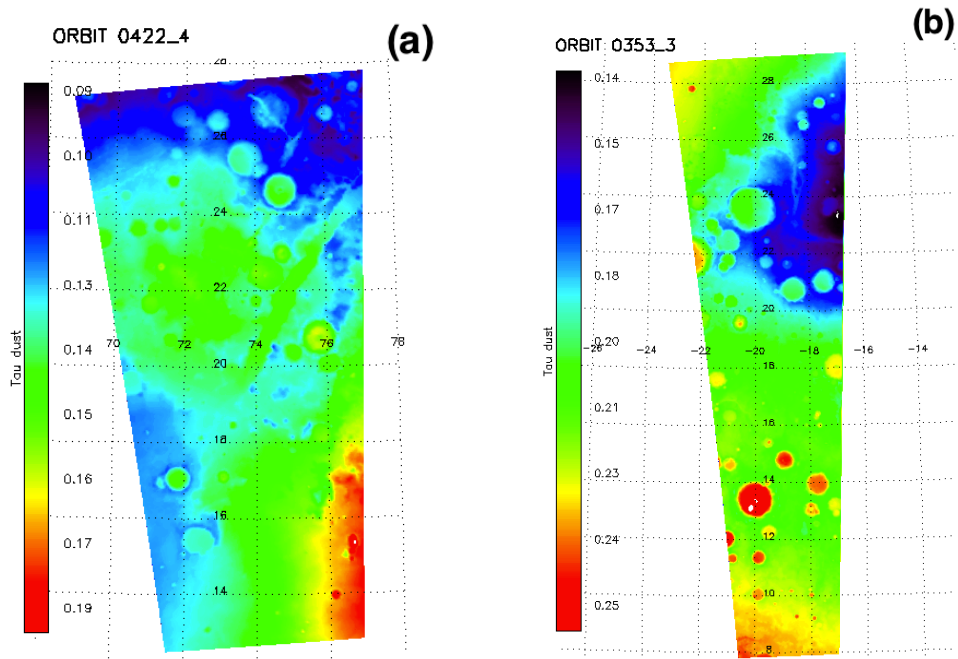
389

390 4.4 Correction for the effect of atmospheric dust

391

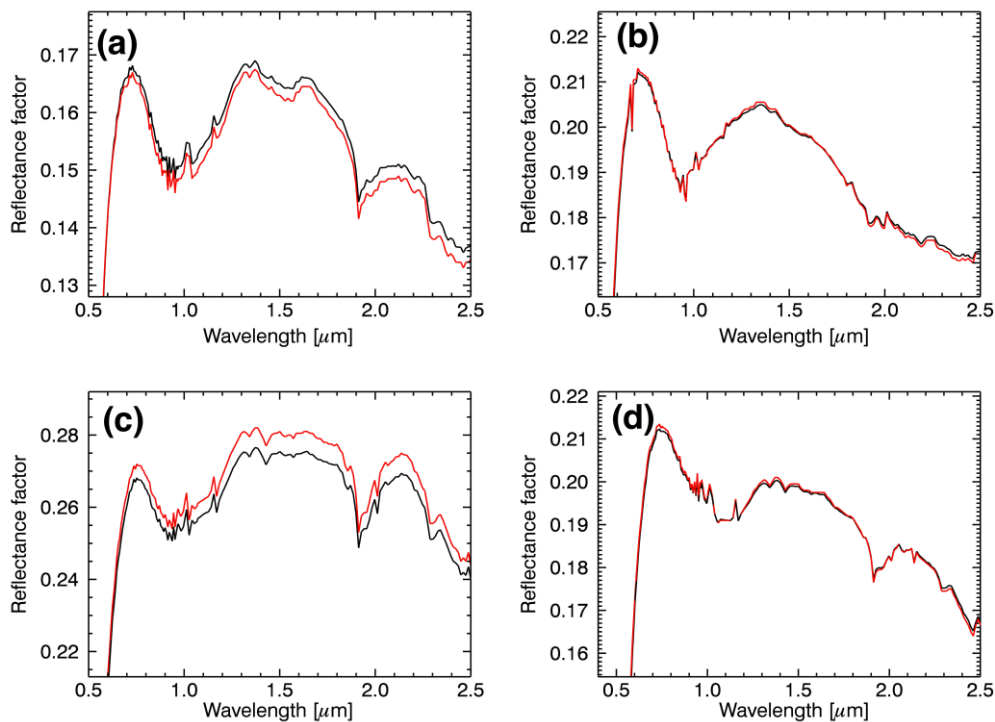
392 Dust is always and everywhere present in the Martian atmosphere showing opacity variation with
 393 season and **location** as described in Smith (2004). Mars experiences global dust storms as well as
 394 local dust storms and small-scale dust devils. Uplifted dust strongly influences the thermal structure
 395 of the atmosphere. During the observational session of orbit 0442_4 the dust optical depth τ (at
 396 1070 cm^{-1}) ranges from 0.1 to 0.2, as reported in MCD and shown in Figure 13a. The dust optical

397 depth is slightly higher for orbit 0353_3 (Figure 13b), especially in the atmospheric column above
398 craters south of 16° of latitude, where τ can be greater than 0.25. We extract the value of dust
399 optical depth from MCD to have the value of τ influencing each spectrum. The dust input scenario
400 is the one called “Mars Year 24” (MY24) designed to mimic Mars as observed by Mars Global
401 Surveyor from 1999 to 2001, a Martian year thought to be typical (MCD, user manual). Vincendon
402 et al. (2007) used a Monte Carlo approach to determine both the aerosol thickness and the surface
403 reflectance factor free from the aerosol contribution at each wavelength in OMEGA near-infrared
404 spectra for high-latitude regions of Mars. We apply the same approach from visible to near-infrared
405 spectral range (from $0.4 \mu\text{m}$ to $2.5 \mu\text{m}$) considering that the observed reflectance factor at a given
406 wavelength is a function of surface reflectance and τ . Taking advantage of this relationship and
407 knowing τ a priori, we use a multiple-scattering radiative transfer code to simulate reflectance
408 factor, assuming the most recent properties for the atmospheric dust (Wolff et al., 2009) and using
409 the observing geometries for each observation. The grain size distribution of dust is described with
410 a log-normal function where the grain effective radius is $1.6 \mu\text{m}$ and the effective variance of
411 distribution is $0.35 \mu\text{m}$. The surface reflectance factor is determined as the value **that** corresponds to
412 the best fit between the observed reflectance factor and the simulated one for each wavelength.
413 The effect of the dust on the spectra depends on the surface reflectance. For dark surfaces the effect
414 of dust is to increase the reflectance while, on contrary, for bright surfaces is to decrease the
415 reflectance. For intermediate values of surface reflectance the effect of atmospheric dust is not
416 distinguishable from that of surface dust. These effects are shown in Figure 14 where two spectra
417 from orbit 0422_4 and two from orbit 0353_3 corrected for the effect of dust are plotted. The
418 displayed surface reflectance shows how the effect of dust can be different for bright (Figure 14a,
419 orbit 0422_4) and dark (Figure 14c, orbit 0353_3) surfaces and how the presence of atmospheric
420 dust cannot be distinguished for intermediate values of surface reflectance (around 0.2, Figure 14b
421 and 14d for orbit 0422_4 and 0353_3, respectively). It is also evident that the narrow spectral
422 features of the surface are not modified by the effect of dust due to scattering, while the continuum
423 is influenced by the dust contribution.



424

425 Figure 13. Maps of dust optical depth (at 1070 cm^{-1}) as extracted from MCD. (a) Orbit 0422_4 and (b) orbit 0353_3.



426

427 Figure 14. (a) Orbit 0422_4: pixel 75, scan 152. (b) Orbit 0422_4: pixel 77, scan 111. (c) Orbit 0353_3: pixel 41, scan
 428 582. (d) Orbit 0353_3: pixel 38, scan 538. The black line is the surface reflectance and the red line is the surface
 429 reflectance corrected for the effect of dust in the atmosphere. The dust optical depths are 0.137 and 0.138 and 0.217 and
 430 0.172 for the shown spectra of orbit 0422_4 and 0353_3, respectively.

431

432 **5. Application of MGM analysis to Martian surface spectra**

433 Removing the atmospheric contribution in the Martian VNIR-IR spectra is crucial to study and map
434 the surface mineralogy from remote sensing data. In this Section we discuss how the Martian
435 surface spectra retrieved by means of the SAS method can be used to study in details the
436 mineralogy of Martian surface, with particular attention to hydrated phases. We spectrally analyse
437 the two OMEGA cubes, from Nili Fossae and Mawrth Vallis, focusing on the retrieving of the
438 Martian mineralogy by using the MGM (Sunshine et al., 1990). In particular, we focus our analysis
439 on those minerals characterized by absorption bands centered at 1.9 μm to 2.3 μm , representative of
440 hydrated minerals, in which spectral range the atmospheric contribution is more important. In order
441 to validate the surface spectra obtained through the SAS method, we apply the MGM deconvolution
442 to both a set of laboratory spectra of minerals of recognized hydrated silicates on Nili Fossae and
443 Mawrth Vallis and to the SAS OMEGA spectra.

444 The MGM is a statistic-base method based on the assumption that different mineral absorptions can
445 be described with a modified Gaussian distribution superimposed on to a continuum. It is widely
446 applied on mineral phases and mixtures analysis, in particular for the electronic absorptions (e.g.,
447 Sunshine et al., 1990; Sunshine and Pieters, 1993, 1998; Klima et al., 2007, 2011; Clenet et al.
448 2011; Serventi et al., 2014submitted). Different papers used also Gaussians models to determine the
449 vibrational overtones present in hydrated silicates, carbonates and sulfates measured in laboratories
450 (see Sgavetti et al., 2015; and references therein). Mustard et al. (2005) showed how pyroxene-rich
451 areas on Mars have wide absorptions at 1 and 2 μm on OMEGA data and how applying the MGM it
452 is possible to separate orthopyroxene from clinopyroxene contribution. Recently, Clenet et al.
453 (2013) applied the MGM to OMEGA data exploring the mafic mineralogy of Syrtis Major. The
454 authors highlighted how the application of MGM on OMEGA data permits to separate the different
455 contribution of mafic minerals and to quantify their parameters.

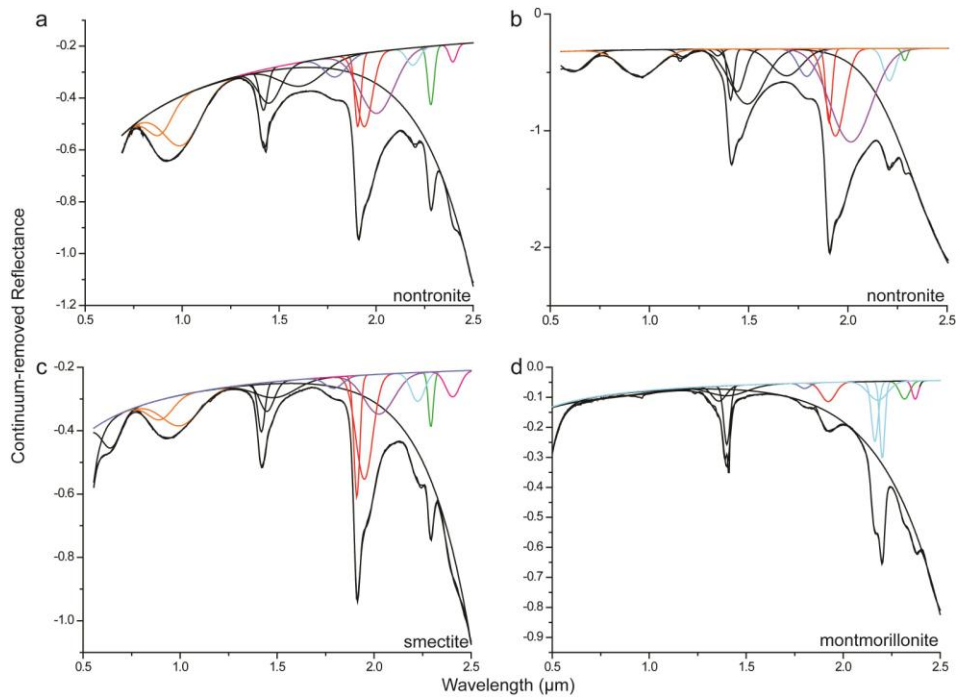
456 Here, we apply the MGM considering:

- 457 1) the continuum as a straight line as function of the wavenumber, with two parameters, the
458 offset and the slope (Sunshine et al., 1990);
- 459 2) each Gaussian is described by three parameters: the band depth (in logarithm of the
460 reflectance), the band center and the band width, or FWHM (both in nanometers).

461 We choose a continuum that model the real strength of the absorption bands (see also Clenet et al.,
462 2011) thus avoiding an horizontal continuum by choosing a fixed, tangent continuum. On the other
463 hand, Gaussians spectral parameters are free to vary. The goodness of the fit is expressed by the
464 RMS (root mean square) value.

465

466 We select spectra of some clay minerals (e.g., nontronite and smectite) from USGS spectral library
467 (Figure 15 and Table 1), which can be considered analogues to Martian phases. Taking into account
468 the literature, which discusses the mineralogy of the selected regions, we consider nontronites,
469 smectites and montmorillonites as laboratory hydrated phases. These minerals belong to the
470 smectite family, already recognized on Martian surface, as in Nili Fossae (Ehlmann et al., 2008) and
471 are characterized by absorption bands comparable with spectra here analysed. Electronic
472 absorptions characterize the 0.5-1.2 μm spectral region and, in particular, bands centered between
473 0.8 and 1.2 μm are due to Fe^{2+} transitions. On the other hand, overtones and combination of modes
474 characterize the longest wavelength. In particular, smectite, nontronite and montmorillonite have
475 the strongest water overtones near 1.41 μm and water combination bands near 1.92 μm . As shown
476 in Ehlmann et al. (2008; and references therein) the absorption at 1.4 μm (due to the OH stretching)
477 depends on the octahedral cations present in crystal structure of hydrated minerals. The stretching
478 occurs at 1.43 μm , at 1.41 μm and at 1.38-1.39 μm if the cation is Fe, Al or Mg, respectively. H-O-
479 H combination stretching and bending vibrations occur near 1.92 μm and 1.97 μm , respectively
480 (Bishop et al., 2008). Weak combination bands have been detected at 2.0 μm for adsorbed water in
481 hydrated minerals. Strong OH combination bands are also present in the 2.2-2.5 μm spectral region,
482 and, as the 1.4 μm absorption, their position is a function of the octahedral cation composition. In
483 general, the OH combination bands occur at 2.17-2.21 μm , 2.29-2.31 μm and 2.32-2.34 μm if Al,
484 Fe^{3+} and Mg are in the octahedral sites, respectively. Al/Fe-OH combination bands occur at 2.24
485 μm . If the cation is the Fe^{2+} the band is centered at 2.35-2.37 μm . Bishop et al. (2002a) interpreted
486 the additional bands between 2.4 μm and 2.5 μm as due to further OH stretching and bending.
487 Bands at 1.6-1.8 μm have not been recognized in the literature, and they can be due to the
488 continuum-removal applied in our deconvolution.



489

490 Fig. 15 MGM deconvolution on laboratory hydrated minerals: a,b) nontronites; c) smectite; d) montmorillonite. Spectra
 491 selected from the USGS spectral library are the black lines; the absorption contributions obtained with the MGM
 492 deconvolution are shown with colored lines.

493

494 As a result we can clearly determine the different absorption contributions on overtone and their
 495 combinations, and differentiate the various phases bearing to the clay minerals by considering the
 496 position of Modified Gaussians.

497 The same MGM approach is also applied on OMEGA surface spectra of the two considered orbits
 498 where hydrated phases were recognized, as derived by both the MO method and the SAS one.
 499 Results are shown in Figure 16 and summarized in Table 1. We find that:

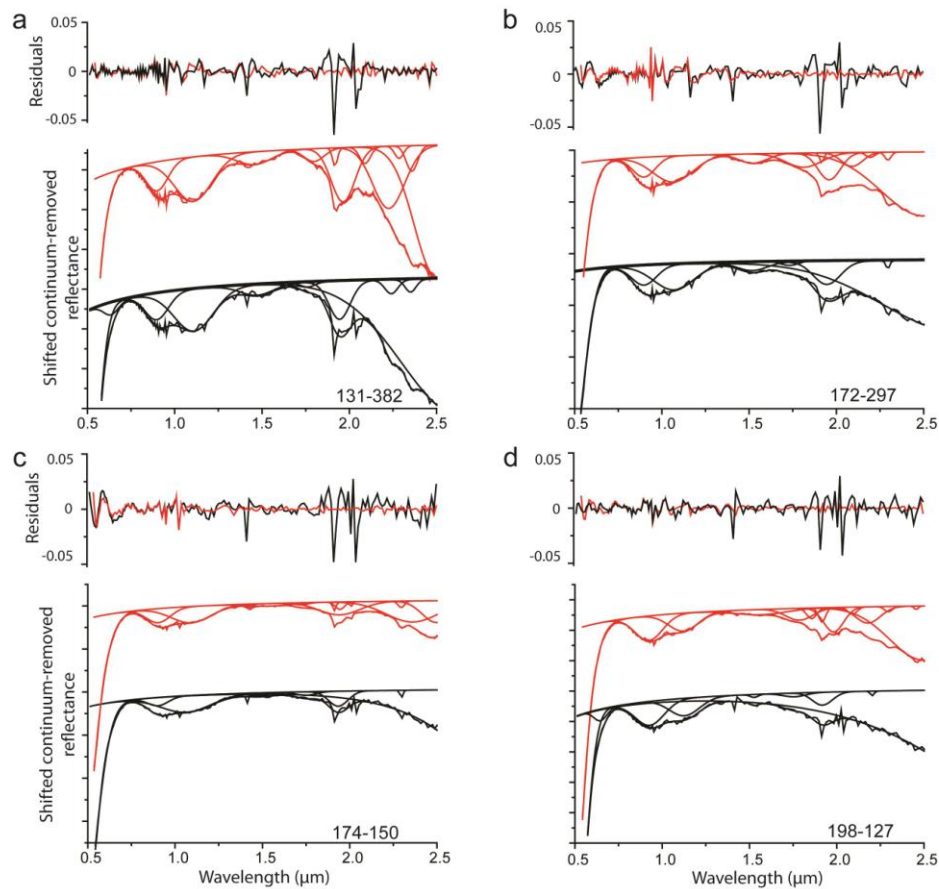
- 500 a) very few differences are present in the 0.5-1.4 μm spectral region, comparing spectra after
 501 application of MO or SAS;
- 502 b) in the NIR range, spectra processed with the SAS method allows to recognized more
 503 absorptions within the composite bands and, therefore, an higher number of Gaussians is
 504 requested with respect to the MO method, likewise for the laboratory spectra dataset.

505 The main differences are in the 1.9-2.1 μm spectral region. In the MO surface spectra, the
 506 absorption bands are described with only two or three Gaussians despite the higher Gaussian
 507 number used for hydrated minerals, and residuals due to atmospheric contribution are high. On the
 508 contrary, in spectra corrected with SAS method, the same spectral region can be described with
 509 five/six Gaussians with a slight variation in position and depth, better fitting the overtone

510 absorptions and revealing differences in hydrated mineralogy or in their abundance. Moreover,
511 spectral residual is five times lower.

512

513



514

515 Figure 16 Figure shows Gaussians and residuals after MGM deconvolution. Black: spectra acquired from images after
516 MO; red: spectra acquired from images after SAS. a,b : Nili Fossae; c,d: Mawrth Vallis.

517

518 It is clear that MGM on laboratory minerals shows deeper bands, explainable with different reasons,
519 such as different particle sizes, presence of darkening agents and mixing effects on a planetary
520 surface, etc.

521 The band centers obtained for the spectra after the SAS correction are comparable with those
522 obtained from laboratory spectra. This indicates that hydrated mineralogy can be evidenced by
523 applying MGM on spectra corrected by SAS, and we have seen that the selected spectra are
524 comparable with the composition indicated in the literature (Ehlmann et al., 2008, 2009; Poulet et
525 al., 2008). Moreover we can model the different absorption processes of these spectra. This aspect
526 allows to better quantify and separate the possible different clay phases. Differences of few

527 nanometers can be due either to a mix of hydrated minerals in the analysed regions or to a slightly
 528 different composition.

529 On the contrary, the lesser number of Gaussians recognized in spectra after MO correction can lead
 530 to difficulties in mineralogical interpretation after MGM deconvolution. In fact, the wider
 531 Gaussians resulting in the spectra after MO correction (Figure 16) do not permit to separate and to
 532 recognize all the vibrational contributions present in the overtone bands, as expected from the
 533 analysis of laboratory data (Figure 15).

534 In conclusion, by decreasing the level of both the atmospheric residuals and random noise in the
 535 OMEGA data when retrieving the surface component, SAS method enable us to improve the
 536 investigation of hydrated mineralogy present in Nili Fossae and Mawrth Vallis by means of MGM.
 537 A higher number of Gaussians can be considered with respect to the previous technique in the 1.8-
 538 2.1 μm spectral range and a better comparison with laboratory data is reached.

539

540

131-382		172-297		174-150		198-127		Nontronite	Nontronite 2	Smectite	montmorillonite	Interpretation
MO	SAS	MO	SAS	MO	SAS	MO	SAS					
0.896	0.898	0.897	0.897	0.902	0.904	0.928	0.923	0.887	0.9519	0.900	0.951	Fe ²⁺
1.109	1.106	1.07	1.064	1.063	1.092	1.128	1.122	1.003		1.005		
1.470	1.455	1.518	1.522	1.485	1.427	1.527	1.568	1.42	1.409	1.419	1.364	OH
								1.45	1.443	1.448	1.392	
					1.537				1.496	1.491	1.401	
								1.617	1.692			
1.762	1.798	1.732		1.751	1.723	1.757	1.786	1.798	1.793	1.793		
			1.813				1.857				1.804	
	1.918		1.916		1.913			1.906	1.904	1.911	1.922	OH
1.944	1.965	1.946	1.959	1.935	1.943	1.918	1.916	1.94	1.937	1.95		
					1.945		1.982					
	2.09		2.09		2.005		2.09	2.005	2.015	2.027		
			2.194				2.179	2.19			2.164	Al-OH
2.241	2.226					2.203			2.209	2.226	2.203	
	2.285	2.294	2.295	2.297	2.296		2.296	2.282	2.286	2.293	2.317	Fe/Mg-OH
2.351	2.359				2.362			2.396			2.373	

541

542 Table. 1 Band centers found by the MGM deconvolution.

543

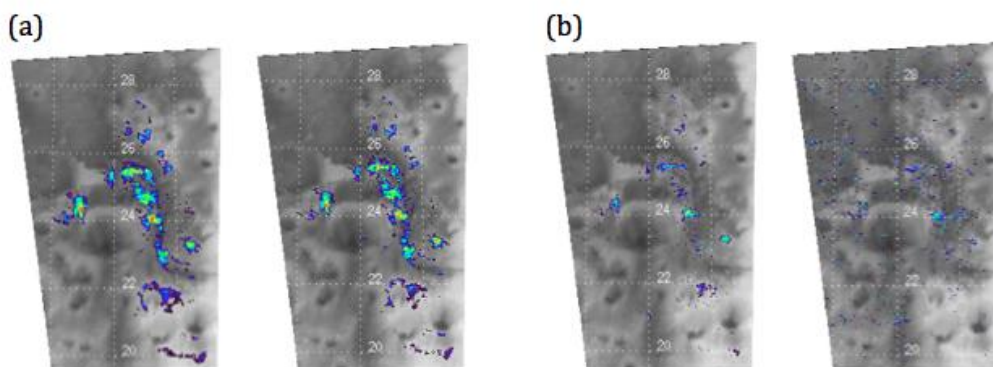
544 6. – SAS method applications

545 By completely separating the atmospheric component from the surface one, the results obtained
 546 with the method described in this work have many scientific implications for the study of the
 547 Martian orbiter data in the infrared spectral range:

- 548 • Since each gas spectral end-member can be isolated and their opacities can be estimated by
 549 means the TT, it is possible to retrieve the geographical distribution of the gaseous
 550 components. In particular the opacities distribution as well as the gaseous column density

551 (if a uniform mixing is assumed with altitude in the atmosphere and the absorption
 552 coefficients are known) can be determined.

- 553 • The final surface spectra we are able to obtain are of great importance, for example, in the
 554 study of ice clouds where the knowledge of each spectral component (including the dust
 555 contribution to the spectra) is crucial to estimate the ice properties.
- 556 • The spectral index maps can be greatly improved, especially for weak mineralogical
 557 absorption bands. In Figures 17a and 17b we compare our spectral index maps with those
 558 obtained with MO method. We consider orbit 0353_3 (Mawrth Vallis) and spectral index
 559 maps at 1.93 μm and 2.3 μm . The comparison shows that, for the 1.93 μm spectral index
 560 maps, the two methods give the same results, while at 2.3 μm the map obtained with SAS
 561 method is considerably improved respect to the one obtained with MO method.
- 562 • Usually, in order to minimize the MO atmospheric residuals and retrieve a smoother surface
 563 relative component to be compared with mineral spectral libraries, the analysis of OMEGA
 564 and CRISM spectra requires the ratio with a featureless surface reflectance measured in a
 565 region very near to the selected area. Hydrated mineralogical features in the OMEGA
 566 surface reflectance spectra retrieved by SAS (in particular in the 1.8-2.1 μm range) show a
 567 better consistency with laboratory data, without necessary rationing the data. The SAS
 568 surface reflectance spectra can be used to deconvolve the contribution of different minerals
 569 in the data, not only those highlighted by the rationing.
- 570 • The lower level of the atmospheric and noise residuals in the retrieved surface reflectances
 571 with SAS method enables us to make a better match with the MGM deconvolution
 572 parameters found for the laboratory spectra of Martian hydrated mineral analogues,
 573 allowing a deeper investigation of this spectral range.



574
 575 Figure 17: (a) Albedo map at 1 μm superimposed with the spectral index maps of the 1.93 μm band obtained
 576 considering surface reflectance with SAS method (on the left, using as threshold the 3σ of Gaussian distribution of
 577 values) and with MO method (on the right, considering a detection threshold of 2%). (b) Albedo map superimposed
 578 with spectral index maps of the 2.3 μm band obtained considering surface reflectances with SAS method (on the left,

579 using as threshold the 3σ of Gaussian distribution of values) and with MO method (on the right, considering a detection
580 threshold of 2%).

581

582 7. – Conclusion

583 The removal of atmospheric contribution from reflectance spectra measured by airborne
584 instruments is crucial to investigate the features of the surface, which are on the same spectral
585 regions of atmospheric components. In particular, the vibrational absorption bands due to water and
586 O-H bound in the near infrared region of the spectrum overlap with atmospheric water and CO₂,
587 compromising the mineralogical deconvolution. The standard processing approach to remove the
588 atmospheric contribution is to divide the surface reflectance data by a scaled atmospheric spectrum
589 measured across Olympus Mons, and to suppress the residual errors by dividing the target spectrum
590 by a low spectral contrast reference spectrum of the same session apparently without any relevant
591 features. This method assumes that any instrumental contaminations, as well atmospheric residuals,
592 affect in the same way the two considered spectra. The SAS method based on the principal
593 component analysis and target transformation removes the noise and atmospheric gaseous
594 components from the reflectance spectra, thus allowing to deeply investigate hydrated minerals on
595 the Martian surface. Moreover, the contribution of dust in the atmosphere is also removed by
596 modeling its effect on each spectrum. We first apply the SAS method on a simulated spectral
597 population in order to evaluate its accuracy and then on two OMEGA orbits where hydrated
598 minerals have been already found. The surface reflectance obtained with the SAS method is almost
599 free from instrumental noise and residuals due to atmospheric components (gases and aerosols) are
600 removed.

601 The surface reflectances obtained for two sessions of observations over Nili Fossae and Mawrth
602 Vallis regions have been investigated by means of MGM, comparing the results obtained from
603 spectra of the same pixel after MO and SAS treatment. In particular, surface spectra showing the
604 hydrated phase have been selected because the diagnostic vibrational absorptions of these minerals
605 are superimposed to the atmospheric absorptions. The information on mineralogy is obtained
606 considering laboratory data, which allows to define the different electronic and vibrational
607 processes to be compared with the measured spectra at Mars. Absorptions between 0.8-1.2 μm can
608 be assigned to electronic Fe²⁺ transitions, both in mafic silicates and in iron-bearing hydrated
609 phases, while absorptions at higher wavelengths reveal the presence in the spectra of overtones of
610 the OH group, in particular Al-OH and Mg-OH overtones. Moreover spectra treated with SAS show
611 a better definition of overtone processes after MGM application, showing a clear reduction of the
612 level of the atmospheric residuals in the 1.8-2.1 μm spectral range. This residual reduction permits

613 to better define the vibration processes indicative of the hydrate minerals present in remote sensing
614 data and improve the comparison with laboratory data.

615 As a further application of our work, we will apply the SAS (including the dust correction) method
616 and MGM to the different surface conditions present on Mars.

617

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621 technical supports.

622

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- We retrieve the surface component from near-IR reflectance spectra.
- We apply the principal component analysis and target transformation to OMEGA spectra.
- Atmospheric dust is removed by means of a radiative transfer model.
- A test spectral population is used to validate the method used in this work.
- MGM analysis shows an improved match of our result with laboratory analogues.