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A new analysis method for the reflectance spectra of silicates using Bayesian estimation

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Introduction: Visible and near infrared (VNIR) reflectance spectroscopy is a very powerful tool to observe planetary surfaces remotely and has revealed a wide variety of information on planetary surfaces [e.g., 1]. Because silicates often exhibit overlapped absorption bands in the VNIR range, they are often deconvolved into multiple simple bands for quantitative analyses.

Conventional MGM Algorithm: One simple approach would be to search for the optimum combination of simple bands that minimize the difference between observed and synthetic spectra by trying every possible parameter set. However, a direct search is usually impractical because it requires an astronomical number of trials. Thus, a more efficient mathematical method is necessary. In previous studies, the steepest descent method has been used frequently to resolve this problem, but this method is not necessarily good at finding the global minimum of a complex function with many local minima. Depending on the initial choice of parameters, an obtained result may be just a local minimum. Furthermore, this mathematical procedure needs to know how many model parameters (e.g., the number of Gaussians for MGM) should be used before the analysis. Generally, a fitting with more Gaussians will lead to a smaller error, but the complexity of the synthetics may become too large (e.g., over fitting).

New MGM Algorithm: In order to resolve these problems, we derived a new MGM algorithm using a Bayesian estimation approach, the exchange Monte Carlo (EMC) method, and the annealing method in this study. The mathematical details and numerical validation of the algorithm used in this study are given by [2,3].

Validation Analyses: In order to examine the validity and applicability of the new MGM algorithm proposed in this study, we conducted actual spectral deconvolution analyses using a series of reflectance spectra, olivine powder samples with different Mg/(Mg+Fe) ratios (mg#) and olivine-pyroxene mixtures with different mixing ratios

The results of our new MGM method indicate that the optimum number of Gaussian bands to reproduce the complex absorption band around 1 micron predicted is three for the reflectance spectra of all the olivine samples. This optimum number is the same as the number estimated empirically by [4]. Furthermore, the trends of the central wavelengths of individual bands band widths and the relative intensities of the three individual bands as functions of mg# are very similar to the results by a conventional MGM [4]. These agreements support that the results of these MGM analyses are not specific to particular datasets or analytical methods but reflect the intrinsic optical properties of olivine.

Though not all Gaussians are detected, most of the deconvolved Gaussians are close to one of the Gaussians of the end-member samples. This will allow us to identify the mineral components within such mixtures. In particular, the bands around 1.2 and 1.03 micron in the mixtures of olivine can be detected when its mixing ratio is as low as 25%.

Conclusion: The above results along with the intrinsic properties of the new algorithm (e.g., little dependence on initial parameter value selection and the capability of finding the optimum number of Gaussians) suggest that method would be appropriate for automated analyses and greatly expand the applicability of MGM greatly, particularly for large volume of spectral datasets obtained for Moon.

References: [1] Pieters, C.M. and P.A.J. Englert (1993) Remote geochemical analysis: Elemental and mineralogical composition; [2] Nagata, K. et al. (2011) Neural Networks, submitted. [3] Sugita, S. et al. (2011) JGR, to be submitted. [4] Sunshine, J.M. and C.M. Pieters (1998) JGR, 103, 13,675.

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