

COMPARING THERMAL INFRARED SPECTRAL UNMIXING ALGORITHMS: APPLICATIONS TO BENNU AND OTHER AIRLESS BODIES.

E. C. Brown¹, K. L. Donaldson Hanna^{1,2}, N. E. Bowles¹, V. E. Hamilton³, B. E. Clark⁴, A. D. Rogers⁵, D. S. Lauretta⁶, and the OSIRIS-REx Team, ¹Atmospheric, Oceanic and Planetary Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford OX1 3PU, UK (eloise.brown@physics.ox.ac.uk), ²Department of Physics, University of Central Florida, FL, USA, ³Department of Space Science, Southwest Research Institute, CO, USA, ⁴Department of Physics & Astronomy, Ithaca College, NY, USA, ⁵Department of Geosciences, Stony Brook, NY, USA, ⁶Lunar and Planetary Laboratory, University of Arizona, Tucson, AZ, USA.

Introduction: The aim of this work is to examine a selection of fitting algorithms for determining composition when applied to the traditional linear unmixing model for thermal infrared (TIR; $\sim 5\text{--}50\ \mu\text{m}$ or $2000\text{--}200\ \text{cm}^{-1}$) laboratory and remote sensing spectra. Here we outline the basic background knowledge required, discuss an alternative approach, and provide comparisons of these different algorithms using a subset of the Origins, Spectral Interpretation, Resource Identification, and Security – Regolith Explorer (OSIRIS-REx) TIR blind test spectra [1]. Current methods have produced geologically relevant mineralogies and abundances for situations with additional prior knowledge (e.g., Mars [2]), however it is uncertain if these methods work similarly in situations with limited prior information. It is therefore important to fully investigate whether such methods are appropriate for observational data that lack additional contextual information (e.g., spacecraft and telescopic data), and to see what new insights a Bayesian approach may bring.

Common approaches for unmixing TIR spectra: Several spectral unmixing algorithms have been developed with varying complexity, many of which have used the least squares technique to find end-members present in a mixture and their corresponding abundances (e.g., [2, 3]). Some of these methods have been adapted to ensure meaningful physical results (i.e., abundances must be non-negative). However, the degree of degeneracy in the retrieved compositional abundances is often unknown, especially in circumstances with relatively poor prior knowledge. When there is limited contextual information and/or noisy data (as is often the case for telescopic observations), the end-member minerals within the chosen spectral library could have multiple assemblages that each produce a statistically good fit to the data (e.g., as measured by the reduced χ^2), thus leading to degenerate results (including, possibly, geologically unlikely compositions). With traditional least squares algorithms, it can be difficult to account for these degenerate solutions, and alternative combinations of end-members may not be fully explored [4].

A Bayesian approach: In this work we adopt Bayesian inference techniques widely used to understand a variety of physical processes and phenomena (e.g., [5]). Such techniques include Markov Chain Monte Carlo (MCMC, [6]) which may be applied to the spectral unmixing problem by exploring the parameter space to determine the most probable end-member mineral abundances, each with an envelope of uncertainty. Sampling techniques such as MCMC are useful as they allow the exploration of a broad range of solutions, subject to the priors, and the analysis of the distribution of possible outcomes. Using a Bayesian perspective can be particularly insightful due to the quantitative inclusion of prior information. In the case of degenerate solutions being more likely (e.g., due to noisy spectra, low spectral contrast, or lack of wider geological context), quantitatively adding *a priori* information allows us to limit the parameter space explored whilst retaining knowledge of how this may affect the final (posterior) retrieved compositions. The input information for each parameter can be based on what is already known about the material (e.g., from the meteorite record) and can include uncertainties on this prior knowledge. Although it is still possible to retrieve unlikely compositions using MCMC, this technique will allow us to better explore possible degenerate solutions.

Data used: The OSIRIS-REx blind test study presented spectral measurements of materials thought to be compositionally analogous to target asteroid (101955) Bennu [1]. Here we use the TIR blind test physical mixtures of well-characterised mineral end-members as we have TIR spectra of both the mixtures and most of the mineral end-members, making it an ideal dataset to compare our Bayesian MCMC algorithm and more commonly used methods.

Future applications: With potential for Bayesian techniques to provide new insights into the quality of the linear fitting model, such alternative algorithms may be applied to additional laboratory data, and to data collected by missions including OSIRIS-REx [7] and the Spitzer Space Telescope [8].

References: [1] Donaldson Hanna K. L. et al. (2019) *Icarus* 319:701-723. [2] Rogers A. D. and Aharonson O. (2008) *JGR* 113:E06S14. [3] Ramsey M. S. and Christensen P. R. (1998) *JGR* 103:577-596. [4] Lapotre M. G. A et al. (2017) *JGR Planets* 122:983-1009. [5] von Toussaint U. (2011) *Reviews of Modern Physics* 83:943-999. [6] Metropolis N. et al. (1953) *J. of Chem. Phys.* 21:1087-1092. [7] Lauretta D. S. et al. (2017) *Space Sci. Rev.* 212:925-984. [8] Werner M. W. et al. (2004) *Astrrophys. J. Supp. Series* 154:1-9.