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TENSOR COMPONENT ANALYSIS AS A TOOL FOR INVESTIGATING DEPTH TRENDS IN CHEM-CAM LIBS DATA FROM GALE CRATER, MARS K. Rammelkamp^{1,2*}, O. Gasnault², O. Forni², E. Dehouck³, C. C. Bedford^{4,5}, J. Lasue², A. Cousin², S. Schröder^{1,2}, R. C. Wiens⁶, N. Lanza⁶. ¹Deutsches Zentrum für Luft- und Raumfahrt, Institut für Optische Sensorsysteme, Berlin, Germany; ²Institut de Recherches en Astrophysique et Planétologie, Toulouse, France; ³LGL-TPE, Lyon, France; ⁴Lunar and Planetary Institute, Universities Space Research Association, Houston, USA; ⁵Astromaterials Research and Exploration Science, NASA Johnson Space Center, Houston, USA; ⁶LANL, Los Alamos, USA; *kristin.rammelkamp@dlr.de

Introduction: ChemCam, the first extraterrestrial laser-induced breakdown spectroscopy (LIBS) instrument on board the Mars Science Laboratory (MSL) [1,2], has been collecting an enormous amount of data since landing in 2012 in Gale crater (> 800 000 single shot spectra of > 29 000 individual targets). With LIBS, a rapid multi-elemental analysis technique, the chemistry of martian rocks and soils can be derived. Typically, a ChemCam LIBS measurement is a raster of 5-25 observation points and at each of these points 30 successive laser shots are done [3]. With each laser shot, material slightly deeper is ablated which allows to track chemical variations with depth. In a recent study using unsupervised clustering on the entire ChemCam dataset measured until sol 2756, six clusters with characteristic compositions were identified [4]. For that study, one averaged LIBS spectrum of all spectra after shot 5 for each observation point was used. The present study is a follow-up of [4] in which we circumvent averaging the spectra of one observation point and include shot-to-shot (STS) trends in the analysis. Matrix decomposition techniques for feature extraction and/or pattern recognition such as principal component analysis (PCA) or non-negative matrix factorization (NMF) are widely used to analyze LIBS data. Those methods take two dimensional matrices as input where, in the case of LIBS data, the column usually corresponds to the measured LIBS point and the rows contain the corresponding spectra. An extension of those decomposition methods to more than two dimensions is tensor component analysis (TCA) [5]. In this study, we apply TCA to ChemCam LIBS data including STS trends as a third dimension. We will focus here on cluster 2 derived in [4] which was referred to as the felsic cluster and for which

we suspect different correlations of elemental emission lines with depth for different types of felsic minerals.

Method: Mainly two approaches for multi-way tensor decomposition exist, the Tucker decomposition and parallel factor analysis (PARAFAC) [5]. We use the latter in this study and in Fig. 1, the principle is shown schematically. The typical data matrix of ChemCam LIBS points and spectrum (wavelength, 6144 channels) is extended by a third dimension associated to the shots (here: 30). In brief, the basic idea is to decompose the tensor in a sum of rank one tensors describing variability along each of the three axes [5,6]. The number of rank one tensors needs to be fixed in advance and they cannot be determined successively like in the case of PCA. In order to prepare the spectra of the felsic cluster [4], observations points with more than 30 shots were excluded resulting in 457 from originally 485 points. All spectra were standardized (mean centered and scaled to unity variance) and shifted to only non-negative values as we apply the non-negative version of PARAFAC. We fixed the number of ranks in this study to 16 which was chosen due to a minimum in the reconstruction error. For the computation, functions provided in python's *TensorLy* [7] package were utilized.

Results:

We will discuss two of the 16 factors in some detail. The first one is factor 2 whose characteristic STS and spectral profiles are shown in Fig. 2 (*top row; left and middle*). The STS profile indicates a significant contribution in the first five shots which strongly decreases and is close to zero after shot 10. Such a trend is expected for superficial contributions which are not part of the underlying rock, such as coatings or dust. Inter-

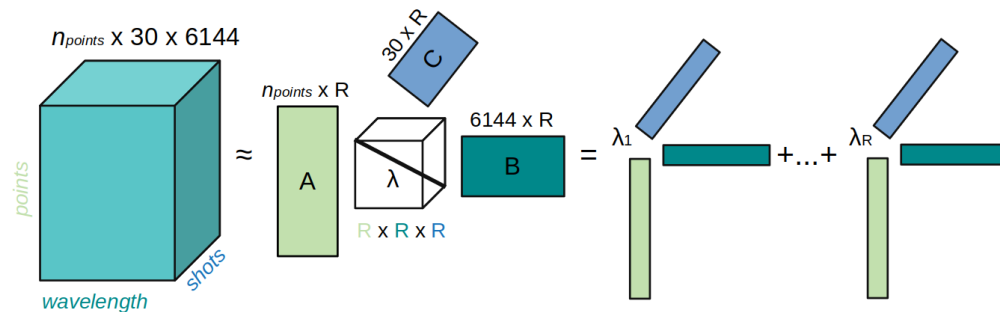


Figure 1: Schematic representation of the PARAFAC tensor decomposition adapted to ChemCam data. The tensor with the three dimensions observation points, wavelength, and shots is decomposed in a sum of rank one tensors. R is the chosen number of rank one tensors and λ values are the weights of each tensor.

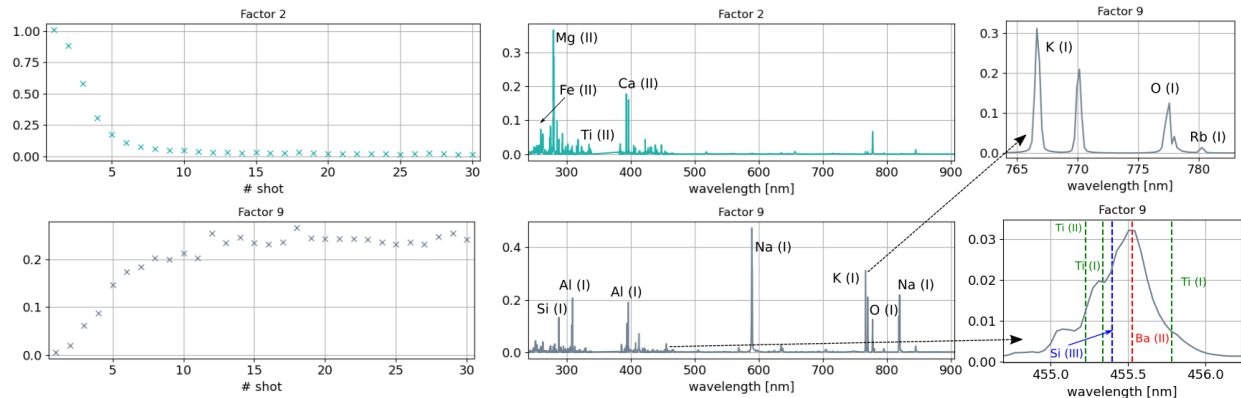


Figure 2: *Left*: STS trends of factors 2 and 9. On factor 2, a decreasing trend until shot 10 is observable, while factor 9 indicates an increase with depth until shot 10. *Middle*: Spectral profile of factors 2 and 9. While factor 2 shows contributions from elements like Mg, Fe, Ti, and Ca, factor 9 is characterized by Si, Al, K, and Na emission lines. *Right*: Zoom to regions on the spectral factor 9 showing contributions of Rb and Ba.

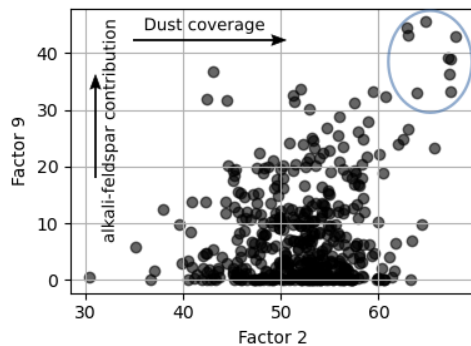


Figure 3: Factor 2 vs. factor 9 scores, each point corresponds to one ChemCam observation point. Higher scores on factor 2 are interpreted to indicate a higher dust coverage and high scores on factor 9 the presence of alkali feldspars. Thus, for example, the points in the blue circle (*Chakonipau* # 1, 4, 5; *Sledgers* # 5, 9; *Bloods_Brook* # 1; *Kinsman* # 2) are expected to be dusty and contain alkali-feldspars.

preting factor 2 as the latter is supported by the emission lines identified in the spectral profile of factor 2 that are typical for dust as observed by ChemCam, such as Mg, Ca, Fe, and Ti [8]. The second factor, we discuss here, is factor 9 whose STS and spectral profiles together with zooms can be found in Figure 2 (*bottom row*). The trend among the shots shows an increase until shot 10 and remains stable for the following shots. The spectral profile shows strong emission lines from the alkaline metals K and Na, as well as Si and Al. This is not unexpected in a dataset which was identified to have dominant contributions from felsic minerals. However, the relative strengths of emission lines and zooms to regions of characteristic trace elements may suggest which kind of felsic mineral is represented by this factor. The zooms on the right site in Fig. 2 show spectral features of Rb and Ba. The latter is superimposed by Si and Ti emission lines, whose positions are marked by colored dashed lines. The correlation of

Ba and Rb in particular with K among the shots, could indicate the presence of alkali-feldspars. The trace elements can substitute K in minerals like alkali-feldspars [9]. In Figure 3, the scores of all points are shown for components 2 and 9. To support the interpretations of both factors, points with particular high or low scores and their imagery (Mascam and ChemCam RMI) were inspected. Indeed, points with low component 2 scores do not show a strong dust coverage and some of them belong to ChemCam rasters on vertical rock surfaces where dust cannot easily accumulate. Points with high scores on both factors such as those in the blue circle in Fig. 3 appear to be dust covered. Additionally, some points belong to the targets *Chakonipau* and *Sledgers* which were identified to contain alkali-feldspars in [9].

Outlook: This first study on TCA for ChemCam LIBS data demonstrates a great potential for the investigation of depth trends in an unsupervised, data-driven fashion. The simultaneous analysis of depth trends of multiple elements can be a great support for mineral identification. In further studies we will investigate more clusters defined in [4], in particular the low SiO₂ cluster 5, which contains points of soil targets but also consolidated rocks. These different types of physical sample matrix usually have different STS trends, which is expected to show up in TCA. This type of analysis is not only relevant and practical for ChemCam data, but also for LIBS data collected at Jezero crater by the SuperCam instrument (Mars 2020/Perseverance rover) and at Utopia Planitia by the MarSCoDe instrument (Tianwen-1/Zhurong rover).

References: [1] Maurice et al. (2012), *SSR*, 170; [2] Wiens et al. (2012), *SSR*, 170; [3] Maurice et al. (2016), *JAAS*, 4; [4] Rammelkamp et al. (2021), *ESS*, 8; [5] Kolda and Bader (2009), *SIAM*, 51; [6] Williams et al. (2018), *Neuron*, 98; [7] Kossaifi et al. (2019), *JMLR*, 20; [8] Lasue et al. (2018), *GRL*, 45; [9] Cousin et al. (2017), *Icarus*, 288