Investigation of neural network architectures for stepwise classification of multi-attribute LIBS spectra under Martian conditions

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Introduction:

Laser-induced breakdown spectroscopy (LIBS) is a spectroscopic technique for analyzing elemental compositions both qualitatively and quantitatively. LIBS uses a pulsed laser to induce a plasma on the surface of a sample. Light emitted by the plasma contains characteristic emission depending on the chemical composition of the target. Since there is no need for direct contact to the sample, LIBS is highly relevant for in-situ exploration of extraterrestrial bodies [1]. The first extraterrestrial LIBS instrument, ChemCam, which is part of the Mars Science Laboratory payload collected more than 800000 single shot spectra since landing in 2012 [2]. In 2021 another two LIBS setups landed on Mars: the MarSCoDe Instrument of China's Tianwen-1 mis-sion [3] and the SuperCam instrument of NASA's Per-severance rover [4].
Besides the favorable applicability of LIBS, the complexity of the underlying physics, as well as high sensibility to experimental conditions, make it challenging to accurately classify and quantify chemical components. This is especially true for in-situ measurements when experimental conditions cannot be controlled. Because of this, machine learning techniques have found numerous applications for analyzing LIBS spectra in recent years. [5, 6]

Method:

In this study, we focus on developing a classification scheme for LIBS spectra measured in our laboratory (read [7] for detailed setup description) in simulated Martian atmospheric conditions. The data set used for our analysis consists of 2500 LIBS spectra obtained from 100 different samples. The goal is to classify LIBS spectra according to different group attributes: Four different Mars simulants [8] (MGS-1, MGS-1C, MGS-1S and JEZ-1) served as a basis for our sample composition, i.e. 625 spectra per Mars simulant. Furthermore, different salts (NaCl, MgCO3, MgSO4 and CaCO3) have been added with varying concentrations (~ 0.5-15%) to simulate a realistic variance of water-deposited salts and cements in Martian sedimentary rocks. To account for varying laser irradiances due to varying sample-to-laser distance, as it is the case for in-situ applications on Mars, each sample was measured with five different laser pulse energies ranging from ~5mJ – 50mJ (6 ns pulse duration and 300 µm laser spot diameter).
Developing a classification algorithm that is able to correctly predict all attributes at once, i.e. the Mars simulant, added salt and the laser energy, is challenging. Therefore, we choose to tackle this classification problem stepwise. We focus on backpropagation neural networks (BNN) as a first choice at each classification step.
In the first step the samples are classified according to their main component, i.e. the Mars simulant. Since each spectrum consists of more than 28000 data points, the dimensionality of the data set was reduced with principal component analysis (PCA) prior to training to improve the efficiency. The PCA scores are then used as input for training a BNN. The highest accuracy is achieved when using the first 15 PCA scores and one hidden layer of size 20. The resulting training and validation accuracy are >98% and >95% respectively. In future work we will include further sub models for stepwise classification of other spectral features such as the laser energy used in the experiment and the salt added to the sample.

References:

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