Investigation of Neural Network Architectures for Stepwise Classification of LIBS Spectra under Simulated Martian Conditions

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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]**. Currently there are three missions mounted with LIBS instruments on Mars, namely ChemCam **[2]**, SuperCam **[3]** an MarSCoDe **[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. For this reason machine learning (ML) techniques such as artificial neural networks (ANN) have found numerous applications for analyzing LIBS spectra in recent years **[5]**.

We are a newly founded junior research group focusing on the developement of innovative data analysis strategies using (ML) algorithms for in-situ LIBS spectroscopic data in order to maximize the scientific return of missions involved in planetary exploration. We are working with data obtained in the laboratory as well as data measured on Mars and plan to incorpoarate physical knowlegde about the LIBS process to impove the performance and explainablity of ML methods.

In a first study, we investigate the performance of different backpropagation neural network (BPNN) architectures for a stepwise classification pipeline of 2500 multi-attributed LIBS spectra measured in the laboratory under simulated Martian atmospheric conditions. Therefore, 100 powdered rock samples have been prepared and measured with our LIBS setup, at the DLR Institute of Optical Sensor Systems in Berlin. These samples consist of four different basaltic Mars simulants **[6]**, which were mixed with four different salts with varying concentrations to simulate a realistic variance of water-deposited salts and cements in Martian sedimentary rock. 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)

In a first step, the samples are classified according to their main component, i.e. the Mars simulant. Before feeding the data to the BPNN, a principal component anaylsis (PCA) was applied in order to reduce the dimensionality of the data. 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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