Neural networks for classification of LIBS spectra under simulated Martian conditions

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LIBS instruments are currently deployed on several Mars missions for in-situ analysis of Martian geochemistry [1,2,3]. In recent years, due to the amount of acquired LIBS data, as well as the complexity of the underlying physics, researchers increased their focus on new data analysis strategies, such as Machine Learning (ML) algorithms. Supervised and unsupervised ML techniques have found numerous applications for both, quantitative and qualitative analysis of LIBS spectra [4,5,6].

In this study, we focus on developing a stepwise classification scheme for multi-attribute LIBS spectra measured in our laboratory (see [7] for detailed setup description) under simulated Martian atmospheric conditions using Back Propagation Neural Networks (BPNN). Therefore, we prepared 100 pressed rock samples (1g pellets), each consisting mainly of one out of four basaltic Mars simulants (MGS-1, MGS-1C, MGS-1S and JEZ-1) [8]. Furthermore, we added one out of four salts (NaCl, $MgCO3$, $MgSO4$ and $CaCO3$) with varying concentration (~0.5-15%) to each sample 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 [1], each sample was measured with five different laser pulse energies ranging from ~5mJ – 50mJ (6 ns pulse duration and 300 µm laser spot diameter). Measuring each sample five times, we ended up with a total of 2500 LIBS spectra, 28507 channels each. Therefore, the data set can be analyzed by different group attributes, i.e. the mars simulant, added salt, concentration of the added salt and/or the laser energy. In summary, we have:

- 625 spectra per mars simulant
- 600 spectra per added salt, 100 samples without salt
- 400 spectra per salt concentration (concentrations ~ [0.5%, 1.0%, 2.5%, 5%, 10.0%, 15.0%])
- 500 spectra per laser energy (laser energies ~ [5.8mJ, 10.8 mJ, 21.4 mJ, 32.9 mJ, 51.0 mJ])

The first step of our classification model focuses on predicting the mars simulant. We use a principal component analysis (PCA) to reduce the dimensionality of the data set from (2500,28507) to (2500,40). The first 15 principal components serve as an input for a BPNN with one hidden layer of size 15 (Adam optimizer, LeakyReLU activation function and batch normalization). The training, validation and test data set sizes were chosen to be 1800, 200 and 500 respectively.

In the second classification step, we build four sub models (one per Mars simulant) and predict the added salts. Each model is again a BPNN with the same architecture as in the first step. The inputs for each model are again the first 16 PCA components. Here, each PCA is done only for samples belonging to one Mars simulant.

For both classification steps we trained a total of 500 models for different train/test split configurations. The ratio of train/test was always the same (1^{st} step: 0.88/0.12, 2^{nd} step: 0.85/0.15), and measurements from the same sample where always kept together. With this benchmark training method we achieve an average train/test accuracy of: 98.78% / 96.51% (1^{st} step) and ~92-98% / ~75-88% (2^{nd} step).

As a first result we observe that the classification of both Mars simulant and salt works best for certain laser energies, i.e. 21.4 mJ and 51.0 mJ. In the future we will provide further statistical analysis of our ensemble/benchmark results.

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