# Investigation of Neural Network Architectures for Stepwise Classification of Multi-Attribute LIBS Spectra under 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, $MgCO_3$, $MgSO_4$ and $CaCO_3$) 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. With this model we achieve a train, validation and test accuracy of ~ 98%, 96% and 96% respectively.

In a next classification step, we plan to build four sub models (one per Mars simulant) and will try to predict the added salts. Also, we will compare the order of classification steps, i.e. classifying the salts first and then the Mars simulant. In either case, the second classification step will be more challenging, since the training data set size is reduced. Furthermore, we will compare our results the conventional classification algorithms such as partial least squares discriminant analysis (PLS-DA).

# REFERENCES

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