**INVESTIGATION OF NEURAL NETWORK ARCHITECTURES FOR CLASSIFICATION OF MULTI-ATTRIBUTE LIBS SPECTRA UNDER SIMULATED MARTIAN ATMOSPHEREIC CONDITIONS.**

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**Introduction:** Currently, LIBS instruments are being used on multiple Mars missions for analyzing the geochemistry of the Martian surface in-situ [1, 2, 3]. In recent years, due to the amount of acquired LIBS data, as well as the complexity of the underlying physics of the technique, researchers increased their focus on new data analysis strategies, such as Machine Learning (ML) algorithms. Both supervised and unsupervised ML techniques have been successfully applied to LIBS spectra for both quantitative and qualitative analysis [4, 5, 6].
In this study, we compare the performance of two Back Propagation Neural Network (BPNN) classification schemes for LIBS data. The two attributes we want to classify are the type of Mars simulant (basaltic rock mixture) of the samples and a salt component. In the first scheme, the Mars simulant and salt classifications are separated into two consecutive BPNN classifiers. In contrast, the second scheme consists of a single multi-label BPNN classifier.

**Sample preparation and data acquisition:** We prepared a total of 100 pressed rock samples (1g pellets), consisting primarily of one of four different basaltic Mars simulants (MGS-1, MGS-1C, MGS-1S and JEZ-1) [7]. We also added one of four different salts (NaCl, $MgCO_3$, $CaSO_4{\times}2(H_2O)$ and $MgSO_4{\times}1(H_2O)$) with varying concentration ( $0.5 - 15\ wt\%$) to each sample to simulate a realistic variance of water-deposited salts and cements in Martian sedimentary rocks. To account for variations in laser irradiance due to differences in sample-to-laser distance, as is the case for in-situ measurements on Mars [1], each sample was measured with five different laser pulse energies ranging from $5mJ$ – $50mJ$ ($6ns$ pulse duration and $300\mu m$ laser spot diameter). Measuring each sample five times (= one experiment), we ended up with a total of 2500 LIBS spectra with 28507 channels each. All measurements were conducted in a dedicated LIBS setup in our laboratory under simulated Martian atmospheric conditions (see [8] for a detailed description of the setup). All this results in a dataset which can be analyzed according to different group attributes, i.e. the Mars simulant, added salt, concentration of the added salt etc. Here we focus on classifying the Mars simulant and salt component.

**Data preprocessing and model architectures:** Before training, we standardized each spectrum by subtracting the mean and dividing by its standard deviation. We then reduced the dimensionality of the dataset using Principal Component Analysis (PCA) from $(2500, 28507)$ to $(2500, D_{in}$, where $D_{in}$ is the input dimension of the BPNN.
Both classification schemes are sketched in Fig.2. All BPNN parameters are shown in Tab.1.
Scheme 1 consists of two classification steps: The first for prediction the Mars simulant (BPNN 1, 4 outputs), and the second predicting the added salt (BPNN 2, 5 outputs: 4 salts + "no salt"). Therefore, we have a total of 5 BPNNs. Note that we did a new PCA for each of the 4 salt classifiers (BPNN 2), indicated by the PCA* in Fig. 2. BPNN 1 and all BPNN 2 were trained for 20 epochs with a learning rate $LR = 0.005$, LeakyReLU activation and Adam optimizer.
The second classification scheme uses one BPNN (BPNN 3) and does a multi-label classification of Mars simulant and salt simultaneously. Therefore, we generated a 9-dimensional one-hot encoded label vector: 4 dims. for the Mars simulants and 5 dims. for the salts (4 salts + "no salt"). BPNN 3 was trained for 250 epochs with a learning rate of $LR = 0.0005$, LeakyReLU activation and Adam optimizer.

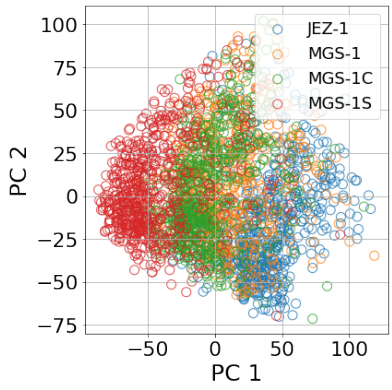


Figure 1: First two PC of the full data set. The different Mars simulants are mainly grouped together but there are overlaps for these two first PC.

| | | $D_{in}$ | Hidden layer size | Dropout rate | BatchNorm | Neg. slope | Batch size |
|---|---|---|---|---|---|---|---|
| Scheme 1 | BPNN 1 | 16 | 15 | × | × | 0.1000 | 25 |
| | BPNN 2 | 16 | 15 | × | × | 0.0075 | 5 |
| Scheme 2 | BPNN 3 | 16 | 30 | 0.2 | ✓ | 0.05 | 128 |

Table 1: BPNN parameters for both classification schemes. Neg. slope is a parameter of the LeakyReLU function.

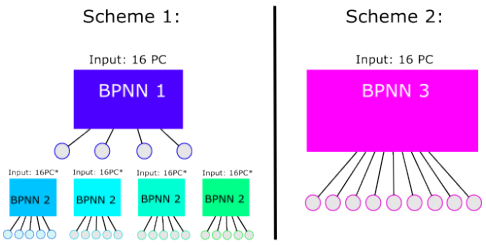


Figure 2: Sketch of both classification schemes. Scheme 1 deploys a step wise approach for classifying the Mars simulant and added salt, while Schem 2 does both simultaneously with a multi-label classification.

**Benchmark training and model evaluation:** Each BPNN was trained using 100 different train-test split configurations. For each configuration, a train-test split ratio of $0.88/0.12$ was chosen. We always kept five measurements from the same experiment in either the train or the test set in order to not distort the results by showing the BPNN data from the same experiment in both sets. Furthermore, the train-test splits where constrained such that all class labels have a roughly uniform distribution, i.e. splits with very unbalanced distributions of Mars simulant and added salts were neglected. The mean test accuracies for correctly predicting a salt, given the Mars simulant has been classified correctly, for both schemes are shown in Tab.2.

| | | JEZ-1 | MGS-1 | MGS-1C | MGS-1S |
|---|---|---|---|---|---|
| Mean acc. [%] | scheme 1 | 74.4 | 70.4 | 80.2 | 67.4 |
| | scheme 2 | 73.3 | 80.7 | 81.6 | 70.3 |

Table 2: Mean test accuracies for predicting a salt, given the Mars simulant is correctly predicted, for both schemes.

From these results, we conclude that there is no gain in splitting up the classification into submodels when using BPNNs. The second scheme actually performs overall slightly better than the step-wise classifier, as can be seen in Tab.2.

**Generalization to newly measured data and outlook:** To assess the generalization ability of our models, we prepared two new samples, consisting of JEZ-1 with NaCl (sample A) and MGS-1 with $MgSO_4 \times 1(H_2O)$ (sample B). Both samples were prepared in the same way as the original samples and measured five times using three different laser energies (out of the five laser energies used in the first measurement cycle). We then projected these spectra into the PCA space used for initial dimensionality reduction and fed the first 16 PC scores into classification Scheme 2. The model did not achieve

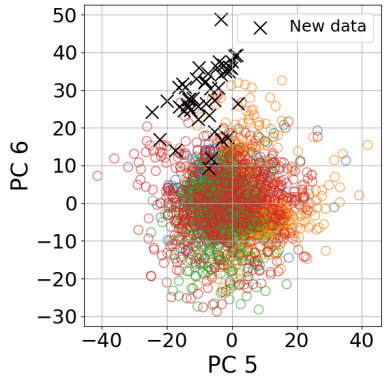


Figure 3: PC 5 and PC 6 for old and new measurements. We projected the new data into the PCA space of the original data set. PC 5 and 6 of the new data show a clear shift relative to the old data.

satisfactory accuracies. For sample A, the Mars simulant prediction accuracy was 47%, the salt prediction accuracy was also 47%, and the accuracy of correctly predicting both was 26.7%. For Sample B, the results were 40.0% (Mars simulant), 6.7% (salt), and 0% (both). This significant difference in performance can be due to two factors:

- The BPNN may be overfitted to the data.
- There may be differences in the chemistry of the Mars simulants or the experimental conditions between the two measurements (which were taken 11 months apart).

Because we did not observe indications of severe overfitting during training, we suspect that the poor performance of the model is due to differences in the data. This is supported by a shift observed in the new scores of PC 5 and PC 6 compared to the old PC scores, as can be seen in Fig. 3. This shift is only present in these two components. When analyzing the loadings of these two PC, we see indications of line shifts, which can be caused by changing wavelength calibration. Further investigation is needed to fully understand this phenomenon. In addition, we will explore convolutional neural network architectures for this classification task.

**References:** **[1]** Maurice, S. et al. (Apr. 2016). In: *Journal of Analytical Atomic Spectrometry* 31 (4), pp. 863–889. ISSN: 13645544. **[2]** Xu, Weiming et al. (Aug. 2021). In: *Space Science Reviews* 217 (5). ISSN: 15729672. **[3]** Maurice, S. et al. (Apr. 2021). **[4]** Li, Lu Ning et al. (June 2021). In: *Spectrochimica Acta - Part B Atomic Spectroscopy* 180. ISSN: 05848547. **[5]** Anderson, Ryan B. et al. (Feb. 2022). In: *Spectrochimica Acta - Part B Atomic Spectroscopy* 188. ISSN: 05848547. **[6]** Rammelkamp, Kristin et al. (Dec. 2021). In: *Earth and Space Science* 8 (12). ISSN: 23335084. **[7]** Cannon, Kevin M. et al. (Jan. 2019). In: *Icarus* 317, pp. 470–478. ISSN: 10902643. **[8]** Schröder, S. et al. (Mar. 2013). In: *Icarus* 223 (1), pp. 61–73. ISSN: 00191035.