MINERALOGICAL CHARACTERIZATION USING NEURAL NETWORKS: COMPOSITION OF MAFIC MINERALS IN MARTIAN METEORITES FROM THEIR SPECTRA

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ABSTRACT

In this study, we test the ability of neural networks to determine the composition of magmatic rocks from their laboratory spectra.

We first describe the structure and behaviour of the multilayer perceptron that we implement and train for quantitative characterization. For that purpose, reference laboratory spectra of mafic minerals from both natural and synthetic samples are used. As their composition in terms of the three mafic minerals, olivine (OL), orthopyroxene (OPX) and clinopyroxene (CPX) are known, those spectra are given as inputs during the learning phase of the neural network.

In the analysis phase, we use the neural network to process spectra acquired on SNCs (Shergottites, Nakhlites, Chassignites) meteorite samples that are considered to be representative of Mars surface. The network outputs mineralogical compositions very quickly, performing only explicit operations.

Our preliminary results show that neural networks are able to quantify mafic minerals, especially in the case of complex mixtures, with much improved computer efficiency and comparable accuracy compared to usual methods. This is very promising regarding future analysis of huge datasets.

Index Terms— Neural, Network, Hyperspectral, Detection, Meteorite

1. INTRODUCTION

Mafic minerals are key components when trying to understand the geological history of planetary bodies like Mars. Indeed, their presence in igneous rocks is directly related to mantle properties and crystallization conditions. They also partially control the nature of the alteration products which could be formed subsequently. In this respect detection of olivine and pyroxenes, and characterization of their respective composition, is an important step that must be done carefully.

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Reflectance spectroscopy, hyperspectral remote sensing in visible/near-infrared is a very powerful tool to achieve this objective. Indeed, olivine and pyroxenes have characteristics broad absorption features near 1 and 2 μm [1, 2] due to the Fe^{2+} electronic transition. During the last decade, imaging spectrometers onboard spacecraft have acquired huge amount of such data and it is actually challenging to process them both quickly and efficiently.

Several techniques (e.g. linear unmixing [3], radiative transfer modeling [4]) aimed at deconvolving absorption bands in terms of mineralogy. Modified Gaussian Model [5] can also be used to quantitatively estimate the chemical composition of each mineral in a rock. Such approach has been successfully applied on OMEGA data [6]. However, the results obtained with those techniques are basically not accurate enough, these methods are time consuming and efforts are still to be done to develop new algorithms. This is why we test in this study the ability of neural networks to determine the composition of minerals from their mafic signatures on laboratory spectra.

2. NEURAL NETWORK IMPLEMENTATION

2.1. Structure of a Neural Network

A neural network is a learning machine which uses a set of scalars as input (the data to analyse) and produces another set of numbers, carefully chosen [7, 8]. In our case, the input vector is the spectrum and the output vector is the modal or the chemical composition (percentage of olivine, clinopyroxene and orthopyroxene, cf. figure 2). Various schemes can be used to connect the input to the output set. We use the multilayer perceptron method in which information propagates forward in the analysis phase and backward in the learning phase through adjacent layers. Each adjacent layers are linked by non-linear weighted connections, as represented in figure 1. At each node, the contributions of all elements of the previous layer are summed up and a threshold is applied. It has been shown that the use of the threshold has a fundamental importance in the learning capacities of the neural network

[9]. This technique is sometimes used to obtain a result in very non-linear problems.

2.2. Training phase of a Neural Network

Before using a neural network on unknown problems, it has to be trained on known problems in a learning phase. The network first learns to reproduce a sufficiently correct output vectors using a set of spectra obtained on synthetic samples with known compositions (the training set). The connexions of the network start from a random state and are organized by a learning algorithm following a uniform gradient descent in the error space. We use the error backpropagation algorithm, which decreases the weights of the connections contributing to "wrong" outputs. We modify the neural weights forcing an uniform convergence on the training set [9]. Thus, at the end of the learning phase, the neural network is able to give a "correct answer" on all the training set. The training is usually the computationally time-consuming phase (about 10 minutes on a single CPU machine in our case).

2.3. Analysis phase of the trained network

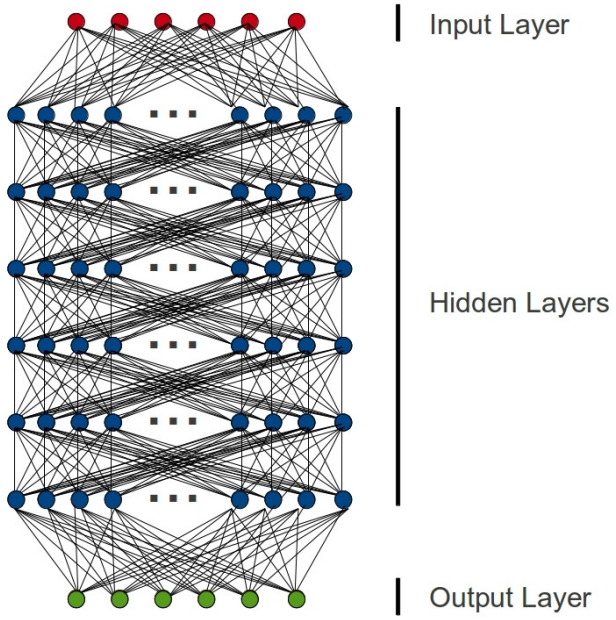
Second, once trained, the neural network can be used on an unknown spectrum and will output a composition only performing explicit operations. The answer of this type of neural network is then almost instantaneous (less than a second on the same machine, mainly due to input/output on the hard drive). To ensure an homogeneous coverage of the output space, we assign a more important weight to the most singular spectra in the back-propagation routine. The weight of each spectra i is defined by $w_i = 1/d_i$, where d_i is the density of training sample in the output space:

$$d_i = \exp\left(-\frac{\frac{1}{N_j}\sum_j (O_i - O_j)^2}{2\ 10^2}\right), \qquad (1)$$

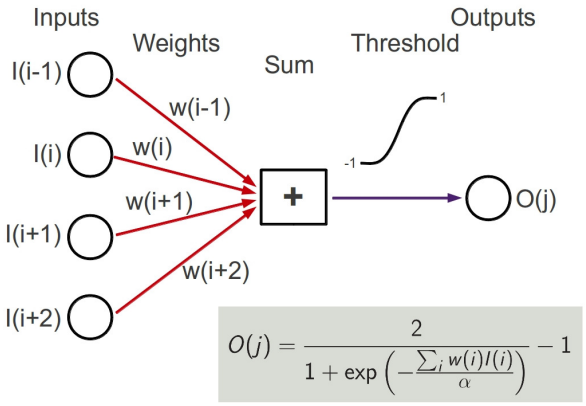
where O_i is the mineralogic or chemical composition (%) of the known spectra and N_j is the number of spectra used in the learning.

Since the structure of a Neural Network is non-linear, one can hardly predict its behavior outside the training set. Once a network is trained, its answer on the training set is within the user-specified tolerance defined during the training. If an unknown input represents a combination of inputs of the training set then the output of the neural network can be seen as an interpolation between different outputs learnt during the training. If an unknown input represents something different from the elements of the training set, then the network tries to extrapolate its answer from its training outputs.

If the unknown input vector is completely different from the inputs on which the network has been trained, it is very unlikely that a correct answer can be obtained. Neural networks are not designed for extrapolation. A completely new situation cannot be learnt without training with the technique



(a) Neural Network Structure (multilayer perceptron). We represent 6 hidden layers as an example, but less layers are generally sufficient to obtain the expected predicting power.



(b) Neuron model (perceptron).

Fig. 1. Schematic representations of (a) a multilayer perceptron and (b) a neuron. The input layer shown in (b) can represent the effective input vector or any previous hidden layer.

we use in this study. A reliable extrapolation can only be expected if the input is "close enough" to the training set, which is hard to quantify since the input is unknown.

In the case of an interpolation, neural networks are known to be able to perform very non-linear operations, which is on purpose for absorption band deconvolving. However, to avoid too non-linear outputs, it is important to keep the learning tolerance in a reasonable range. Neural networks can usualy be forced to exactly reproduce the training outputs. Yet, in such case, the connections between layers have lost all smoothness and the network is not able to interpolate or extrapolate anymore. To avoid this problem, we stopped the learning phase when the average output error reaches 10 %.

3. TRAINING AND TESTING DATA SETS

All training spectra come from the Brown/RELAB library. Most of them have already been used in [10] to improve MGM approach and a reference list of RELAB files can be found there. We select the wavelength range between 0.46 and 2.60 μm while keeping full spectral resolution (6.6 nm). We remove the first order approximation of each spectrum to give an input signal as insensitive as possible to acquisition conditions and sample physical state to the neural network.

Our neural network has been trained on a set of 190 spectra, some of them being representative of mixtures while others are representative of mono-mineral samples with various chemical compositions (mafic minerals only). Because of the limitations of available laboratory measurements, very few ternary mixtures are included in the learning set. We assign a more important weight to these ternary mixtures in the learning phase. To do this, we apply the synapses penalties with different magnitudes, according to the density of input samples in the training set (see eq. 1). An isolated spectrum in the mineralogic composition space of the training set have more importance than a spectrum closely surrounded by a large number of neighbors.

To test our neural network, we choose to use spectra of SNCs as those meteorites may be the most representative samples of Mars surface measurable in laboratory. SNCs have been intensively studied and their mineralogical compositions are well known from independent analytical laboratory measurements (e.g. [11] and references therein). We here used a set of 11 spectra, representative of the different families of SNCs.

4. RESULTS ON SNCS

Figures 2 and 3 show the results of the neural network on the testing set (spectra of the SNCs meteorites). To explore the reproductibility of the solution, we trained 10 identical neural networks with different initial neural weights. All networks used here have only one hidden layer with 40 neurons.

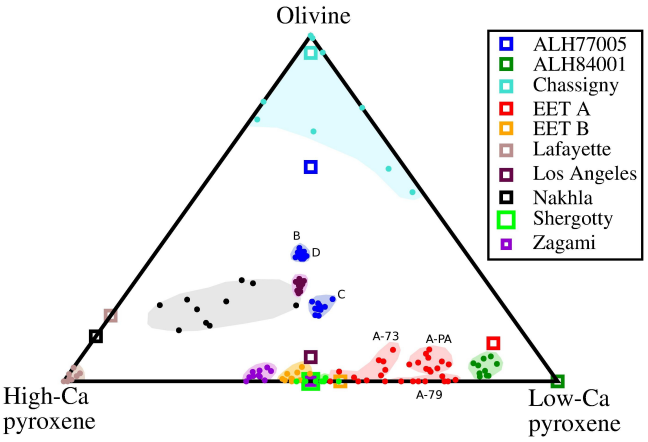


Fig. 2. SNCs modal compositions estimated using neural networks (dots) compared to literature (squares, from [11]). Neural network is tested with different initial neural weights so several dots are reported for each SNCs (see text for details). When different spectra exist for one SNC, results are distinguished using labels around the colored fields.

Figures 2 and 3 show that the outputs of the networks (represented by colored dots) are concentrated in different localized areas for each spectrum.

Figure 2 shows the outputs of the network as the OL-CPX-OPX compositions of the tested spectra compared to the average range expected for each meteorite (from [11]). The position of the points in the triangle represents the mineralogic composition between the three poles. The points located on the edges are bimodal. The different compositional classes revealed by the network are shaded using the same colors as the corresponding color dots. The network is clearly able to detect pure and mixed compositions with a satisfactory reproductibility. Discrepencies can nevertheless occur, especially when a mineral is much less abundant than the other. This may be directly related to the absorption features which could be masked in a mixture spectra and implies as other deconvolution techniques to take detection thresholds into account.

Figure 3 shows the chemical composition of clinopyroxenes and olivines detected in each meteorite, using an other version of the neural network, trained for chemical composition only. The composition of meteorites with very low clinopyroxene contents are very scattered and thus not depicted in the top part of the figure 3 (similarly, we plot only high olivine content outputs in the bottom part). Work is still ongoing considering the orthopyroxene component. Although the tested samples have similar CPX compositions, the neural network is still able to distinguish tendencies within the spectra. Localized compositional areas are clearly identified and all of them fall within the expected trends from laboratory measurements [11]. However, iron content in olivine is almost always overestimated (10 to 20 %).

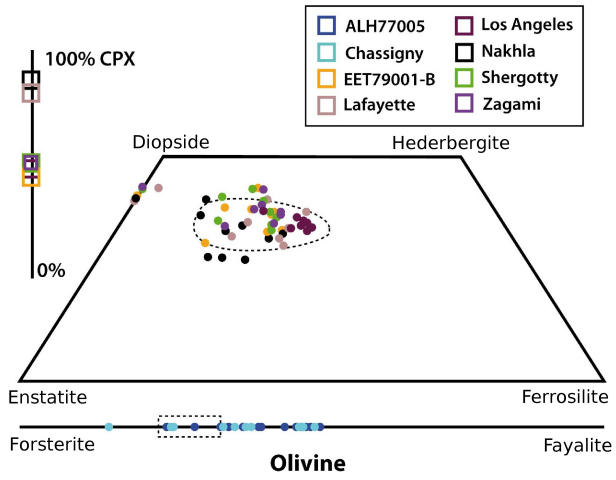


Fig. 3. Chemical compositions of two individual mafic minerals in SNCs estimated using neural networks (dots) and compared to literature (dashed lines, from [11]). The composition of clinopyroxenes is depicted on the top trapeze and olivine composition is shown on the bottom line. Clinopyroxene modal abundances in the meteorites are also reported.

The scattering of the outputs of the network actually seems to be a good indicator of mineralogic enrichment and provides a way to quantify the uncertainty of the output of the neural network.

5. CONCLUSIONS

The neural network we developed in this study show promising results on SNCs. Indeed, only using laboratory data as a training set (i.e., partial coverage of the whole range of possibility), we are able to detect and characterize each mineral phase in an unknown spectrum.

The neural network approach used in this study is relatively easy to implement and the weight connections recorded at the end of the learning phase are very light. The most important limitation of this kind of approach lies in the potential limitation of data available to train the neural network. Yet, we show here that once a sufficient amount of training spectra is collected, a multilayer perceptron network is comparable to much computationaly intensive inverse techniques like the Modified Gaussian Method.

In a next step, we will implement our neural network within an automated procedure which will analyze each spectra of individual CRISM image. CRISM [12] is an imaging spectrometer onboard MRO (NASA) for exploring different environments of Planet Mars. This implies to deal with some additional difficulties (noise, weak absorption features, complex photometry). Then, we should be able to process very quickly and efficiently large amounts of data required to do high precision geology for a large number of sites in the red Planet.

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