

ARTIFICIAL NEURAL NETWORKS AS A TOOL FOR PROGNOSIS OF CHEMICAL AND MINERAL COMPOSITION OF LUNAR SOILS FROM SPECTRAL MEASUREMENTS. V. V. Korokhin¹, Yu. G. Shkurov¹, D. G. Stankevich¹, C. Pieters², and U. Mall³, ¹Astron. Institute of Kharkov National Univ. 35 Sumska St., Kharkov, 61022, Ukraine, dslpp@astron.kharkov.ua, ²Geological Sciences, Brown Univ., Providence, RI 02912, USA. ³Max Plank Institute for Solar System Research, 2 Max Plank St., Katlenburg-Lindau, 37189, Germany.

Introduction: Lunar Soil Characterization Consortium (LSCC) data give a unique opportunity to study direct links between spectral characteristics and the chemical/mineral composition of lunar soils [1,2]. These links can be used for a prognosis of the composition of the lunar surface with spectral observations of the Moon. Preliminary results using maria samples were described in [3]. In this work we exploit the whole LSCC dataset including highland samples to evaluate two different statistical approaches. We compare below a linear and a nonlinear regression approach; the latter uses artificial neural networks.

Data preparation: We start with transformation of reflectance $A_i(\lambda)$ into extinction spectra $k_i(\lambda)$, using a spectral model [4]. Then we reduce the number of spectral characteristics using principal component analysis (PCA) and find a statistically optimal description of spectral data. As is known, PCA gives a system of eigenfunctions, $\varphi_q(\lambda)$, that allow any given spectrum to be described as a series with a minimal number of terms:

$$k_i(\lambda) = \bar{k}(\lambda) + \sum_{q=1}^Q a_{i,q} \varphi_q(\lambda), \quad (1)$$

where $a_{i,q}$ are the expanding coefficients for the i -th spectrum, and $\bar{k}(\lambda)$ is the average spectrum of the whole spectra dataset, Q is the number of used eigenfunctions (factor's number); Q may be significantly less than the number of points in initial spectra, because the $a_{i,q}$ decrease very rapidly with increasing q .

We have carried out the investigation to find an optimal value of Q , which is defined, first of all, by the level of noise in spectra. We used the technique described in [5]. The result show that $Q = 6-8$ is optimal for the measured spectra with noise level 1-3%.

I. Multiple linear regression (MLR) approach: We assume that a linear relationship exists between the compositional parameters $P_{k,i}$ (e.g., TiO_2 or pyroxene abundance) and the set of PCA coefficients $a_{i,q}$ derived for each spectrum of the set with formula (1):

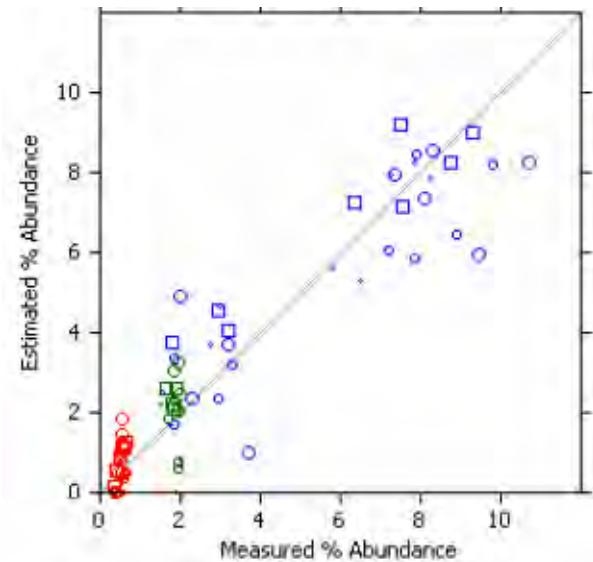
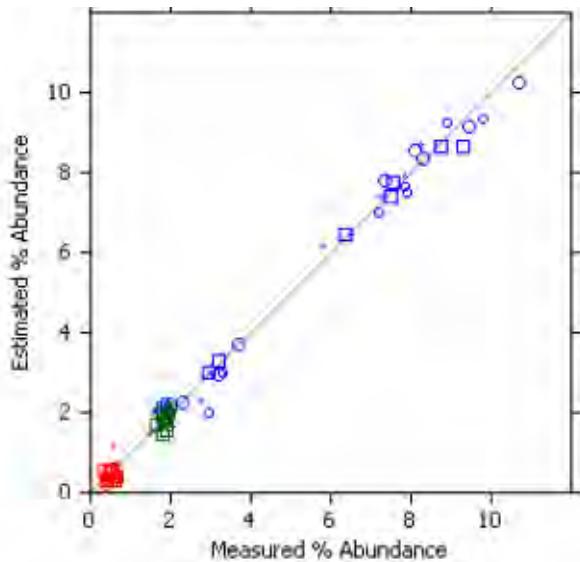
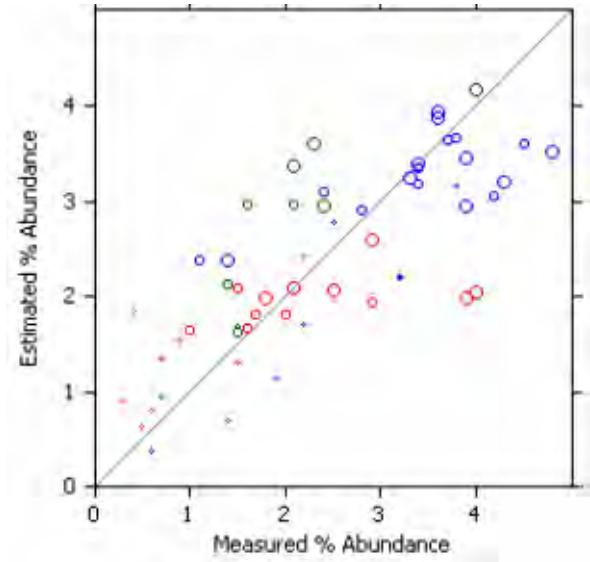
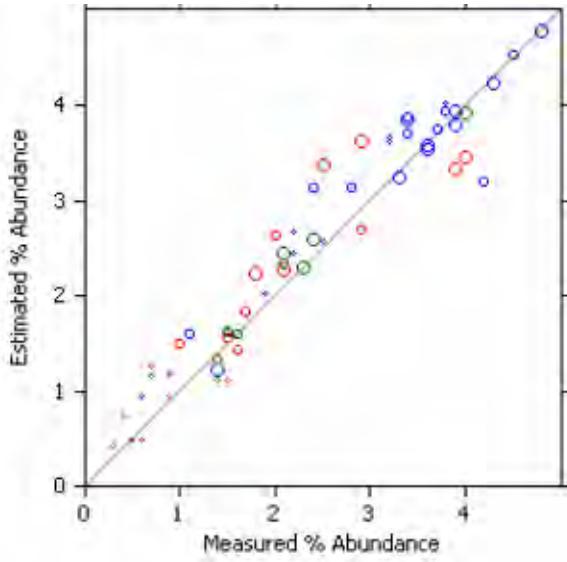
$$P_{k,i} = w_{0,k} + \sum_{q=1}^Q w_{q,k} a_{i,q}, \quad (2)$$

where $w_{q,k}$ are the loading (weight) coefficients which are the same for all spectra for a given composition parameter, Q is the number of eigenfunctions used. We find the loading coefficients using the classical minimal least-squares method.

To evaluate how well this approach can predict composition, correlation diagrams of measured versus MLR estimated have been used. Examples of such diagrams for abundances of TiO_2 and olivine are shown in Figs. 1 and 2 (blue, red, green symbols are used respectively for maria, Apollo-14, and Apollo-16 highland samples). Size of the circles corresponds to the size-particle fractions (small: $<10 \mu m$, middle: $10-20 \mu m$, large: $20-45 \mu m$); rectangles designate bulks ($<45 \mu m$). In the ideal case all points should lie on the diagonal line. The data on the plots show the dispersion around the diagonals. The prognosis quality can be characterized with the correlation coefficient for estimated and measured abundances.

For some composition components, e.g., FeO and total pyroxene, the correlation coefficients are relatively high (0.98 and 0.94, respectively), but for others (e.g., SiO_2 and olivine) they are poor. The latter may indicate that either the parameters correlate with optical properties only weakly or the assumption on linearity of the relationships is not correct.

II. Nonlinear regression approach using artificial neural networks: There is a computation technique which allows finding empirical relations in systems with any number of parameters without any restrictions on character of these relations. This is the artificial neural networks (ANN) approach. There are many sorts of neural networks for different applications. However the so-called multilayer perceptron [6] with errors back propagation teaching method [7] is most suitable for our tasks. We use a perceptron with one hidden layer and with four neurons for studying the links between $a_{i,q}$ and composition parameters. The input layer contain the number of neurons is equal to the PCA factors Q (6 used in our case), the output layer have one neuron. Results of using an ANN for the composition prognosis are shown in Figs. 3 and 4. One can see that an ANN regression gives more perfect prediction than the linear MRL approach (cf. Figs. 1 and 3 and Fig. 2 and 4). Partially this can be related to the fact that the number of formally independent combinations of the input parameters is much higher in the ANN case than in the MRL one. Nevertheless the accounting for any nonlinearity should also significantly contribute to the result.

Fig. 1. TiO_2 . MLR prediction ($Q = 6$). $k = 0.93$.Fig. 3. TiO_2 . ANN prediction. $k = 0.99$.Fig. 2. Olivine. MLR prediction ($Q = 6$). $k = 0.78$.Fig. 4. Olivine. ANN prediction. $k = 0.96$.

Conclusions: We compared two statistical techniques for prognosis of lunar surface composition using the LSCC data that give a unique opportunity to study correlations between spectral characteristics of lunar soil and abundance of chemical and mineral components. Using the ANN technique allows us to study empirical links between spectral characteristics of lunar soil and composition parameters without any restrictions on the character of these relations. This appears to provide better quality of prediction as compare to MLR analysis. The results of our work may be a useful for strategy in the analysis of lunar spectra obtained with spacecraft spectrometers of current (SMART-1) and especially future (Chandrayaan) missions.

This work was supported by CRDF (grant UKP2-2614-KH-04).

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