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NEURAL NETWORK-BASED SPECTRAL UNMIXING OF SUPERCAM INFRARED SPECTRA. A. M. Zastrow¹ (a.m.zastrow@lanl.gov), S. M. Clegg¹, A. M. Ollila¹, E. B. Flynn¹, J. R. Johnson², C. Pilorget³, S. Le Mouélic⁴, T. Fouchet⁵, F. Poulet³, C. Royer⁶, E. Dehouck⁷, N. Randazzo⁸, A. Brown⁹, C. Quantin-Nataf⁷, A. Cousin¹⁰, S. Maurice¹⁰, and R. C. Wiens¹¹. ¹Los Alamos National Laboratory, ²Johns Hopkins University Applied Physics Laboratory, ³Institut d'Astrophysique Spatiale, ⁴Laboratoire de Planétologie et Géosciences, ⁵Observatoire de Paris, ⁶LATMOS, CNRS, France, ⁷Université Claude Bernard Lyon 1, ⁸University of Alberta, ⁹Plancius Research, ¹⁰Institut de Recherche en Astrophysique et Planétologie, ¹¹Purdue University.

Introduction: Spectral unmixing is the process of determining the components of a mineral mixture and their abundances based on their spectra. Many spectral unmixing algorithms have been developed, which range from simple linear models to more complex non-linear models. In this work, we use a neural network approach to spectral unmixing and apply it to near-infrared (NIR) spectra from the SuperCam instrument on the Mars 2020 rover [1].

We are using neural networks for unmixing because they are particularly adept at learning the non-linearity of a given system. In the NIR spectral range, mixing is non-linear due largely to volume scattering (wherein incoming light interacts with multiple interfaces in a medium before being reflected out to a detector) [2]. Therefore, the expectation is that a neural network will be able to learn the non-linearity of the system better than traditional modeling approaches.

Datasets: SuperCam is one of the science instruments on the Mars 2020 rover, with several capabilities for determining geochemistry and mineralogy. We are focusing on data from the infrared spectrometer, with a spectral range of ~ 1.3 to $2.6 \mu\text{m}$ and 256 spectral channels. There are many minerals with diagnostic absorptions in the SuperCam wavelength range, and there have been many NIR lab studies of those minerals and their mixtures that are relevant to Mars.

Spectral library. Our spectral library is made up of NIR data measured at the Reflectance Laboratory at Brown University (RELAB, <https://pds-speclib.rsl.wustl.edu>). Our current spectral library contains 26 Mars-relevant minerals (or, in machine learning terms, classes), including primary silicates, phyllosilicates, carbonates, sulfates, iron oxides, etc. There are approximately 200 single mineral spectra of grain sizes ranging from <45 to $>250 \mu\text{m}$, 300 binary mixtures, and 100 mixtures of three or more components. The library is not exhaustive and is currently being expanded.

Neural Network Architecture: Our model is a basic multi-layer convolutional neural network (CNN) [3]. In CNNs, “kernels” of different sizes move across the spectra, allowing the network to consider nearby spectral channels concurrently when learning the features of the data. This approach is particularly

useful with spectral data since absorption bands cover multiple spectral channels and the value of each channel is dependent on the channels around it. Not only does the network learn the features that are diagnostic of each mineral, but it importantly learns which features distinguish between different minerals.

Our network consists of two 1D convolutional layers each with Rectified Linear Unit (ReLU) activations (where $f(x) = x$ if $x > 0$, else $f(x) = 0$), batch normalization and max pooling layers, followed by two fully connected layers (every neuron in the layer is connected to every neuron in the next layer) with ReLU activations.

The network is used for two tasks: classification (which minerals) and regression (their abundances). For the classification model, the final layer is a fully connected layer with a Sigmoid activation. This produces output values between 0 and 1 that represents the probability that a given class is present in the mixture. If the output probability for a class is greater than 0.5, we consider the model to have positively identified that class as being present. For the regression model, the final layer is a fully connected layer with no activation. We have not put any other restrictions on the regression model, e.g., forcing output values to be between 0 and 1 or add up to 1 (nor do we plan to in the future).

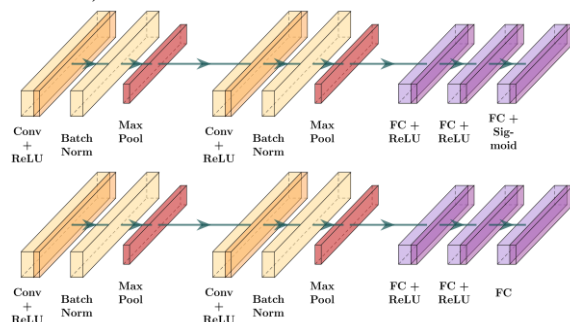


Figure 1. Top row: classification network. Bottom row: regression network. The two networks are trained separately, but with the same training data.

Data Augmentation: The key to our neural network is its training data. For the network to successfully learn how to identify mixtures, it needs to see many (many) examples of mixture spectra in the training process. It would require a great undertaking

to make all the possible mixtures of interest in the lab and measure them and we would still need more data to train with. Therefore, we use synthetic mixture data calculated from physics-based models to train our model and lab mixture data to test it. Specifically, we use the Hapke analytical model [2] to create the training data from single mineral spectra. The Hapke model we use only takes the incidence and emission angles of the measurements as inputs. Other parameters (e.g., porosity, grain size, roughness, etc.) are not included. This is the data generation process:

1. Randomly select a spectrum from a random class (some minerals have more than one spectrum, typically a grain size variation).
2. Repeat step 1 for as many components as desired in the mixture (2 or 3) and assign each component an abundance (summing to 1).
3. Calculate a mixed spectrum.

Training Process: We create a new set of 800 random synthetic mixture spectra in every epoch to train the model. We run the model for 10,000 epochs and select the best model based on the multi-label accuracy (for classification) or root mean squared error (RMSE, units of % abundance, for regression) on the binary lab mixtures in our spectral library.

Selection Criteria: We are being conservative in what we consider as “reliable” predictions from the model based on their performances on the lab spectra

(~98% accuracy and ~7% abundance RMSE [4]). For classification, output probabilities greater than 0.5 are considered as positive identifications. We then pair those results with abundance predictions from the regression model greater than 15%.

Application to SuperCam Data: Presented here are results from 5505 atmospherically corrected NIR spectra from sol 28 to 1142 with no saturation or power failures. For completeness, we have run our model on all spectra, regardless of potential shadowing of the targets. The figure below shows abundance results for carbonate, olivine, and low-Ca pyroxene superimposed on various spectral parameters (described in Figure 2). Our results show good agreement with the spectral parameters; for example, carbonate abundances increase as the 2.32 and 2.53 band depths increase (top left), low-Ca pyroxene predictions have high LCPINDEX2 [5] values (bottom left), and olivine abundances increase as the slope from 1.3 to 1.8 increases (bottom right).

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References: [1] Fouchet et al. (2022) *Icarus*, 373, 114733. [2] Hapke (2012) *Theory of Refl. and Emit. Spec.* [3] Zastrow & Flynn (2023) *CoDA, Statistical Analysis & Data Mining*, in review. [4] Zastrow et al. (2024) *LPSC LV*, Abst. #2375. [5] Viviano et al. (2014) *JGR-Planets*.

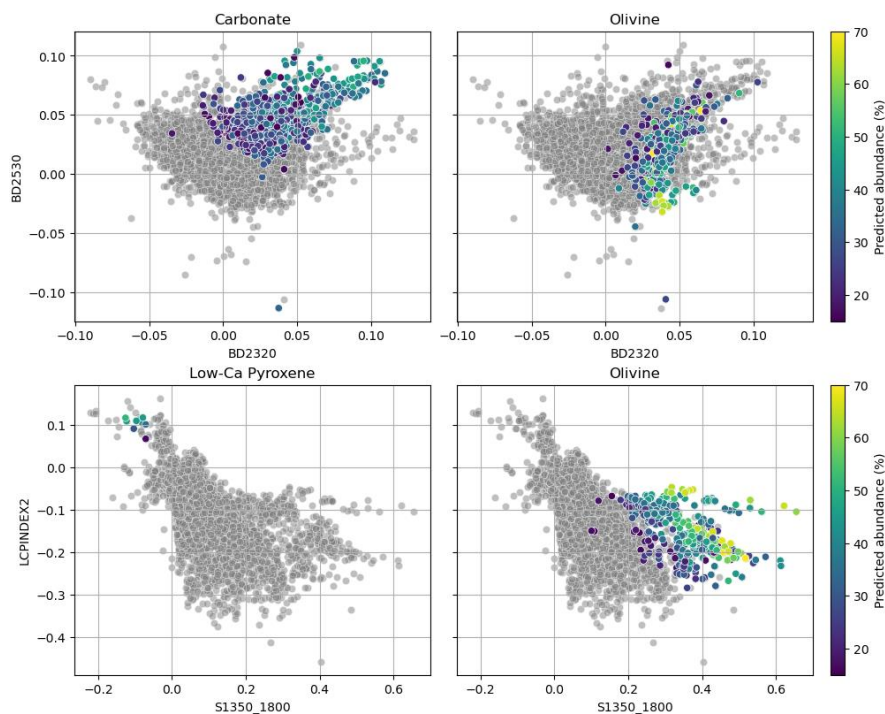


Figure 2. Predicted model abundances superimposed on spectral parameters. Top left: carbonate; top right: olivine; bottom left: low-Ca pyroxene; bottom right: olivine. Spectral parameters, top row, x-axis: band depth at 2.23 μm ; y-axis: band depth at 2.53 μm ; bottom row, x-axis: slope from 1.35 to 1.8 μm ; y-axis: low-Ca pyroxene index from [5]. Same colormap for all plots.