AUTOMATIC CLASSIFICATION OF MINERAL SPECTRA. S. T. Ishikawa[1] and V. C. Gulick[2], [1] NASA Ames/EAP/University of California Santa Cruz (Sascha.T.Ishikawa@nasa.gov), [2] NASA Ames/SETI Institute (Virginia.C.Gulick@nasa.gov).

Introduction: We present a robust, autonomous mineral classification method using Raman spectra. Our study shows that mineral classifiers built with artificial neural networks can be trained, using spectral data acquired by in situ Raman spectroscopy, to accurately distinguish among key minerals for characterizing the composition of igneous rocks. These minerals include olivine, quartz, plagioclase, potassium feldspar, mica, and several pyroxenes. On average, our classifier performed with 83 percent accuracy on unseen data; quartz and olivine, as well as the pyroxenes, were classified with 100 percent accuracy. In addition to identifying diagnostic bands and shapes, our classifier was able to incorporate fluorescence patterns into its classification scheme thereby improving the accuracy of results.

Background: Raman spectroscopy provides rapid, non-invasive mineralogical analyses. Samples can be scanned with a laser and analyzed in situ without being moved and without the need for preparation, such as grinding or pulverizing. For example, Haskin et al. (1997) used a manual "point cloud" method for quantifying the relative abundance of minerals in rock samples using in situ Raman spectroscopy with reported acquisition times between 30 and 45 seconds per spectrum. This approach is appealing because it provides a method for compositional analysis of samples as they are found, without alteration. Furthermore, the mineralogical analysis can be performed an unlimited number of times, and can be automated.

Traditional methods of automatic or semi-automatic Raman analysis use properties of observed spectral bands, such as shape and peak location, by fitting functions (e.g. polynomials or splines) to the bands in order to extract relevant features, which are then used to compare spectra.

Experimental Setup: The minerals we used in this study help to discriminate between felsic and mafic igneous rocks. Mafic igneous rocks are enriched in iron, magnesium, calcium and sodium, but are lower in silica. They are enriched in the minerals biotite, olivine, pyroxene, amphibole and plagioclase feldspar. However, felsic igneous rocks are enriched in silica, aluminum, and potassium and therefore contain higher percentages of the minerals quartz, muscovite, and potassium feldspars.

We used a Concurrent Analytical Inc. Raman spectrometer with an excitation wavelength of 852 nm to measure spectra of minerals in our collection. Our instrument has a resolution of 1.8 cm^{-1}, a spectral range of 456.1-1638.8 cm^{-1}, and a spot size of ~50 microns.

The spectra were acquired manually under controlled conditions. Each sample was shielded from ambient light by placing it in a dark enclosure. During the acquisition process the probe was initially placed within 1-2 cm from the sample surface. The focus of the excitation laser was manually adjusted until the signal strength was at its strongest, which coincides with the focal length of the laser beam.

Spectra were selected from six key mineral groups that can be used to identify igneous rocks. These groups are quartz, potassium feldspar, plagioclase feldspar, mica, pyroxene, and olivine. We processed the spectra as follows. First, we used linear interpolation to ensure uniform wavelength intervals. Second, we derivatized the spectra by replacing the spectra with their first derivative to suppress lower frequency spectral artifacts such as fluorescence, which can obscure important spectral bands. Third, we applied a smoothing filter using the Savitzky-Golay algorithm to attenuate the noise that was introduced during the derivatization process. Fourth, we normalized the spectral response values to account for variations in spectral intensity by re-scaling the values to the range [0,1]. Lastly, we utilized the multivariate technique of principal components analysis (PCA) to reduce the dimensionality of the data prior to training a machine learning classifier. Between 80 and 90 percent of the variance in the spectral data was captured using the first three principal components (see Figure 1).

A neural network, implemented by the multilayer perceptron (MLP) algorithm in the WEKA machine learning library, was used to learn the spectral data from training set. A 10-fold cross-validation procedure was used during training, which made efficient use of a limited number of samples. Furthermore, it enabled us to optimize various parameters (e.g. smoothing values and the number of PCs) before testing on unseen data. However, since the training and validation samples are drawn from the same dataset, there is some over-fitting (the reported accuracy will likely be higher than when using a separate testing set).

Application to other Spectral data sets: To further test the robustness of our algorithm, we used spectra from the RRUFF mineral database [5], a website that archives Raman spectra of mineral samples collected from various sources. We are also currently testing our algorithm on other spectral data sets as we expect our approach to perform well under any type of spectral data (e.g. Raman, reflectance, XRD, LIBS, etc.)

provided that each category of minerals or elements has reasonably distinct spectral signatures. Note, however, that we were able to demonstrate that an artificial neural network is able to learn the subtle differences, beyond simple Raman band positions and general shape, that are not as easily perceived by humans.

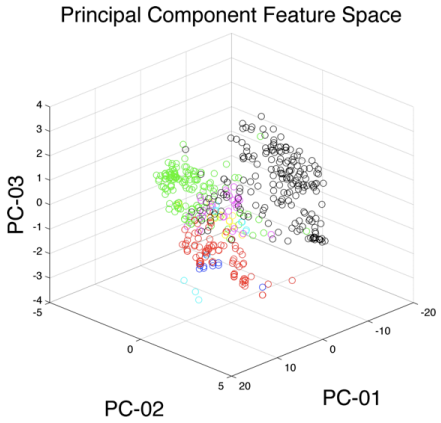

Figure 1. Distribution of mineral spectra in principal component feature space. Note the clustering of different colored points, which correspond to different mineral groups, e.g. pyroxene (balck), olivine (green), plagioclase (red).

Results: We evaluated our trained classifier using a separate test set of data "unseen" by the classifier. We were able to classify pure minerals by their mineral groups with an average accuracy of 83 percent.

The tables below provide, called *confusion matrices*, summarize the classification accuracies by providing information on how often an item was misclassified as something else. The rows indicate the total distribution of mineral classifications in a class of minerals given by the row header. The sum of the cells in each row indicates the total number of items belonging to a given class. The sum of the shaded diagonal cells indicates the total number of correct classifications.

	QTZ	*KSP*	*PLA*	*PYX*	*MCA*	*OLI*	*%*
QTZ	3	0	0	0	0	0	100
KSP	0	16	4	0	0	0	80
PLA	0	2	10	0	0	0	83
PYX	0	1	0	12	1	0	85
MCA	0	0	0	0	1	0	100
OLI	0	1	0	1	0	8	80

Table 1. Summary of classification performance of our neural network that was trained with Raman spectral data from our mineral collection. On average, the classifications were correct 83 percent of the time.

	QTZ	*KSP*	*PLA*	*PYX*	*MCA*	*OLI*	*%*
QTZ	5	0	0	0	0	0	100
KSP	0	9	1	0	0	0	90
PLA	0	17	4	0	1	0	18
PYX	0	0	0	45	0	0	100
MCA	0	0	0	2	9	0	81
OLI	0	0	0	0	0	14	100

Table 2. Summary of classification performance of our neural network that was trained with Raman spectral data from the RRUFF mineral library. On average, the classifications were correct 80.4 percent of the time.

Lastly, we provide preliminary results using the same method of mineral classification applied to reflectance spectra from the RELAB Spectral Library. A 10-fold cross-validation procedure was used during training; however, due to the sparcity of some minerals we were unable to generate a separate test set.

	QTZ	*KSP*	*PLA*	*PYX*	*MCA*	*OLI*	*%*
QTZ	10	0	0	0	0	0	100
KSP	0	7	3	0	0	0	70
PLA	0	4	5	0	0	0	50
PYX	0	0	1	8	0	1	80
MCA	0	0	1	0	9	0	90
OLI	0	0	1	0	0	9	90

Table 3. Summary of classifications during a 10-fold cross-validation procedure.

Conclusions. Our results from both the RRUFF Raman spectra as well as the RELAB reflectance spectra suggest difficulties distinguishing between plagioclase feldspars and potassium feldspars (K-spars). For example, 77 percent of plagioclase spectra in the RRUFF test set were incorrectly classified as K-spar. These trends are likely due to the chemical similarities between both minerals. Interestingly, however, these trends are absent in results from using our own Raman spectra due to predictable patterns of fluorescence in our spectrometer. Therefore, our classifier is capable of leveraging a particular response from the instrument to improve classification, which provides further demonstration of its robustness.

Acknowledgments: The study also used reflectance spectra from the RELAB spectral website at Brown University.

References: [1] Haskin, L. A., Wang, A., Rockow, K. M., Jolliff, B. L., Korotev, R. L., Viskupic, K. M., 1997. Journal of Geophysical Research 102(E8), pp. 19,293–19,306. [2] Ishikawa, S. T., Hart, S. D., Gulick, V. C. American Geophysical Union, Fall Meeting 2010, abstract #IN51A-1137. [3] Hall, M., Frank, E., Holmes, G., Pfahringer, B., Reutemann, P., Ian, H. SIGKDD Explorations 11(1), pp. 10-18, 2009. [5] Downs, R. T. 19th General Meeting of the International Mineralogical Association in Kobe, Japan. O03-13, 2006.