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Automated Remote Sensing with Near Infrared Reflectance Spectra: Carbonate Recognition

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Abstract. Reflectance spectroscopy is a standard tool for studying the mineral composition of rock and soil samples and for remote sensing of terrestrial and extraterrestrial surfaces. We describe research on automated methods of mineral identification from reflectance spectra and give evidence that a simple algorithm, adapted from a well-known search procedure for Bayes nets, identifies the most frequently occurring classes of carbonates with reliability equal to or greater than that of human experts. We compare the reliability of the procedure to the reliability of several other automated methods adapted to the same purpose. Evidence is given that the procedure can be applied to some other mineral classes as well. Since the procedure is fast with low memory requirements, it is suitable for on-board scientific analysis by orbiters or surface rovers.

Keywords: reflectance spectroscopy, mineralogy, artificial intelligence, Bayes nets, TETRAD, carbonates, mars

1. Introduction

The identification of surface composition from reflectance spectra has traditionally relied on two methods. The older of the two is a direct examination of spectra by experts, seeking lines or bands characteristic of particular substances, sometimes taking account of overall luminosity of the spectrum, and sometimes, with computational aids, taking account of the shapes of bands. The standard alternative is simultaneous linear regression of an unknown

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spectrum against a library of known spectra for candidate materials; a number of spectral libraries have been compiled which can be used for this purpose. Some neural net procedures have also been used to analyze spectral data, typically not for identifying surface composition directly, but rather for finding bounded regions of similar composition in an array of point spectra from a "visual" field. Other automated techniques have been explicitly used to identify surface composition of minerals and rocks, including a Bayesian technique described below. However, despite its numerous applications for planetary and terrestrial exploration and for various military purposes, we have found no published systematic (or unsystematic) study comparing automated classification of reflectance spectra to human expert classification of reflectance spectra, nor any systematic comparative study of alternative automated procedures. Using a both laboratory and field data sets, this paper provides such comparisons.

So far as planetary exploration is concerned, reflectance spectroscopy techniques have already shown themselves to be useful. Near-infrared reflectance spectroscopy (from approximately 0.4 μm to 2.5 μm) in particular has offered geologists an important potential source of petrological information for planetary, satellite and other solar system exploration. Lightweight, low-power commercial instrumentation is available, detailed physical models have been developed (e.g. Hapke, 1993), and such data is routinely used by geological spectroscopists in practical mineral classification (see, for example, Chapters 3, 14, 16, 20, and 21 of Pieters and Englert (1993) and references therein). Were such instruments coupled with intelligent software for mineral classification from spectra, the resulting system could be used for either remote sensing or surface based studies, reducing data storage and information transmission requirements and aiding autonomous, rational, scientifically-informed decisions by robot explorers about further directions for exploration and data acquisition.

This interest in planetary exploration motivates an examination of the problem of determining whether rock or soil samples contain carbonates and, in particular, whether such samples contain either of the most frequently occurring forms of carbonate material—calcite or dolomite. Carbonate identification is interesting for extra-terrestrial exploration, because carbonates are typically formed by processes—such as deposition from water—that could indicate an historical environment that once supported life. We therefore, focus on the task of carbonate identification. We compare the reliabilities of (a) an expert human spectroscopist, (b) an expert system that models human expert procedures, and (c) a variety of automated techniques, including linear regression, each with various resampling and cross-validation techniques, on the task of carbonate identification from visual to near infrared reflectance spectra. All of our tests of data mining procedures use the same library of spectra for training or reference. A variety of data sets are used for testing, including laboratory and field spectra obtained under various conditions.

In our tests, an adaptation of the PC algorithm (Spirtes et al., 1993, 2000) implemented in the TETRAD II program (Scheines et al., 1994) for constructing causal Bayes nets from data, combined with appropriate data selection and data preprocessing, performed more reliably than any other automated procedure we have tested. We will refer to this procedure as the "modified PC" or "modified Tetrad" algorithm. In some tests this procedure was more informative than a human expert spectroscopist and almost as reliable, and in other tests the procedure performed almost as well as human experts with access both to physical samples and to measured spectra of the physical samples. These claims are made more precise in the data summaries given below. We additionally compare various preprocessing and data selection procedures, and, through an experiment comparing expert human performance and machine performance, we investigate the likelihood that our techniques can be successfully applied to other classes of minerals.

2. Preprocessing of data

Raw spectral data are preprocessed in our analysis in a variety of ways to produce data that can usefully be analyzed by automated techniques.

First, raw spectral data are converted to intensities by comparing them to spectra from standard white samples measured under the same conditions. To compensate for the varying power function of sunlight, digitalized spectra, taken in the field, are automatically divided by the spectrum of a white reference surface placed near the target, and these ratios are recorded for a number of channels—826 channels in the instrument used in this study.[1] These ratios are the intensities of the spectral measurements for their respective channels. Different instruments covering the same wavelength interval may use distinct wavelength channels, and comparisons of field spectra taken with one instrument to laboratory spectra taken with another instrument require that the channels for one of the instruments be used to interpolate values for the channels used in the other instrument. This interpolation ensures that data submitted to identification algorithms utilize the same set of wavelengths throughout.

Second, anomalous lines are removed from the spectrum. For various reasons, at some wavelengths the output of a spectroscope in the field may have out-of-range intensity values. For example, water vapor in the atmosphere often creates anomalous absorption lines around 1.9 μm. These lines within each spectrum can be removed by computational preprocessing, or they can be removed by hand, or the spectra themselves can be tested automatically for extreme variation and extremal spectra rejected altogether for analysis. We use the latter two procedures—removing anomalous lines by hand and rejecting spectra with extremal variation—for spectra taken in the field in the experiments described in this paper.

Third, hull differences of the spectrum are calculated. After any elimination of out-of-range channels, the intensities for each of the remaining channels in a spectrum can then be subjected to interpretation either directly—the data are the "raw" spectral intensities—or after transformation. The most common transformation fits a piece-wise linear "hull" around the extremal points of hills and valleys of the spectrum and computes, for each channel, the difference between the spectral intensity at that channel and the numerical value of the hull at that channel on the intensity scale. The "hull difference" values are then subjected to analysis. An alternative but less successful procedure is to compute first differences among intensities in successive channels. We have found that a suitably loose hull difference works best.

The effects of different preprocessing procedures are illustrated by analyses of the spectrum of a rock taken near Silver Lake, CA; the results are shown in Table 1. The composition of the rock was analyzed by two procedures, using the raw spectra, hull differences, and first differences, with and without water lines removed. One of the procedures was linear regression with a reference library of laboratory spectra from the Jet Propulsion Laboratory

Table 1. Analyses of the spectrum of a sample taken near Silver Lake, CA, known to contain dolomite and calcite and described as "dolomite with calcite veins." Only minerals with positive regression coefficients are shown.

Water lines removed			Water lines included	
Tetrad	Stepwise regression	Data treatment	Stepwise regression	Tetrad
Calcite	Calcite	None	Calcite	Dolomite
Dolomite	Cyclosilicate		Dolomite	
			Cyclosilicate	
Calcite	Calcite	Hull difference	Calcite	Dolomite
Dolomite	Dolomite		Dolomite	Cyclosilicate
	Cyclosilicate		Cyclosilicate	
	Arsenate		Arsenate	
Dolomite	Cyclosilicate	First difference	Cyclosilicate	None
	Cerussite			

(Grove et al., 1992) and the STEPWISE procedure in Minitab. The other procedure was the modified PC algorithm, to be explained later in this paper. The target rock was subsequently identified by an expert as "dolomite with calcite veins," and chemical testing showed both dolomite and calcite composition.[2]

3. Data selection

In addition to preprocessing methods, further decisions were made about which regions of the spectrum to accept for purposes of automatic processing. When analyzing the spectrum from an unknown source to determine its composition, three data selection protocols are used:

1. Accept the entire spectrum, after removing any channels with out-of-range values.
2. Accept only channels in a particular interval or union of intervals, when the purpose is to recognize a particular component, or class of components, if present, and this component, or class of components, is known to exhibit a distinctive spectral features in this particular wavelength interval or set of intervals.
3. Detect only particular spectral bands or lines characteristic of particular components of interest, if present.

The advantage of the first strategy is evidently that it uses all of the data, but if only parts of the spectrum provide a distinctive signal for a mineral class, use of the entire spectrum may be a disadvantage. The advantage of the second strategy is that it makes efficient use of background knowledge to focus on the informative part of the spectral signal; the disadvantage is that the procedure reduces the size of the data set, which sometimes makes statistical procedures inapplicable, as we will illustrate in subsequent sections. The third strategy also makes use of background knowledge, but lines and bands characteristic of the spectrum of a pure mineral may be shifted or masked in the spectrum from a surface of mixed composition.

4. A field test of automated procedures and data selection protocols

In the winter of 1999, NASA scientists conducted field tests of a robot and instruments in and about Silver Lake, California, a dry lake bed in the Mojave Desert (Stoker et al., 2001). Among the instruments was a near-infrared spectrometer (Johnson et al., 2001). Spectra were taken, usually in situ, of rocks and soils; the spectra were identified as carbonates or non-carbonates both by the field geologists, from physical observations of the specimens and their spectra, and by a group of geologists located remotely at NASA Ames, who used both the spectra and the descriptions of the field experts (Gazis and Roush, 2001). Paul Gazis at NASA Ames provided software to correct instrumental artifacts and to filter out spectra that, typically because of atmospheric effects, were too noisy to process. After this pre-processing, 21 spectra remained; 13 samples were identified as carbonates and 8 samples identified as non-carbonates by the field geologists. Subsequently, eight of the 21 samples were analyzed by standard petrographic techniques. All eight analyses agreed with the judgements of the field geologists and the remote geologists.

The data were analyzed using the following combinations of procedures. (The details of the procedures, and their rationales, are explained in the next section.)

1. The modified PC algorithm, seeking to recognize any carbonates, using a restricted interval of wavelengths with intensity patterns characteristic of carbonates.
2. The modified PC algorithm, seeking to identify carbonates from calcites and dolomites only, using a restricted interval of wavelengths with intensity patterns characteristic of carbonates.
3. The modified PC algorithm, seeking to recognize any carbonates, using all wavelengths available from the instrument.
4. The modified PC algorithm, seeking to recognize only calcites and dolomites, using all wavelengths available from the instrument.
5. Linear regression, seeking to recognize the presence of any carbonates using all wavelengths available from the instrument.
6. Linear regression, seeking to recognize the presence of any carbonates using all wavelengths available from the instrument, but reporting only components with positive regression coefficients.
7. Linear regression, seeking to recognize carbonates from calcites or dolomites only, using all wavelengths available from the instrument.
8. Linear regression, seeking to recognize carbonates for calcites or dolomites only, using all wavelengths available from the instrument, but reporting only components with positive regression coefficients.
9. An expert system seeking to recognize the presence of any carbonates from a triple of lines around 2.3 μm. (Gazis and Roush, 2001)

Because this data set has been incompletely described in at least two other published reports, we give its composition in full in Tables 2 and 3. The field group's name for each sample is given in the leftmost columns of the tables.

The number of samples correctly estimated to contain or not contain carbonates, given at the bottom of each column, is based on the assumption that the expert field identifications

Table 2. Carbonate identifications of field spectra from Baker, CA using the modified PC algorithm.

Sample	Field expert ID	Modified PC ID (all carbonates; 2.0–2.5 μm)	Modified PC ID (calcite or dolomite only; 2.0–2.5 μm)	Modified PC ID (calcite or dolomite only; 0.4–2.5 μm)	Modified PC ID (all carbonates; 0.4–2.5 μm)	Laboratory ID
Emperor #1	C	C	C	C	C	C (90%) NC (10%)
Emperor #2	C	C	C	C	C	C (90%) NC (10%)
T 103	NC	NC	NC	NC	NC	NA
T 105	NC	NC	NC	C	C	NA
T 106	C	C	C	C	C	NA
Endolith	C	C	C	C	C	C (93%) NC (7%)
Tubular-tabular	NC	NC	NC	NC	C	NC (100%)
Arroyo disturbed	C	NC	NC	C	C	C (20%) NC (80%)
Arroyo undisturbed	C	C	C	C	C	C (25%) NC (75%)
C3PO	C	C	C	C	C	NA
Chewie	NC	C	NC	NC	C	NA
Jabba	C	C	C	C	C	NA
Jawa	C	C	C	C	C	NA
Lando	C	C	C	C	C	C (93%) NC (7%)
Luke	C	C	C	C	C	NA
R2D2	C	C	C	C	C	C (78%) NC (22%)
Solo	C	C	C	C	C	NA
Tarken	NC	NC	NC	NC	NC	NA
Vader	NC	NC	NC	C	C	NA
Valentine	NC	NC	NC	C	C	NC (100%)
Yoda	NC	NC	NC	NC	C	NA
Total correct		19	20	18	15	

The first column shows the nickname given to each sample for purposes of analysis. The second column shows the carbonate ID of the rock by an expert in the field. Columns 3 through 6 display carbonate identifications using the modified PC algorithm, with different preparations of spectra and different criteria for carbonate identification. In columns 3 and 4, all spectra are hull differenced and then truncated to the interval [2.0, 2.5]; in columns 5 and 6, the spectra are hull differenced but not truncated. In columns 3 and 6, a sample is counted as a carbonate if the modified PC algorithm returns a set of minerals which contains any carbonate from among the 15 large-grain carbonates in the JPL mineral data set; in columns 4 and 5, a sample is counted as a carbonate only if the modified PC algorithm returns a set containing a calcite or a dolomite. Column 7 shows the results (where laboratory testing is available).

Table 3. Carbonate identifications of field spectra from Baker, CA using the simultaneous linear regression algorithm in Minitab.

Sample	Field expert ID	Regression ID (all carbonates; 0.4–2.5 μm)	Regression ID (all carbonates with positive coefficient; 0.4–2.5 μm)	Regression ID (calcite or dolomite only; 0.4–2.5 μm)	Regression ID (calcite or dolomite only, with positive coefficient; 0.4–2.5 μm)	Expert system ID	Laboratory ID
Emperor #1	C	C	C	C	C	C	C (90%) NC (10%)
Emperor #2	C	C	C	C	C	C	C (90%) NC (10%)
T 103	NC	C	C	C	C	NC	NA
T 105	NC	C	C	C	C	NC	NA
T 106	C	C	C	C	C	C	NA
Endolith	C	C	C	C	C	C	C (93%) NC (7%)
Tubular-tabular	NC	C	C	C	NC	NC	NC (100%)
Arroyo disturbed	C	C	C	C	C	NC	C (20%) NC (80%)
Arroyo undisturbed	C	C	C	C	C	C	C (25%) NC (75%)
C3PO	C	C	C	C	C	C	NA
Chewie	NC	C	C	NC	NC	NC	NA
Jabba	C	C	C	C	NC	NC	NA
Jawa	C	C	C	C	NC	C	NA
Lando	C	C	C	C	C	C	C (93%) NC (7%)
Luke	C	C	C	C	C	C	NA
R2D2	C	C	C	C	C	NC	C (78%) NC (22%)
Solo	C	C	C	C	C	NC	NA
Tarken	NC	C	NC	C	NC	NC	NA
Vader	NC	C	C	C	C	NC	NA
Valentine	NC	C	C	C	NC	NC	NC (100%)
Yoda	NC	C	C	C	C	NC	NA
Total correct		13	14	14	15	17	

Column 1 shows the nickname given to each sample for purposes of analysis. Column 2 shows the carbonate ID of the rock by an expert in the field. Columns 3 through 6 display carbonate identifications using linear regression, with different criteria for carbonate identification. In columns 3 and 5, samples are counted as carbonates if when regressed onto the JPL library at least one of the JPL carbonates has a significant regression coefficient; in columns 4 and 6, this regression coefficient must be not only significant but also positive. Also, in columns 3 and 4, a sample is counted as carbonate if when regressed any of the JPL carbonates has a significant regression coefficient; in columns 5 an 6, only significant regression coefficients for calcites and dolomites are counted. Column 7 shows the identification by the expert system used in the study, and column 8 shows the results (where available) of laboratory testing.

represent the truth. This is a reasonable assumption because expert field identifications rely on both physical examination of samples and examination of measured spectra and, where tested, agree with laboratory analyses of the samples. Assuming that remote expert classifications represent the truth would change values only for samples 'jawa' and 'R2D2,' increasing the scores of two regression procedures by 1 and the score of the expert system by 2. All data were hull differenced for all procedures. For a more detailed description of the expert system referred to here, see Gazis and Roush (2001). A team from the Jet Propulsion Laboratory has also classified the Silver Lake spectra with a neural net (Gilmore et al., 2000). Their report of their results is unclear in essential respects, but they report the identification of only eight carbonates.

These results suggest that the modified PC procedure, in combination with a data filter restricting the set of wavelengths used as a data, outperforms the other eight procedures considered and is nearly as good as expert identification in the field using physical examination and spectra—without the filter, the modified PC procedure overfits almost as badly as regression and is inferior to an expert system modeling an expert spectroscopist. Why all of this should be so, and why the regression procedure is not combined with the same data filter, and, finally, whether these suggestions hold up under further tests, is discussed in the following sections.

5. Descriptions of the automated procedures

5.1. Multiple regression

The regression procedure takes each channel wavelength as a unit and uses the value of the intensity of the target rock at each measured wavelength as the dependent variable. The independent variables are the intensities of each of the 135 large-grain mineral samples in the JPL library of reflectance spectra, at the same wavelengths. The 135 minerals are divided into 17 classes, one of which is the carbonate class, with 15 minerals, including 3 dolomites and 2 calcites.[3]

In the regression procedure using all carbonates, a carbonate is recorded as present if any of the 15 carbonates in the JPL library has a significant regression coefficient, using a 0.05 significance level. In the regression procedure using only calcites and dolomites, a carbonate is recorded as present if any of the five calcites or dolomites has a significant regression coefficient, using a 0.05 significance level. In the regression procedures requiring a positive sign, a carbonate is reported present if a carbonate mineral has a significant positive coefficient. In only one case was the result very sensitive to the significance level (an increase in the significance level to 0.054 would have resulted in the misclassification of 'Chewie' as a carbonate using either of the two regression procedures that identify carbonates through calcites and dolomites.) Otherwise, variations in the significance level between 0.100 and 0.010 would have made no difference in the regression results.

Note that regression suffers from three difficulties, one structural and two statistical, which make it an inferior procedure in many applications:

1. Consider any two regression variables, X_1, X_2 among a set $\mathbf{C}$ of candidate causes of an outcome variable Y. Suppose X_1 and X_2 are correlated due to factors that influence both

X_1 and X_2 values but are not themselves in **C**. Suppose, finally, that another factor U, not included in **C**, influences both Y and X_2. Then, even if X_1 has no influence on Y, and even if there is no correlated error between X_1 and Y, and even if all common influences on X_1 and Y are included among the variables in **C**, for sufficiently large sample sizes the partial regression coefficient for X_1 will (almost certainly) have a significant value. The phenomenon is sometimes called conditional correlated error. In the present application, it can result in the identification of minerals that are not, in fact, components of the source.

2. Simultaneous linear regression computes the partial regression coefficient of a variable X_1 effectively by conditioning (assuming a Normal distribution) on all other regressors in the regressor set **C**—in our application, conditioning on all of the other 134 minerals in the JPL library. While any one of these variables may be only loosely correlated with X_1, together they may be highly correlated with X_1. In that case, the covariation of X_1 and Y after partialing out the variation in Y due to other factors in **C** may be effectively zero. In the present application, multicollinearity can result in failing to identify a true component of the source.
3. The variance of the estimates of a simple regression coefficient is a function of the sample size. The variance of the estimates of a partial regression coefficient is a function of sample size and the number of other candidate causes, or regressors—that is, a function of the cardinality of **C**. The bigger the sample size and the smaller the number of other regressors, the smaller the variance. Assuming a Normal distribution, the trade off is one for one: adding an extra regressor variable is equivalent in its effect on the variance to reducing the sample size by one unit. In the present application, reducing the number of channels used for data analysis increases the variance of the estimates of regression coefficients. In the extreme case in which the number of variables is greater than the sample size, regression is ill-defined, and standard regression packages will not run at all. In our application, regression procedures will not run using the JPL library as the regressor set **C** and restricting the data to the channels with wavelengths in the interval [2.0 μm, 2.5 μm].[4]

Several remedies to this last difficulty can be considered. The wavelength interval [2.0 μm, 2.5 μm], in this case, is chosen because previous work on carbonate spectra shows that this region has distinctive spectral features for carbonates. We could search for a larger range of wavelengths optimal for regression procedures in this application. We could eliminate some of the minerals in the JPL library from the set of possible components of the source, but that would decrease the reliability of the procedure when those components or spectrally similar components are actually present in the source. We could use a stepwise regression procedure, but other experiments with small samples have found stepwise regression less reliable than the procedure used here (Spirtes et al., 1993, 2001). A better solution to this problem is available—viz., the algorithm described in the next subsection.

5.2. *The modified PC algorithm*

All three of the problems cited above with linear regression stem from a single structural feature of the regression procedure, linear or otherwise. In estimating the influence of a variable X on the outcome Y, regression conditions simultaneously on all other candidate variables—i.e., all of the other members of **C**. That is, in our (rather conventional, but not textbook) use of regression, we test the null hypothesis that X has no influence on Y (or is not a component of Y) by using the distribution of a test statistic that is conditioned on all other members of **C**.

There is an alternative procedure that minimizes the number of variables that must be conditioned on. It takes as input a set of background variables $\mathbf{C} = \{X_1, X_2, \ldots, X_n\}$ together with a target variable Y not in **C** and dynamically eliminates variables from **C** using conditional independence facts, calculated from data. Variables are eliminated which are independent of Y conditional on subsets of other remaining variables in **C**, where the cardinality m of the subsets increases in size ($m = 0, 1, 2, \ldots$) until no more variables can be eliminated from **C**. More formally:

Modified PC Algorithm:

Given set **C** of background variables and target variable Y:

1. for each X_i in **C**, test the hypothesis that the correlation of X_i with Y is zero; if the correlation of X_i with Y is zero, $\mathbf{C} := \mathbf{C} - \{X_i\}$;
2. for each X_i in **C**, and for each $X_j \neq X_i$ in **C**, test the hypothesis that the correlation X_i with Y, controlling for X_j, is zero; if the correlation of X_i with I_t controlling for X_j is zero, $\mathbf{C} := \mathbf{C} - \{X_i\}$;
3. for each X_i in **C** and each X_j, $X_k \neq X_i$ in **C** test the hypothesis that the correlation X_i with Y, controlling for X_j, X_k is zero; if the correlation of X_i with I_t controlling for X_j, X_k is zero, $\mathbf{C} := \mathbf{C} - \{X_i\}$;

... and so on, until no more members of **C** can be removed. Return **C**.

This procedure may be understood intuitively as a application of the theory of search for graphical causal models (Spirtes et al., 1993, 2001), applied in this case to produce a directed graph representing a hypothesis about the mineral composition of a source.

If n members of **C** are actually components of Y, no more than n variables must be conditioned on simultaneously. If, for example, three minerals in the JPL library are actual components of a sample, a large number of statistical tests will be done, but none of the tests will require controlling for more than three variables—in no test will the sample size effectively be reduced by more than 4, in contrast to multiple regression in which the sample size is reduced by 134. For that reason, unlike multiple regression, the procedure can be used with the JPL library with the reduced data set using only intensities in channels for wavelengths in the interval [2.0 μm, 2.5 μm].

This procedure is subject to the statistical objection that no confidence intervals or error probabilities can be calculated (see Robins et al., 1999; Spirtes et al., 2000). But, unlike regression, there is a proof that the procedure—under specified assumptions—is asymptotically correct, and in simulation studies the procedure is much more reliable than best subsets procedures (Spirtes et al., 1993). While confidence intervals have important uses, if the choice is between a procedure with confidence intervals that is known to be asymptotically invalid and is unreliable in real applications and in simulation studies and with small samples, or an asymptotically correct procedure found to be reliable but admitting no confidence intervals, we prefer the latter.

6. Test with laboratory spectra

Because the sample size in the field test is small and the samples are all from a single site, the procedures tested above need to be tested as well on a separate and preferably larger data set. The Johns Hopkins University (JHU) has assembled a library of reflectance spectra for a variety of solid and powdered rock samples.[5] Each spectrum in the JHU rock library is accompanied by a description of the petrology of the sample. Because mineralogical nomenclature is so varied, these descriptions do not generally identify sample components either as among the 135 specific minerals represented in the JPL library (e.g., calcite, dolomite, etc.) or as among the 17 general mineral classes into which the JPL library is classified (e.g., carbonates, phyllosilicates, etc.). Assignment of JHU samples to the 17 general JPL mineral classes on the basis of the petrological descriptions alone requires expert knowledge.

Using the JHU petrology descriptions, but without access to the sample spectra, Ted Roush of NASA Ames determined which of the 17 JPL mineral classes is represented in each of the 192 JHU rock samples. Since the rocks were not pure minerals, they could each belong to more than one of the 17 general mineral classes. 92 of the samples were judged to contain some form of carbonate. These assignments of JHU minerals to carbonate class were then used as ground truth in tests of reliabilities of various procedures for mineral classification.

Each of the procedures applied to the field test data was applied to the JHU samples as well, except that, in place of the expert system based on Roush's own procedures in identifying carbonates from spectra, Roush himself—without access to the petrological descriptions of the samples—attempted to identify samples with carbonate components. The results of these analyses are summarized in Table 4.

We recognized that among the machine classification algorithms available in the artificial intelligence literature, there may be classifiers that perform better than the modified PC algorithm. To search for such procedures, we used the Model 1 program, a commercial program that uses a training set—in our study, the JPL library—to assess the performance of a large number of algorithms.[6] We tested one of the best-scoring algorithms found by Model 1 on the JHU library. The procedures among which Model 1 searched included include linear regression, cross-validated linear regression, logistic regression, cross validated logistic regression, backpropagation on a neural network, cross-validated backpropagation, CART (classification and regression trees), naïve Bayes, and other procedures.

The Model 1 program found that a cross-validated logistic regression procedure performed best on the JPL library (a simple linear regression procedure performed worst). When used on a test set to identify a target variable with a particular algorithm—in our case to identify samples in the JHU library containing carbonates—Model 1 listed the samples in order from those most likely to contain carbonate (according to the algorithm tested) to those least likely and reported how far down in the ordering one must go for any specific number of correct identifications. The result for 36 correct carbonate identifications is shown in the next to right-most column of Table 4. Results for other selections are similarly poor.

Table 4. Comparison of tetrad, regression, Model 1, and human expert on the task of identifying samples with carbonate components among the JHU rock samples.

	Procedure									
	TA	TACR	TCD	TCDR	RAC	RACP	RCD	RCDP	M1	HE
Number of carbonates identified	58	63	42	41	192	191	154	176	73	25
Number of carbonates correctly identified	38	47	36	38	92	91	79	90	36	24
Number of noncarbonates misidentified as carbonates	20	16	6	3	100	100	75	86	37	1
Number of carbonates misidentified as noncarbonates	54	45	56	54	0	1	13	2	56	68
Total number of errors	74	61	62	57	100	101	88	88	93	69
Prob (carb | carb predicted)	0.66	0.60	0.90	0.93	0.48	0.48	0.51	0.51	.49	0.96
Prob (carb predicted | carb)	0.41	0.51	0.39	0.41	1.00	0.99	0.86	0.98	.39	0.26

TA = Tetrad all carbonates 0.4–2.5; TACR = tetrad all carbonates 2.0–2.5; TCD = tetrad calcite or dolomite 0.4–2.5; TCDR = tetrad calcite or dolomite 2.0–2.5; RAC = regression all carbonates (any coefficient); RACP = regression all carbonates (positive coefficient only); RCD = regression calcite and dolomite, any coefficient; RCDP = regression calcite and dolomite, positive coefficients only; M1 = Model 1; HE = human expert.

These results show the same pattern as in the field test. Regression procedures are essentially useless, and one would do roughly as well flipping a coin to decide whether the source of a spectrum contains carbonate. Like the expert system in the field trials, the human expert is conservative and has (almost) no false positive carbonate identifications, but correctly identifies only limestones and marbles, but the expert also has the largest collection of false negatives. As in the field tests, the modified PC algorithm identifying carbonates through calcite or dolomite and restricted to the wavelength interval [2.0 μm, 2.5 μm], stands out—its false positive rate is almost as small as the human expert's, but its false negative rate is substantially smaller. The best procedure that the (very expensive) Model 1 program could find was dramatically inferior.

7. Carbonate composition from a scene

Roush and his colleagues at Ames Research Center obtained 640 spectra by scanning a scene consisting of rocks of varying composition placed in a square soil bed. The spectra were taken from a short distance away from the site, using a white reference placed by the nearest rock. One of the rocks was limestone, a carbonate; others included a cement block with very low and indeterminate limestone content, a bright sulphate rock, and rocks of other composition. These spectra were classified for carbonate identification at Ames by least squares procedures, with the Gazis and Roush expert system and, independently, by Roush from the spectra. The details of these analyses will appear elsewhere. The results of the modified Tetrad classification, using a 2.0–2.47 μm data filter (because of signal noise at the extreme long wave length end of the spectrum), a 10 box boxcar smoother, hull differencing,

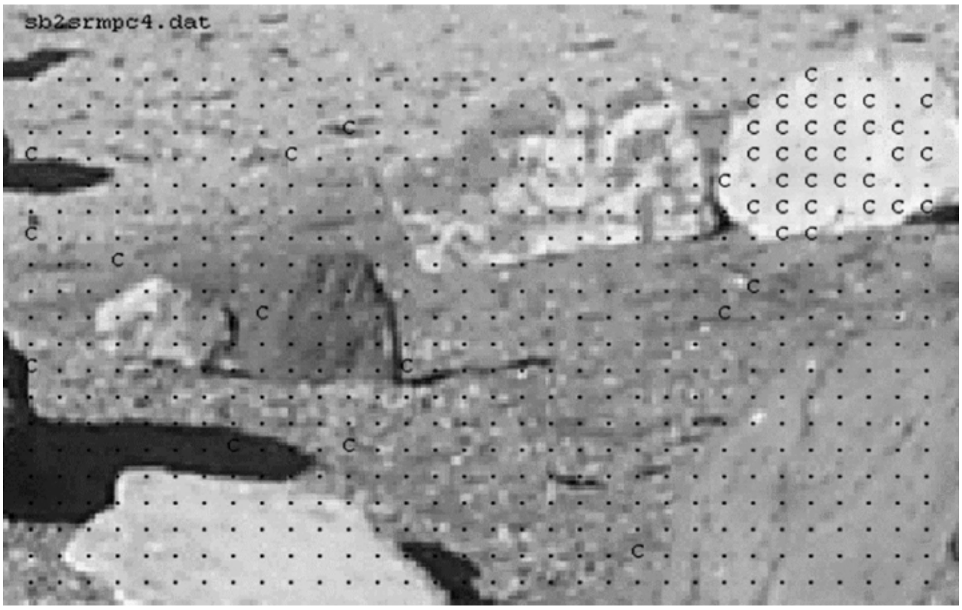


Figure 1. Identification of pixels containing carbonates (C) and not containing carbonates (·) in a 20 × 32 pixel scene using the modified PC algorithm. For details, see text.

a .01 significance level for independence tests, and eliminating the comparatively rare carbonate, cerussite, from the JPL reference library (because in the spectral interval allowed by the data filter, its spectrum matches a sulphate) is shown in figure 1. The white rock in the upper right hand corner is limestone.

8. Experiments with variable white reference location

Because the power spectrum of the sun varies with place and time, reflectance spectra require comparison of the reflected light from a surface with that reflected from a white reference surface. In laboratory studies, and in the laboratory and field studies so far reported here, the reference is placed at or near the target sample. But remote sensing requires that the white reference be near the spectroscope and remote from the target. We have been able to find no study of the accuracy of deconvolution algorithms in this deployment.

We obtained commercial floor tiles respectively of terra cotta (silicate), marble (a carbonate), and granite. Each tile had a rough side and a smooth side. Repeated measurements, four of each side, were made of the reflectance spectra of these tiles at NASA Ames Research Center, under two conditions. In one condition, the white reference was placed next to the tiles, 28 feet from the spectrometer. In the other, the white reference was placed 2 feet in front of the spectrometer, and the target tiles were in the former position, 28 feet from the instrument. The data were then analyzed with the expert system referred to previously and the modified Tetrad procedures with 2.0–2.43 μm data filter, no hull differencing, 20

Table 5. Ames test of mineral identification with varied location of white reference.

	Reference at target	Reference at instrument
Ames expert system	2 of 8 carbonates No false positives	2 of 8 carbonates No false positives
Tetrad, 2.0–2.4 μm .05 significance	7 of 8 carbonates 4 false positives	7 of 8 carbonates 1 false positive
Tetrad 2.0–2.4 μm .01 significance	7 of 8 carbonates 2 false positives	7 of 8 carbonates 3 false positives

box boxcar smoothing, using two significance levels for independence tests. The results are shown in Table 5.

9. Other mineral classes: A human expert baseline and a John Henry experiment

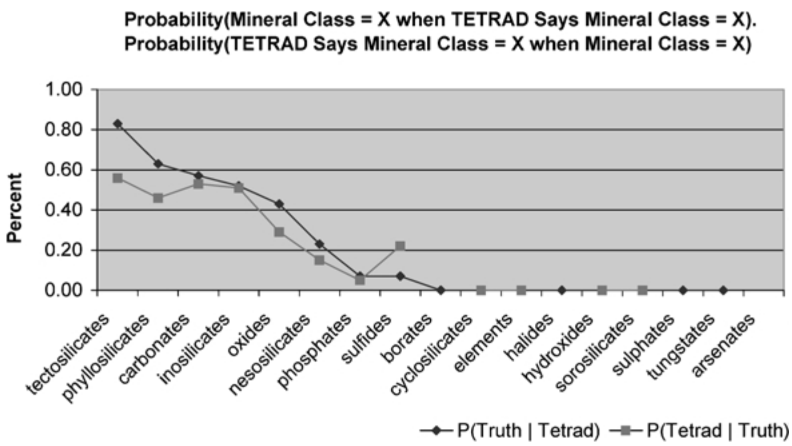
Many other minerals or mineral classes other than carbonates are of scientific interest or of interest in terrestrial or Martian exploration. To investigate whether automated procedures can approximate human expertise for other mineral classes, we obtained an experimental human expert baseline and compared it with the performance of the modified Tetrad program with no data filter.

Roush examined 191 JHU spectra stripped of identifiers and attempted to determine, for each of the 17 JPL mineral classes, which classes were present in the JHU source. He had unlimited time and was free to use any reference works or computer aids he wished. In the event he spent about 12 hours on the task over 4 days. The modified PC algorithm was then run on the same spectra, using the entire 0.4 μm–2.5 μm spectrum, hull differenced, at 0.05 significance for independence tests, and outputting any of the 17 JPL classes if a representative of that class was found for a sample. For eight of the seventeen JPL mineral classes, no representative, or no more than two representatives, were present in the JHU library, and for those classes the experiment is of no significance. The results are shown graphically in figures 2(a) and (b).

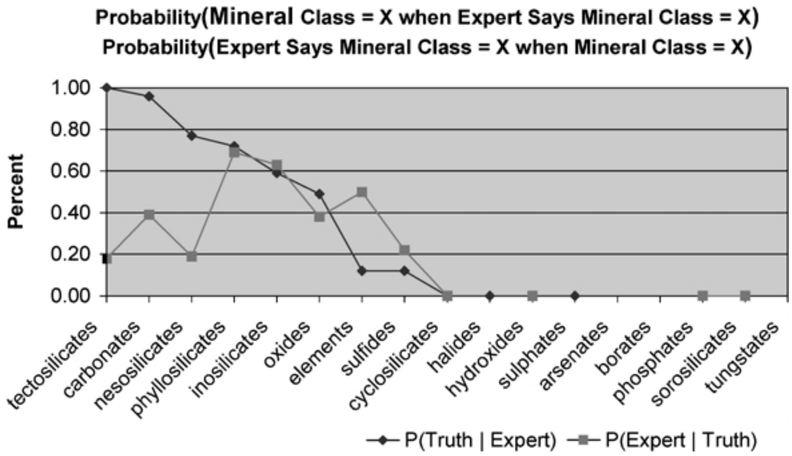
For tectosilicates, phyllosilicates and inosilicates the positive identifications of the human expert have significant reliability, and can be approximated (with more false positives and fewer false negatives) by the modified PC algorithm. We have reason to hope, therefore, that subclasses of these mineral groups can be distinguished, and informative spectral regions found, for which the machine procedures will be useful. The problem is to find informative data filters for each class, if they exist.

10. Automated construction of data filters

Moody et al. (2001) describe two methods for locating data filters for a given mineral class. One procedure bins the intensities of library spectra at each frequency and computes the information about the given class at each spectral interval. A second procedure partitions



(a)



(b)

Figure 2. Graph (a) shows the conditional probability that rocks contain minerals belonging to a certain class, given that the modified PC algorithm ("TETRAD") identifies them as containing minerals belonging to that class. The reverse conditional probabilities are shown as well. Graph (b) shows the conditional probability that rocks contain minerals belonging to a certain class, given that the expert of the experiment described in Section 9 ("Expert") identifies them as containing minerals belonging to that class. The reverse conditional probabilities are shown as well. The rock spectra being identified in each case are the 192 rock spectra from the Johns Hopkins University Spectral Library.

the 4.0–2.5 mm spectral region into intervals and codes each interval as an allele value (present or absent) in a genetic algorithm, using the modified tetrad algorithm to evaluate fitness.

The information algorithm is sensitive to the number of bins used, and the genetic algorithm is sensitive to the number of elements of the partition—the number of genes—used.

Best results in the experiments were obtained with a genetic algorithm with ten genes. An interval for carbonates corresponding closely to the 2.0–2.5 mm region was found, and reasonably well-defined intervals were also found for inosilicates. Other mineral classes and subclasses have not been explored.

11. Discussion

In less formal experiments we have used the JPL library as a training set and the JHU library as a test set to explore a number of other approaches to automated mineral classification from reflectance spectra, with little success. Kohenen self-organizing maps and AutoClass yield interesting classifications of the JPL spectra, but they generally do not correspond to standard mineral classifications of geological interest. The problem of identifying mineral composition from reflectance spectra seems as if it could fruitfully be treated by neural net techniques, and that was our initial approach. In 1996 we generated training data for a network with four hidden nodes by taking random linear combinations of JPL spectra and we testing the trained network on JHU data. JPL investigators have subsequently used a similar approach. We trained networks for carbonate identification but found that the networks did not perform well if the test data contained significant fractions of minerals not in the training set. A further problem is that in reality the reflectance spectra of rocks, soils and other materials are not in general linear or even additive functions of the spectra of their component minerals, and such training procedures therefore lack realistic training sets.

We have attempted carbonate identification with two Support Vector Machine programs available online ("MySvm" and "SvmLight"). Treating labels as continuous produced some promising results superficially similar to those reported here. However, with labels treated as discrete, as they are treated for the algorithms reported above, neither program converged at all, no matter which general purpose kernel was used.

It may well be that boosting techniques, or carefully chosen kernels for Support Vector Machines, or something else altogether that we have not considered, will improve on the results reported here for the modified PC algorithm with appropriate data filters, but for the present the modified PC algorithm seems to be the best available procedure for the identification of carbonate content in minerals and perhaps for the identification of other mineral class content as well. The algorithm can be improved in various ways, for example by resolving ambiguities—such as that between cerussite and certain sulphates—within the range admitted by a data filter by comparing spectral regions excluded by the data filter.

Executables and source code for all of the algorithms described in this paper, except the Gazis-Roush expert system and proprietary Model 1 algorithms, can be downloaded from http://www.phil.cmu.edu/rockspec. Data sets described in this paper can be downloaded from the same location.

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Notes

1. The spectral channels for the JPL library range in wavelength from 0.400 μm to 2.500 μm. They increase by 0.001 μm from 0.400 μm to 0.800 μm and then by 0.004 μm from 0.800 μm to 2.500 μm, for a total of 826 channels.
2. We thank Dawn Robinson and Ray Arvidson of Washington University for the petrological analysis of this sample.
3. The JPL mineral library contains spectra for 160 different minerals, each of which is measured at from one to three different powder grain sizes. Of these 160 minerals, 135 minerals are measured at the large grain size (125–500 μm). It is this set of 135 large grain spectra which is used as a background library.
4. In this case, the number of variables is 135 and the sample size is equal to the number of channels in the interval [2.0 μm, 2.5 μm] for the JPL library = 126.
5. The JHU spectral library contains many more spectra than just these 192 rock spectra, including spectra for soils and plants, but our interest was just in the rock spectra. The rock spectra were of six types: (1) solid igneous, (2) powdered igneous, (3) large grain powdered metamorphic, (4) small gain powdered metamorphic, (5) large grain powdered sedimentary, and (6) small grain powdered sedimentary.
6. Model 1 is currently distributed by the Unica Corporation under the name “Affinium Model.”

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