OF SPECTRAL MIXTURES

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N86-11626

ABSTRACT

A technique is outlined that tests the hypothesis that AIS image spectra are produced by mixtures of surface materials. This technique allows separation of AIS images into concentration images of spectral endmembers (e.g., surface materials causing spectral variation). Using a spectral reference library it was possible to uniquely identify these spectral endmembers with respect to the reference library and to calibrate the AIS images.

INTRODUCTION

A primary objective for interpretation of multispectral images is to identify the direct physical factors causing spectral variation on the ground. We demonstrate in this paper that a spectral mixture model makes possible the identification of image spectra, assuming that there is a linear relationship between image spectra and a library of reference spectra. Modeling spectral mixtures reduces the dimensionality of the spectral data and leads to inferences regarding the spatial interrelation of spectral classes that have been delineated using conventional classification techniques.

Two AIS image scenes from Cuprite, Nevada were analyzed against a reference library of laboratory spectra. The first image is from August 1983 (RUN ID101) and the second July 1984 (RUN ID403). All analyses were limited to the wavelength range of 2.1 µm to 2.4 µm comprising 32 spectral channels. The reference library spectra were obtained from field samples collected from the Cuprite area. They included a variety of altered rhyolites containing opaline silica, kaolinite, and alunite, and samples of soils, playa, desert varnish, and green and dry vegetation. The laboratory spectra were taken using a Beckman DK2-A spectrophotometer.

An initial objective of our analysis was to determine the spectral endmembers and their abundances among the laboratory samples, using the method described by Smith et al. (1985). The endmembers are defined as those spectra from the reference library that when linearly combined (linear mixture model) can form all other spectra. Endmembers must have an abundance of 1 and the computed endmember abundances for all other spectra must be between 0 and 1. Based on the eigenvalues of spectra in the 2.1 to 2.4 µm region there are six potential endmembers among the Cuprite samples: opaline silica, desert varnish, alunite, kaolinite, and playa, and green vegetation. A plot of the transformed spectra by the two primary eigenvectors is depicted in Fig. 1. These plots indicate the compositional trends for the reference samples. A major objective is to determine to what extent the variation observed in the reference spectra is present in the image spectra.
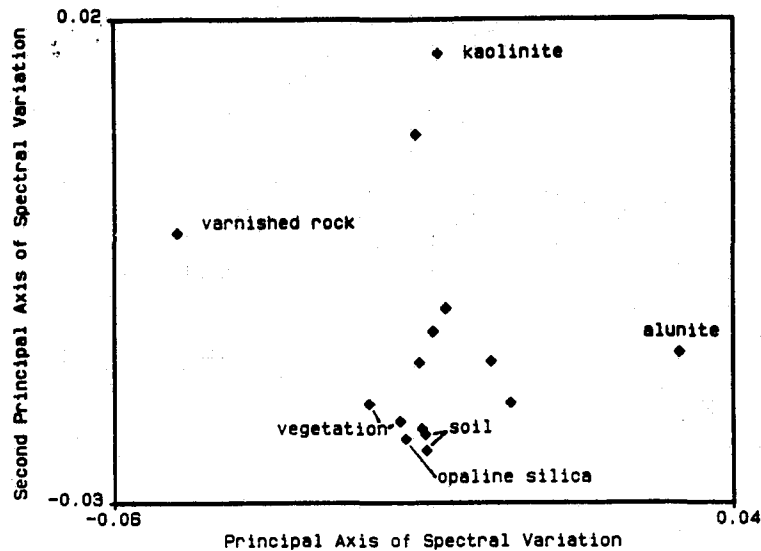
Fig. 1. The linear transformation of laboratory spectra of field samples onto the first two principal axes of variation. Prospective endmember spectra are those nearest the outside boundaries.

COMPARISONS OF NORMALIZED SPECTRA

For the image spectra we also determine how many endmembers are required to predict all other image spectra given the previously stated constraints. However, unlike the laboratory spectra, the image spectra include variation from the surface orientation, atmospheric absorption, etc. Thus, some of the endmember spectra resolved from the image may represent factors that are not associated with mixing of the spectra of the surface materials. Three unknown spectral endmembers were found for the 32 wavelength bands of 2.1 to 2.4 μm using the calibrated energy normalized image of August 1983. Here, normalized spectra are computed by dividing each reflectance by the sum of the reflectances over the wavelength interval of analysis. Mixtures of these image-derived endmembers model all image spectra to nearly within the instrumental error. Further comparisons need only consider these endmember spectra and their uniqueness in causing the observed spectral variation. To compare the image spectra with the reference spectra it is necessary to calibrate the image data.

To first order, we select a linear model that maps flux density measurements of the surface to reflectance measurements from a laboratory spectrophotometer, i.e.,

$$G_b (DN_b + A_b) = \sum_{i=1}^{n} (f_n R_{nb}) \tag{1}$$

where G_b is the gain for band b, A_b the offset for band b, DN_b is the image brightness value for band b, f_n the fraction of endmember n, and R_{nb} the reflectance of endmember n for band b. The G_b's can be different for each wavelength band. If the image is correctly calibrated the G_b coefficients can be reduced to one by normalizing both image and reference spectra by the sum of flux densities or reflectances over the

32 wavelengths. Using the 32 channels from 2.1 μm to 2.4 μm of Cuprite (August, 1983 image) an optimal solution of spectral mixtures providing correspondence in spectral variation between the image and the reference library was determined to include alunite, kaolinite, and playa silt. Using normalized spectra we could not differentiate between the playa silt, opaline silica, or vegetation in the 2.1 to 2.4 μm range.

The use of normalized spectra with a simple calibration model does support the hypothesis that image spectra are produced by mixtures of surface materials. The disadvantages of this approach are that if the attenuations are poorly corrected due to instrument-calibration errors and/or atmospheric uncertainties, then solutions based on the spectral library may be wrong. Also, much of the spectral variation is lost from normalizing the spectra by whatever method, and thus may result in more than a single physical explanation (i.e., reduce the uniqueness) of the source of spectral variation. Optimally, it is desired to have a technique that validates the atmospheric corrections and instrumental calibration assumptions as well as providing a unique solution to the source of spectral variation.

ABSOLUTE SPECTRAL COMPARISONS CALIBRATED TO TWO OR MORE REFERENCE AREAS

Given laboratory measurements of representative samples, the gains and offsets expressed in Equation 1 could be calculated directly by hypothesizing analogous image and laboratory spectra. This requires that pixels exist in the image that encompass spectrally pure and homogeneous areas on the ground (training areas) and that such spectra also exist in the reference library. To determine the gains in Equation 1, we perform a linear search of the reference library solving for the attenuations (G_b) for each spectrum. For a given mixture model of n spectral endmembers in an image, the validity of the attenuations is determined from the compositional abundances and rms errors and should ideally appear as in Table 1. Note that at this point we introduce illumination intensity (shade) as a spectral endmember (Adams et al., 1985).

Table 1. The optimal pattern of reference and library endmember abundances if the calculated attenuations (G_b) are valid.

Abundance of Reference Spectra	Abundances of Image Endmember:		Illumination Intensity	rms error
	Spectrum A	Spectrum B		
Sample A	1.0	0.0	0 - 1	0
Sample B	0.0	1.0	0 - 1	0
Sample C . . .	0 - 1	0 - 1	0 - 1	0

For the July, 1984 uncalibrated AIS image two training areas were selected representing a fan containing varnished rhyolites (varnished spectrum) and "kaolinite hill" (kaolinite spectrum). Searching the spectral reference library for the optimum calibration, as defined above, resulted in a single solution (Table 2) that matches the above matrix pattern. The search through the reference library included

140 reference spectra of minerals and vegetation in addition to the spectra of samples collected from Cuprite. Abundances that are less than zero and greater than one indicate spectral variation that is greater than that of the sample for which the attenuation coefficients were computed. The model could be changed to incorporate the reference spectrum endmember having the greatest degree of variance, which would result in all positive fractions with values between zero and one, similar to the ideal pattern of Table 1.

Table 2. An Optimal mixture model fit of the Cuprite, Nevada (July, 1984) uncalibrated AIS image. This model provided the best fit for the major source of spectral variation in the image.

| Abundance of Reference Spectra | Abundance of Image Spectra: | | | |
| | | | Illumination | |
	Varnished	Kaolinite	Intensity	rms error
Varnished Rhyolite #1	1.0	0.0	0.0	0.00
Kaolinite #2	0.0	0.6	0.4	0.01
Kaolinite #1	0.0	0.9	0.1	0.02
Varnished Rhyolite #3	1.6	-0.4	-0.2	0.01
Varnished Rhyolite #2	1.1	0.2	-0.3	0.02

Unlike the example using normalized spectra, the above procedure provides a means of calibrating an image absolutely with respect to illumination intensity, and thus resolves the effects due to both surface orientation and self-shading of surface materials. The illumination intensity is a spectral endmember analogous to the endmembers of the surface materials. An image of the illumination intensity provides qualitative evidence of the validity of the model by depicting topographical features. From this calibration, it was possible to determine that the albedo of the most likely spectral reference endmember was associated with the playa silt. The opaline silica and vegetation spectra that were similar to the playa when normalized are distinct and separable when spectral variation due to illumination intensity was removed and comparisons made on non-normalized spectra.

Vertical striping occurred in the endmember abundance images, and is a result of assuming that all vertical lines had equal attenuation coefficients (G_b). This is true to a first approximation, but for extraction of the minor absorption features characteristic of minerals such as alunite and kaolinite these differences in gain must be exact. The presence of the vertical striping indicates the calibration proposed by Equation 1 is not valid in the case of the AIS images, where each vertical line can have a different gain and offset as well as each wavelength band.

ABSOLUTE SPECTRAL COMPARISONS CALIBRATED TO MIXTURES OF ENDMEMBERS

Reference (training) areas of spectrally pure materials do not always exist on the pixel scale in an image. More typically all pixels contain spectral mixtures. A more generalized approach requires only that the mixture space in the spectral library exist in the image. For

the simple case of two mixture components in an image the following equations are applicable:

$$G_s \, G_b \, DN_{e1b} = f_{1a} \, R_{e1b} + (1 - f_{1a}) \, R_{e2b} \qquad (2)$$

$$G_b \, DN_{e2} = f_{1b} \, R_{e1b} + (1 - f_{1b}) \, R_{e2b} \qquad (3)$$

G_b is the gain for band b, G_s a gain due to differential illumination of the image endmembers, DN_{e1b} and DN_{e2b} are the 16-bit image brightness values for two spectral endmembers e1 and e2 in the raw data AIS image, f_{1a} and f_{1b} are the fractions of reference spectra that mix to form the image spectra, and R_{e2} and R_{e1} are the library reflectances of two reference spectra at band b. Our objective is to identify those combinations of spectra in the reference library that provide a solution to the fractions in Equations 2 and 3 and to determine how unique the solution is with respect to the reference library. The example is based on two spectra for simplicity; however, multiple spectra were actually used. By algebraic manipulation of Equations 2 and 3, one can solve for the mineral abundances (f_{1a} and f_{1b}) independent of the gains G_b. Since the fractions should be constant at each wavelength for a given mixture of materials, the 32 wavelength bands from the AIS image allow a least squares fit (or coefficient of variation) to be determined for each fraction from any combination of two library reference spectra. By searching the spectral library using all combinations of two spectra in the reference library we can rank solutions by their fit to all 32 bands. For the Cuprite images this search procedure also led to the spectra of kaolinite and varnished rhyolite.

It is also possible to use Equations 2 and 3 to test the assumption that the calibration gains and offsets are spatially equal as well as to compute them. In the previous example we found that this assumption was not valid. Spatial gains and offsets can be calculated by identifying the spectral endmembers in each line independently. For an image with two spectral endmembers Equations 2 and 3 can then be applied to solve for the gains G_b between each line rather than between the image and the reference library. It is not necessary that all endmembers be represented in the image spectra from line to line, but at least two of the endmembers must be present.

CONCLUSIONS

We have demonstrated an approach using spectral mixture models and a spectral reference library that identifies the origin of spectral variation in AIS images. To make use of the spectral library it was necessary to separate the effects of spectral variation in the image that were not due to surface materials, e.g., illumination intensity, atmospheric attenuation, and instrument calibration. The Cuprite image was modeled successfully as spectral playa silt, kaolinite, alunite, and shade. These materials form spectral endmembers in the 2.1 to 2.4 μm range, whereas other samples are spectral endmembers in other wavelength regions (e.g., green vegetation in the 0.4 to 1.1 μm range).

The alignment of image and reference library spectral endmembers provides evidence that linear spectral mixtures are applicable to organizing the high spectral-spatial resolution of AIS images. The inverted approach to calibration presented here does not rely on ·

statistical assumptions or local parameter uncertainties in removing effects due to atmospheric attenuation and instrumental calibration, and so provides an independent test on the applied calibrations.

REFERENCES

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