

Spectral Identification of Minerals using Imaging Spectrometry Data: Evaluating the Effects of Signal to Noise and Spectral Resolution using the Tricorder Algorithm

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INTRODUCTION

The rapid development of sophisticated imaging spectrometers and resulting flood of imaging spectrometry data has prompted a rapid parallel development of spectral-information extraction technology. Even though these extraction techniques have evolved along different lines (band-shape fitting, endmember unmixing, near-infrared analysis, neural-network fitting, and expert systems to name a few), all are limited by the spectrometer's signal to noise (S/N) and spectral resolution in producing useful information. This study grew from a need to quantitatively determine what effects these parameters have on our ability to differentiate between mineral absorption features using a band-shape fitting algorithm. We chose to evaluate the AVIRIS, HYDICE, MIVIS, GERIS, VIMS, NIMS, and ASTER instruments because they collect data over wide S/N and spectral-resolution ranges. The study evaluates the performance of the Tricorder algorithm (Clark and Swayze, this volume) in differentiating between mineral spectra in the 0.4-2.5 μm spectral region. The strength of the Tricorder algorithm is in its ability to produce an easily understood comparison of band shape that can concentrate on small relevant portions of the spectra, giving it an advantage over most unmixing schemes, and in that it need not spend large amounts of time reoptimizing each time a new mineral component is added to its reference library, as is the case with neural-network schemes. We believe the flexibility of the Tricorder algorithm is unparalleled among spectral-extraction techniques and that the results from this study, although dealing with minerals, will have direct applications to spectral identification in other disciplines.

METHOD

We decided to model only single-component mineral spectra because they allow us to establish the absolute minimum S/N and spectral resolution necessary to distinguish between mineral species. This type of simplified model was adopted with the understanding that multicomponent spectra will require even higher S/N and resolution because of overlapping absorptions and weaker band strengths due to dilution by the other mixture components. Minerals from seven mineral groups (alunite, calcite, chlorite, hematite, kaolinite, montmorillonite, and muscovite) were chosen for evaluation based on the presence of easily detected spectral features and common occurrence at the ground surface. All of these minerals have either Fe charge-transfer and crystal field bands in the VIS/NIR region or OH^- , Metal-OH, H_2O , CO_3^{2-} , and SO_4^{2-} vibrational features in the NIR region. Some of the minerals have features in both regions.

A bidirectional-reflectance spectrum of each mineral was first deconvolved to the spectral resolution of each imaging instrument, and then scaled random noise was added. Signal to noise is defined here as 50 percent reflectance divided by the standard deviation of the gaussian-noise spectrum, with standard deviation uniform at all wavelengths. To make our determinations statistically accurate, we generated over 20,000 noisy spectra for each convolved mineral spectrum. The S/N levels varied from 1 to 500 as did the number of noisy spectra at each level: 400 for the high S/N levels and up to two thousand at the low S/N levels. These spectra were then analyzed by the Tricorder algorithm and the best matching library mineral spectra chosen for each noisy-spectrum. Tricorder fits the noisy spectra to over 120 library mineral spectra (convolved to the noisy spectrum resolution) by first removing the continuum from diagnostic spectral regions of both the noisy spectrum and library spectra, and then least-squares scaling each library spectral absorption to the corresponding continuum-removed region in the noisy spectrum. During the process of scaling, a linear correlation coefficient, which we

call the "fit," is generated for each library mineral comparison. The mineral with the highest fit is chosen as the best spectral match. Tricorder determines the fit of each library mineral spectrum by individually fitting all the diagnostic absorptions in the library spectrum to the noisy spectrum and then calculating an overall fit by weighting each individual fit by its absorption-feature's area.

Because random noise can make a mineral's spectral features resemble those of other minerals and because this effect is magnified as S/N decreases, we expected Tricorder to choose several different mineral matches, especially at the low S/N levels. We also expected Tricorder to make correct identifications at high S/N levels. Tricorder gave the results that we expected at these S/N extremes. Of particular interest is the S/N region where Tricorder first starts to make incorrect identifications. By plotting the percentage of correct identifications versus S/N level, we can determine precise S/N levels at which the algorithm has a given percent accuracy in identifying this mineral at a given spectral resolution. By plotting the individual incorrect mineral identifications versus S/N we can determine which minerals are most likely to start spectrally resembling the noisy spectrum as S/N decreases. For example, calcite is misidentified 1 out of 9 times at a S/N of 13 at AVIRIS resolution. Stated another way, with Tricorder, we are able to spectrally recognize calcite 90 percent of the time at a S/N of 13 at AVIRIS resolution. The other 10 percent of the time we would either identify calcite as epidote, nontronite, hectorite, dolomite (each of which have strong 2.3- μm absorptions) or classify the noisy spectrum as having NO MATCH in the spectral library. As spectral resolution decreases this 90 percent identification level occurs at progressively higher S/N levels.

By compiling the S/N levels for each imaging spectrometer at which 90 percent of the identifications of a mineral are correct, we can quantitatively assess the effects of S/N and spectral resolution for each imaging spectrometer. Preliminary work shows that Tricorder's ability to correctly identify a mineral increases with increasing S/N and spectral resolution.