AUTOMATIC CONTINUUM ANALYSIS OF REFLECTANCE SPECTRA

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ABSTRACT

A continuum algorithm based on a "Segmented Upper Hull" method (SUH) is described. An upper hull is performed on segments of a spectrum defined by local minima and maxima. The segments making a complete spectrum are then combined. The definition of the upper hull allows the continuum to be both concave and/or convex, adapting to the shape of the spectrum under study. The method performs multiple passes on a spectrum by segmenting each local maximum to minimum and performing an upper hull. The algorithm naturally adapts to the widths of absorption features, so that all features are found, including the nature of doublets, triplets, etc. The algorithm is also reasonably fast on common minicomputers so that it might be applied to the large data sets from imaging spectrometers.

INTRODUCTION

Data from imaging spectrometers requires fast analysis of the continuum and features in a spectrum. To date, analyses of such data have not employed the analysis techniques used on reflectance spectra obtained in the laboratory. For laboratory spectra, the analyst chooses continuum tie points and uses an algorithm to derive the continuum based on straight line segments or a curve such as a cubic spline. Some researchers have used the "upper convex hull" method (Green and Craig, 1985) for automatic determination of a continuum on Airborne Imaging Spectrometer (AIS) data. However, the upper convex hull is limited to spectra having certain characteristics (which happened to be common in the limited spectral coverage in AIS data) and is not always applicable. For example, in snow (water ice), the continuum in the near infrared is concave (e.g. Clark, 1981) and cannot be analyzed using the upper convex hull. Other spectra appear to have portions of the spectrum requiring a concave continuum (e.g. see alunite, Figure 1A, 1.3 to 2.2 μm and the examples of kaolinite in Green and Craig [1985] in the 2.2-μm region). As imaging spectrometer data with greater spectral coverage become available, more sophisticated continuum analysis is necessary. A continuum analysis should adapt to different types of absorptions present in a spectrum, such as very broad bands like that in olivine near 1 μm to the very sharp absorptions seen in OH-bearing minerals, and spectra with combinations of both sharp and broad absorptions.

AUTOMATIC CONTINUUM ANALYSIS

We approached the problem by analyzing how a spectroscopist chooses a spectrum, and modified it to use a method that can be both

fast and consistent in a computer algorithm. The algorithm is best described by example.

First the upper hull is determined (Figure 1A) on the original spectrum. The upper hull is derived by first finding the maximum in the entire spectrum (the "global maximum"), and then finding the line segments that bound the spectrum so that all points lie on or below the hull. The spectrum is divided into two segments on each side of the global maximum and treated independently. The local maximum away from the global maximum is found next for a spectral segment. A line is then computed between the global maximum and the local maximum. The data are divided by the continuum and checked to see if any points have values greater than 1. If a point does, this a relative peak and is marked as a new continuum tie point, and a new continuum is computed. This process is repeated until no points fall above the continuum. The local maximum becomes the new global maximum and the process of finding the next local minimum and local maximum is repeated until each end of the spectrum is reached. The method allows the continuum to be both concave and convex, but does not allow the slope to change sign or equal zero except at the global maximum.

An example of an upper hull is shown in Figure 1A and the continuum removed data in Figure 1B. Note how the hull follows local maxima to produce a continuum that is both convex and concave. The upper convex hull would have produced a straight line from 1.3 to 2.26 μm having major minima near 1.4, 1.8 and 2.2 μm and between them local maxima all below the continuum. The SUH presented here greatly reduces this problem. Also, the SUH method can be extended to analyze the fine structure that occurs in many absorption features.

Next, the continuum removed spectrum (e.g. Figure 1B) is divided into spectral segments bounded by continuum tie points (where data = 1.0 in the continuum removed spectrum). An example of tie points are labeled a and c in Figure 2A. Then, the minimum between the two tie points is found (labeled b in Figure 2A). The segment a-b is treated as an isolated spectrum and the upper hull derived. Segment b-c is treated likewise. Thus, there are two "Segmented Upper Hulls" that converge on the local minimum. The local maxima closest to the minimum on each side (labeled x and y on Figure 2A) are connected by a straight line. The data are divided by the continuum and checked to see if any points fall above the continuum and if so, the continuum tie points adjusted.

If there are no local minima between the data = 1.0 continuum tie points and the minimum, then the continuum was fully removed in the last iteration. Therefore, the continuum is defined to follow the data through the band (e.g. Figure 2A, bands near 1.75 and 2.3 μm).

The continua derived for the segments are spliced together and the spectrum is divided by the resulting continuum (Figure 2B, solid line). This continuum removed spectrum is then treated as a new spectrum and again fed to the SUH routine. The iterative process continues until a straight line is derived (e.g. Figure 2C).

The SUH routine will naturally follow the maximum data points, thus each small minimum due to noise fluctuations could be treated as a band. We chose to reject any minimum below a threshold and force the continuum to follow these small variations. The threshold is chosen in one of two ways: the standard deviation error bar value if it exists (as it does from our lab spectrometer) or a constant value chosen by the user (we chose a default of 1%).

The iterative SUH routine has been tested on laboratory spectra and laboratory spectra convolved to AVIRIS sampling intervals and resolution. The greatest number of iterations was found to be 3 in the case of alunite. The upper hull on the original spectrum counts as the first iteration. Three iterations take about ½ second of cpu time on an HP9000/500 series cpu (where processing speed is between a VAX 750 and 780 VMS system with floating point accelerator) on complicated spectra like the alunite. However, we have yet to optimize the code, so this value represents an upper limit to the possible compute time. The alunite analysis produced 17 minima between continuum tie points.

Our next step is to analyze each minimum for band position, width, asymmetry, depth and continuum level. That algorithm is already written and will be integrated with the SUH routine. The resulting output of the combination will be a list of spectral features. The continuum removal plus feature analysis is estimated to take less than 1.5 seconds of cpu time per AVIRIS spectrum on the HP9000, so that an entire AVIRIS 550x550 pixel scene can be analyzed in about 5 days of cpu time.

CONCLUSIONS

A fast, reliable continuum analysis routine has been formulated using the upper convex hull routine on segments of a spectrum. The speed of the routine is such that it is feasible to run on existing minicomputers on large amounts of data such as from AVIRIS.

Correlation of the feature analysis with a database of known features derived from laboratory spectra will result in maps of mineral occurrence. The non-selective nature of the algorithm will also select absorptions due to vegetation, atmospheric absorptions and any other natural or unnatural objects in the scene. The algorithm is not sensitive to the strength of the absorptions (except that they must be above the noise level) so that if features due to a particular mineral are present but weak due to low abundance or masking by opaques, it can still be identified. The algorithm might also be used on spectra in other wavelength regions such as the mid-infrared.

Images could be produced using "spectral intensity" (the depths of the absorption bands relative to those of the pure mineral) of specific minerals. The spectral intensity is correlated to the abundance and grain sizes of the minerals in the optical surface.

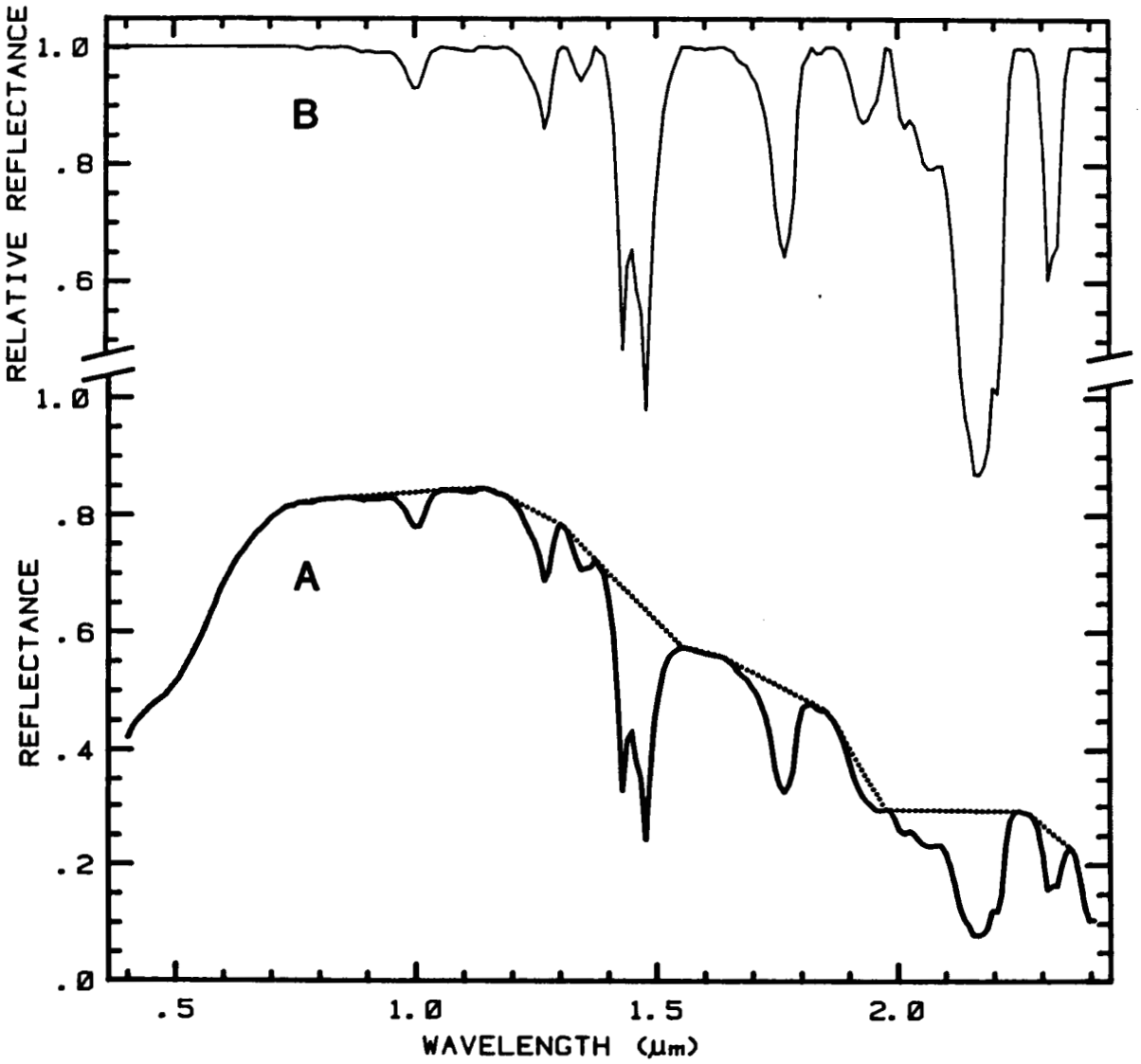

Figure 1. The reflectance spectrum of alunite convolved to AVIRIS resolution is shown with the upper hull (dotted line in A) and the reflectance divided by the upper hull continuum (B).

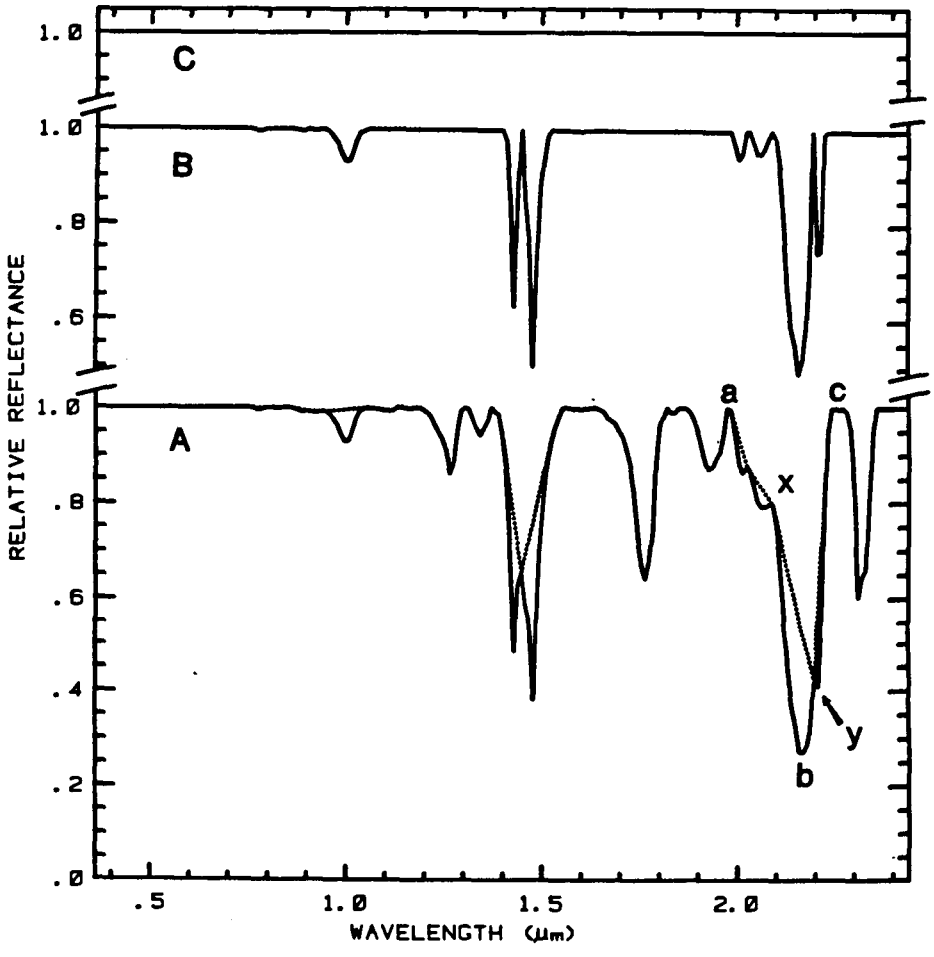

Figure 2. The "Segmented Upper Hull" (SUH) is shown for the second iteration (A, dotted line) compared to the continuum removed first iteration (A, solid line). The third iteration SUH is shown in B, but it overlies the continuum removed second iteration data so when the third iteration SUH is divided into the data a straight line is derived (C). Each iteration analyzes finer structure associated with the complex absorption bands until the continuum removed data equals 1.0.

REFERENCES

Clark, R.N. (1981) Water frost and ice: The near-infrared spectral reflectance 0.65-2.5 μm, *J. Geophys. Res.*, **86**, 3087-3096.

Green, A.A. and Craig, M.D. (1985) Analysis of aircraft spectrometer data with logarithmic residuals, in Proceedings of the Airborne Imaging Spectrometer Data Analysis Workshop, April, 1985, (G. Vane and A. Goetz, eds.) JPL Publication 86-35, 111-119.