SPECTRAL VARIABILITY AND ANALYSIS PROCEDURES FOR HIGH RESOLUTION REFLECTANCE DATA

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ABSTRACT:

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Hyperspectral data (0.4 - 2.5 μm reflectance data at 0.01 μm resolution) are considered for both surface and aircraft data sets representing soils, vegetation, and other common surfaces. Both types of data are well described by 20-30 spectral shapes, although minerals may require a larger number due to sharp absorption features at the longer wavelengths. This suggests that, in contrast with research studies, operational applications do not require 200 or more spectral measurements at 0.01 μm resolution to obtain the useful information in reflectance data. Comparison of surface and aircraft observations shows that the types of shapes are similar, except for known atmospheric water vapor features in the aircraft spectra. It thus should be possible to estimate water vapor corrections in remotely sensed reflectance data using relatively broad band $(0.04 \mu m)$ spectral observations.

KEY WORDS: Hyperspectral, Spectral Collections, AVIRIS, Basis functions

1. INTRODUCTION

Recent advances in instrumentation, combined with interest in global environmental assessment, have prompted the development of high spectral resolution sensors which provide imagery with large numbers of spectral bands. The AVIRIS instrument (Vane, 1987) is a good example, obtaining data in 224 spectral bands in the range 0.4-2.5 $\mu \rm m$ for an image swath more than 600 pixels wide. This discussion follows closely that of the previous meeting of this symposium (Price, 1991), applying a newer methodology which has been developed to address the expansion of spectra in basis functions (Price, 1993) when the number of such functions becomes relatively large, i.e. > 15. We first review the description by spectral basis functions, then apply the formalism to collections of surface/laboratory spectra, then to AVIRIS imagery, and then describe the relationship between the two types of spectra, where the systemmatic difference (atmospheric water vapor) is readily identified.

2. DESCRIPTION OF HYPERSPECTRAL DATA BY BASIS FUNCTIONS

Let $\mathbf{x}^{\alpha}(\lambda)=(\mathbf{x}_{1}^{\alpha},\ \mathbf{x}_{2}^{\alpha},\ \dots \mathbf{x}_{n}^{\alpha})$ represent a measured spectrum for the set of n wavelength values $\lambda=(\lambda_{1},\ \lambda_{2},\ \lambda_{3},\ \dots \lambda_{n})$, with superscript α denoting the individual sample. Throughout we shall work with reflectance spectra, i. e. the ratio of reflected to incident radiation, as this eliminates effects of local illumination conditions and facilitates comparison of spectral collections from many laboratories. For remote sensing applications the illumination source is usually the sun. We shall describe visible to near infrared spectra (0.4 to 2.5 μ m) by a set of spectral basis functions:

$$\mathbf{x}^{\alpha} \approx \sum_{i=1}^{M} S_{i}^{\alpha} \boldsymbol{\varphi}_{i}(\lambda),$$
 (1)

where the basis functions $\varphi(\lambda_1,\ \lambda_2,\ \lambda_3,\ \ldots \lambda_n)$ are spectral shapes, as defined from statistical analysis of a collection of spectra, and the coefficients S_i^α are wavelength integrals over specific band limits for the original measurements \mathbf{x}^α . Each basis function φ_i has an associated spectral interval $[\lambda_i(\min),\ \lambda_i(\max)]$ representing the domain of integration for determining the coefficients S_i . Thus each φ has essentially unit value in its spectral interval (more precisely has mean value of 1.0 in this interval), then decreases according to the degree of wavelength correlation in the ensemble of measured spectra. The expansion represents successive approximations to the original spectra. Evidently the number of basis functions M which is required to describe the \mathbf{x}^α to within very small residuals must be much less than the spectral dimensionality n, or else the expansion is not useful. In this section we describe first the definition and properties of the expansion, where the formalism for obtaining a set of basis functions φ by a single set of computations has been described in Price, 1993.

2.1 Definition and Properties of the Expansion

From inspection we know that most visible to near infrared reflectance spectra vary in a relatively smooth fashion, implying that correlations exist between measurements at nearby wavelengths. Thus a measurement in a limited spectral range provides information about values over a interval. Let $\delta \mathbf{x}_i^{\alpha}$ be the difference between a measured spectrum and the sum through term i of the expansion, and S_i^{α} be the average of $\delta \mathbf{x}_i^{\alpha}$ over the interval $[\lambda_i(\min), \lambda_i(\max)]$

$$S_{i}^{\alpha} = \frac{1}{\left[\lambda_{i}(\max) - \lambda_{i}(\min)\right]} \int_{\lambda_{i}(\min)}^{\lambda_{i}(\max)} \delta x_{i}^{\alpha} d\lambda$$
 (2)

At the beginning $\delta \mathbf{x}_1 = \mathbf{x}$. Because the value of \mathbf{S}_i is correlated with the value of $\delta \mathbf{x}$ over a wider range, we define the basis function $\boldsymbol{\varphi}_i$ by

$$\varphi_{\hat{1}}(\lambda) = \langle \delta x_{\hat{1}} S_{\hat{1}} \rangle / \langle (S_{\hat{1}})^2 \rangle. \tag{3}$$

where the brackets represent an ensemble average, e. g. < x > = 1/N $\sum_{\alpha=1}^{N}$ \mathbf{x}^{α} . From the definition of S, the normalization of $\boldsymbol{\varphi}$ is

$$\frac{1}{\left[\lambda_{i}^{(\max)-\lambda_{i}^{(\min)}}\right]} \int_{\lambda_{i}^{(\min)}}^{\lambda_{i}^{(\max)}} \varphi_{i}(\lambda) d\lambda = \frac{1}{\left[\lambda_{i}^{(\max)-\lambda_{i}^{(\min)}}\right]} \int_{\lambda_{i}^{(\min)}}^{\lambda_{i}^{(\max)}} \langle \delta \mathbf{x}_{i}^{S} \rangle / \langle (S_{i}^{(\infty)})^{2} \rangle d\lambda = 1 \quad (4)$$

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so that φ has a mean value of one within the integration interval. At each iteration level i the residual vector $\delta \mathbf{x}_i^\alpha$ is approximated by $\delta \mathbf{x}_i^\alpha \approx S_i^\alpha \ \varphi_i(\lambda)$, leaving a new residual $\delta \mathbf{x}_{i+1}^\alpha$. Then the procedure moves to $\delta \mathbf{x}_{i+1}$. From the definition $\delta \mathbf{x}_i$ and all higher order residuals have the value zero somewhere within the wavelength interval $d\lambda_i$. Thus successive residuals $\delta \mathbf{x}_i$ pass through zero at more and more wavelength values as the order of the expansion increases, and the magnitude of the residuals $\int (\delta \mathbf{x})^2 d\lambda$ decreases. Illustrations of basis functions may be found in Price, 1990 and 1992.

The criterion for terminating the selection of spectral bands is based on the comparison of the residuals with the noise present in the ensemble of spectra. Let percent error ${\tt E}$ be defined by

$$E(M) = 100% \cdot \left\langle \int \left(\mathbf{x} - \sum_{i=1}^{M} S_{i} \varphi_{i}\right)^{2} d\lambda \right\rangle / \left\langle \int \left(\mathbf{x}^{2}\right) d\lambda \right\rangle$$
 (5)

where the integral extends over the wavelength range of interest, excluding the regions of strong water vapor absorption in the atmosphere at 1.35 to 1.47 μm and 1.81 to 2.02 μm , since these are not usable for airborne and satellite observations. For terminating the expansion in basis functions we generally require E(M) \leq 0.01%, or less for high signal to noise data, as, for example laboratory spectra. This value 0.01% corresponds to the noise level at a measurement signal to noise ratio of 100:1, e. g. to a mean square reflectance error of 0.2% at 20% reflectance. However while some collections of laboratory and field reflectance spectra are relatively noisy, others are nearly free of random variations at the 0.01 μm scale. Also some data sets have higher noise at the upper and lower ranges of the observed spectrum and lower noise in the midrange (0.6-1.3 μm). Thus a simple condition on residuals is not sufficient to guarantee that all spectral features are described.

3. APPLICATION TO SURFACE AND LABORATORY SPECTRA

When carrying out statistical processing one must utilize as general a data set as possible in order to include variability reasonably expected in satellite or aircraft data. For this analysis a number of collections of spectra have been studied, including soils, vegetation, and igneous and sedimentary rocks. Many of these data sets have become available only recently. The first two data sets do not span the full range 0.40-2.50 $\mu\mathrm{m}$ like the others, but they are the most complete spectral data sets available for describing conventional agriculture. We describe the data sets briefly:

1. Agricultural crops. This collection (Biehl, et al., 1984) contains approximately 1400 field spectra from soybeans, corn, and winter wheat, with a few observations of sunflowers and alfalfa and bare soil, taken throughout several growing seasons. In the era of these measurements field spectrometers were less advanced. The useable interval was 0.50-2.31 μm , with the water vapor intervals (1.35-1.47 and 1.80-2.02 μm) deleted due to low signal. These spectra have been discussed previously (Price, 1990, 1992). During this analysis it was found by comparison with vegetation spectra from the other collections that some data from 1978 were corrupted by drift of one of the two detectors due to temperature changes. (C. Daughtry and L. Biehl, private communication, 1992). Elimination of these spectra left a total of 1276.

- 2. Soils, principally from the United States (Stoner, et al., 1980). These 564 spectra represent soil samples obtained by the U. S. Department of Agriculture's Soil Conservation Service, plus a few from foreign countries. Laboratory spectra were measured with soils at field capacity, which tends to reduce spectral variability. The measurement range was 0.55-2.32 $\mu \mathrm{m}$.
- 3. Selected vegetation species. These and subsequent spectra were obtained for the interval 0.4-2.5 μm . The 597 laboratory spectra represent four species (Pinus coulteri coulter pine, Ceanothus crassifolius Torr. ceanothus, Salvia mellifera Greene. black sage, and Adenostoma fasciculatum Hook & Arn. chamise) in a variety of modes leaves, stems, flowers, fruits, needles, etc, under varying conditions of fresh/drying/dead. The spectra were originally obtained in order to assess potential moisture status determination methods (Cohen, 1991a, 1991b), 1991c)
- 4. Spectral diversity (Satterwhite and Henley, 1991). This collection of 285 samples is the best single spectral survey for a variety of surfaces, including trees, shrubs, grasses, soils, and rocks. Both field and laboratory spectra are included, with emphasis on spectra from arid and semiarid environments. The collection is too varied to be summarized here.
- 5. Vegetation. These 24 laboratory spectra, of high quality but undocumented, represent mainly leaves of trees and bushes: sassafras, locust, red oak, yew, poplar, etc. (D. Krohn, private communication, 1991).
- 6. Water. Two spectra for sea water and lake water are included in the 5S spectral code (Tanre et al., 1990).
- 7. Sedimentary rocks. These 160 laboratory spectra from sedimentary rocks in the western U. S. have been documented for potential geologic applications (Lang, et al., 1990) Many of the identified absorption bands fall in the regions which we exclude due to atmospheric water vapor absorption.

Table 1 presents 19 recommended bands for characterizing the seven spectral collections, where water vapor regions are excluded, as are the regions 0.4-0.55 μ m and 2.31-2.50 μ m, based on the limitations of the LARS data.

Table 1. Recommended bands for the seven spectral collections (μm)

0.55-0.60	0.76-0.79	1.20-1.28	2.03-2.09
0.61-0.65	0.80-0.93	1.29-1.34	2.10-2.16
0.66-0.68	0.94-1.02	1.48-1.55	2.17-2.22
0.69-0.71	1.03-1.13	1.56-1.70	2.23-2.31
0.72-0.75	1.14-1.19	1.71-1.80	

These 19 spectral bands describe the ensemble very well, in the sense that E is reduced to a value of 0.004%. When the full range 0.40 - 2.5 $\mu \rm m$ is considered we must eliminate data sets 1 and 2 (LARS spectra), which do not describe the short and long wavelength regions. For the full spectral domain we find that 22 spectral bands are sufficient to describe the ensemble, with a residual of E = 0.003%. Thus we conclude that approximately 20 spectral intervals are sufficient to describe data sets 1-7, representing commonly observed materials such as soils, vegetation and rocks, at least to the extent that the available data sets are representative. The addition of minerals and man made materials (not described here) introduces considerably more localized spectral variability, and many more bands are required. Whether most mineral types occur frequently at large enough scale to be seen in satellite data is unknown, but may be examined through the study of AVIRIS data.

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4. APPLICATION TO AVIRIS IMAGERY

Twenty eight AVIRIS scenes were selected using the quick look data at the Jet Propulsion Laboratory. They were transformed to apparent reflectance by dividing by the solar constant. The description of spectra in terms of reflectance as opposed to radiance greatly equalizes the wavelength dependence. However it increases the effect of noise.

Table 2 lists the data sets used, and the scene type. The selection largely spans the natural variability represented in the AVIRIS data sets, with the exception of clouds. The two spruce forest scenes (920616B and 920615B) are for overlapping areas, as was discovered only during image processing.

Table 2. AVIRIS Data Scenes and Surface Types

Flight	Run	Scene	Catalog name	type of scene
920602A	9	8	Moffett Field	suburb, shallow water
920826B	3	2 80	Maricopa farm	agriculture
920828B	13	1	Los Alamos	geology, town
920827B	2	5	Rodgers Dry Lake	geology
921119B	9	8	Tampa Bay	city, water
920603B	2	3	Cuprite	geology
920826B	5	1	Camp Pendleton	water, military base
920615B	2	3	Harvard Forest	forest
920612B	2	5	Indian Pines	agriculture, forest
920531C	6	1	Death Valley	geology
920603B	14	3	Cima volcanic field	geology
920708B	1	2	Gainesville, FL	lake, vegetation
920819B	2	1	Denver	suburb, agriculture
920828B	2	5	San Juan Mtns	snow, geology
920602A	6	2	Jasper Ridge	suburb, vegetation
920826B	4	1	Fort Huachuca	a.f.base, geology
920616B	2	1	Spruce forest	forest, clear cuts
920820B	6	1	Pleasant Grove	agriculture
921117D	2	30	Jackson, TN	agriculture, forest
921119B	5	4	Tampa Bay	island, shallow water
920826B	6	2	San Joaquin	agriculture
920531C	2	1	Owens Valley	geology
920820B	7	1	Dunnigan, CA	agriculture
920819B	10	14	San Berdardino	agriculture
920708B	5	1	Gainesville, FL	town, vegetation
920621C	2	1	Blackhawk Island	ag, forest, water
920615B	8	1	Spruce forest	forest, clear cuts
920820B	8	3	Davis, Webster	agriculture, town

Since 28 AVIRIS images represent 4 gigabytes of data an efficient analysis strategy was needed. First a scene showing considerable variability in surface types (Moffet Field) was analyzed. It was found that 9 variables (spectral intervals) described E to within 0.1%. Then a 1% sample of the 28 scenes (every 100th pixel) was analyzed. Finally, the basis function expansion to level 20 was subtracted out from each scene to select "bad" pixels, with the worst 1% in terms of residuals being saved from each. Then these were added to the original 1% sample, so that the significance of poorly described spectra was multiplied by a factor of 50. Even this requires only approximately 20 basis functions to describe the AVIRIS signal very well, as illustrated in table 3.

Table 3. Variables Required to Meet Varying Accuracies

Accuracy (100-E)	<pre># variables Moffet field</pre>	<pre># variables 1% sample</pre>	<pre># variables 1% sample +1% bad</pre>
(100 1)	(1 scene)	(28 scenes)	(28 scenes)
90%	1	1	1
99%	3	3	4
99.9%	9	8	12
99.95%		15	19
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The recommended spectral bands are presented in table 4.

Table 4. Recommended bands for the 28 AVIRIS scenes (µm)

0.40-0.44	0.75-0.85	1.17-1.22	1.57-1.71	2.26-2.31
0.48-0.55	0.90-0.93	1.23-1.28	1.97-1.99	2.41-2.47
0.60-0.68	0.97-0.99	1.29-1.31	2.07-2.08	2.48-2.50
0.69-0.70	0.99-1.08	1.43-1.48	2.09-2.16	
0 72-0 74	1.11-1.16	1 50-1 56	2 21-2 24	

Finally, each of the coefficient images ($S_{\rm i}$) for each of the 28 scenes was studied visually. Small variance images (i>23) still showed signals at a level of a few tenths of a percent. Possible explanations include instrument noise, spectral misregistration, broad atmospheric variations between images (aerosols), and true scene to scene variability. Little or no evidence was found for isolated surface types with extraordinary spectral features such as minerals.

5. COMPARISON OF SURFACE AND AVIRIS SPECTRA: THE EFFECT OF THE ATMOSPHERE

There exists a systematic difference between the shapes described by the basis functions for surface/laboratory spectra, and those derived from AVIRIS data. This difference is due to water vapor absorption features in the AVIRIS spectra. The sample sizes for the data sets are disproportionate, consisting of a few thousands of surface spectra, and almost 10 million AVIRIS spectra. Therefore we have used all the surface spectra plus a sample of the AVIRIS spectra, with a larger number of AVIRIS spectra because these have not been corrected for atmospheric absorption or solar zenith angle, and thus have lower "effective" reflectances. By combining these data sets, with the regions of strong water absorption (defined previously) omitted, we find that the weak absorption features in the AVIRIS spectrum represent the third most important shape variable (basis function) in the ensemble. However since our goal is to invert AVIRIS spectra to obtain spectra having the same shapes as surface spectra, we select spectral intervals which are suitable for describing both types, then identify a spectral band which specifies the atmospheric effect. Thus using 11 bands at (0.40-0.49, 0.50-0.70, 0.71-0.73, 0.74-0.83, 0.97-1.11, 1.23-1.34, 1.48-1.54, 1.55-1.77, 2.03-2.14, 2.15-2.36, and $2.41-2.50\mu\text{m}$), we can describe both surface and AVIRIS spectra very well, except in the regions of strong water vapor absorption. Are these 11 broad band intervals sufficient to provide a reasonable estimate of reflectance in regions where atmospheric water vapor causes a difference from ground values, as is required for estimation of atmospheric water vapor, and for possible identification of surface types? By calculation on the surface ensemble we may compare this approach with the Continuum Interpolated Band Ratio (CIBR) and the Narrow/Wide (N/W) algorithms, as discussed in Carriere and Conel (1993). The CIBR method averages spectral values at 0.88 μm and 1.10 μm to

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instrument en images lence was es such as estimate the value at 0.94 μm , while the N/W method takes the ratio of a 0.03 μm wide band to a 0.07 μm wide band centered on 0.94 μm to estimate the strength of atmospheric absorption. By analysis of the surface data we find that the 11 relatively broad bands describe this region fairly well: The CIBR yields a root mean square error at 0.94 of 1.3%, the N/W an error of .6%, and the expansion in basis functions an error of 1.2%. Thus we conclude that the procedure used here yields a reasonable estimate of surface reflectance in regions of moderate water vapor absorption. For measurement of the water vapor effect we add a spectral channel at 1.12-1.15 μm . Figure 1 illustrates the first basis function derived by using 11 surface basis functions, then selecting the interval $1.12-1.15\mu\mathrm{m}$ as the observation band.

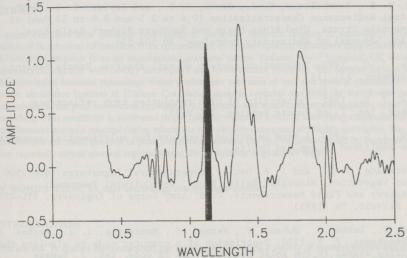


Figure 1. Basis function describing atmospheric attenuation of AVIRIS data as compared to surface spectra. Spectral band is $1.12\text{-}1.15\mu\text{m}$, while peaks at 0.94, 1.38 and 1.95 are due to spectral correlations. The regions of strong absorption are unsatisfactory for water vapor estimation because they are also highly variable (also due to water) in the ground spectra.

6. CONCLUSION

From examination of approximately 3000 laboratory and field spectra and 28 AVIRIS scenes it appears that approximately 20-25 measurements are adequate to define the spectral variability of most natural surfaces, excepting minerals. Thus improvement of the Thematic Mapper, in terms of spectral bands, is recommended. It also appears possible to simplify treatment of atmospheric effects for comparing remotely sensed spectra with a spectral library.

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