ABUNDANCE ESTIMATION OF SPECTRALLY SIMILAR MINERALS

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ABSTRACT

This paper evaluates a spectral unmixing method for estimating the partial abundance of spectrally similar minerals in complex mixtures. The method requires formulation of a linear function of individual spectra of individual minerals. The first and second derivatives of each of the different sets of mixed spectra and the individual spectra are determined, at signal-to-noise ratios of 50:1, 200:1 and 500:1. The error is minimized by means of simulated annealing. Experiments were made on several different mixtures of selected end-members, which could plausibly occur in real situations. We conclude that in the method proposed, the use of the original and first order derivatives provides a valuable contribution to unmixing procedures provided the signal-to-noise ratio is between 50:1 and 200:1. When the signal-to-noise ratio increases, the second derivative of the observed spectrum and the second derivatives of the end-member spectra give most precise estimates for the partial abundance of each end-member. This can often be seen when the signal-to-noise ratio is of the order 500:1.

Index Terms— abundance, unmixing, derivatives, signal-to-noise ratio, spectrally similar, hyperspectral

1. BACKGROUND AND OBJECTIVE

Spectral unmixing of hyperspectral remote sensing images is proving useful in determining abundances of different minerals. Most spectral unmixing techniques are variants of algorithms involving matrix inversion [1, 2, 3, 4]. A major problem in spectral unmixing is the non-orthogonality of end-members. Theories behind this are becoming well-established [5, 1].

The ability to estimate abundances in complex mixtures through spectral unmixing techniques is further complicated when considering very similar spectral signatures [6]. It is known that iron-bearing oxide/hydroxide/sulfate minerals have similar spectral signatures. When considering a mixture of the iron-bearing oxide/hydroxide/sulfate minerals, the complexity of estimating these abundances would be related to (a) selection of end-members of iron-bearing oxide/hydroxide/sulfate minerals based on only image data (for a "true" remote sensing case), (b) estimation of partial abundances of end-members and (c) the signal-to-noise ratio (SNR) of the image.

This paper addresses the following two questions, (a) how could estimates of abundances of spectrally similar iron-bearing oxide/hydroxide/sulfate minerals in complex mixtures be obtained using hyperspectral data? and (b) what is the effect of the proposed method based on the SNR of the image?

To address the above two questions, a spectral mixture was generated with varying linear proportions of individual spectra of a set of iron-bearing oxide/hydroxide/sulfate minerals. The set of end-members is commonly associated with sulphide-bearing mine wastes. Prior to unmixing, the mixed spectrum was first subjected to smoothing, using B-Splines, as the derivatives will not necessarily exist in the case of nonsmooth curves. Hyperspectral images, for example DAIS, HyMap and Hyperion each have very different SNR's. In this paper I therefore used SNR of 500:1, 200:1 and 50:1 to see the effect of the proposed method in terms of its accuracy.

The first and the second derivatives were then calculated for the different mixed spectrum and the individual spectra of the minerals. In [6] it has been shown that most pairs of the derivatives for individual spectra have lower correlation coefficients than the pairs of original individual spectra. The sum and the variance, of the difference between the estimated and actual mixed spectrum is minimized by means of simulated annealing.

2. METHOD OF SPECTRAL UNMIXING

Spectral unmixing is a deconvolution process for estimating the contribution of individual e ($e = 1, \ldots, ||E||$) component spectra to an observed spectrum containing a set M of unknown $||M||$ spectral end-members, where $E \subset M$, $||E||$ and $||M||$ are the number of end-member spectra in E and in M, respectively. Each component spectrum e, which can be derived from a spectral library, consists of L discrete wavelengths λ_l ($l = 1, \ldots, L$). It is denoted by $R^e = (R^e(\lambda_1), \ldots, R^e(\lambda_L))$, where $R^e(\lambda_l)$ is the reflectance value at wavelength λ_l.

An observed spectrum $U = (U(\lambda_1), \ldots, U(\lambda_L))$ is assumed to be a linear combination of the $||M||$ end-members plus an error term. It is difficult, if not impossible, to model U for all possible components or end-members in a complex spectral mixture. Instead an exhaustive set of end-members of interest (subset E of M) is considered. The proportion contribution of each of these end-members can then be estimated.

The details of this method can be found in [6]. The advantage of the method proposed in [6] is (i) the fractional abundance is between 0 and 1, (2) the total abundance due to end-members in E is at most equal to 1, and (3) the method does not require matrix inversion in deriving a solution. Comparisons for this study was made using the sum of the variance of the differences between the observed spectrum and the end-member spectra (VarSpec), the sum of the variance of the differences between the first derivatives of the observed spectrum and the first derivatives of the end-member spectra (VarDeriv) and the sum of the variance of the differences between the second derivatives of the observed spectrum and the second derivatives of the end-member spectra (Var2Deriv). These functions were then minimized through simulated annealing [7].

3. END-MEMBER SPECTRA AND SYNTHETIC MIXTURES

Synthetic spectral mixtures were created to test the proposed spectral unmixing methodology and its accuracy with several different SNR's. Four secondary iron-bearing oxide/hydroxide/sulfate minerals that could from pyrite-rich mine wastes were selected to compose a set of end-members, namely: ferrihydrite; copiapite; jarosite and goethite. Although each secondary iron-bearing oxide/hydroxide/sulfate mineral within a weathering sulfide-bearing mine waste shows distinctive spectral features in the 0.4–2.5 μm regions of the electromagnetic spectrum, this study was limited to the spectral range 0.5–1.1 μm, because this is where most of the iron-bearing oxide/hydroxide/sulfate minerals of interest have many and strong spectral features.

The individual spectrum of each of the four end-members was selected from the USGS spectral library [8] and then linearly mixed with each other according to some proportions of each end-member. The mixed spectrum was then degraded to an approximate 15 nm spectral resolution. Error from the Uniform distribution was then added to the spectra. The resampling was performed (a) to simulate data with lower spectral resolution hyperspectral sensors (e.g., HyMap, DAIS, etc.) as compared to the spectral resolution of the original end-members in the library, (b) to reduce dimensionality of the data, and (c) because it is a practical technique found effective for prediction of different soil properties [9]. It is acknowledged, however, that spectral channel degradation potentially increases correlation between end-members, which would undermine spectral unmixing [1]. For this reason, it is proposed and demonstrated to "decorrelate" end-members using either their first or their second derivative.

Experiments were made on several different mixtures of selected end-members, which could plausibly occur in real situations: (a) the observed spectrum is a pure end-member spectrum and is included in the set of end-members considered for unmixing ($R^e \in E$); (b) the observed spectrum is a pure end-member spectrum but is excluded (because, e.g. not identified or not known) in the set of end-members considered for unmixing ($R^e \in M \backslash E$); (c) the observed spectrum is a mixture of end-member spectra and all end-members are included in the set of end-members considered for unmixing (all $R^e \in E$) and (d) the observed spectrum is a mixture of end-member spectra and some end-members are excluded (for similar reasons as in (b)) in the set of end-members considered for unmixing (some $R^e \in M \backslash E$). For (c) and (d), two simple mixtures of the end-member spectra were considered, namely, mixed spectrum 1 with 50% goethite and 50% jarosite, and mixed spectrum 2 with 15% goethite, 25% jarosite, 25% copiapite and 35% ferrihydrite (the figures can be seen in [6]). For each mixture, error from the $U(-0.02, 0.02)$, $U(-0.005, 0.005)$ or $U(-0.002, 0.002)$ was added, with corresponding SNR of 50:1, 200:1 or 500:1, respectively, in the visible to near infrared regions. Note that (c) also considers the case where the mixed spectrum results from a smaller set of end-members in E. This is useful if prior information suggests including end-members in the set E, when in fact these end-members does not contribute to the mixed spectrum. The resulting abundance for these end-members, in such a case, should then be equal to zero.

Note also that prior to unmixing, the mixed spectra were first subjected to smoothing as the derivatives will not necessarily exist in the case of non-smooth curves. Graphs of the end-member spectra and the mixed spectra can be found in [6] and is not repeated here.

4. ABUNDANCE ESTIMATION FROM SPECTRA

Tables 1–3 show the results of the experiments using observed spectra, first and second derivatives of spectra, using VarSpec, VarDeriv and Var2Deriv [6] and SNR of 50:1, 200:1 or 500:1.

If the observed spectrum is a pure end-member, and is included in the set of end-members considered for unmixing, application of the proposed method is able to estimate abundance of all materials in set E (table 1) with a high degree of accuracy, with estimated abundance ≥ 0.73 for the correct end-member and ≤ 0.19 for an incorrect end-member. These estimates are further increased as the SNR increases, with estimated abundance ≥ 0.90 for the correct end-member and ≤ 0.06 for an incorrect end-member for SNR of at least 200:1. Abundance estimates by using the first derivative of the spectra are comparable to the abundance estimates by using the original spectra at a SNR of 50:1 (slight decrease for goethite and ferrihydrite). As the SNR increase to 200:1, the abundance estimates by using the first derivative of the spectra is more accurate than the abundance estimates by using the original spectra in most cases. Abundance estimates by using the second derivative of the spectra are much worse when compared to the abundance estimates by using the original or first derivative spectra at a SNR of 50:1. As the SNR increases to 500:1, the abundance estimates by using the second derivative is more accurate than the abundance estimates by using the original and first derivative spectra in most cases.

If the observed spectrum is a pure end-member, but is excluded from the set of end-members considered for unmixing, application of the proposed method results in estimated abundances of the materials with poor accuracies. Estimated abundances vary between 0.01 and 0.92 for the correct end-member (see the columns $M \backslash E$) and between 0.00 and 0.92 for an incorrect end-member. It is interesting to note that the results are very similar across the various SNR but there is a substantial improvement when using the second derivative of the spectra as opposed to the observed spectra or even the first derivative of the spectra (table 1). The exception was for jarosite, where both the SNR and higher order derivatives had virtually no effect (in terms of improvement) on the estimates.

If the end-member spectra contributing to the observed mixed spectrum are included in the set of end-members considered for unmixing (all $R^e \in E$), the estimated abundances increases as the SNR increases. High accuracies can be observed for the first derivative of the spectra when the SNR is at least 200:1 and for the second derivative of the spectra when the SNR is at least 500:1 (table 2).

If some end-member spectra contributing to the observed spectrum are excluded from the set of end-members considered for unmixing (some $R^e \in M \backslash E$), estimated abundances have a low accuracy for each end-member (table 3). What is noticeable, is that the accuracies remain fairly consistent for the various SNR but there seems to be a slight improvement in using the second derivative of the spectra as opposed to the original or first derivative of the spectra. Using the second derivative with a SNR of 500:1 produced the most accurate abundance estimates.

5. CONCLUSIONS

We conclude that in the method proposed, the use of the original and first order derivatives provides a valuable contribution to unmixing procedures provided the SNR is between 50:1 and 200:1. When the SNR increases, the second derivative of the observed spectrum and the second derivatives of the end-member spectra give most precise estimates for the partial abundance of each end-member. This can often be seen when the SNR is of the order 500:1.

Table 1. Estimated mineral abundance based on the observed, first derivative and second derivative spectra of a pure end-member of iron-bearing minerals with SNR of 50:1, 200:1 and 500:1. The dash (—) indicate that the end-member spectrum was excluded from the set E of end-members considered for unmixing.

Known abundance				Estimated abundance														
Goe	Jar	Cop	Fer	SNR of 50:1					SNR of 200:1					SNR of 500:1				
				Goe	Jar	Cop	Fer	$M\backslash E^1$	Goe	Jar	Cop	Fer	$M\backslash E^1$	Goe	Jar	Cop	Fer	$M\backslash E^1$
End-member spectrum included in E																		
Using observed spectra																		
1.00	0.00	0.00	0.00	0.73	0.06	0.00	0.19	0.02	0.90	0.03	0.00	0.06	0.01	0.97	0.00	0.01	0.01	0.01
0.00	1.00	0.00	0.00	0.00	0.94	0.01	0.03	0.02	0.01	0.94	0.03	0.00	0.02	0.03	0.94	0.03	0.00	0.00
0.00	0.00	1.00	0.00	0.00	0.04	0.93	0.00	0.03	0.01	0.02	0.94	0.00	0.03	0.01	0.01	0.94	0.01	0.03
0.00	0.00	0.00	1.00	0.05	0.00	0.00	0.92	0.03	0.01	0.01	0.00	0.96	0.02	0.01	0.01	0.00	0.97	0.01
Using 1st derivative spectra																		
1.00	0.00	0.00	0.00	0.67	0.06	0.06	0.20	0.01	0.91	0.02	0.03	0.01	0.03	0.97	0.01	0.00	0.00	0.02
0.00	1.00	0.00	0.00	0.00	0.98	0.01	0.00	0.01	0.00	0.95	0.01	0.02	0.02	0.00	0.94	0.03	0.01	0.02
0.00	0.00	1.00	0.00	0.03	0.01	0.95	0.00	0.01	0.02	0.00	0.95	0.02	0.01	0.00	0.04	0.92	0.00	0.04
0.00	0.00	0.00	1.00	0.02	0.00	0.00	0.90	0.08	0.02	0.00	0.00	0.91	0.07	0.01	0.00	0.01	0.93	0.05
Using 2nd derivative spectra																		
1.00	0.00	0.00	0.00	0.45	0.00	0.15	0.37	0.03	0.88	0.00	0.06	0.01	0.05	0.95	0.01	0.01	0.01	0.02
0.00	1.00	0.00	0.00	0.00	0.52	0.46	0.00	0.02	0.00	0.93	0.01	0.02	0.04	0.01	0.94	0.01	0.01	0.03
0.00	0.00	1.00	0.00	0.00	0.17	0.46	0.00	0.37	0.00	0.00	0.99	0.00	0.01	0.00	0.01	0.98	0.01	0.00
0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.93	0.07	0.01	0.00	0.00	0.97	0.02	0.01	0.00	0.01	0.97	0.03
End-member spectrum excluded in E																		
Using observed spectra																		
1.00	0.00	0.00	0.00	—	0.26	0.00	0.73	0.01	—	0.27	0.00	0.69	0.04	—	0.27	0.00	0.69	0.04
0.00	1.00	0.00	0.00	0.40	—	0.59	0.00	0.01	0.42	—	0.57	0.00	0.01	0.45	—	0.54	0.00	0.01
0.00	0.00	1.00	0.00	0.00	0.36	—	0.00	0.64	0.00	0.37	—	0.00	0.63	0.00	0.38	—	0.00	0.62
0.00	0.00	0.00	1.00	0.91	0.00	0.00	—	0.09	0.92	0.00	0.00	—	0.08	0.92	0.00	0.00	—	0.08
Using 1st derivative spectra																		
1.00	0.00	0.00	0.00	—	0.29	0.00	0.61	0.10	—	0.29	0.00	0.57	0.12	—	0.28	0.00	0.58	0.14
0.00	1.00	0.00	0.00	0.21	—	0.78	0.00	0.01	0.26	—	0.73	0.00	0.01	0.28	—	0.71	0.00	0.01
0.00	0.00	1.00	0.00	0.00	0.44	—	0.00	0.56	0.00	0.44	—	0.00	0.56	0.00	0.44	—	0.00	0.56
0.00	0.00	0.00	1.00	0.22	0.00	0.00	—	0.78	0.21	0.00	0.00	—	0.79	0.22	0.00	0.00	—	0.78
Using 2nd derivative spectra																		
1.00	0.00	0.00	0.00	—	0.08	0.03	0.66	0.23	—	0.17	0.00	0.46	0.37	—	0.28	0.00	0.57	0.15
0.00	1.00	0.00	0.00	0.22	—	0.77	0.00	0.01	0.38	—	0.60	0.01	0.01	0.40	—	0.58	0.01	0.01
0.00	0.00	1.00	0.00	0.00	0.30	—	0.00	0.70	0.00	0.25	—	0.00	0.75	0.00	0.31	—	0.00	0.69
0.00	0.00	0.00	1.00	0.05	0.03	0.00	—	0.92	0.06	0.03	0.00	—	0.91	0.05	0.03	0.00	—	0.92

^{1} represents the set of end-member spectra that are in the exhaustive set containing all possible end-member spectra but excluding the end-member spectra used for unmixing.

Table 2. Estimated mineral abundance based on the observed, first derivative and second derivative spectra of mixtures containing known proportions of four iron-bearing minerals with SNR of 50:1, 200:1 and 500:1. The end-member spectrum is included in the set E consider for unmixing.

Goe	Jar	Cop	Fer	Goe	Jar	Cop	Fer	$M\backslash E^1$
	Known abundance				Estimated abundance			
				Using observed spectra				
				SNR of 50:1				
0.50	0.50	0.00	0.00	0.47	0.46			0.07
0.50	0.50	0.00	0.00	0.17	0.37	0.00	0.32	0.14
0.15	0.25	0.25	0.35	0.03	0.58	0.00	0.33	0.06
				SNR of 200:1				
0.50	0.50	0.00	0.00	0.49	0.50			0.01
0.50	0.50	0.00	0.00	0.46	0.50	0.02	0.01	0.01
0.15	0.25	0.25	0.35	0.06	0.28	0.24	0.41	0.01
				SNR of 500:1				
0.50	0.50	0.00	0.00	0.49	0.50			0.01
0.50	0.50	0.00	0.00	0.44	0.52	0.00	0.03	0.01
0.15	0.25	0.25	0.35	0.15	0.25	0.24	0.35	0.01
				Using 1st derivative spectra				
				SNR of 50:1				
0.50	0.50	0.00	0.00	0.11	0.53			0.36
0.50	0.50	0.00	0.00	0.15	0.30	0.11	0.43	0.01
0.15	0.25	0.25	0.35	0.02	0.50	0.09	0.38	0.01
				SNR of 200:1				
0.50	0.50	0.00	0.00	0.50	0.49			0.01
0.50	0.50	0.00	0.00	0.45	0.49	0.00	0.05	0.01
0.15	0.25	0.25	0.35	0.10	0.27	0.24	0.38	0.01
				SNR of 500:1				
0.50	0.50	0.00	0.00	0.50	0.49			0.01
0.50	0.50	0.00	0.00	0.47	0.49	0.02	0.00	0.02
0.15	0.25	0.25	0.35	0.13	0.25	0.25	0.35	0.02
				Using 2nd derivative spectra				
				SNR of 50:1				
0.50	0.50	0.00	0.00	0.00	0.31			0.69
0.50	0.50	0.00	0.00	0.09	0.12	0.24	0.40	0.15
0.15	0.25	0.25	0.35	0.01	0.21	0.30	0.39	0.09
				SNR of 200:1				
0.50	0.50	0.00	0.00	0.51	0.44			0.05
0.50	0.50	0.00	0.00	0.50	0.38	0.11	0.00	0.01
0.15	0.25	0.25	0.35	0.08	0.14	0.39	0.38	0.01
				SNR of 500:1				
0.50	0.50	0.00	0.00	0.51	0.49			0.00
0.50	0.50	0.00	0.00	0.51	0.49	0.00	0.00	0.00
0.15	0.25	0.25	0.35	0.13	0.25	0.25	0.35	0.02

[1] represents the set of end-member spectra that are in the exhaustive set containing all possible end-member spectra but excluding the end-member spectra used for unmixing.

Table 3. Estimated mineral abundance based on the observed, first derivative and second derivative spectra of mixtures containing known proportions of four iron-bearing minerals with SNR of 50:1, 200:1 and 500:1. The dash (—) indicate that the end-member spectrum was excluded from the set E of end-members considered for unmixing.

Goe	Jar	Cop	Fer	Goe	Jar	Cop	Fer	$M\backslash E^1$
	Known abundance				Estimated abundance			
				Using observed spectra and				
				SNR of 50:1, 200:1 and 500:1 respectively				
0.15	0.25	0.25	0.35	0.60	0.25	—	—	0.15
0.15	0.25	0.25	0.35	0.59	0.24	—	—	0.17
0.15	0.25	0.25	0.35	0.59	0.23	—	—	0.18
				Using 1st derivative spectra and				
				SNR of 50:1, 200:1 and 500:1 respectively				
0.15	0.25	0.25	0.35	0.23	0.35	—	—	0.42
0.15	0.25	0.25	0.35	0.08	0.40	—	—	0.52
0.15	0.25	0.25	0.35	0.09	0.39	—	—	0.52
				Using 2nd derivative spectra and				
				SNR of 50:1, 200:1 and 500:1 respectively				
0.15	0.25	0.25	0.35	0.05	0.22	—	—	0.73
0.15	0.25	0.25	0.35	0.00	0.31	—	—	0.69
0.15	0.25	0.25	0.35	0.05	0.30	—	—	0.65

[1] represents the set of end-member spectra that are in the exhaustive set containing all possible end-member spectra but excluding the end-member spectra used for unmixing.

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