Unmixing of spectrally similar minerals

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CSIR Built Environment
Logistics and Quantitative Methods (LQM)

Meraka Seminar Presentation 2009

Outline

1. Background and Research Question
2. Method of spectral unmixing
3. End-member spectra and synthetic mixtures
4. Results
5. Conclusions

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The Problem

- Most spectral unmixing techniques are variants of algorithms involving matrix inversion.
- Major problem in spectral unmixing is the non-orthogonality of end-members.
- Ability to estimate abundances in complex mixtures through spectral unmixing techniques – complicated when considering very similar spectral signatures.
- Iron-bearing oxide/hydroxide/sulfate minerals have similar spectral signatures.
- How could estimates of abundances of spectrally similar iron-bearing oxide/hydroxide/sulfate minerals in complex mixtures be obtained using hyperspectral data?

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Old method: problem

Linear Spectral Mixture Analysis (LSMA): The observed spectrum U for any given pixel in the scene is expressed as:

$$U \quad = \quad Rp + \epsilon \quad \text{where} \sum_{i=1}^{n} p_i = 1 \text{ and } 0 \leq p_i \leq 1$$

and R is a matrix of which each column corresponds to an endmember, p is a column vector that denotes the abundances and ϵ denotes the residual term.

Minimize: $\displaystyle\sum_{i=1}^{n} \epsilon_i^2 = \sum_{i=1}^{n} \left(\sum_{j=1}^{m} (R_{i,j} \times p_i) - U_i \right)^2$

Solution: $\hat{p} = \left(R^T R\right)^{-1} R^T U$

New method: solution

Suppose M is an exhaustive set of endmembers and $E \subset M$ is a set of endmembers under consideration for unmixing. Each component spectrum $e \in E$ 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.

The observed spectrum U for any given pixel in the scene is expressed as:

$$U \;=\; \begin{bmatrix} R^E \\ R^{M\setminus E} \end{bmatrix} \times \begin{pmatrix} p^E & p^{M\setminus E} \end{pmatrix} + \epsilon \quad \text{where} \sum_{e=1}^{||E||} p_e \leq 1 \text{ and } 0 \leq p_e \leq 1$$

Accordingly, a spectrum at λ_l can be modeled as

$$\widehat{U}(\lambda_l) = \sum_{e=1}^{||E||} p_e R^e(\lambda_l) + p_0 R^{M\setminus E}(\lambda_l)\,, \qquad (1)$$

where $0 \leq p_e \leq 1$, $p_0 + \sum_{e=1}^{||E||} p_e = 1$ and $0 \leq p_0 \leq 1$.

The difference between the estimated and actual spectra at λ_l equals

$$\omega_l = U(\lambda_l) - \sum_{e=1}^{||E||} p_e R^e(\lambda_l)\,. \qquad (2)$$

Minimization of some function of ω_l, e.g. $\mathrm{SumSpec} = \sum_{l=1}^{L} |\omega_l|$ or $\mathrm{VarSpec} = \mathrm{var}(\omega_l)$ results in estimates for p_e.
Alternatively: Use either the differences in the first derivative or the second derivative instead of the actual differences. The difference in the first derivative between an estimated and an actual spectrum at λ_l is

$$\omega_l' = \frac{\Delta U(\lambda_l)}{\Delta \lambda_l} - \sum_{e=1}^{||E||} p_e \left(\frac{\Delta R^e(\lambda_l)}{\Delta \lambda_l} \right)\,, \qquad (3)$$

where $\Delta x_l = x_{l+1} - x_l$. Minimization of a loss function of equation 3, e.g. $\mathrm{SumDeriv} = \sum_{l=1}^{L-2} |\omega_l'|$ or $\mathrm{VarDeriv} = \mathrm{var}(\omega_l')$, results in estimates of p_e.
The minimization is achieved through simulated annealing, using either SumSpec, SumDeriv, VarSpec or VarDeriv as the fitness function to optimize.

Simulated annealing is a general optimization method of a fitness function $\phi(\omega)$ – depends on p_e. Starting with a random configuration of p_e, $\phi(\omega^0)$ is calculated. Let ω^i and ω^{i+1} represent two solutions with fitness $\phi(\omega^i)$ and $\phi(\omega^{i+1})$. Configuration ω^{i+1} is derived from ω^i by randomly replacing one point p_j of ω^i by a new point p_k in $\left[0, 1 + p_j - \sum p_e\right]$, so that $\sum p_e \leq 1$. A probabilistic acceptance criterion decides whether ω^{i+1} is accepted or not i.e.

$$P_c(\omega^i \rightarrow \omega^{i+1}) = \begin{cases} 1, & \text{if } \phi(\omega^{i+1}) \leq \phi(\omega^i) \\ \exp\left(\dfrac{\phi(\omega^i) - \phi(\omega^{i+1})}{\mathbf{c}}\right), & \text{if } \phi(\omega^{i+1}) > \phi(\omega^i) \end{cases} \tag{4}$$

where **c** denotes a parameter and is reduced by a factor of 0.95, thereby decreasing the probability of accepting inferior moves. Reduction stops when the process stabilizes. A transition takes place if ω^{i+1} is accepted. Next, a solution ω^{i+2} is derived from ω^{i+1}, and the probability $P_c(\omega^{i+1} \rightarrow \omega^{i+2})$ is calculated with a similar acceptance criterion as equation 4. The fitness function will be one of SumSpec, VarSpec, SumDeriv or VarDeriv.

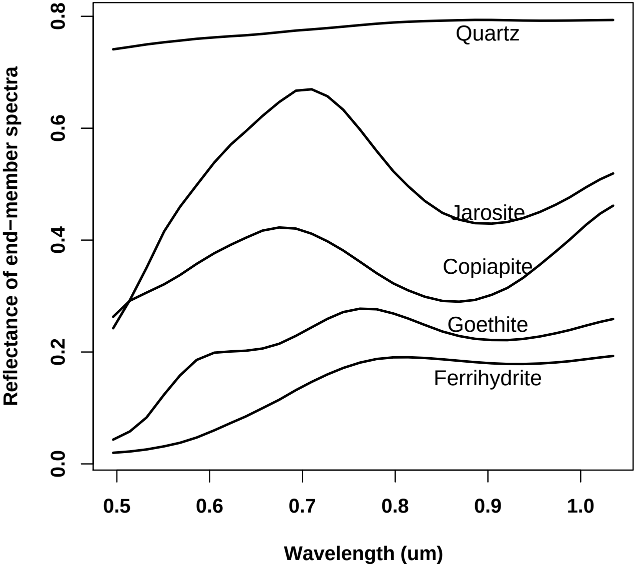

Figure: Five end-members spectra from USGS library, resampled to DAIS VIR region

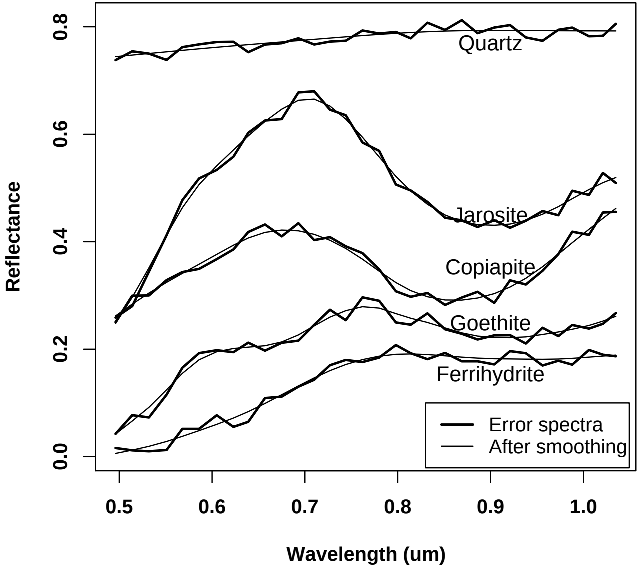

Figure: Five end-members spectra with error from the $U(-0.02, 0.02)$ distribution. Smoothing was applied to the spectra.

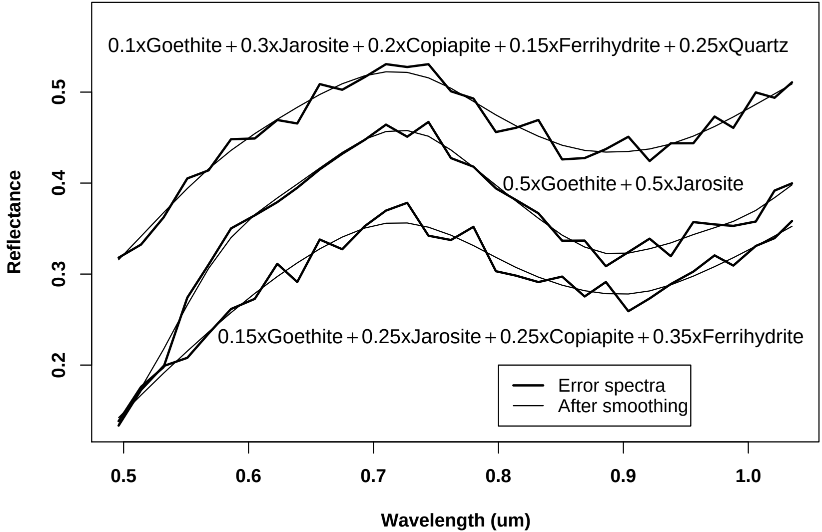

Figure: Mixed spectra with error from the $U(-0.02, 0.02)$ distribution. Smoothing was applied to the spectra.

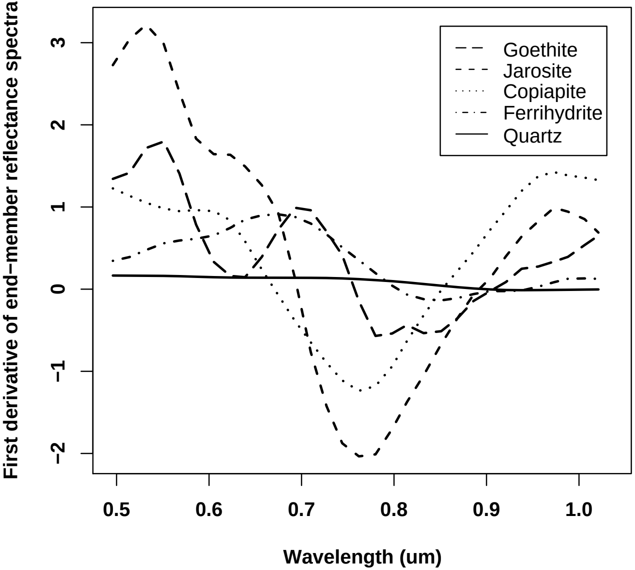

Figure: First derivative of end-member spectra after applying smoothing.

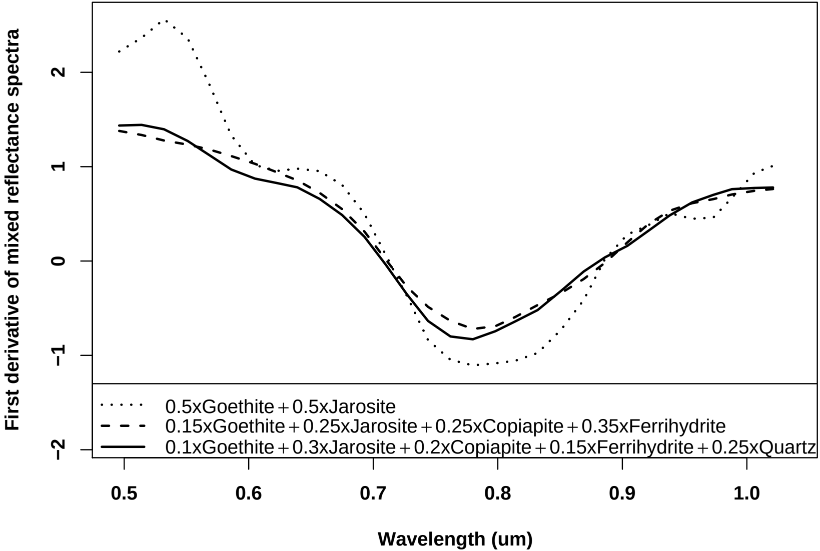

Figure: First derivative of mixed spectra after applying smoothing.

Table: Abundance: Using observed spectra & SumSpec.

Known abundance				Estimated abundance				
Goe	Jar	Cop	Fer	Goe	Jar	Cop	Fer	$M \backslash E$
End-member spectrum included in E								
1.00	0.00	0.00	0.00	0.78	0.03	0.05	0.14	0.00
0.00	1.00	0.00	0.00	0.03	0.94	0.00	0.01	0.02
0.00	0.00	1.00	0.00	0.03	0.06	0.89	0.02	0.00
0.00	0.00	0.00	1.00	0.03	0.00	0.01	0.92	0.04
End-member spectrum excluded from E								
1.00	0.00	0.00	0.00	—	0.25	0.00	0.64	0.11
0.00	1.00	0.00	0.00	0.00	—	1.00	0.00	0.00
0.00	0.00	1.00	0.00	0.01	0.68	—	0.00	0.31
0.00	0.00	0.00	1.00	0.71	0.00	0.00	—	0.29
Mixtures								
0.50	0.50	0.00	0.00	0.48	0.51	—	—	0.01
0.50	0.50	0.00	0.00	0.40	0.52	0.01	0.05	0.02
0.15	0.25	0.25	0.35	0.66	0.30	—	—	0.04
0.15	0.25	0.25	0.35	0.20	0.26	0.23	0.29	0.02

Table: Abundance: Using observed spectra & VarSpec.

Known abundance				Estimated abundance				
Goe	Jar	Cop	Fer	Goe	Jar	Cop	Fer	$M \backslash E$
End-member spectrum included in E								
1.00	0.00	0.00	0.00	0.90	0.02	0.00	0.08	0.00
0.00	1.00	0.00	0.00	0.07	0.91	0.00	0.00	0.02
0.00	0.00	1.00	0.00	0.02	0.01	0.94	0.00	0.03
0.00	0.00	0.00	1.00	0.03	0.00	0.01	0.92	0.04
End-member spectrum excluded from E								
1.00	0.00	0.00	0.00	—	0.26	0.00	0.69	0.05
0.00	1.00	0.00	0.00	0.43	—	0.57	0.00	0.00
0.00	0.00	1.00	0.00	0.01	0.38	—	0.00	0.61
0.00	0.00	0.00	1.00	0.97	0.00	0.01	—	0.02
Mixtures								
0.50	0.50	0.00	0.00	0.49	0.50	—	—	0.01
0.50	0.50	0.00	0.00	0.35	0.54	0.01	0.09	0.01
0.15	0.25	0.25	0.35	0.55	0.24	—	—	0.21
0.15	0.25	0.25	0.35	0.14	0.25	0.23	0.34	0.04

Table: Abundance: Using 1st derivative spectra & SumDeriv.

Known abundance				Estimated abundance				
Goe	Jar	Cop	Fer	Goe	Jar	Cop	Fer	$M\backslash E^1$
End-member spectrum included in E								
1.00	0.00	0.00	0.00	0.87	0.02	0.00	0.06	0.05
0.00	1.00	0.00	0.00	0.00	0.94	0.06	0.00	0.00
0.00	0.00	1.00	0.00	0.01	0.04	0.91	0.00	0.05
0.00	0.00	0.00	1.00	0.07	0.01	0.00	0.86	0.06
End-member spectrum excluded from E								
1.00	0.00	0.00	0.00	—	0.33	0.00	0.66	0.01
0.00	1.00	0.00	0.00	0.48	—	0.51	0.00	0.01
0.00	0.00	1.00	0.00	0.00	0.45	—	0.01	0.54
0.00	0.00	0.00	1.00	0.33	0.00	0.00	—	0.67
Mixtures								
0.50	0.50	0.00	0.00	0.48	0.51	—	—	0.01
0.50	0.50	0.00	0.00	0.46	0.48	0.05	0.01	0.00
0.15	0.25	0.25	0.35	0.27	0.32	—	—	0.41
0.15	0.25	0.25	0.35	0.09	0.24	0.26	0.39	0.02

Table: Abundance: Using 1st derivative spectra & VarDeriv.

Known abundance				Estimated abundance				
Goe	Jar	Cop	Fer	Goe	Jar	Cop	Fer	$M \backslash E^1$
End-member spectrum included in E								
1.00	0.00	0.00	0.00	0.90	0.00	0.03	0.07	0.00
0.00	1.00	0.00	0.00	0.01	0.92	0.04	0.01	0.02
0.00	0.00	1.00	0.00	0.01	0.07	0.92	0.00	0.00
0.00	0.00	0.00	1.00	0.08	0.00	0.00	0.89	0.03
End-member spectrum excluded from E								
1.00	0.00	0.00	0.00	—	0.28	0.00	0.56	0.16
0.00	1.00	0.00	0.00	0.31	—	0.68	0.00	0.01
0.00	0.00	1.00	0.00	0.00	0.46	—	0.00	0.54
0.00	0.00	0.00	1.00	0.27	0.00	0.00	—	0.73
Mixtures								
0.50	0.50	0.00	0.00	0.44	0.53	—	—	0.03
0.50	0.50	0.00	0.00	0.45	0.52	0.02	0.01	0.00
0.15	0.25	0.25	0.35	0.05	0.40	—	—	0.55
0.15	0.25	0.25	0.35	0.07	0.27	0.24	0.37	0.05

Table: Correlation coefficient between pairs of original spectra, pairs of first derivative of spectra and pairs of second derivative of spectra.

Original spectra:

	goethite	jarosite	copiapite	ferrihydrite
goethite	1.00			
jarosite	0.67	1.00		
copiapite	0.43	0.72	1.00	
ferrihydrite	0.86	0.29	0.16	1.00

1st derivative (lower △) & 2nd derivative (upper △):

	goethite	jarosite	copiapite	ferrihydrite
goethite	1.00	0.35	-0.14	0.22
jarosite	0.71	1.00	0.43	0.18
copiapite	0.35	0.79	1.00	-0.02
ferrihydrite	0.44	0.24	-0.15	1.00

This study resulted in four main conclusions.

- Abundances of spectrally similar minerals in mine wastes can be estimated with relatively high accuracy by unmixing of first derivatives of target spectra, in which contributing components are decorrelated.
- Simulated annealing proved efficient in minimizing variance of the difference spectrum to estimate abundance of spectrally similar minerals.
- Higher accuracy of abundance estimates is gained when end-member spectra contributing to target spectra is included.
- The choice to use the original spectra, the first or second derivatives spectra depends on the signal-to-noise ratio of the sensor device. Higher signal-to-noise ratios allows better accuracy in the abundance estimation by using higher order derivatives.