A methodology to unmix spectrally similar minerals using high order derivative spectra

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Outline

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Overview of hyperspectral remote sensing

Hyperspectral sensors

- record the reflectance in many narrow contiguous bands
- various parts of the electromagnetic spectrum (visible - near infrared - short wave infrared)
- at each part of the electromagnetic spectrum results in an image

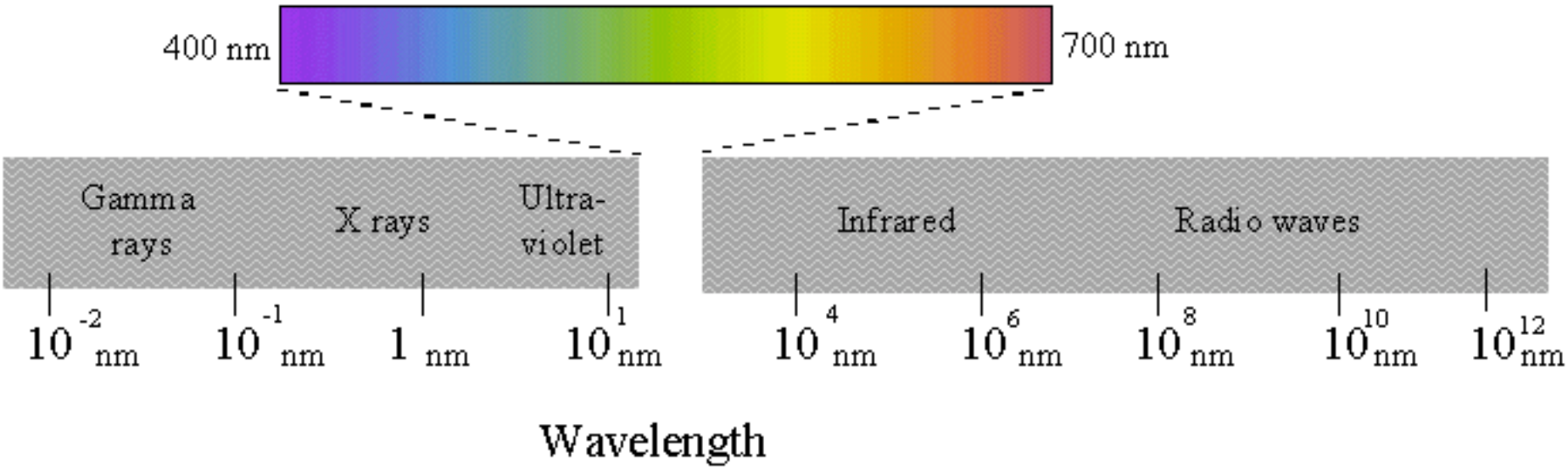

Figure: Spectral Range

Overview of hyperspectral remote sensing (cont. . .)

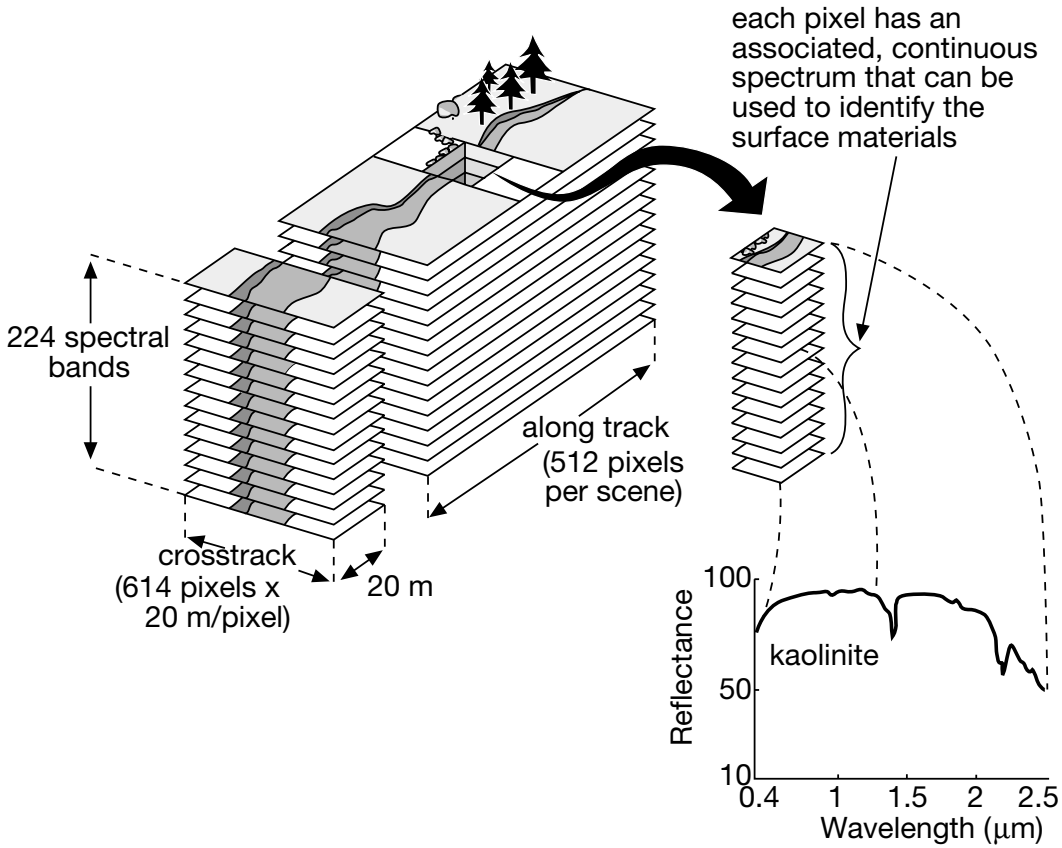

Figure: Hyperspectral cube

Overview of hyperspectral remote sensing (cont. . .)

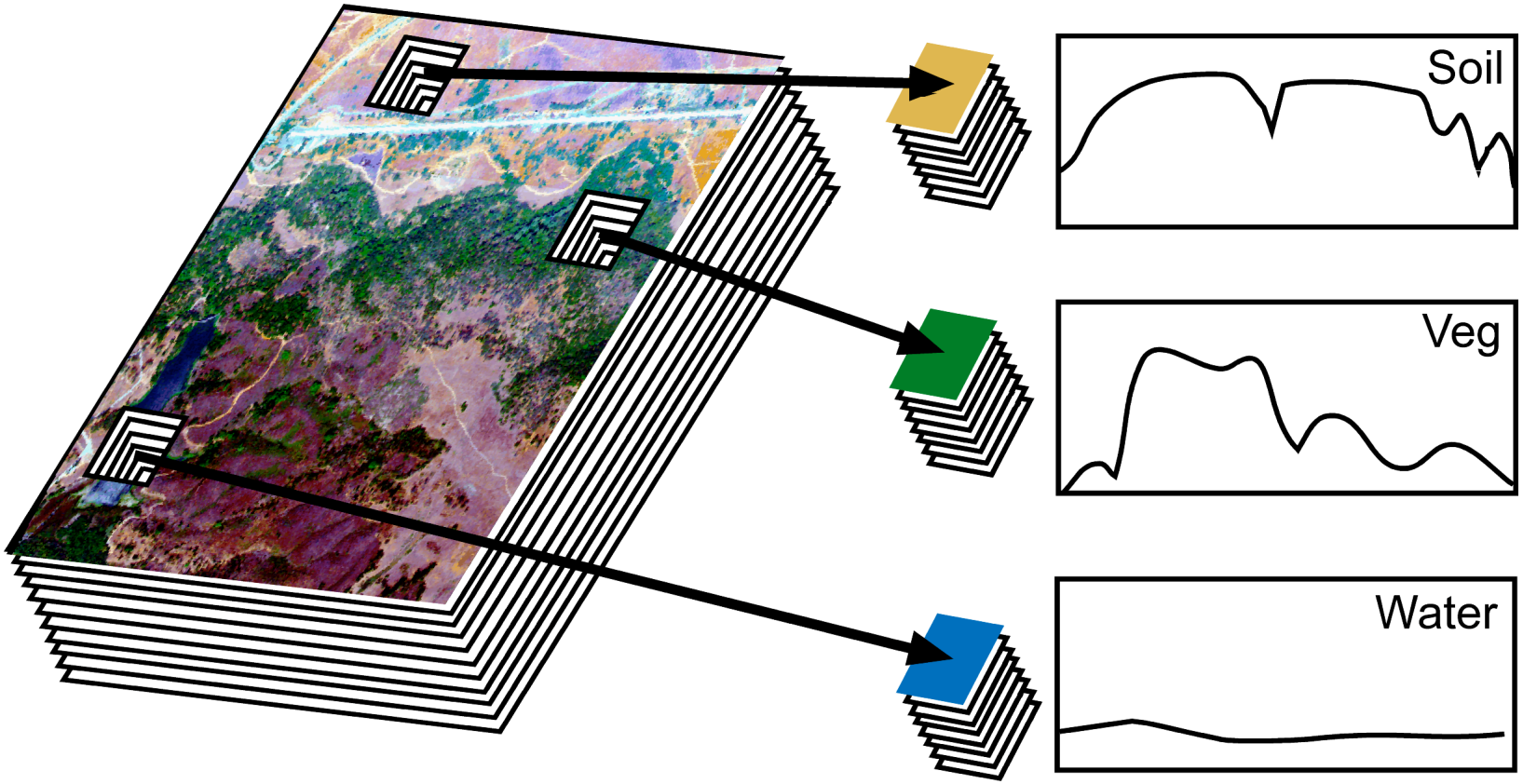

Figure: Pixels in hyperspectral image

Overview of hyperspectral remote sensing (cont. . .)

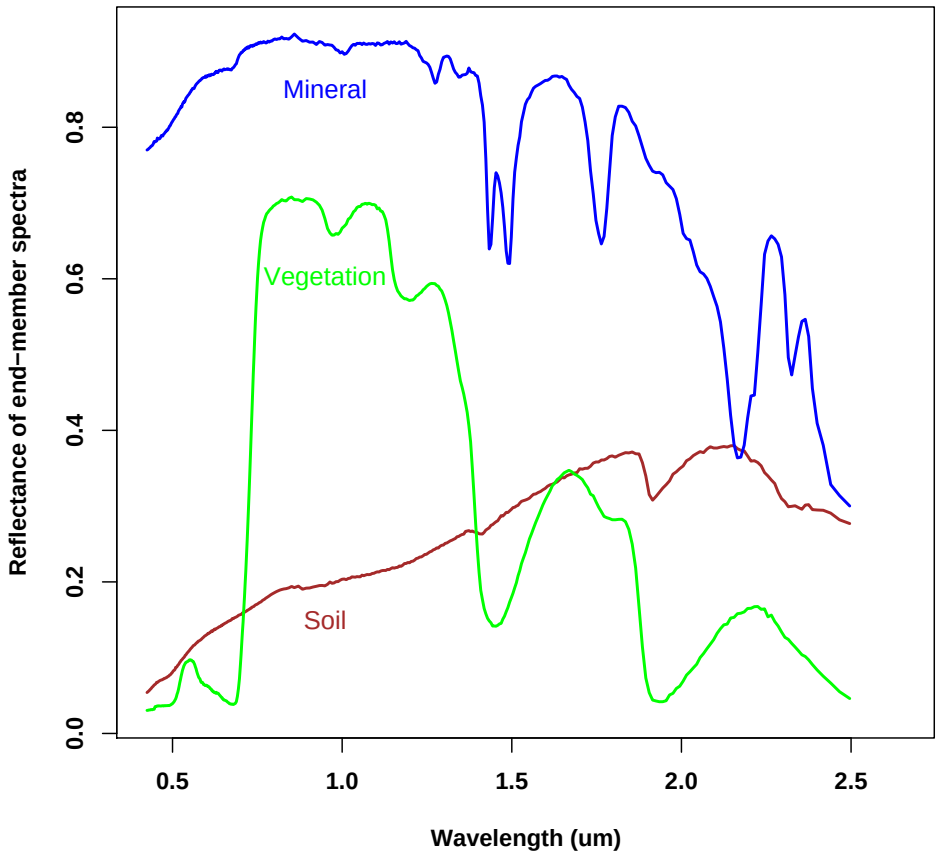

Figure: Example of 3 different spectral signatures

If research could be as easy as eating a chocolate cake . . .

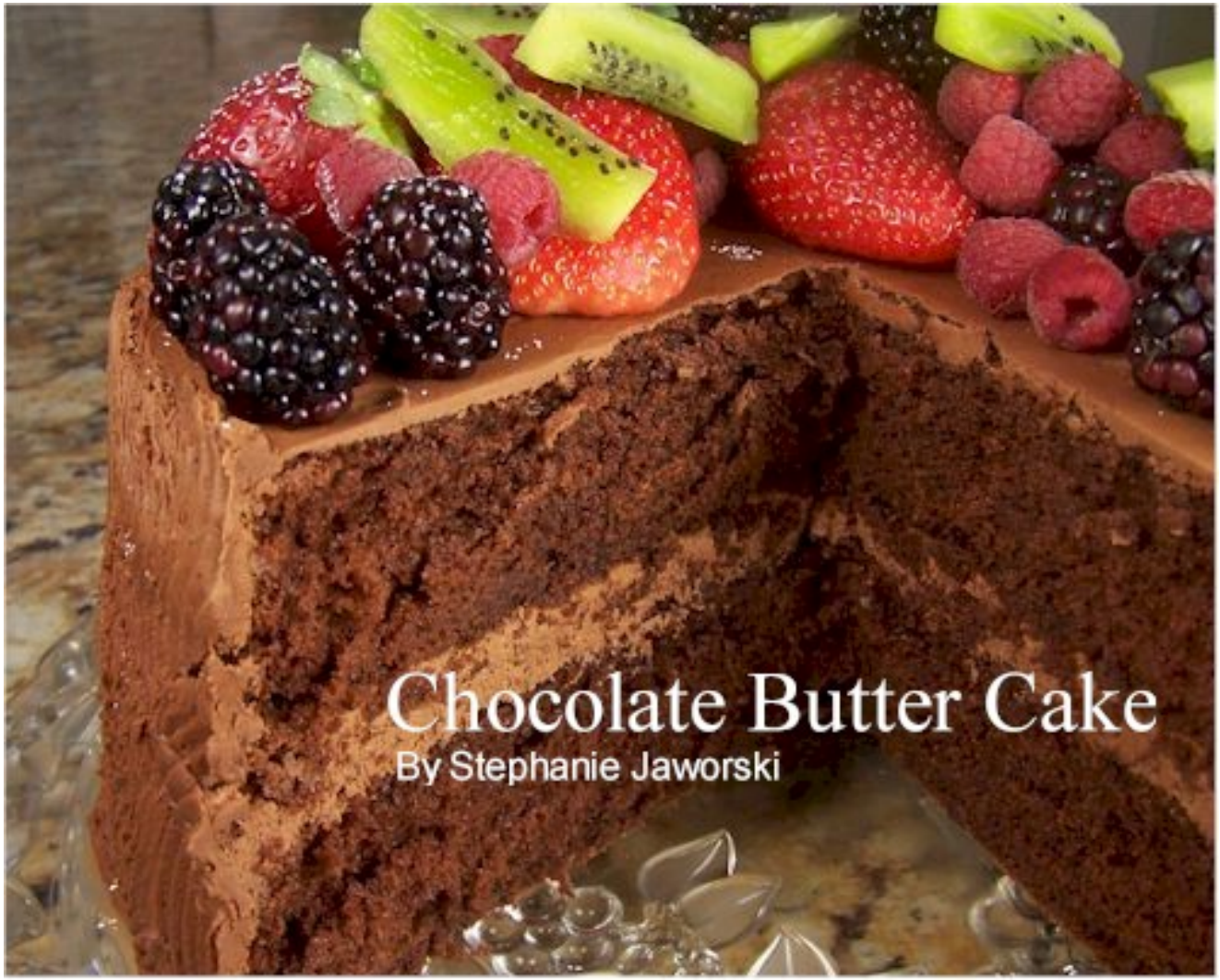

Figure: Can you guess the ingredients for this chocolate cake?

Ingredients	Quantity
unsweetened chocolate	
unsweetened cocoa powder	
boiling water	
flour	
baking powder	
baking soda	
salt	
unsalted butter	
white sugar	
eggs	
pure vanilla extract	
milk	

Table: Chocolate cake ingredients

Ingredients	Quantity
unsweetened chocolate	120 grams
unsweetened cocoa powder	28 grams
boiling water	240 ml
flour	315 grams
baking powder	2 teaspoons
baking soda	1 teaspoon
salt	1/4 teaspoon
unsalted butter	226 grams
white sugar	400 grams
eggs	3 large
pure vanilla extract	2 teaspoons
milk	240 ml

Table: Chocolate cake ingredients

What is spectral unmixing?

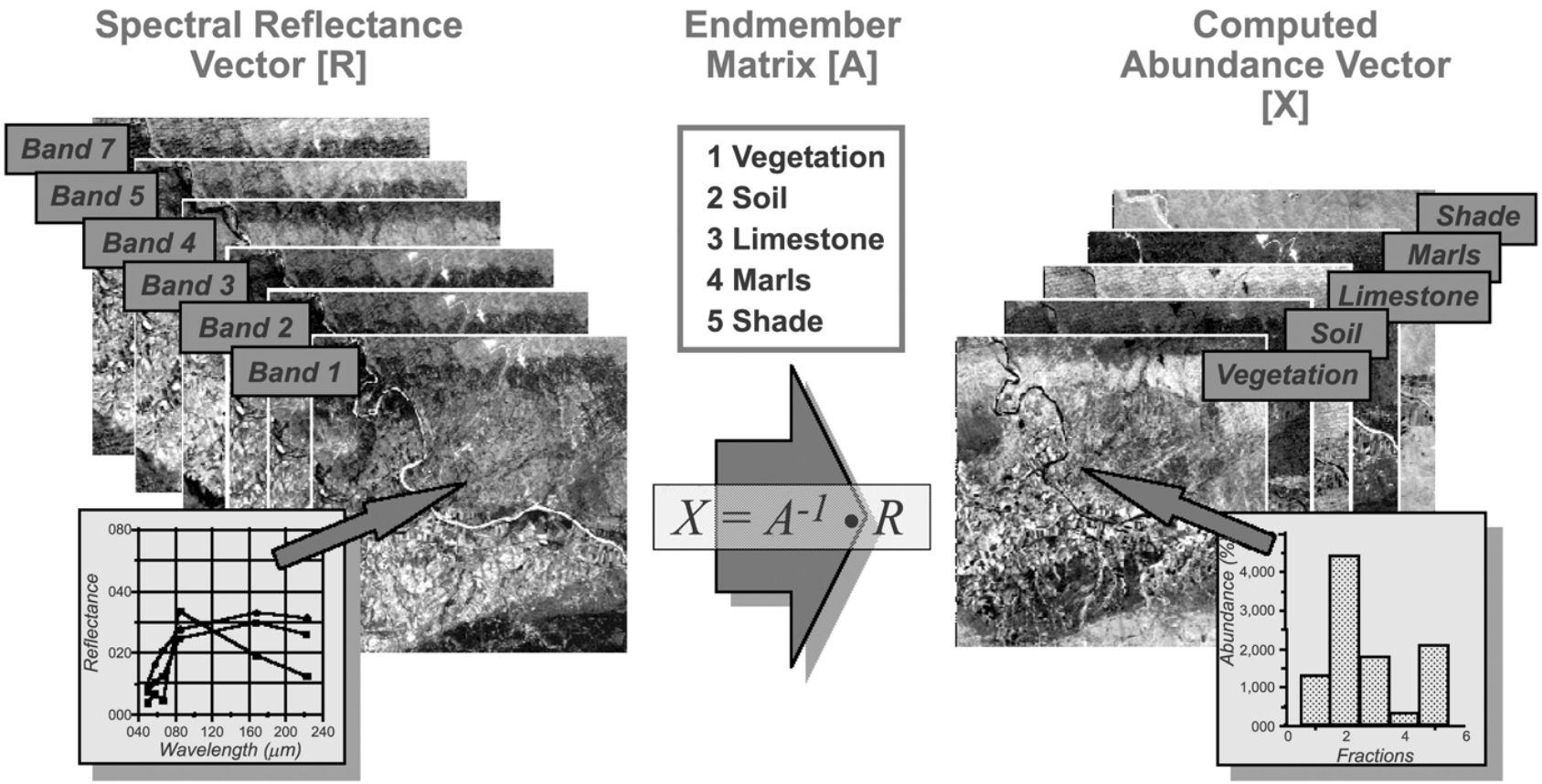

Figure: The concept of unmixing – taken from
`http://www.emeraldinsight.com/fig/0830140104006.png`

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?

Old method: problem

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

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

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

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

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

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

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

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

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

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 $\mathbf{c}$ 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.

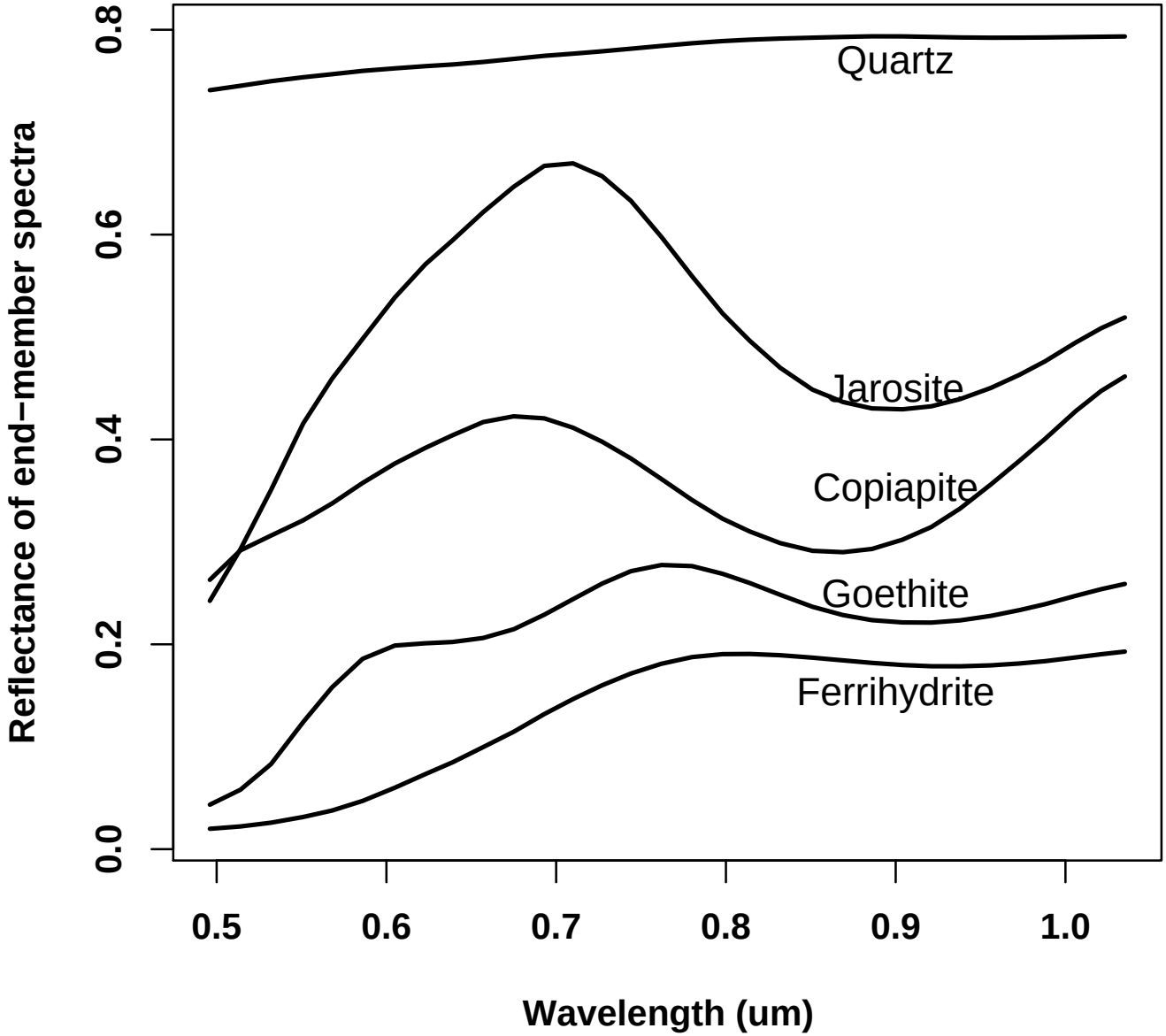

Figure: Five end-members spectra from USGS library, resampled to DAIS VIR region

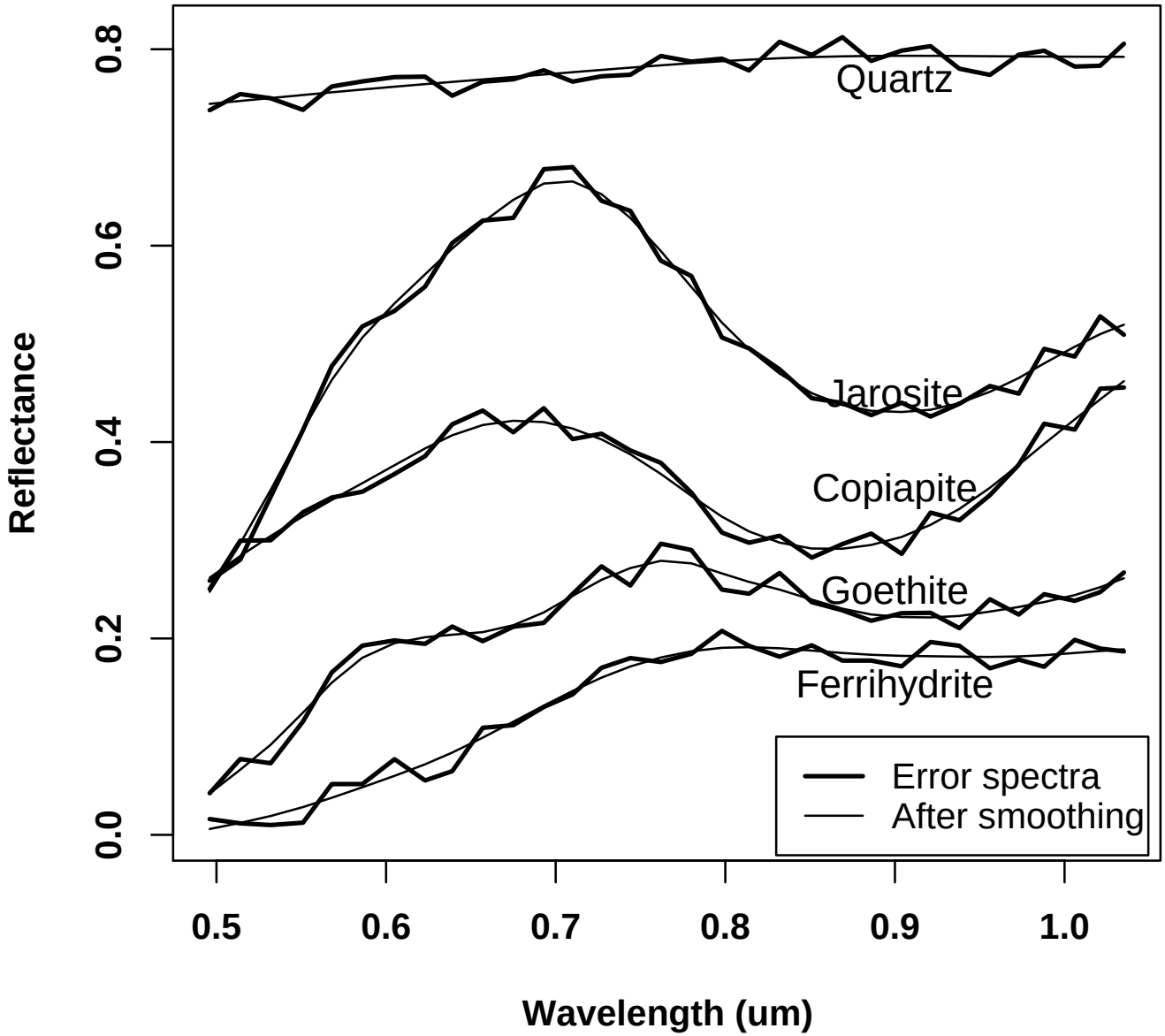

Figure: Five end-members spectra with error from the $U(-0.02, 0.02)$ distribution. Smoothing was applied to the spectra.

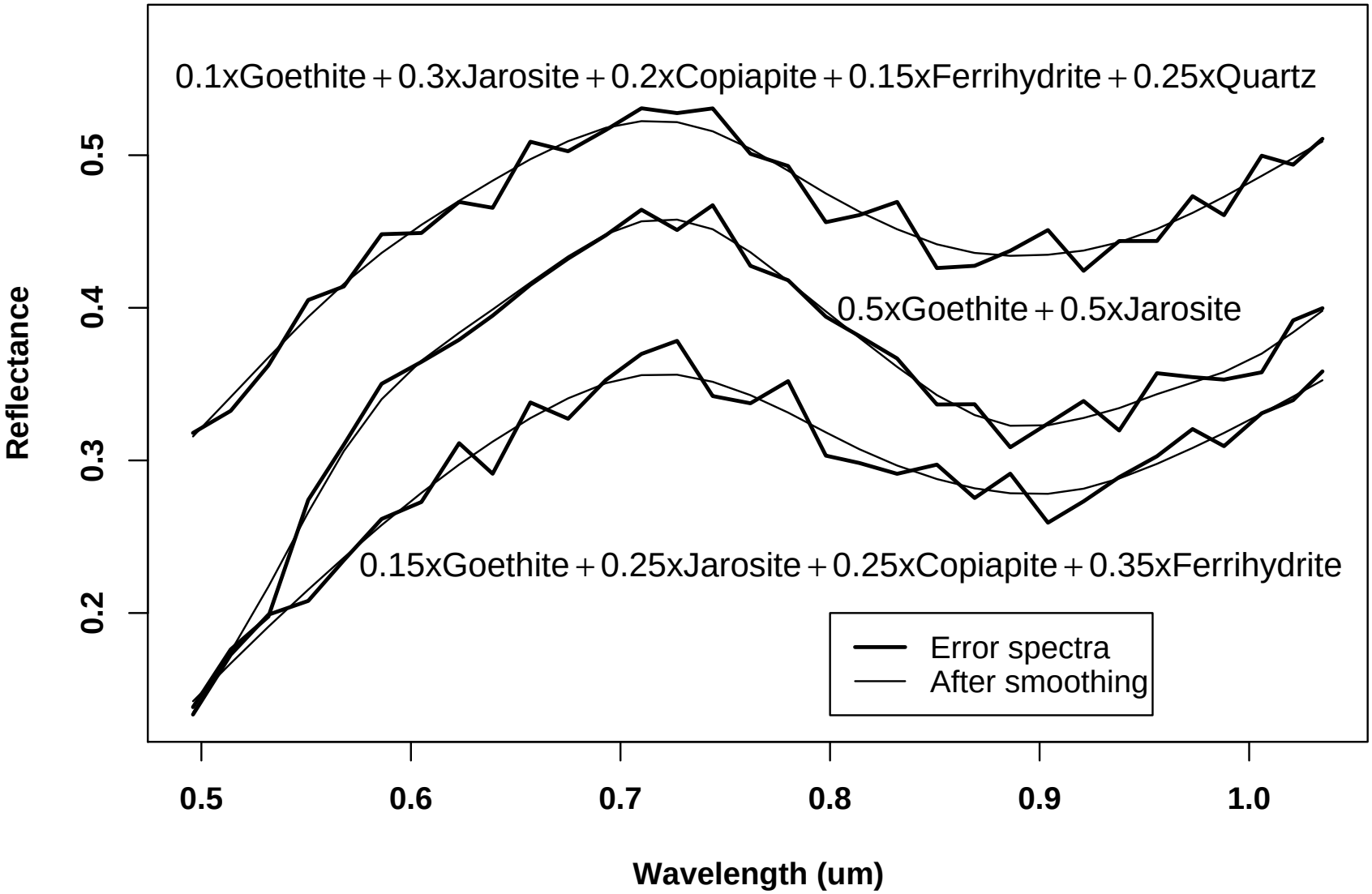

Figure: Mixed spectra with error from the $U(-0.02, 0.02)$ distribution. Smoothing was applied to the spectra.

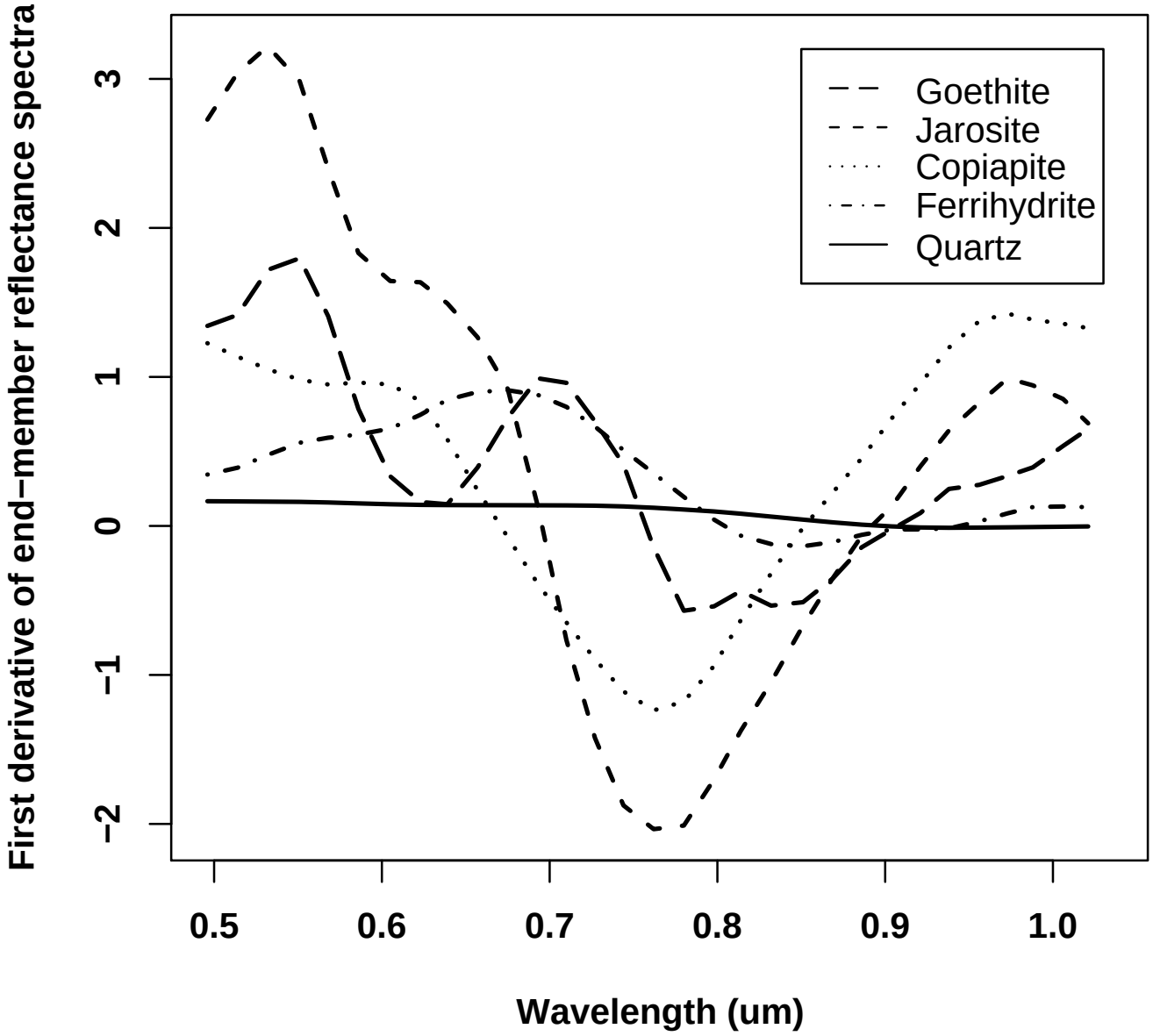

Figure: First derivative of end-member spectra after applying smoothing.

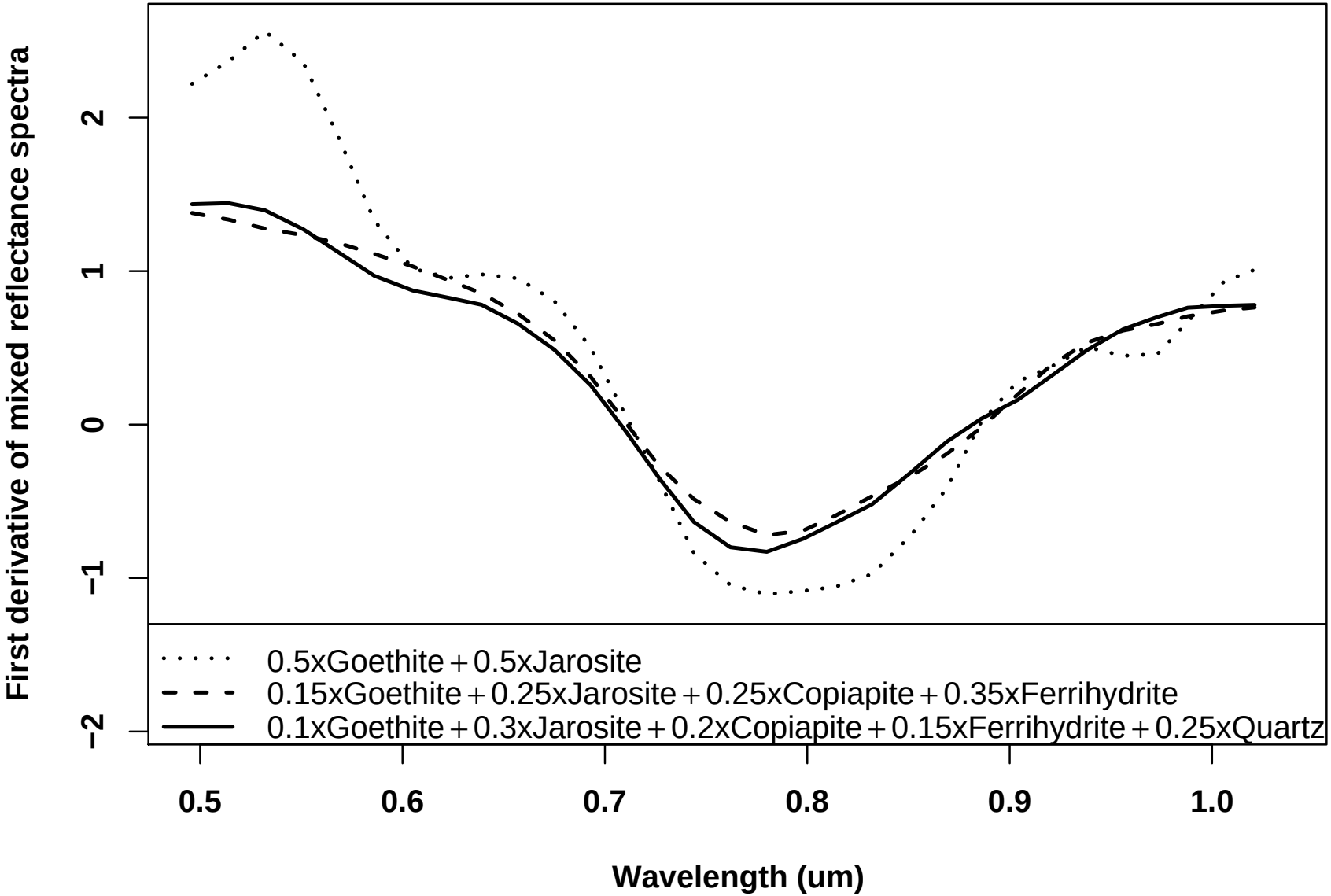

Figure: First derivative of mixed spectra after applying smoothing.

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 $\triangle$) & 2nd derivative (upper $\triangle$):

	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.

More details: Debba *et. al.* (2006). Abundance estimation of spectrally similar materials by using derivatives in simulated annealing, *IEEE Geoscience and Remote Sensing*, vol. 44, no. 12, 3649–3658.

The Problem

- What is the effect of the proposed method based on the SNR of the image?

Table: Abundance: End-member spectrum included in E for SNR of 50:1

Known abundance				Estimated abundance				
Goe	Jar	Cop	Fer	Goe	Jar	Cop	Fer	$M \setminus E$
Using observed spectra								
1.00	0.00	0.00	0.00	0.73	0.06	0.00	0.19	0.02
0.00	1.00	0.00	0.00	0.00	0.94	0.01	0.03	0.02
0.00	0.00	1.00	0.00	0.00	0.04	0.93	0.00	0.03
0.00	0.00	0.00	1.00	0.05	0.00	0.00	0.92	0.03
Using 1st derivative spectra								
1.00	0.00	0.00	0.00	0.67	0.06	0.06	0.20	0.01
0.00	1.00	0.00	0.00	0.00	0.98	0.01	0.00	0.01
0.00	0.00	1.00	0.00	0.03	0.01	0.95	0.00	0.01
0.00	0.00	0.00	1.00	0.02	0.00	0.00	0.90	0.08
Using 2nd derivative spectra								
1.00	0.00	0.00	0.00	0.45	0.00	0.15	0.37	0.03
0.00	1.00	0.00	0.00	0.00	0.52	0.46	0.00	0.02
0.00	0.00	1.00	0.00	0.00	0.17	0.46	0.00	0.37
0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.93	0.07

Table: Abundance: End-member spectrum included in E for SNR of 200:1

Known abundance				Estimated abundance				
Goe	Jar	Cop	Fer	Goe	Jar	Cop	Fer	$M \setminus E$
				Using observed spectra				
1.00	0.00	0.00	0.00	0.90	0.03	0.00	0.06	0.01
0.00	1.00	0.00	0.00	0.01	0.94	0.03	0.00	0.02
0.00	0.00	1.00	0.00	0.01	0.02	0.94	0.00	0.03
0.00	0.00	0.00	1.00	0.01	0.01	0.00	0.96	0.02
				Using 1st derivative spectra				
1.00	0.00	0.00	0.00	0.91	0.02	0.03	0.01	0.03
0.00	1.00	0.00	0.00	0.00	0.95	0.01	0.02	0.02
0.00	0.00	1.00	0.00	0.02	0.00	0.95	0.02	0.01
0.00	0.00	0.00	1.00	0.02	0.00	0.00	0.91	0.07
				Using 2nd derivative spectra				
1.00	0.00	0.00	0.00	0.88	0.00	0.06	0.01	0.05
0.00	1.00	0.00	0.00	0.00	0.93	0.01	0.02	0.04
0.00	0.00	1.00	0.00	0.00	0.00	0.99	0.00	0.01
0.00	0.00	0.00	1.00	0.01	0.00	0.00	0.97	0.02

Table: Abundance: End-member spectrum included in E for SNR of 500:1

Known abundance				Estimated abundance				
Goe	Jar	Cop	Fer	Goe	Jar	Cop	Fer	$M \setminus E$
Using observed spectra								
1.00	0.00	0.00	0.00	0.97	0.00	0.01	0.01	0.01
0.00	1.00	0.00	0.00	0.03	0.94	0.03	0.00	0.00
0.00	0.00	1.00	0.00	0.01	0.01	0.94	0.01	0.03
0.00	0.00	0.00	1.00	0.01	0.01	0.00	0.97	0.01
Using 1st derivative spectra								
1.00	0.00	0.00	0.00	0.97	0.01	0.00	0.00	0.02
0.00	1.00	0.00	0.00	0.00	0.94	0.03	0.01	0.02
0.00	0.00	1.00	0.00	0.00	0.04	0.92	0.00	0.04
0.00	0.00	0.00	1.00	0.01	0.00	0.01	0.93	0.05
Using 2nd derivative spectra								
1.00	0.00	0.00	0.00	0.95	0.01	0.01	0.01	0.02
0.00	1.00	0.00	0.00	0.01	0.94	0.01	0.01	0.03
0.00	0.00	1.00	0.00	0.00	0.01	0.98	0.01	0.00
0.00	0.00	0.00	1.00	0.01	0.00	0.01	0.97	0.03

Table: Abundance: End-member spectrum excluded in E for SNR of 50:1

Known abundance				Estimated abundance				
Goe	Jar	Cop	Fer	Goe	Jar	Cop	Fer	$M \setminus E$
Using observed spectra								
1.00	0.00	0.00	0.00	—	0.26	0.00	0.73	0.01
0.00	1.00	0.00	0.00	0.40	—	0.59	0.00	0.01
0.00	0.00	1.00	0.00	0.00	0.36	—	0.00	0.64
0.00	0.00	0.00	1.00	0.91	0.00	0.00	—	0.09
Using 1st derivative spectra								
1.00	0.00	0.00	0.00	—	0.29	0.00	0.61	0.10
0.00	1.00	0.00	0.00	0.21	—	0.78	0.00	0.01
0.00	0.00	1.00	0.00	0.00	0.44	—	0.00	0.56
0.00	0.00	0.00	1.00	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
0.00	1.00	0.00	0.00	0.22	—	0.77	0.00	0.01
0.00	0.00	1.00	0.00	0.00	0.30	—	0.00	0.70
0.00	0.00	0.00	1.00	0.05	0.03	0.00	—	0.92

Table: Abundance: End-member spectrum excluded in E for SNR of 200:1

Known abundance				Estimated abundance				
Goe	Jar	Cop	Fer	Goe	Jar	Cop	Fer	$M \setminus E$
Using observed spectra								
1.00	0.00	0.00	0.00	—	0.27	0.00	0.69	0.04
0.00	1.00	0.00	0.00	0.42	—	0.57	0.00	0.01
0.00	0.00	1.00	0.00	0.00	0.37	—	0.00	0.63
0.00	0.00	0.00	1.00	0.92	0.00	0.00	—	0.08
Using 1st derivative spectra								
1.00	0.00	0.00	0.00	—	0.29	0.00	0.57	0.12
0.00	1.00	0.00	0.00	0.26	—	0.73	0.00	0.01
0.00	0.00	1.00	0.00	0.00	0.44	—	0.00	0.56
0.00	0.00	0.00	1.00	0.21	0.00	0.00	—	0.79
Using 2nd derivative spectra								
1.00	0.00	0.00	0.00	—	0.17	0.00	0.46	0.37
0.00	1.00	0.00	0.00	0.38	—	0.60	0.01	0.01
0.00	0.00	1.00	0.00	0.00	0.25	—	0.00	0.75
0.00	0.00	0.00	1.00	0.06	0.03	0.00	—	0.91

Table: Abundance: End-member spectrum excluded in E for SNR of 500:1

Known abundance				Estimated abundance				
Goe	Jar	Cop	Fer	Goe	Jar	Cop	Fer	$M \setminus E$
				Using observed spectra				
1.00	0.00	0.00	0.00	—	0.27	0.00	0.69	0.04
0.00	1.00	0.00	0.00	0.45	—	0.54	0.00	0.01
0.00	0.00	1.00	0.00	0.00	0.38	—	0.00	0.62
0.00	0.00	0.00	1.00	0.92	0.00	0.00	—	0.08
				Using 1st derivative spectra				
1.00	0.00	0.00	0.00	—	0.28	0.00	0.58	0.14
0.00	1.00	0.00	0.00	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	0.00	0.00	1.00	0.22	0.00	0.00	—	0.78
				Using 2nd derivative spectra				
1.00	0.00	0.00	0.00	—	0.28	0.00	0.57	0.15
0.00	1.00	0.00	0.00	0.40	—	0.58	0.01	0.01
0.00	0.00	1.00	0.00	0.00	0.31	—	0.00	0.69
0.00	0.00	0.00	1.00	0.05	0.03	0.00	—	0.92

Table: Abundance: Mixtures for SNR of 50:1, 200:1 and 500:1 using observed spectra

Known abundance				Estimated abundance				
Goe	Jar	Cop	Fer	Goe	Jar	Cop	Fer	$M \backslash E$
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

Table: Abundance: Mixtures for SNR of 50:1, 200:1 and 500:1 using first derivative spectra

Known abundance				Estimated abundance				
Goe	Jar	Cop	Fer	Goe	Jar	Cop	Fer	$M \backslash E$
				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

Table: Abundance: Mixtures for SNR of 50:1, 200:1 and 500:1 using second derivative spectra

Known abundance				Estimated abundance				
Goe	Jar	Cop	Fer	Goe	Jar	Cop	Fer	$M \backslash E$
				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

Table: Abundance: Mixtures and end-member spectrum excluded in E

Known abundance				Estimated abundance				
Goe	Jar	Cop	Fer	Goe	Jar	Cop	Fer	$M \setminus E$
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

This study resulted in two main conclusions.

- 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.

More details: Debba *et. al.* (2009). Abundance estimation of spectrally similar minerals. *In Proceedings of 2009 IEEE International Symposium on Geoscience and Remote Sensing*. July 13–17, 2009 Cape Town, South Africa. Accepted.

Recommendations

- Solve the problem statistically.
- Use feature selection or feature extraction techniques for dimensionality reduction on the set of original spectra and higher order derivatives.

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