





BUILDING A HYPERSPECTRAL LIBRARY AND ITS INCORPORATION INTO SPARSE UNMIXING FOR MINERAL IDENTIFICATION

Thanh Bui^{1,2}, Beate Orberger^{3,4}, Simon B. Blancher¹, Ali Mohammad-Djafari⁴, Henry Pilliere⁵, Anne Salaun¹, Xavier Bourrat⁶, Nicolas Maubec⁶, Thomas Lefevre⁵, Celine Rodriguez¹, Antanas Vaitkus⁷, Saulius Grazulis⁷, Cedric Duée⁶, Dominique Harang⁵, Thomas Wallmach¹, Yassine El Mendili⁸, Daniel Chateigner⁸, Mike Buxton⁹, Monique Le Guen¹⁰

 Eramet Research, Eramet Group, Trappes, France; 2) L2S, CNRS, Centrale Supélec, Université Paris-Saclay, France; 3) GEOPS-Université Paris Sud-Paris Saclay, Orsay, France; 4) Catura Geoprojects, Paris, France; 5) ThermoFisher Scientific (TFS), Artenay, France;
BRGM, Orléans, France; 7) Vilnius University Institute of Biotechnology, Vilnius, Lithuania; 8) CRISMAT-CNRS, Normandie Université, Caen, France; 9) Delft University of Technology, Delft, The Netherlands; 10) Eramet Nickel Division, Eramet Group, Trappes, France













Contents

- Introduction
- Hyperspectral library
- Sparse unmixing techniques
- Results
- Conclusions and perspectives



SOLSA project

H2020 SOLSA (Sonic Online and Sample Analysis) project aims at constructing an analytical expert system for on-line-on-mine-real-time mineralogical and geochemical analyses on sonic drill cores.





Nickel laterites

- Ni resources:
 - Sulfide ores 0
 - Ni laterites \cap
- Ni laterites
 - Consitute 60 70% of the \cap world's Ni resources
 - Reach 60% of total Ni \cap production in 2014
 - Contribute 20 30% of the Ο total Co supply.

Butt *et al.*, 2013





Three nickel laterite ore types, based on the dominant minerals hosting Ni: ٠

Ores	Mean grades of Ni	Principle ore minerals	% of total Ni laterite resources	Position in lateritic profiles
Oxide	1.0 – 1.6 wt%	Goethite, absolane, lithiophorite	60%	Mid to upper saprolite and upwards to the plasmic zone
Hydrous Mg silicate	1.44 wt%	Serpentine, talc, chlorite, sepiolite	32%	Mid to lower saprolite
Clay silicate	1.0 – 1.5 wt%	Smectite, saponite	8%	Mid to upper saprolite



SOLSA ID A system

SWIR (1000 – 2500 nm) camera



5



Thanh M. BUI

6



Hyperspectral imaging for mineralogy identification

Note: if the deepest absorption is in the AIOH waveband, absorptions at these wavelengths will include SECONDARY AIOH absorptions of that mineral

ecules [Dominant absorption features
ЭН	1400nm (1550nm and 1750- 1850nm in some minerals)
ater	1400nm and 1900nm
ЮН	2160-2228nm
OH	2230-2295nm
gOH	2300-2370nm
CO ₃	2300-2370nm (and also at L870nm, 1990nm and 2155nm)
OH ater IOH 2OH gOH CO ₃	1400nm (1550nm and 1750- 1850nm in some minerals) 1400nm and 1900nm 2160-2228nm 2230-2295nm 2300-2370nm 2300-2370nm (and also at 1870nm, 1990nm and 2155nm)



Crystallinity variations -> shape variations Compositional variations -> wavelength shifts

Pontual et al. 1997





- Statistical approaches (Debigion et al. 2008 ; Altmann et al., 2015)
 - The likelihood: data generation models
 - Priors: constraints on the endmembers
- Geometrical approaches (Nascimento et al., 2005; Bioucas-Dias et al. 2009)
 - The observed hyperspectral vectors: simplex set whose vertices correspond to the endmembers.
- Sparse regression



 $\min_{X} ||AX - Y||_{F}^{2} + \lambda ||X||_{2,1} \quad subject \ to: X \ge 0, \ \mathbf{1}^{T} X = 1$

- The observed image signatures can be expressed in the form of linear combinations of a number of pure spectral signatures known in advance (spectral library).
- Unmixing amounts to finding the optimal subset of signatures in a spectral library that can best model each mixed pixel in the scene.
- The sparse unmixing exploits the usual very low number of endmembers (maximum of 4, Berman *et al.*, CSIRO, 2017) present in real images, out of a spectral library.



Hyperspectral library

- Other libraries (e.g., USGS) may not contain spectra of pure minerals.
- We wish to include spectra that are collected with our instruments used in our operational exploration.
- Minerals found in Ni laterites in New Caledonia may not be present in other libraries.





Hyperspectral library

- Rock and mineral samples provided ٠ by BRGM, ERAMET and the National Museum of Natural History, France
- Spectra extraction: ENVI 5.4 and G-MEX by taking into account the wavelength positions and the relative intensities of the absorption features.



1400

1600

1800

Wavelength (nm)

2000

Spectral Profile

2200

2400











Sparse unmixing techniques

CLSUnSAL (Collaborative sparse unmixing by variable splitting and augmented Lagrangian):
$$\begin{split} \min_{X} \|AX - Y\|_{F}^{2} + \lambda \|X\|_{2,1} \\ subject \ to: \ X \geq 0, \ \mathbf{1}^{T} X = 1 \end{split}$$

SUnSAL (Sparse unmixing by variable splitting and augmented Lagrangian):
$$\begin{split} \min_{X} \|AX - Y\|_{F}^{2} + \lambda \|X\|_{1,1} \\ subject \ to: \ X \geq 0, \ \mathbf{1}^{T} \ X = 1 \end{split}$$

FCLS (Fully contrained least squares):

 $\min_{X} ||AX - Y||_{F}^{2}$ subject to: $X \ge 0$, $\mathbf{1}^{T} X = 1$

The optimization is based on the alternating direction method of multipliers (ADMM)

Bioucas-Dias *et al.*, 2010 Iordache *et al.*, IEEE Trans, 2014 Afonso *et al.*, IEEE Trans, 2011



Hyperspectral library

37 spectra representing 21 minerals have been collected: ankerite, calcite, dolomite, magnesite lizardite, nepouite, antigorite, chrysotite, saponite, montmorillonite, nontronite, kaolinite, pimelite, talc, sepiolite,

alunite, asbolane, chromite, diaspore, enstatite, forsterite







Simulated data: SNR = 40 dB



Signal to reconstruction error (SRE) ratio:

$$SRE = 10 \log \frac{E \|\boldsymbol{x}\|^2}{E \|\boldsymbol{x} - \hat{\boldsymbol{x}}\|^2}$$

К	FCLS		SUnSAL		CLSUnSAL	
	SRE	Time	SRE	time	SRE	time
2	14.24	0.022	14.94	0.254	16.74	0.228
3	6.41	0.019	7.45	0.259	11.95	0.230
4	5.25	0.022	7.07	0.499	7.16	0.453

FCLS: Fully constrained least squares

SUnSAL: Sparse unmixing by variable splitting and augmented Lagrangian

CLSUnSAL: Collaborative sparse unmixing by variable splitting and augmented Lagrangian





Data acquired from a serpentinized harzburgite sample

1 cm

RGB image







0.8

0.6

0.4

0.2

0

Proportion (abundance) of each mineral:









Thanh M. BUI

19

Computation time: 4 mins



Data acquired from a serpentinized harzburgite sample



RGB image



QEMSCAN results



Thanh M. BUI



Computation time: 4 mins



Conclusions and perspectives

Wavelength (nm)

- Using our hyperspectral library, the CLSUnSAL provided the highest accuracy.
 - Need to improve the computation time.
 - Incorporate the spatial context to the unmixing problem
- The library is constantly extended
 - 257 spectra have been extracted for 49 minerals
- A graphic user interface is under development
- Machine learning classification approaches have been implemented.



Fhanh M. BUI



Thank you for your attention!





SOLSA project

H2020 SOLSA (Sonic Online and Sample Analysis) project aims at constructing an analytical expert system for on-line-on-mine-real-time mineralogical and geochemical analyses on sonic drill cores.





SOLSA software



Hyperspectral classification and unmixing techniques are being integrated



VNIR/SWIR camera parameters

Parameters	FX10 VNIR	SWIR OLES30
Spectral range (nm)	400 - 1000	1000 - 2500
Spectral bands	224	288
Spectral FWHM (nm)	5.5	12
Spatial sampling	1024	384
FOV (degree)	38	17
Maximum frame rate (fps)	330	450
Exposure time range (ms)	0.1 – 20	0.1 – 20
Aperture	1.7	2
Focal length (mm)	15	30
Measurement distance (m)	0.118	0.316
Field of View (mm)	81.26	94.45
Spatial resolution (um)	79.36	245.97
Depth of Field (mm)	1.91	9.64





Spectral classification using machine learning techniques





Spectral classification - results

540 samples (randomly selecting 360 for training, 180 for testing);

C-SVC, C = 100; RBF, γ = 0.999

Iteratively evaluated in 50 times

Features	Training (%)	Testing (%)
SAM	99.97 ± 0.07	99.56 ± 0.60
Filtered spectra	100	99.64 ± 0.55
Continuum removal	100	98.62 ± 0.84
Filtered spectra + PCA	99.97 ± 0.07	99.29 ± 0.78
Continuum removal + PCA	99.70 ± 0.28	98.02 ± 1.08



66 mm

Spectral classification - results

Goethite



Hematite 2 Hematite 1 Magnetite 2 Chromite Magnetite 1 Chromite Chromite Chromite Chromite



Goethite Hematite 2 Hematite 1 Olivine, Chromite

Chromite Magnetite 1 Chromite Chromite Chromite

28





Hyperspectral classification



Accuracy: 0.888



Gradient boosting machines: n_estimators=500, max_features=15

Accuracy: 0.892

