Mineral Identification And Characterization: An Integrated Approach For Hyperspectral Image Processing

R. Rialland (CEA)
R. Marion (CEA)
C. Soussen (L2S)
V. Carrère (LPGN)

Context:

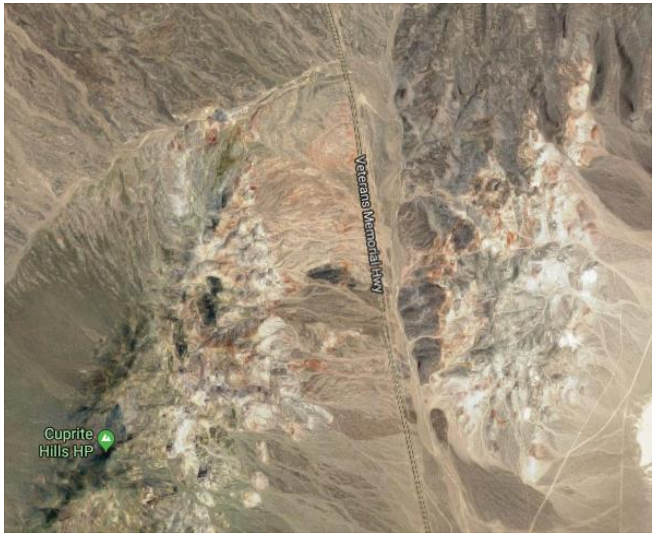
- Provide information on industrial activities conducted in a factory and on their impact on the surrounding environment
- Study mineralogy of areas of geological interest

Objectives:

- Identify, characterize and map minerals from a hyperspectral image

Constraints:

- Diversity of areas and minerals of interest
- Extraction of mineral information from reflectance spectra
- Limits from the database:
  - Spectra are acquired with several sensors (laboratory/airborne/space-borne)
  - Comparison with the spectra in the database



Cuprite (Nevada – USA)

Mountain Pass (California – USA)

OUTLINE

FROM MINERALOGY TO SPECTROSCOPY

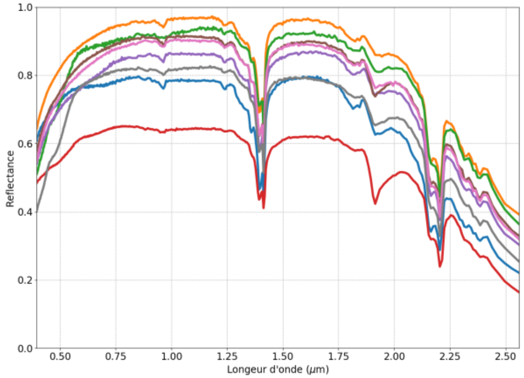
How is a mineral defined?

- Chemical composition
- Arrangement of the atoms (crystal lattice)
- Physico-chemical, mechanic and optical properties

Reflectance spectrum of a mineral:

- Spectral range: VNIR - SWIR [0.4 – 2.5] µm
- Continuum: humidity and surface roughness of the substrate (scattering)
- Absorptions: composition, concentration

⇒ It makes the identification and the characterization of the mineral possible



Kaolinite ($Al_2Si_2O_5(OH)_4$) and associated reflectance spectra

STATE OF THE ART[1] AND MAIN ISSUES

- <u>Supervised / knowledge-based</u> (band ratios, MGM procedure[4,5,6] , Tetracorder[3], etc.)

→ *A priori* knowledge
→ Mineral identification by metrics
→ Spectral mixtures

- <u>Supervised / data-driven</u> (PLSR, MTMF[2], etc.)

→ *A priori* knowledge
→ Mineralogical information exploitation

- <u>Learning-based</u> (ANN, Random Forest, etc.)

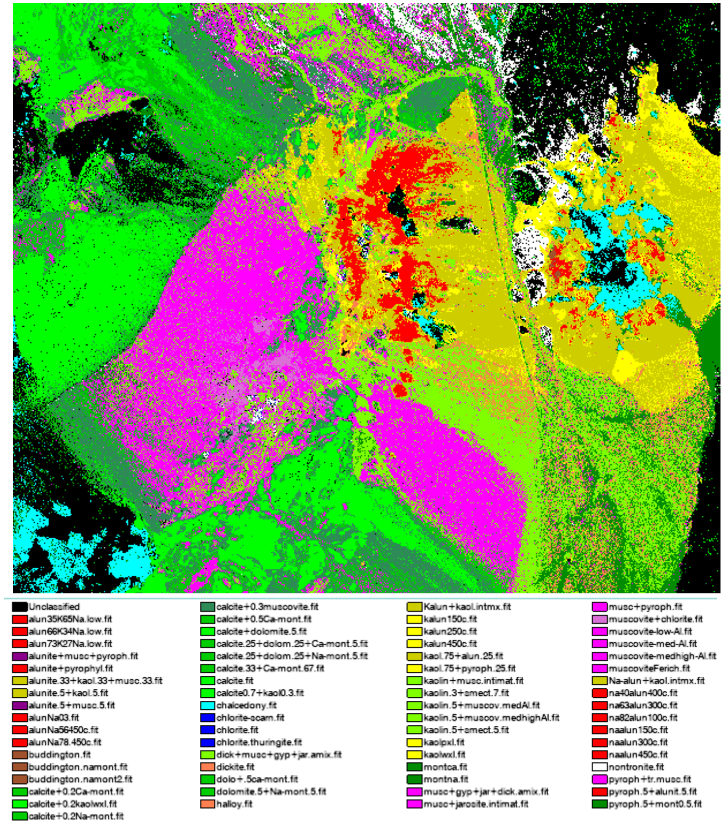
→ Several minerals study
→ Mineralogical information exploitation

- <u>Unsupervised</u> (Minimum wavelength mapper[7], k-means, etc.)

→ Mineralogical information exploitation
→ Database management

- <u>Unmixing</u> (linear mixing model, etc.)

→ Several minerals study
→ Spectral mixtures

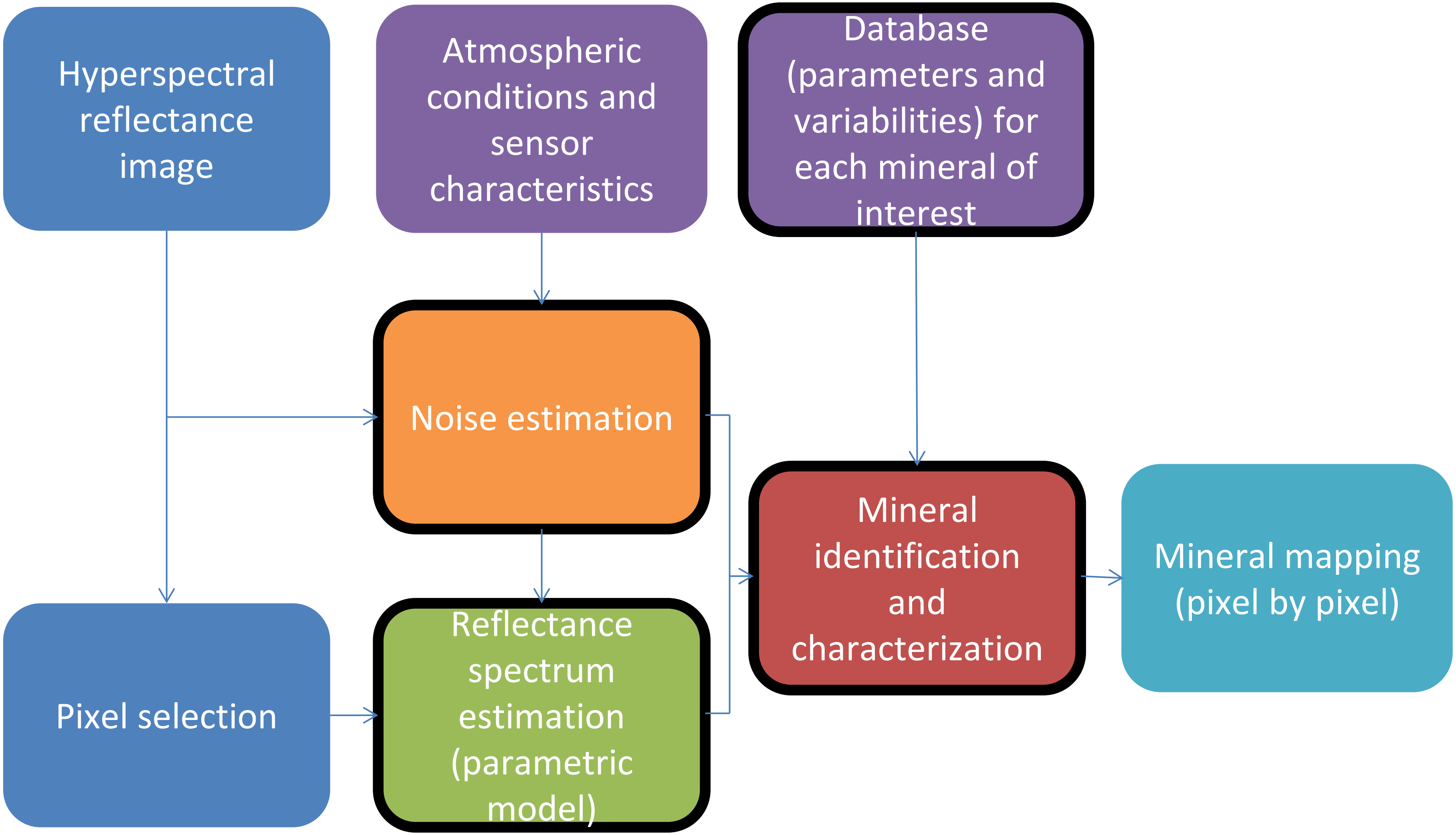


<u>Cuprite mineral map (Tetracorder) over the range [2.1 – 2.4] µm</u>

[1] Asadzadeh *et al.*, 2016
[2] Kruse *et al.*, 2003
[3] Swayze *et al.*, 2014
[4] Lothodé, 2016
[5] Brossard *et al.*, 2016
[6] Marion *et al.*, 2018
[7] Bakker *et al.*, 2011

⇒ We propose to modify the AGM procedure to automatically identify, characterize and map minerals without any prior knowledge

EVOLUTION OF THE AGM PROCEDURE



EGO MODEL[1,2] (EXPONENTIAL GAUSSIAN OPTIMIZATION)

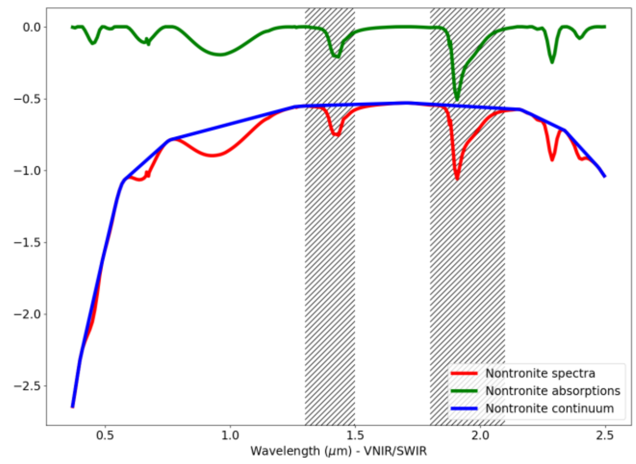
Objective:

- Parametric model (continuum and absorptions) for the logarithm of reflectance spectra

$$\ln \rho(\lambda) = C(\lambda) + \sum_{i}^{N} G_i(\lambda)$$

$$C(\lambda) = c_0 + c_1.\lambda^{-1} + G_{UV}(\lambda) + G_{EAU}(\lambda)$$

$$G_i(\lambda) = S_i.e^{-\frac{1}{2}\left(\frac{\lambda-\mu_i}{\sigma_i - k_i(\lambda-\mu_i)}\right)^2}$$



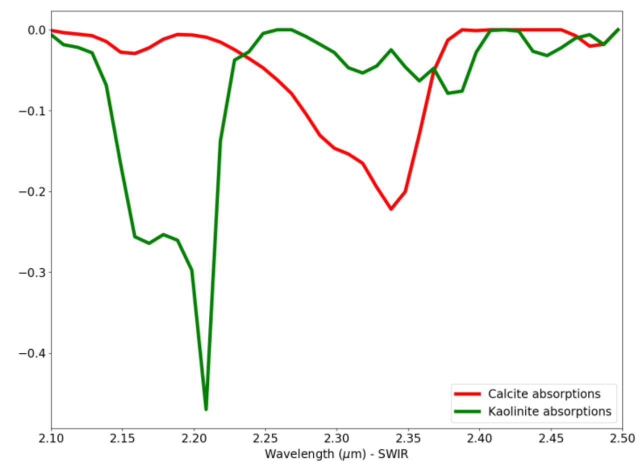
Nontronite spectrum from USGS with associated continuum and absorptions

Why is this model well adapted ?

- Absorptions shapes:
  - VNIR (wide and shallow), SWIR (narrow and deep)
  - Asymmetry (ex: calcite)

Estimation issues:

- Number of estimated Gaussians
- Gaussians asymmetries and absorptions doublets
- Joint estimation of continuum and absorptions



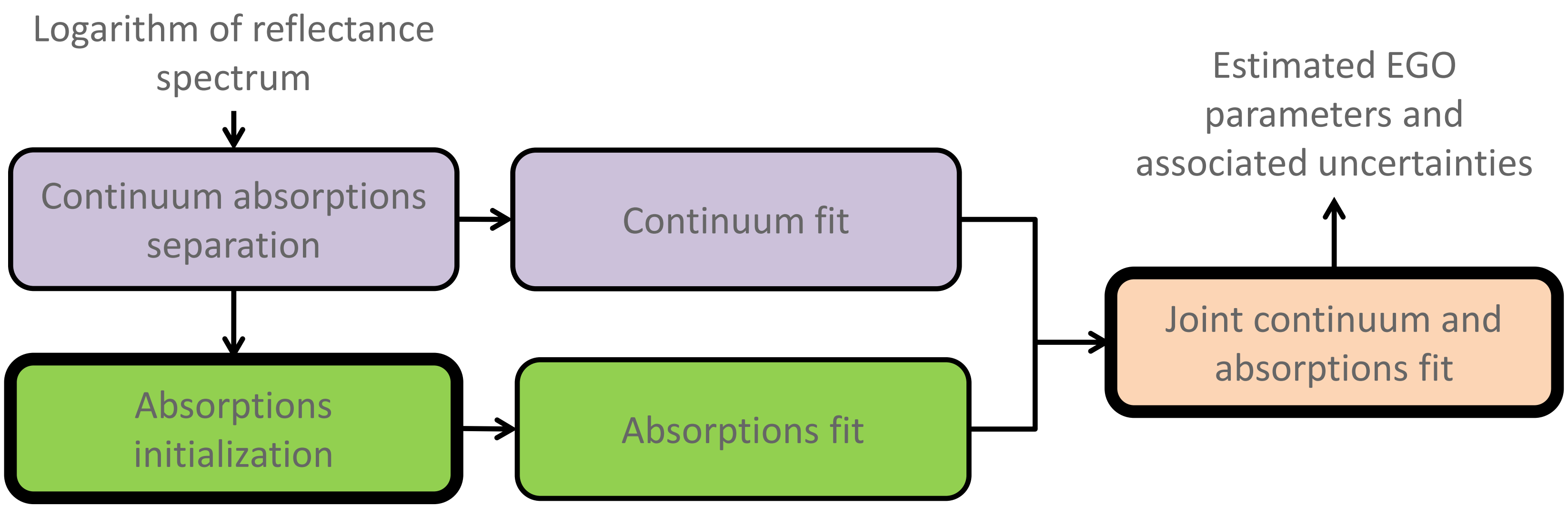
Calcite and kaolinite absorptions from USGS

[1] Pompilio *et al.*, 2009 [2] Pompilio *et al.*, 2010

Preprocessing:

- Image noise estimation and characterization: signal dependent model[1]
- Spectral mask (atmospheric water vapor)

Reflectance spectrum estimation procedure:



⇒ Continuum removal: Clark et Roush[2]
⇒ Absorptions initialization: NNOMP[3]
⇒ Continuum and absorptions fit: non-linear least squares
⇒ Joint continuum and absorptions fit: optimal estimation[4]

[1] Acito *et al.*, 2011
[2] Clark *et al.*, 1984
[3] Bruckstein *et al.*, 2008
[4] Tarantola, 2005

NNOMP[1,2] (NON-NEGATIVE ORTHOGONAL MATCHING PURSUIT)

$$\ln \rho(\lambda) = C(\lambda) + \sum_{i}^{N} G_i(\lambda)$$

$$G_i(\lambda) = S_i . e^{-\frac{1}{2}\left(\frac{\lambda-\mu_i}{\sigma_i - k_i(\lambda-\mu_i)}\right)^2}$$

Objectives:

- Estimate the number of Gaussians
- Initialize Gaussians parameters (depth, center, width)

Problem formulation:

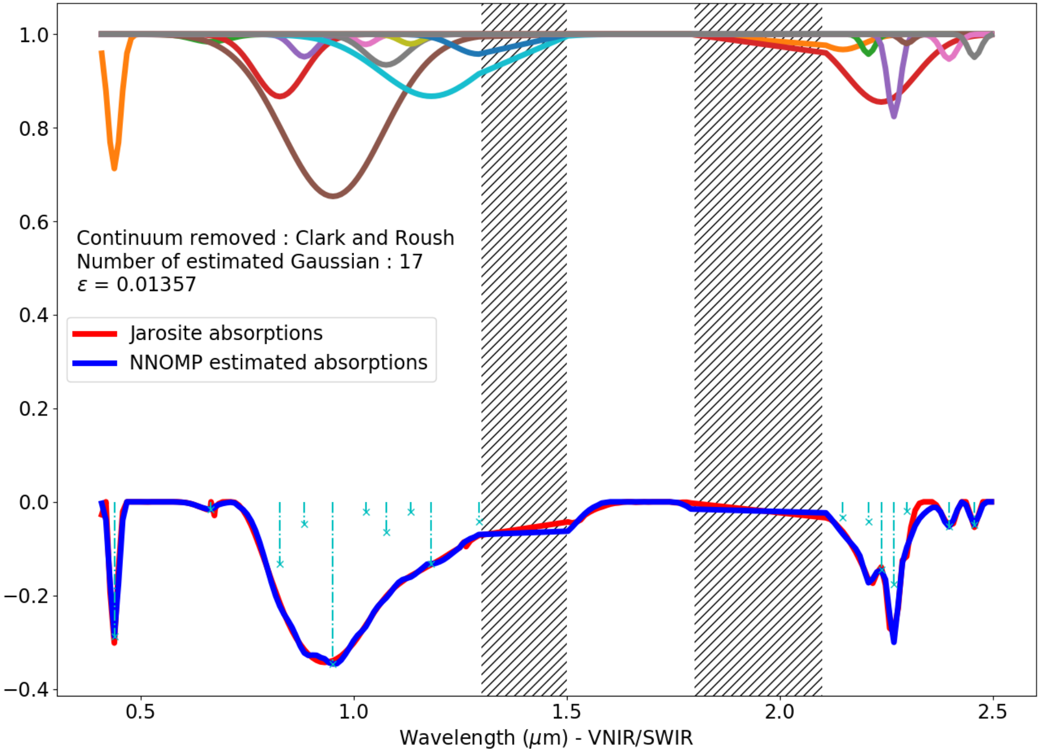
- Gaussians dictionary $\mathcal{H}$ (center and width discretization)
- Find $\boldsymbol{x}$ sparse minimizing the following problem:

$$\min_{x>0, \|x\|_0 \leq K} \|\log \rho - \mathcal{H}\mathbf{x}\|_2^2$$

Stopping criterions:

- Maximal number of Gaussians (K)
- MDLc (Minimum Description Length corrected) calculated for each added Gaussian (j):

$$\min_{j} \left\{ \log \epsilon(S_j) + \frac{\log(N_\lambda)\left(|S_j| + 1\right)}{N_\lambda - |S_j| - 2} \right\}$$



Jarosite absorptions from USGS spectral library and initialization with NNOMP

[1] Bruckstein *et al.*, 200 8 [2] Nguyen *et al.*, 2017

OPTIMAL ESTIMATION[1]

$$\ln \rho(\lambda) = C(\lambda) + \sum_{i}^{N} G_i(\lambda)$$

$$C(\lambda) = c_0 + c_1 . \lambda^{-1} + G_{UV}(\lambda) + G_{EAU}(\lambda)$$

$$G_i(\lambda) = S_i . e^{-\frac{1}{2}\left(\frac{\lambda - \mu_i}{\sigma_i - k_i(\lambda - \mu_i)}\right)^2}$$

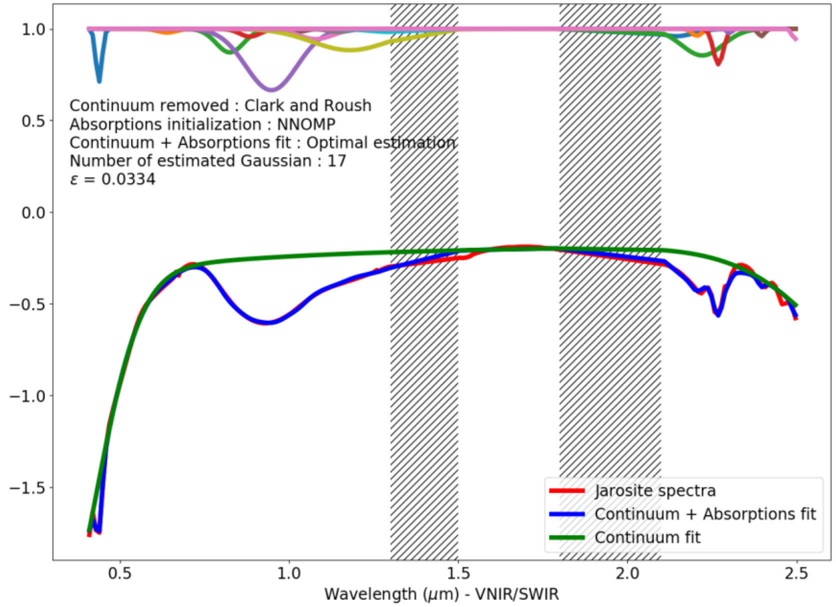
Objectives:

- Joint continuum and absorptions fit to the logarithm of the reflectance
- The number of Gaussians is fixed
- Estimate uncertainties

Problem formulation:

- Minimize a cost function which depends on a measurement error and a prior estimation on the parameters θ

$$\chi^2(\theta) = \frac{1}{2}(\theta - \theta_{init})^T S_a^{-1}(\theta - \theta_{init}) + \frac{1}{2}(\ln \rho(\lambda) - EGO(\lambda,\theta))^T S_\varepsilon^{-1}(\ln \rho(\lambda) - EGO(\lambda,\theta))$$



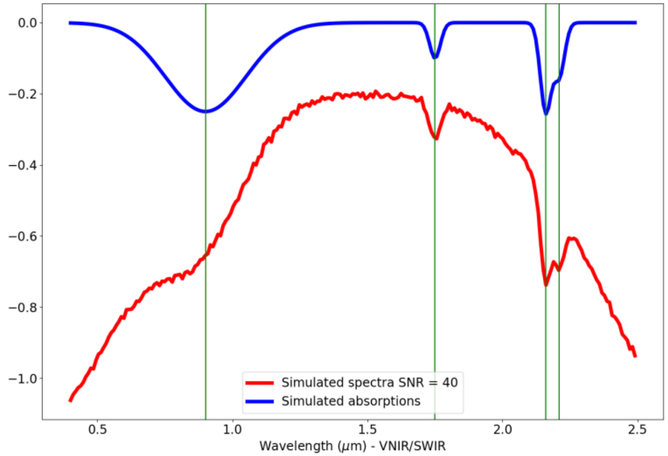
Jarosite spectrum from USGS spectral library and fit with optimal estimation

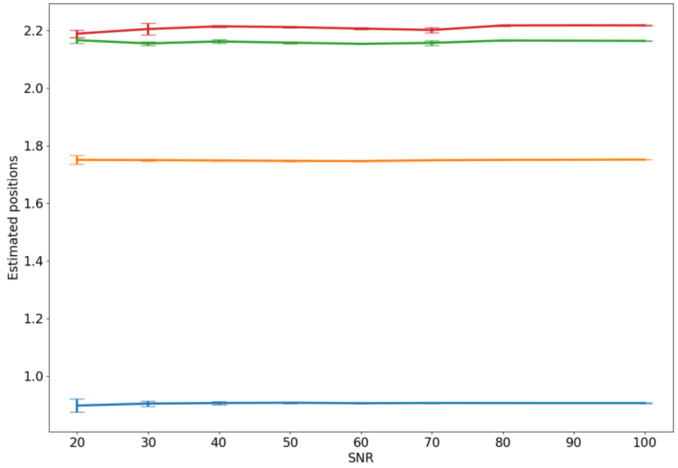
Results:

- Difficulties to estimate the asymmetry
- Uncertainties can be estimated for each EGO parameter

[1] Tarantola, 2005.

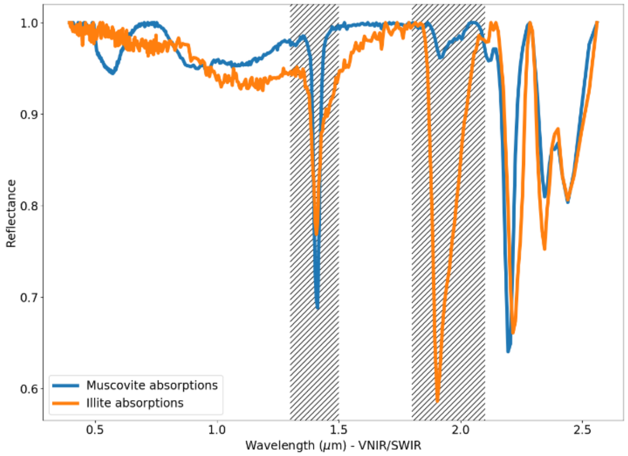
Validation with noise:





Simulated spectra with 4 absorptions and estimated positions with different SNR

Potential of using uncertainties for mineral identification and characterization:



Muscovite and illite spectra from USGS spectral library

- ⇒ Close absorptions (doublets) detection
- ⇒ Separation and identification of muscovite and illite using uncertainties on estimated positions

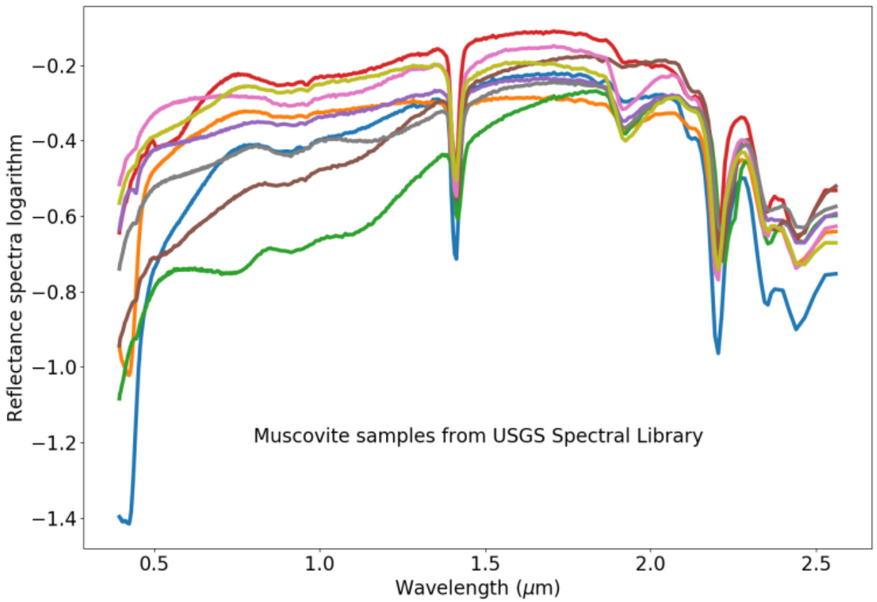
IDENTIFICATION PROCEDURE: DATABASE CREATION

Minerals of interest (~ 30 minerals):

- Clays (kaolinite, illite, montmorillonite, etc.)
- Carbonates (calcite, dolomite, etc.)
- Sulfates (alunite, jarosite, etc.)
- Rare earth elements (bastnaesite, monazite, etc.)
- Etc.

Database creation:

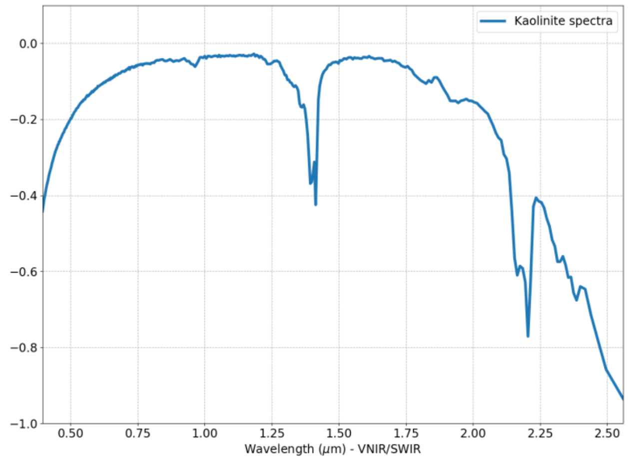
- Reflectance spectra database
- EGO parameters database (mean and standard deviation) for each mineral
- Same reflectance spectra estimation procedure



Diagnostic absorptions	Mean	Standard deviation
Absorption around 2.20µm	Center = 2.2066 Amplitude = - 0.3795 Width = 0.0214 Asymmetry = - 0.0908	Center = 0.0078 Amplitude = 0.0623 Width = 0.0027 Asymmetry = 0.0386
Absorption around 2.34µm	Center = 2.35071 Amplitude = - 0.1800 Width = 0.02837 Asymmetry = - 0.1525	Center = 0.0041 Amplitude = 0.0416 Width = 0.0042 Asymmetry = 0.0486
Absorption around 2.43µm	Center = 2.44962 Amplitude = - 0.15734 Width = 0.0388 Asymmetry = -0.03575	Center = 0.0044 Amplitude = 0.0334 Width = 0.0050 Asymmetry = 0.0878

Main idea:

- For each mineral of the database, create an expert rule based on the EGO parameters database



Kaolinite spectrum from USGS spectral library

Example of kaolinite:
⇒ diagnostics doublet AlOH absorptions (2.16 and 2.21 µm)
⇒ secondary absorptions (2.31, 2.35 and 2.38 µm)
⇒ absorption's depths

- Comparison between expert rule parameters (mean and standard deviation) and estimated parameters (estimation and uncertainties) => Gaussian distributions comparison
- A score is given for each expert rule

⇒ Adaptable solution for identification and characterization
⇒ Deal with spectral mixtures (not validated yet)

[1]Poli *et al.*, 2018

CONCLUSION AND FUTURE WORKS

Conclusions:

1) Automatic and modular procedure able to extract mineralogical information from reflectance spectra based on a physical model

2) Estimation procedure makes possible the physical interpretation of retrieved parameters

3) Mineral identification (and characterization) procedure using expert rules (expert system)

Future works:

1) Improvement and validation of the EGO model estimation procedure on simulated and real spectra

2) Application and validation of the identification/characterization procedure for spectral mixtures

3) Mineral characterization (abundance, grain size, humidity, etc.) and application on various study cases