Automatic Detection of Diagnostic Absorption Features for Mineral Identification Using Continuous Wavelet Transform

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What am I looking for?

About 10 minerals of interest presenting absorptions features in the solar domain (VNIR/SWIR)

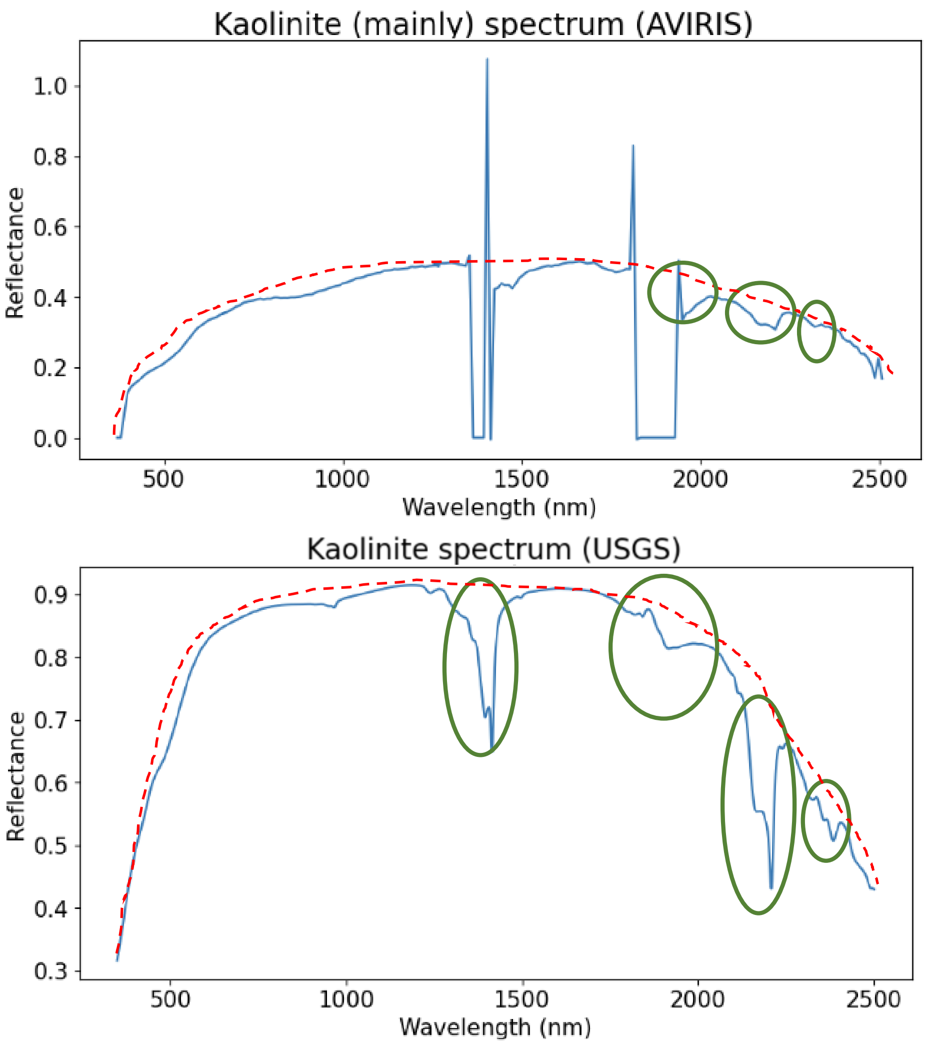
Type	Silicate Structure	Mineral Group	Example	VNIR	SWIR
Silicates	Inosilicates	Amphibole	Actinolite	Possible	Good
		Pyroxene	Diopside	Moderate	Moderate
	Cyclosilicates	Tourmaline	Elbaite	None	Good
	Nesosilicates	Garnet	Grossular	Possible	Possible
		Olivine	Forsterite	Possible	Possible
	Sorosilicates	Epidote	Epidote	None	Good
	Phyllosilicates	Mica	Muscovite	None	Clear
		Chlorite	Clinochlore	None	Good
		Clay Minerals	Illite	None	Good
			Kaolinite	None	Good
	Tectosilicates	Feldspar	Orthoclase	None	None
			Albite	None	None
		Silica	Quartz	None	Possible
Non-Silicates	Carbonates	Calcite	Calcite	None	Moderate
		Dolomite	Dolomite	None	Moderate
	Hydroxides		Gibbsite	None	Good
	Sulphates	Alunite	Alunite	Possible	Good
			Gypsum	None	Good
	Borates		Borax	None	Moderate
	Halides	Chlorides	Halite	Uncertain	Uncertain
	Phosphates	Apatite	Apatite	Possible	Possible
	Hydrocarbons		Bitumen	Possible	Moderate
	Oxides	Hematite	Hematite	Good	None
		Spinel	Chromite	None	None
	Sulphides		Pyrite	Possible	None

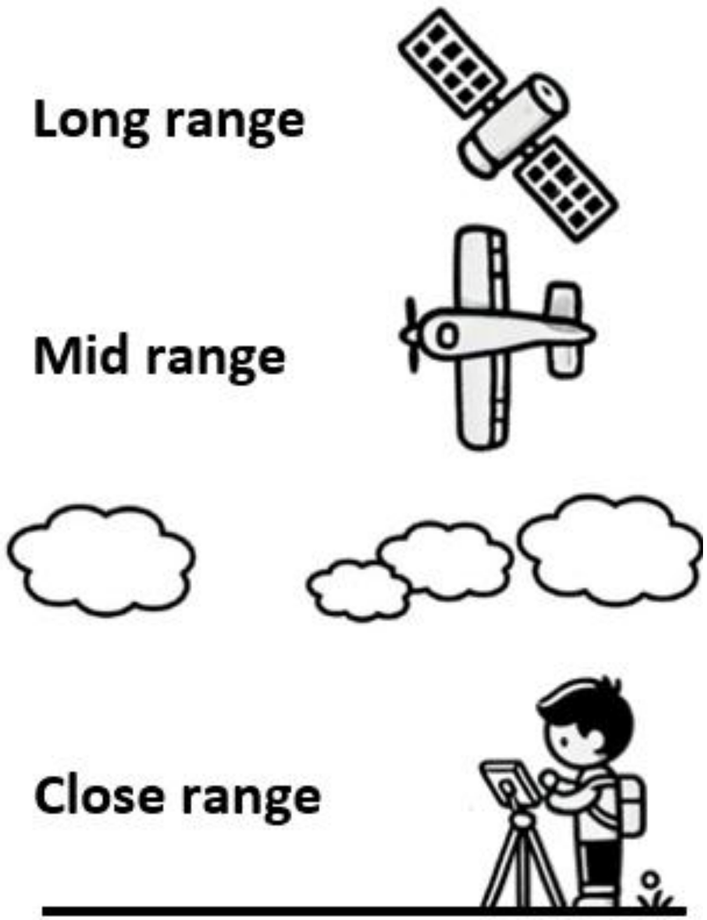
Clear	Most suitable region for mineral identification
Good	Good response but mixtures can influence mineral characterization
Moderate	Moderate but better mineral responses in other regions
Possible	Selective response possible but mineral identification difficult
None	Non-Diagnostic responses or no responsiveness of mineral in region
Uncertain	Available spectral data insufficient to assess identification potential

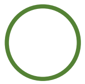
Source : Terracore

Spectroscopic data

Example of kaolinite







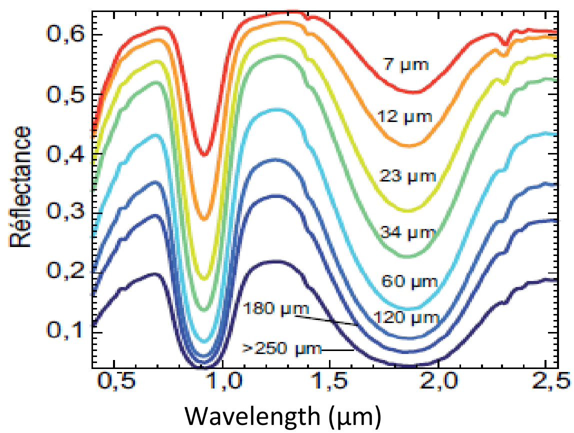
Absorption bands = Chemical effects

Continuum = Physical effects

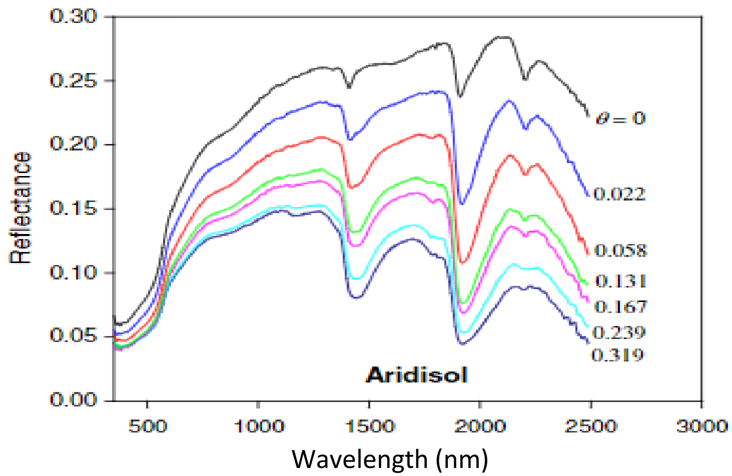
Factors affecting reflectance spectra

- **Acquisition chain:** camera calibration, acquisition geometry …
- **Environmental conditions:** illumination (direct/diffuse), adjacency effects …
- **Physical properties:** grain size and shape, porosity, surface roughness (shadows) …
- **Chemical properties :** mineralogical composition, water, organic matter, pollutant …

Average grain size [1]



Water content [2]

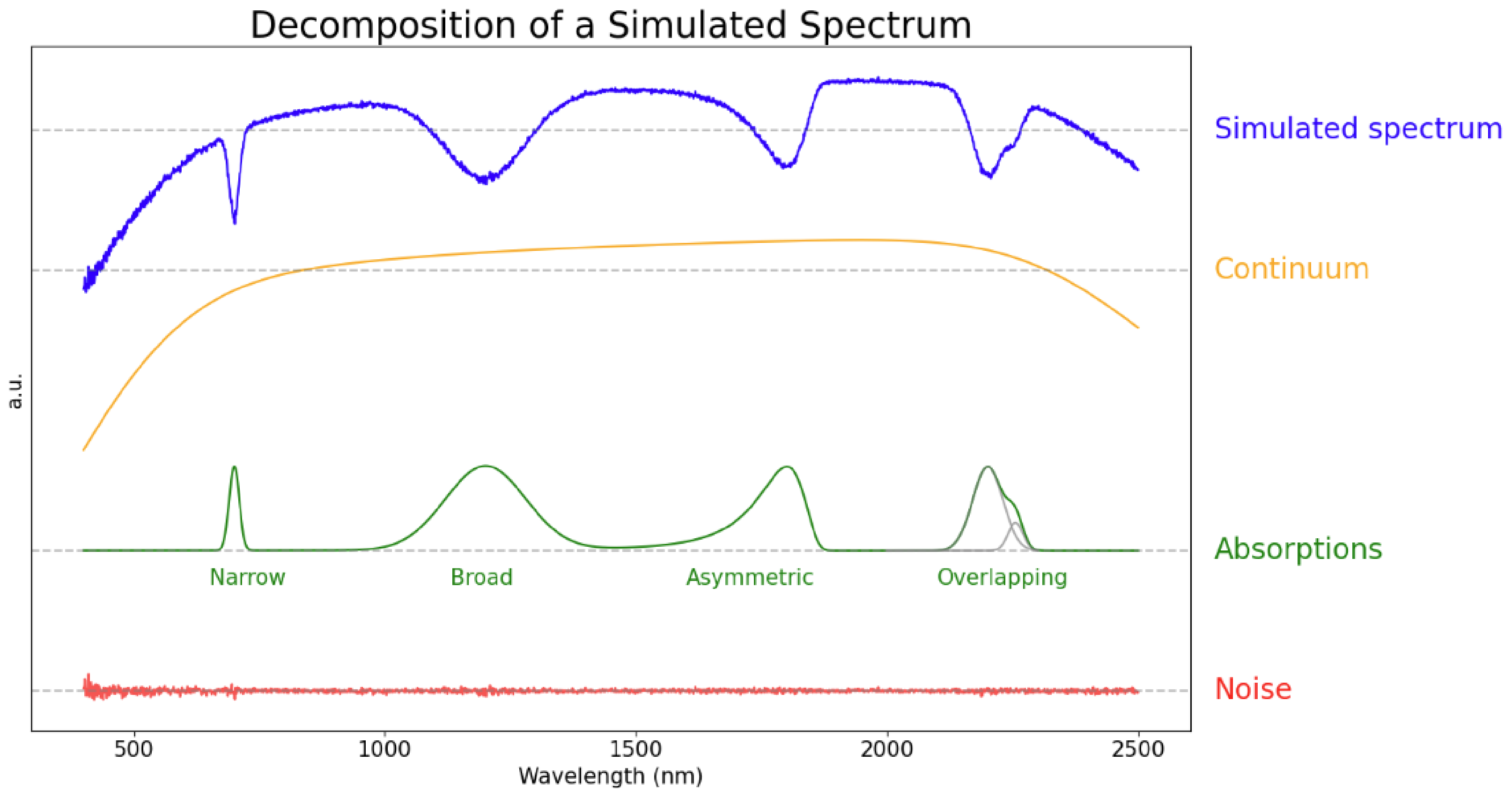


[1] Verpoorter (2009)
[2] Sadeghi et al. (2015)

Spectral deconvolution

Objectives: reduce data dimensionality, minimize the impact of noise, mitigate correlations between parameters, and improve parameter interpretability.

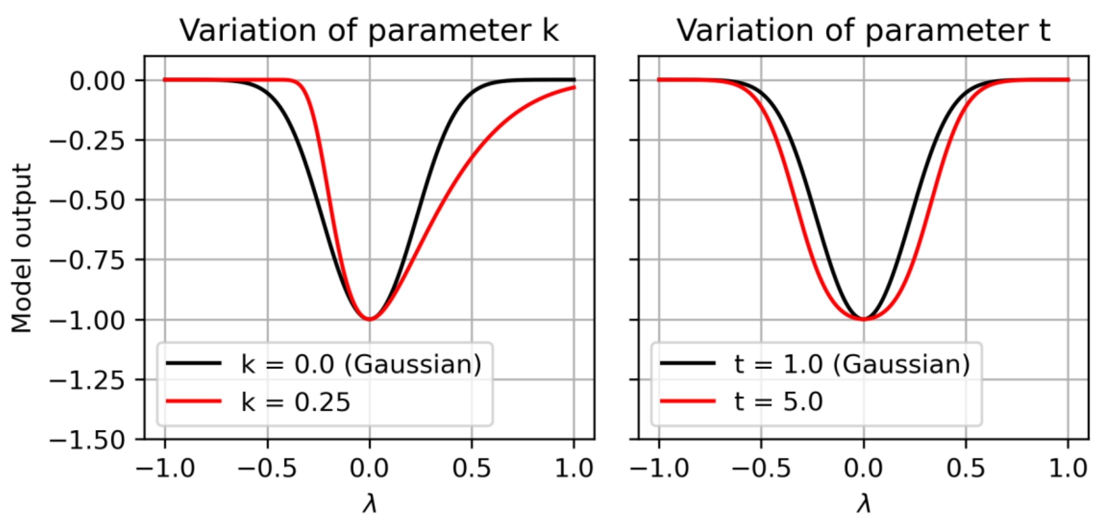
Logarithm of the reflectance spectrum $$\ln \rho(\lambda, \theta) = c(\lambda, \theta_c) - \sum_{i=1}^{N} G(\lambda, \theta_{G_i}) + n(\lambda)$$



Absorption model: EGO (Exponential Gaussian Optimization) [3]

$$G(\lambda, \theta_G) = -\frac{s}{1 - e^{-\frac{1}{2}t}} \left[1 - e^{-\frac{1}{2}\left(t e^{-\frac{1}{2}\left(\frac{\lambda - \mu}{\sigma\left(1 + \tanh\left(\frac{k}{\sigma}(\lambda - \mu)\right)\right)} \right)^2} \right)} \right]$$

5 parameters:
- Amplitude s
- Position μ
- Width σ
- Asymmetry k
- Flatness t

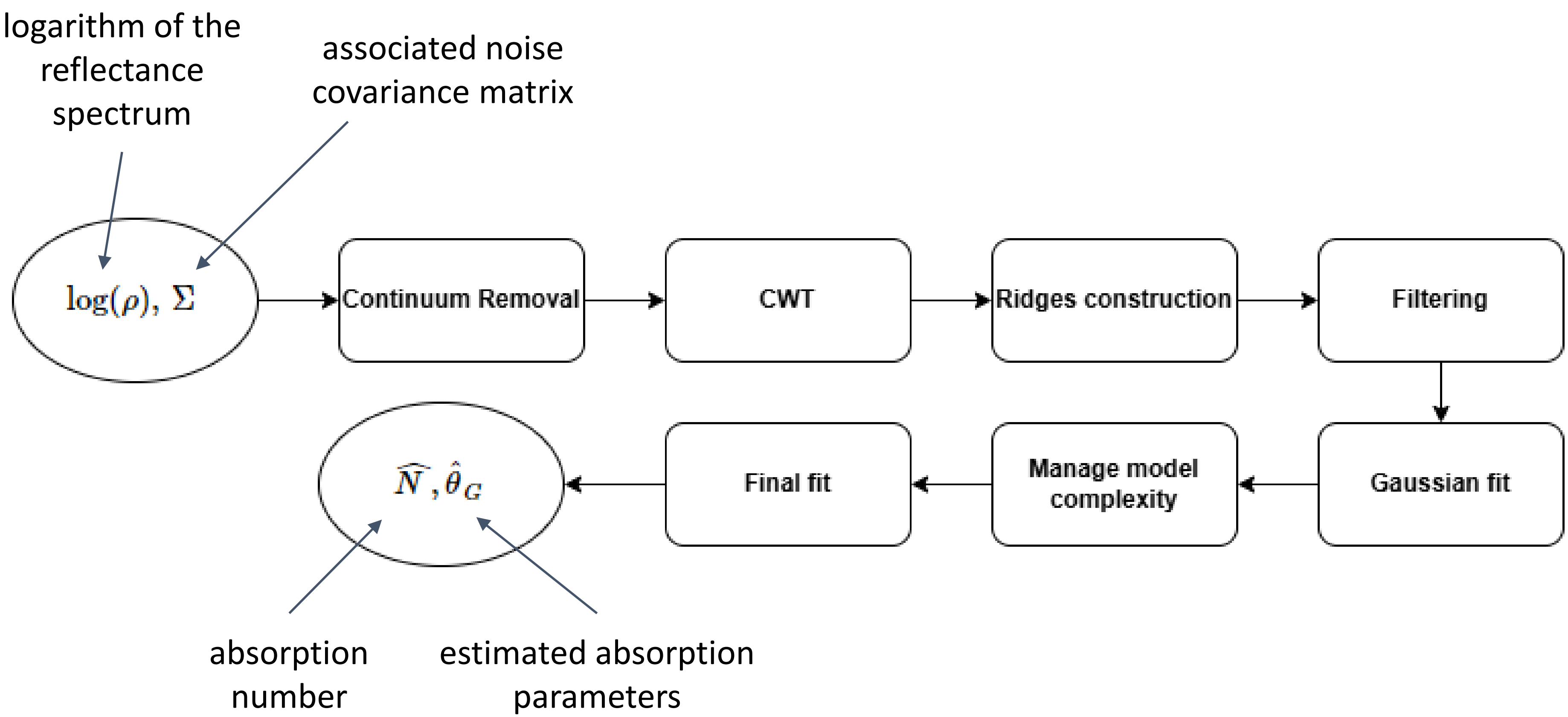


~1000 wavelengths → A few dozen parameters

8 + 5N parameters
(8 for the continuum, 5N for the absorptions)

[3] Pompilio et al. (2009)

EGO Fitting Procedure



Wavelet transform

2D matrix of wavelet coefficients

$$C(a, b) = \int_R f(t) w_{a,b}(t) \mathrm{d}t$$

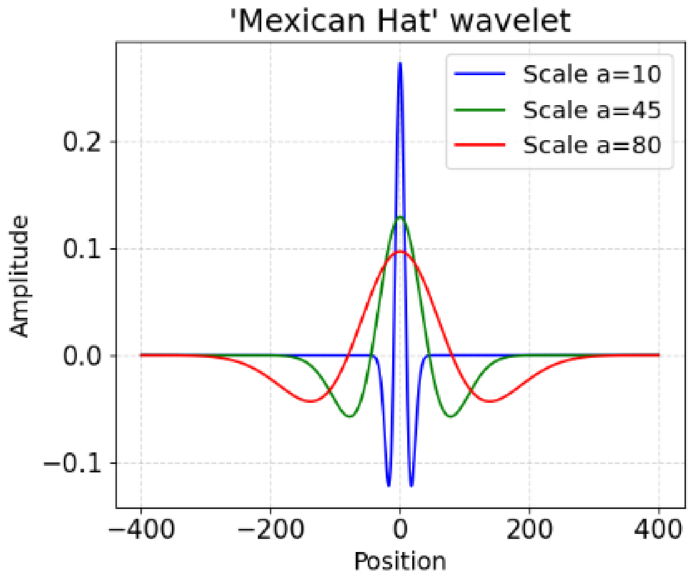
Scaled and translated wavelet

$$w_{a,b}(t) = \frac{1}{\sqrt{a}} w\left(\frac{t-b}{a}\right), \quad a \in R^+ - \{0\},\ b \in R$$

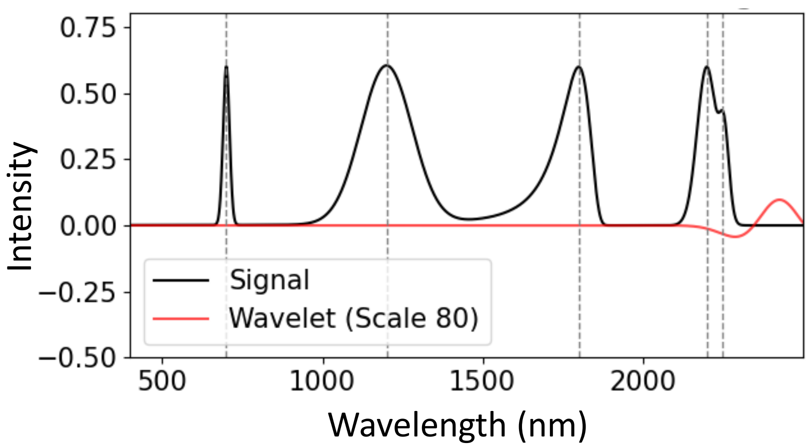
Mother wavelet: Mexican Hat

$$\varphi(x) = \frac{2}{\sqrt{3}} \left(\frac{1}{\pi}\right)^{\frac{1}{4}} (1 - x^2) e^{-\frac{x^2}{2}}$$

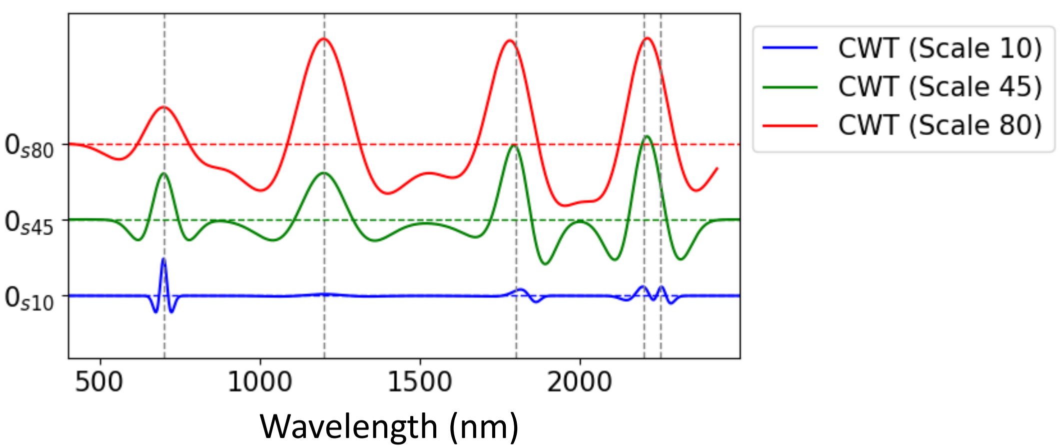
f(t): signal; a: scale factor; b: translation; w(t): mother wavelet



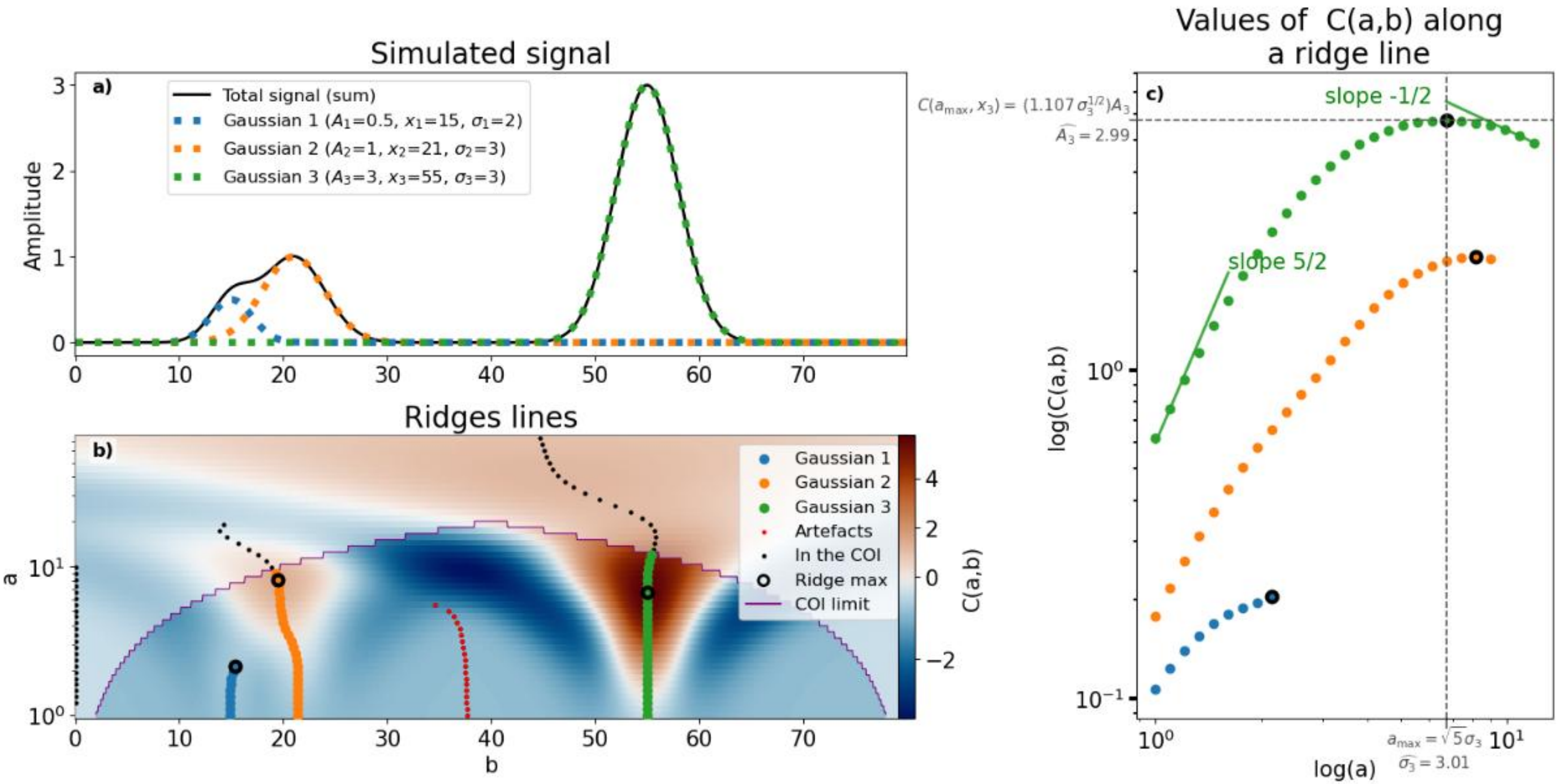
Convolution of the wavelet and the signal



Wavelet coefficients

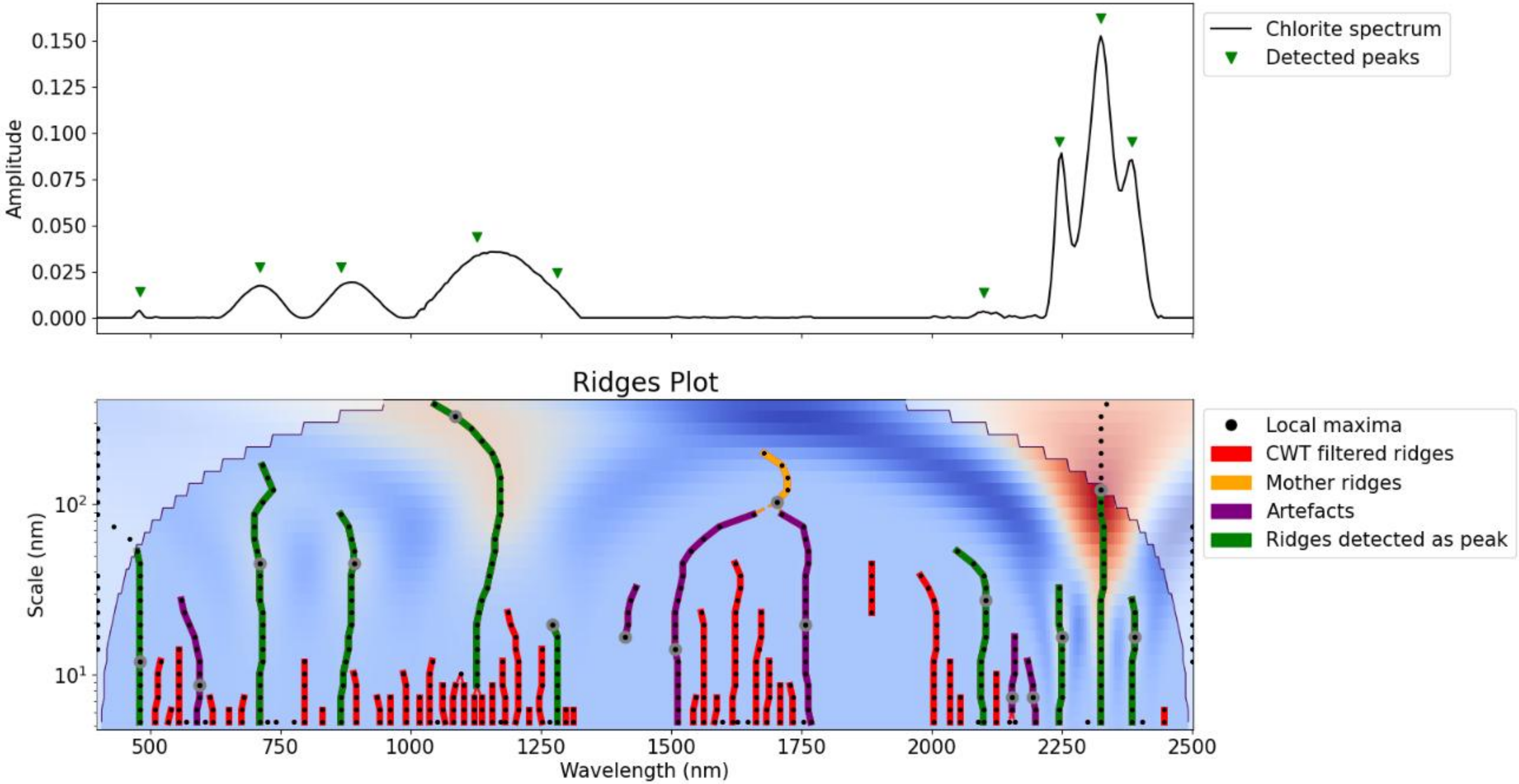


Ridge detection



Filtering

- in wavelet space
- with ridge geometry
- in signal space

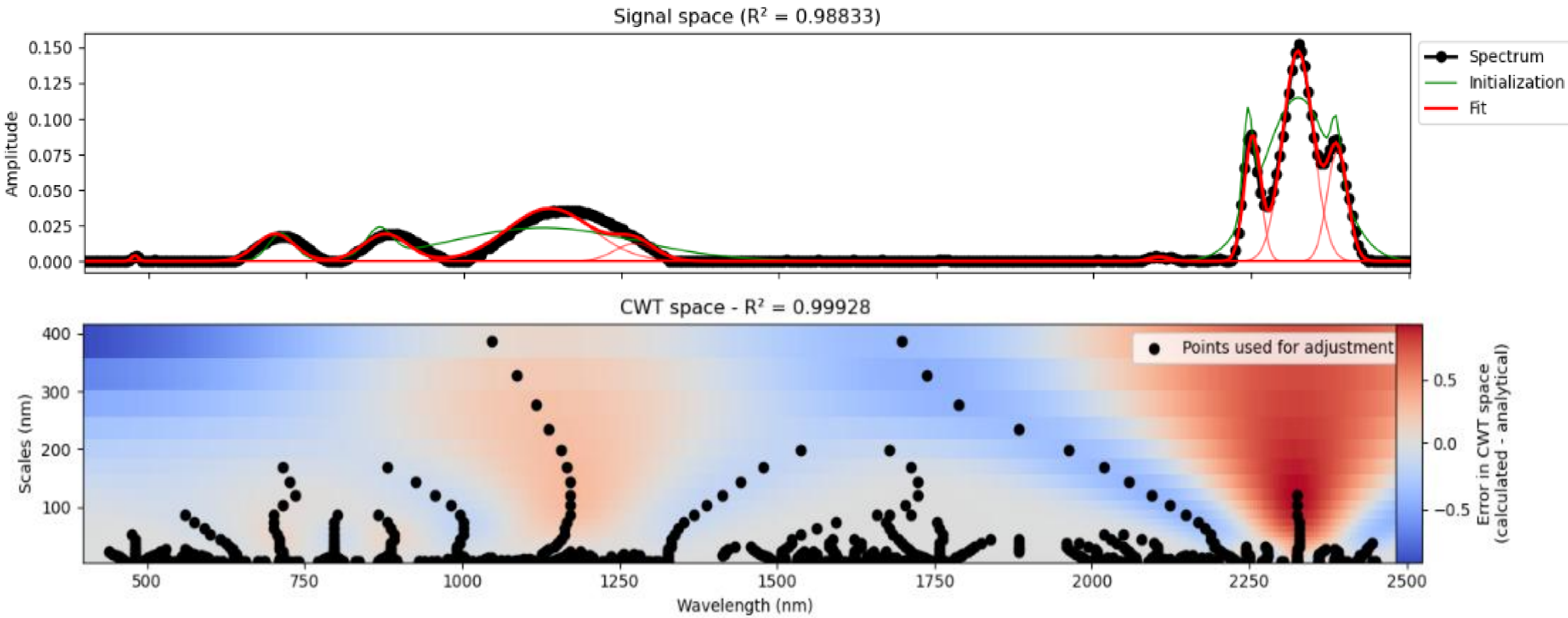


Gaussian fit

Analytical equation of the wavelet transform of a sum of gaussians:

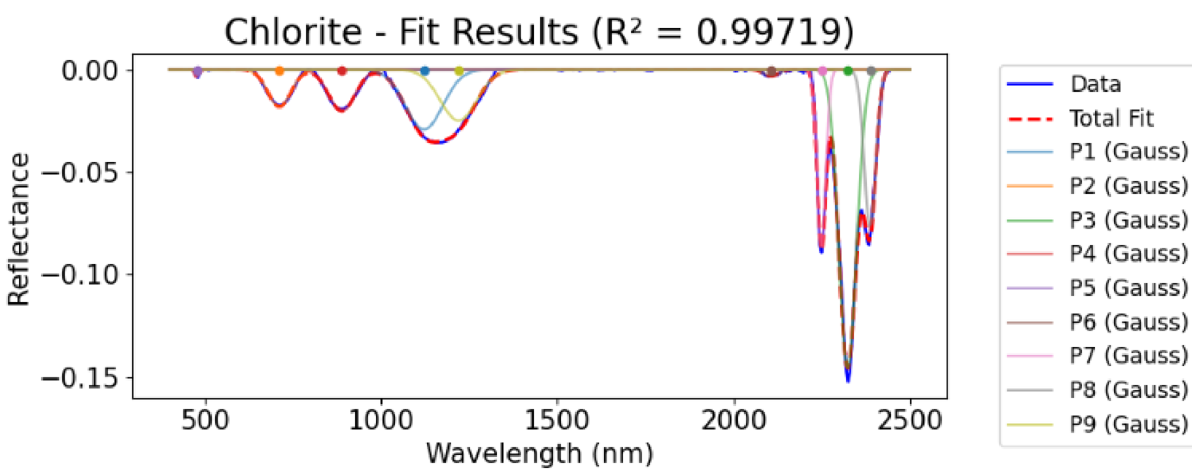
$$C(a,b) = \frac{2\sqrt{2}}{\sqrt{3}}\pi^{\frac{1}{4}}a^{5/2}\sum_{i=1}^{N} A_i \frac{\sigma_i}{(\sigma_i^2 + a^2)^{3/2}}\left[1 - \frac{\Delta_i^2}{\sigma_i^2 + a^2}\right]e^{\left(-\frac{\Delta_i^2}{2(\sigma_i^2+a^2)}\right)}, \quad \Delta_i = b - x_i$$

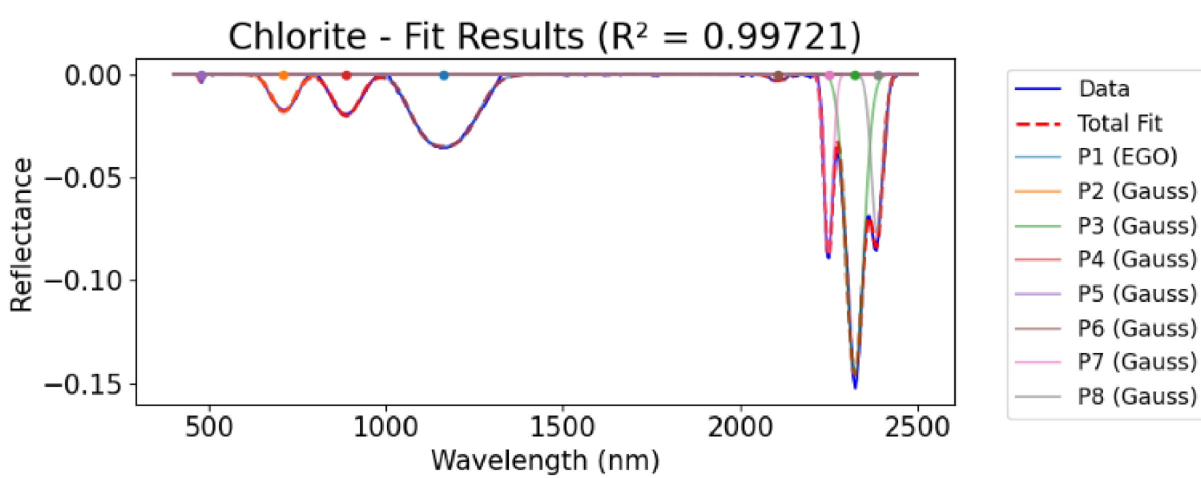
N : gaussian number
a : cwt scale
b : cwt position
σ : gaussian width
x : gaussian position
A : gaussian amplitude



Manage model complexity

Can peaks be merged ?
Is it necessary to add a skewness or flattening parameter to the peak?



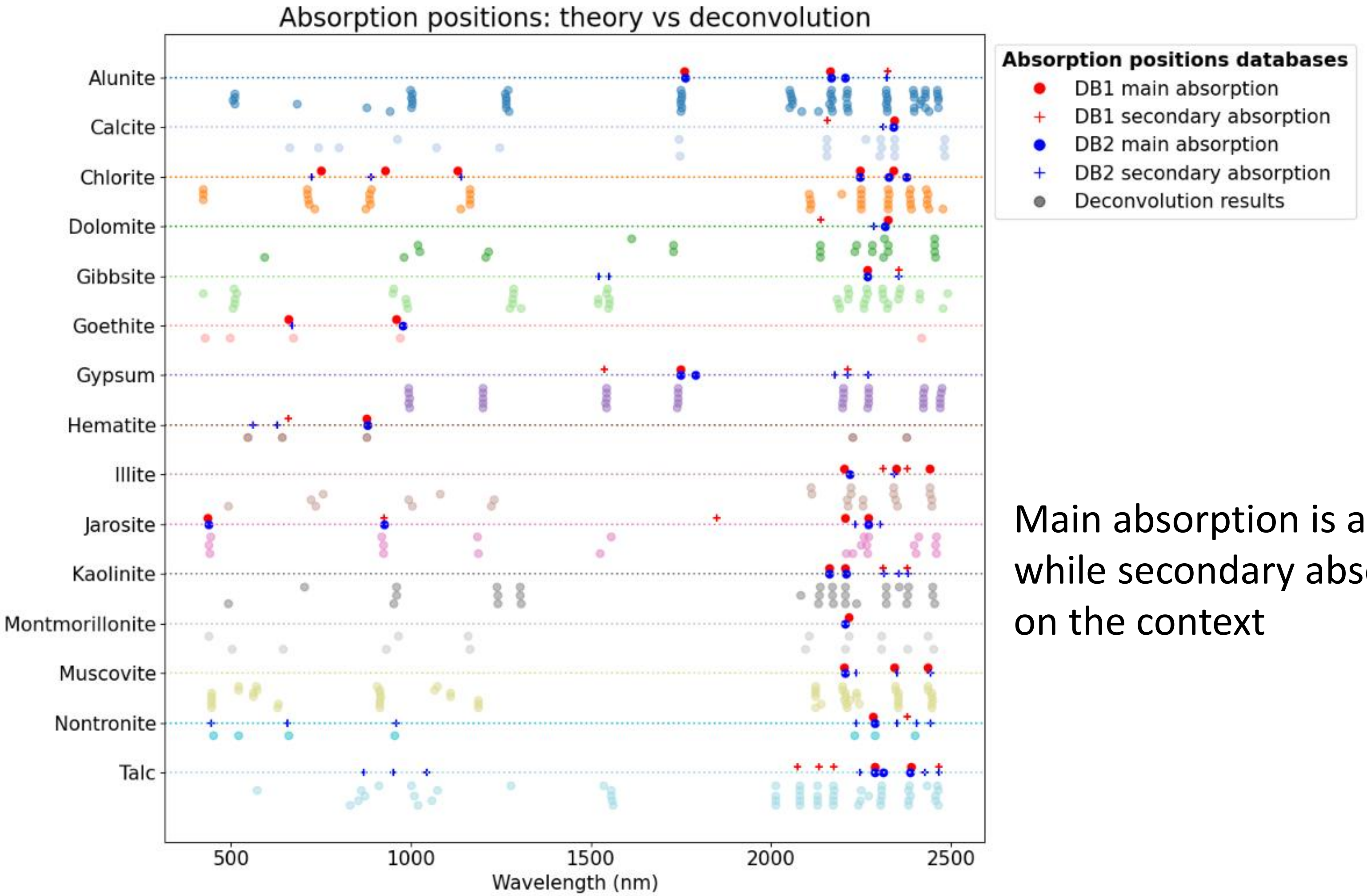


AIC comparison on local model:

2 Gaussian vs 1 EGO model
→ select EGO model if $\Delta_{AIC} > 3$

Mineral Classification

Fuzzy logic provides an interpretable decision inspired by the expertise of spectroscopists



Main absorption is always present, while secondary absorption depends on the context

Conclusions and perspectives

Conclusions:

- Algorithm applicable to different types of data
- Noise taken into account
- Fast (~1s per spectrum)
- Overlaps handled effectively

Perspectives:

- Minerals classification using fuzzy logic
- Understanding and quantifying the impact of moisture content on model parameters (detection limits)
- Developing robust models for mineral quantification that account for these effects

Bibliography

[1] Verpoorter, C. (2009). *Télédétection hyperspectrale et cartographie des faciès sédimentaires en zone intertidale: application à la Baie de Bourgneuf* (Doctoral dissertation, Université de Nantes).

[2] Sadeghi, M., Jones, S. B., & Philpot, W. D. (2015). A linear physically-based model for remote sensing of soil moisture using short wave infrared bands. *Remote Sensing of Environment*, *164*, 66-76.

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[4] Rialland, R. (2021). Télédétection hyperspectrale pour l'identification et la caractérisation de minéraux industriels (Doctoral dissertation, Université Paris-Saclay).