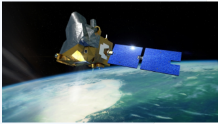
Estimating Spectral Responses of Spectrometers by solving a Nonlinear Inverse Problem



Jihanne EL HAOUARI, *University of Toulouse, TéSA*
Jean-Yves TOURNERET, *University of Toulouse, TéSA*
Herwig WENDT, *University of Toulouse, CNRS*
Christelle PITTET, *CNES*
Jean-Michel GAUCEL, *Thales Alenia Space*

May 15th, 2024

1. Introduction

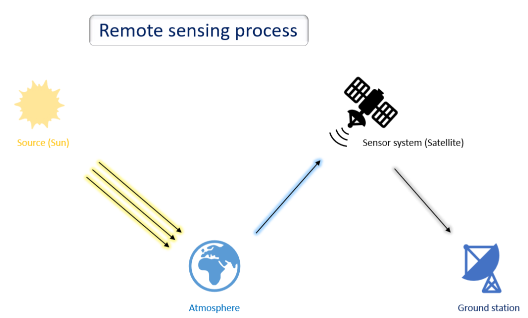
Context

- Climate change challenges
- Need to accurately determine the CO_2 concentrations at the Earth surface
- MicroCarb mission

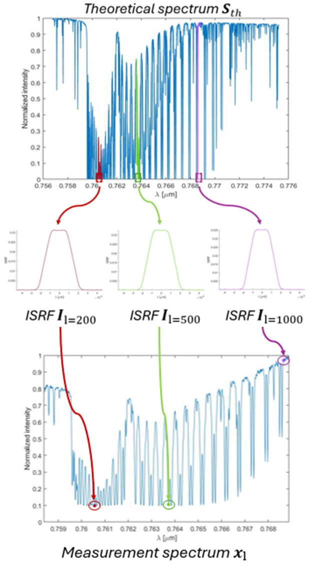
1. Introduction

Context

- Remote sensing to determine the concentration of CO_2 from the measured spectra
- Calibration process: accurate estimates of the Instrument Spectral Response Functions (ISRFs)



1. Introduction



Estimation of the ISRFs
An ill-posed problem

For each wavelength λ_ℓ

- 1 observation $x_\ell \in \mathbb{R}^+$
- 1 ISRF $\boldsymbol{I}_\ell \in \mathbb{R}^{N+1}$
- 1 nonlinear function f_ℓ

$$x_\ell = f_\ell(< \boldsymbol{s}_{th,\ell}, \boldsymbol{I}_\ell >) \qquad (1)$$

$\boldsymbol{s}_{th,\ell}$ known

$\boldsymbol{I}_\ell$ unknown

f_ℓ unknown

2. ISRF estimation without radiometric errors

Forward model

$$x_\ell = f_\ell(< \boldsymbol{s}_{th,\ell}, \boldsymbol{I}_\ell >)$$

f_ℓ - unknown radiometric errors (see later)

x_ℓ measurements

$\boldsymbol{s}_{th,\ell}$ known

$\boldsymbol{I}_\ell$ unknown

2. ISRF estimation without radiometric errors

Forward model

$$s_\ell = < \boldsymbol{s}_{th,\ell}, \boldsymbol{I}_\ell >$$

s_ℓ measurements

$\boldsymbol{s}_{th,\ell}$ known

$\boldsymbol{I}_\ell$ unknown

2. ISRF estimation without radiometric errors

Assumption: ISRFs $\boldsymbol{I}_\ell$ vary little from ℓ to $\ell+1$

Use of sliding window of $L+1$ measurements around λ_ℓ

- $\boldsymbol{S}_{th,\ell} = [\boldsymbol{s}_{th,\ell-\frac{L}{2}}, \ldots, \boldsymbol{s}_{th,\ell+\frac{L}{2}}] \in \mathbb{R}^{(L+1)\times(N+1)}$
- $\boldsymbol{s}_\ell = [s_{\ell-\frac{L}{2}}, \ldots, s_{\ell+\frac{L}{2}}] \in \mathbb{R}^{L+1}$

Observation model (matrix form)

$$\boldsymbol{s}_\ell = \boldsymbol{S}_{th,\ell}\boldsymbol{I}_\ell$$

Assumptions on ISRFs $\boldsymbol{I}_\ell$:

- Smooth
- Positive valued

2. ISRF estimation without radiometric errors

Gaussian model [Beirle2017]

$$\boldsymbol{I}_{\ell,\beta_{\mathrm{G}}}(x) = A_{\mathrm{G}}\ \exp\left(-\frac{(\lambda_\ell - x - \mu_{\mathrm{G}})^2}{2\sigma_{\mathrm{G}}^2}\right), \quad x \in \boldsymbol{\Delta} \qquad (2)$$

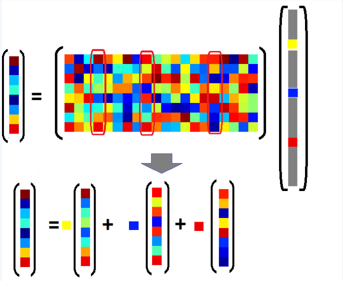
$\boldsymbol{\Delta}$ wavelength grid, $\beta_{\mathrm{G}} = (A_{\mathrm{G}}, \mu_{\mathrm{G}}, \sigma_{\mathrm{G}}^2)^T$ -parameters

Super-Gaussian model [Beirle2017]

$$\boldsymbol{I}_{\ell,\beta_{\mathrm{SG}}}(x) = A_{\mathrm{SG}}\ \exp\left(-\left|\frac{\lambda_\ell - x - \mu_{\mathrm{SG}}}{w_{\mathrm{SG}}}\right|^{k_{\mathrm{SG}}}\right), \quad x \in \boldsymbol{\Delta} \qquad (3)$$

$\beta_{\mathrm{SG}} = (A_{\mathrm{SG}}, \mu_{\mathrm{SG}}, w_{\mathrm{SG}}, k_{\mathrm{SG}})^T$-parameters

2. ISRF estimation without radiometric errors



Sparse representation of ISRFs

- Dictionary $\mathbf{\Phi} \in \mathbb{R}^{(N+1)\times N_D}$ (SVD of representative ISRFs)

$$\boldsymbol{I}_\ell \approx \boldsymbol{I}_\ell^K = \mathbf{\Phi}\boldsymbol{\alpha}_\ell = \sum_{k=1}^{K} \alpha_k \mathbf{\Phi}_{\gamma_k} \qquad (4)$$

$$\boldsymbol{s}_\ell \approx \boldsymbol{S}_{th,\ell}\boldsymbol{I}_\ell^K = \mathbf{\Psi}_\ell\boldsymbol{\alpha}_\ell \qquad (5)$$

where $\mathbf{\Psi}_\ell = \boldsymbol{S}_{th,\ell}\mathbf{\Phi}_\ell \in \mathbb{R}^{(L+1)\times N_D}$

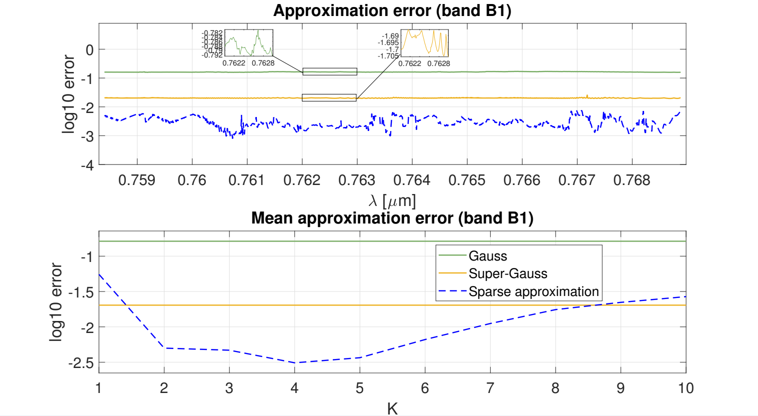
Optimization problem

$$\arg\min_{\boldsymbol{\alpha}_\ell} L(\boldsymbol{\alpha}_\ell, \mu) = \arg\min_{\boldsymbol{\alpha}_\ell} ||\boldsymbol{s}_\ell - \mathbf{\Psi}_\ell\boldsymbol{\alpha}_\ell||_2^2 + \mu||\boldsymbol{\alpha}_\ell||_0 \qquad (6)$$

Solved using Orthogonal Matching Pursuit (OMP)

2. ISRF estimation without radiometric errors

Numerical results

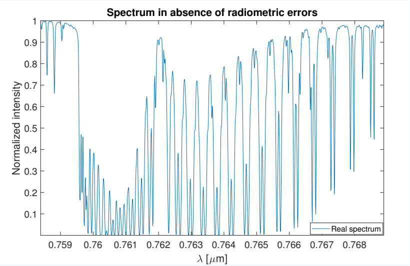


Competitive performance of sparse approximation

3. Nonlinear inverse problem

Forward model

$$\boldsymbol{s}_\ell = \boldsymbol{S}_{th,\ell}\boldsymbol{l}_\ell \quad (7)$$



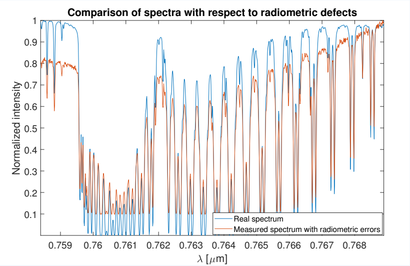
3. Nonlinear inverse problem

Forward model

$$\boldsymbol{x}_\ell = f_\ell(\boldsymbol{s}_\ell) = f_l(\boldsymbol{S}_{th,\ell}\boldsymbol{I}_\ell) \tag{7}$$

$$= g_\ell(\boldsymbol{S}_{th,\ell}\boldsymbol{I}_\ell; \boldsymbol{\theta}_\ell) \tag{8}$$

$\boldsymbol{\theta}_\ell$ - a parameter vector



Radiometric errors (function f_ℓ)

- 1 function per pixel ℓ
- Physical phenomena modeled
  - Linear gains
  - Dark current
  - Non-linear gains

3. Nonlinear inverse problem

Problem in presence of radiometric errors

1. $f_\ell = g_\ell(\cdot; \boldsymbol{\theta}_\ell)$ only depends on the pixel ℓ, not on the spectrum
2. $g_\ell(\cdot; \boldsymbol{\theta}_\ell)$ is differentiable
3. Use of Q theoretical spectra
4. $\boldsymbol{x}_\ell^{(q)} \in \mathbb{R}^{L+1}$, $q = 1, ..., Q$

$$\text{Find } (\hat{\boldsymbol{\theta}}_\ell, \hat{\boldsymbol{I}}_\ell) = \arg\min_{\boldsymbol{\theta}_\ell, \boldsymbol{I}_\ell} ||\boldsymbol{x}_\ell - g_\ell(\boldsymbol{S}_{th,\ell} \boldsymbol{I}_\ell; \boldsymbol{\theta}_\ell)||_2^2$$

$\boldsymbol{S}_{th,\ell}$ known

$\boldsymbol{x}_\ell$ - measurements

3. Nonlinear inverse problem

Optimization problem

$$(\hat{\boldsymbol{I}}_\ell, \hat{\boldsymbol{\theta}}_\ell) = \arg \min_{(\boldsymbol{I}_\ell, \boldsymbol{\theta}_\ell)} \sum_{q=1}^{Q} ||\boldsymbol{x}_\ell^{(q)} - g_\ell(\boldsymbol{S}_{th,\ell} \boldsymbol{I}_\ell; \boldsymbol{\theta}_\ell)||^2 \tag{9}$$

Use of sparse representation to model $\boldsymbol{I}_\ell$

3. Nonlinear inverse problem

Notations for the Q theoretical spectra

- $\boldsymbol{x}_\ell = [\boldsymbol{x}_\ell^{(1)}, \ldots, \boldsymbol{x}_\ell^{(Q)}] \in \mathbb{R}^{Q(L+1)}$
- $\boldsymbol{s}_\ell = [\boldsymbol{s}_\ell^{(1)}, \ldots, \boldsymbol{s}_\ell^{(Q)}] \in \mathbb{R}^{Q(L+1)}$
- $\boldsymbol{\Psi}_\ell = [\boldsymbol{\Psi}_\ell^{(1)}, \ldots, \boldsymbol{\Psi}_\ell^{(Q)}] \in \mathbb{R}^{Q(L+1)\times(N_\mathrm{D}+1)}$

3. Nonlinear inverse problem

Iterative estimation method

- Initial ISRF estimation
  - g_ℓ = identity
  - $\hat{\boldsymbol{s}}_\ell = \boldsymbol{\Psi}_\ell \hat{\boldsymbol{\alpha}}_\ell$ (OMP)
- Step 1: Estimation of radiometric errors
  - $\hat{\boldsymbol{\theta}}_\ell = \arg\min_{\boldsymbol{\theta}_\ell} ||\boldsymbol{x}_\ell - g_\ell(\boldsymbol{\Psi}_\ell \hat{\boldsymbol{\alpha}}_\ell; \boldsymbol{\theta}_\ell)||_2^2$
- Step 2: Correction of radiometric errors
  - $\hat{\boldsymbol{s}}_\ell = \arg\min_{\boldsymbol{s}_\ell} ||\boldsymbol{x}_\ell - g_\ell(\boldsymbol{s}_\ell; \hat{\boldsymbol{\theta}}_\ell)||_2^2$
- Step 3: Re-estimation of $\hat{\boldsymbol{\alpha}}_\ell$ from corrected measurements
  - $\hat{\boldsymbol{s}}_\ell = \boldsymbol{\Psi}_\ell \hat{\boldsymbol{\alpha}}_\ell$ (OMP)

3. Nonlinear inverse problem

Simplification for separable nonlinearity

General forward model

$$\boldsymbol{x}_\ell = g_\ell(\boldsymbol{S}_{th,\ell}\boldsymbol{I}_\ell; \boldsymbol{\theta}_\ell) \tag{10}$$

Separable model for g_ℓ

$$g_\ell(z, \boldsymbol{\theta}) = \sum_{p=0}^{P} g_\ell^{(p)}(z)\ \theta_\ell(p) \tag{11}$$

Application to forward model

$$\boldsymbol{x}_\ell = \sum_{p=0}^{P} g_\ell^{(p)}(\boldsymbol{S}_{th,\ell}\boldsymbol{I}_\ell)\ \theta_\ell(p) \tag{12}$$

3. Nonlinear inverse problem

Example: polynomial model

$$g_\ell^{(p)}(z) = z^p, \quad p = 0, ..., P \tag{13}$$

Application to forward model

$$\boldsymbol{x}_\ell = \sum_{p=0}^{P} (\boldsymbol{S}_{th,\ell} \boldsymbol{I}_\ell)^p \ \theta_\ell(p) \tag{14}$$

Iterative estimation method

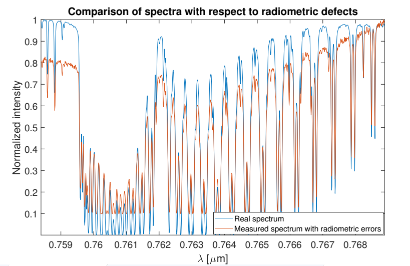
- Step 1: Radiometric errors - polynomial coefficients
  - $\hat{\boldsymbol{\theta}}_\ell = \arg\min_{\boldsymbol{\theta}_\ell} ||\boldsymbol{x}_\ell - \sum_{p=0}^{P} (\boldsymbol{S}_{th,\ell} \boldsymbol{I}_\ell)^p \ \theta_\ell(p)||_2^2$
- Step 2: Correction - zeroes of polynomials
  - $\hat{\boldsymbol{s}}_\ell = \arg\min_{\boldsymbol{s}_\ell} ||\boldsymbol{x}_\ell - \sum_{p=0}^{P} \boldsymbol{s}_\ell^p \ \theta_\ell(p)||_2^2$

4. Numerical experiments

Data description

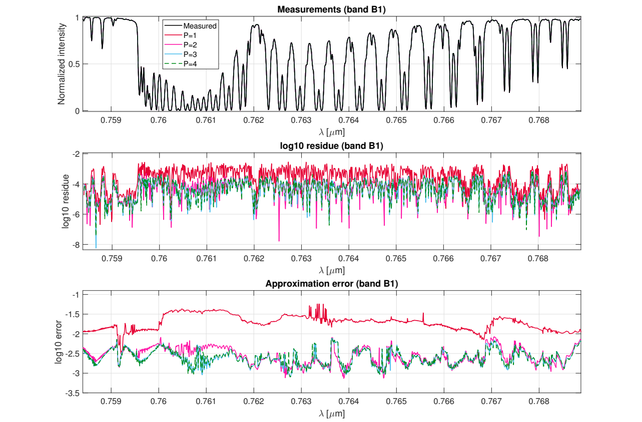
Simulated data for MicroCarb mission

- Theoretical spectra obtained with 4A/OP radiative transfer software
- Radiometric errors modeled as polynomials of degree 3



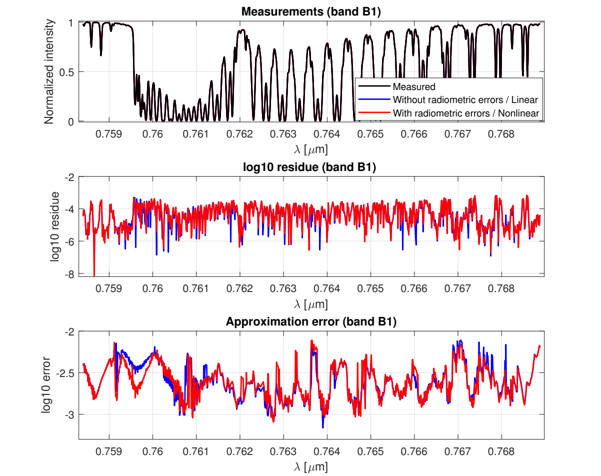
4. Numerical experiments

Estimation performance vs polynomial orders ($P \in 1, 2, 3, 4$)



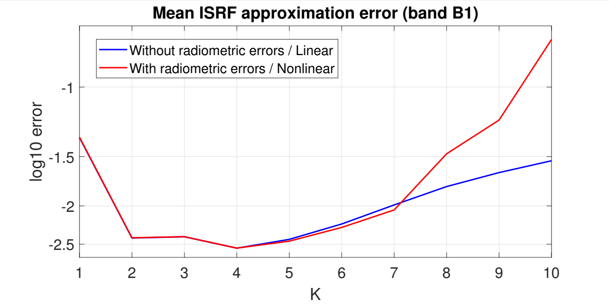
4. Numerical experiments

Nonlinear case versus linear case



4. Numerical experiments

Nonlinear case versus linear case



similar performance for $K \in \{1, \ldots, 7\}$

Conclusion

- ISRF estimation using a sparse representation
- Joint estimation of measurement nonlinearities and the ISRF using an iterative algorithm
- Competitive performance

Prospects

- Analyses of other degradations (spectral shifts, stray light...)
- Potential interest of machine learning methods (neural networks) to learn the nonlinearities from data