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Retrieval of surface emissivity from FORUM-EE9 simulated measurements: optimization of constraints

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Forum mission

FORUM (Far-infrared Outgoing Radiation Understanding and Monitoring):

- Fourier Transform Spectrometer (FTS);
- End-to-end (E2E) simulator;
- 9th ESA's Earth Explorer mission (EE9);
- Complete emission spectrum at the top of the atmosphere (TOA) \rightarrow unique picture of the Earth's radiative budget;
- ▶ $100 1600 \text{ cm}^{-1}$ region of the atmosphere (FIR and part of MIR) \rightarrow more than 95% outgoing longwave flux lost by our planet.

Targets:

- Upper Troposphere and Lower Stratosphere Water Vapor;
- Surface emissivity in polar and dry regions ;
- Cirrus clouds characteristics.

Final aim: improving the accuracy of climate models

Direct and inverse problem

Direct problem: from the atmospheric status vector x find the simulated spectrum y = F(x), with F known as **forward model**.

Inverse problem: from the measured spectrum y find the parameter vector x (retrieval vector) which minimizes ||y - F(x)||.



Direct problem

Radiative transfer equation (homogeneous mean, fixed frequency ω):

Lambert-Beer law + Planck law

$$\frac{d}{dx}I(x) = -\rho(x)\alpha(x)I(x) + \rho(x)\alpha(x)B(T(x)),$$

where:

- I is the intensity of light ray;
- x is the coordinate along the direction of the light beam;
- $\blacktriangleright \rho \alpha$ is the attenuation coefficient;
- ▶ B(T(x)) is the Planck function depending on the temperature T.

Continuous solution for the altitude layer from 0 to x_N :

$$I(x_N) = I(x_0)e^{-\int_0^{x_N}\rho(x)\alpha(x)dx} + \int_0^{x_N}\rho(x)\alpha(x)B(T(x))e^{\int_x^{x_N}\rho(x')\alpha(x')dx'}dx$$

Inverse problem: determine an estimate of *x* from the measurements *y*.

The inverse problem is very **ill-conditioned**.

Given a Gaussian measurement error $\varepsilon = y - F(x)$, with $S_y = \mathbb{E}[\varepsilon \varepsilon^t]$. Suppose there is an apriori estimate x_a of x with error $\varepsilon_a = x - x_a$ and $S_a = \mathbb{E}[\varepsilon_a \varepsilon_a^t]$. We can compute:

$$P(y, x_{a}) = \frac{1}{(2\pi)^{\frac{n}{2}}|S_{a}|} e^{\frac{(x_{a} - x)^{t}S_{a}^{-1}(x_{a} - x)}{2}} \frac{1}{(2\pi)^{\frac{m}{2}}|S_{y}|} e^{\frac{(y - F(x))^{t}S_{y}^{-1}(y - F(x))}{2}}.$$

where:

- \triangleright |...| is the determinant of A;
- *n* is the dimension of *x*;
- \blacktriangleright *m* is the dimension of *y*.

Inverse problem and Optimal Estimation method

We can rewrite P as:

$$P(y, x_a) = \frac{1}{(2\pi)^{\frac{n+m}{2}} |S_a| |S_y|} e^{-\frac{1}{2} \left[(x_a - x)^t S_a^{-1} (x_a - x) + (y - F(x))^t S_y^{-1} (y - F(x)) \right]}$$

Optimal estimation method for the inversion:

The maximization of the probability that a given parameter vector is compatible with the measurements is equivalent to the minimization of the quantity:

$$\chi^{2}(x) = (x_{a} - x)^{t} S_{a}^{-1}(x_{a} - x) + (y - F(x))^{t} S_{y}^{-1}(y - F(x)).$$

The minimization

Gauss-Newton method (GN) + Levenberg-Marquardt technique (LM):

$$\begin{aligned} x_{k+1} &= x_k + \left(\mathcal{K}_k^t \mathcal{S}_y^{-1} \mathcal{K}_k + \mathcal{S}_a^{-1} + \alpha_k \operatorname{diag}(\mathbf{K}_k^t \mathbf{S}_y^{-1} \mathbf{K}_k) \right)^{-1} \\ & \cdot \left[\mathcal{K}_k^t \mathcal{S}_y^{-1} (y - \mathcal{F}(x_k)) + \mathcal{S}_a^{-1} (x_a - x_k) \right], \end{aligned}$$

where k is the iteration index, α_k is the Marquardt parameter at iteration k and $K_k = \nabla F(x_k)$.

Why LM?

- the damping term α_k helps in the inversion of the matrix to be computed;
- ► for large values of α_k , $x_{k+1} x_k$ goes to $-\frac{\nabla \chi^2(x)}{\alpha(x)}$, which is a descend direction for the cost function.

Drawback: premature convergence.

Surface emissivity

Emissivity of the surface of a material:

effectiveness in emitting energy as thermal radiation (visible radiation and infrared radiation).

Each body re-emits part of the energy that reaches it in the form of thermal energy, and reflects the rest.

For the energy conservation law:

 $E_{absorbed} + E_{reflected} = E_{incident}.$

Emissivity (ϵ) and **Reflectivity** (r) are defined as:

$$\epsilon = \frac{E_{absorbed}}{E_{incident}},$$
$$r = \frac{E_{reflected}}{E_{incident}},$$
$$\epsilon + r = 1.$$

Iterative Variable Strength regularization (IVS)

Aim: Regularization of the retrieved surface emissivity profile.

Why?

No correlations in the a-priori VCM to avoid cross-talks between spectral ranges with different sensitivity to surface emissivity \rightarrow better reconstruction in the transition intervals \rightarrow oscillations in the retrieved profile.

Method:

It is an a-posteriori regularization consisting in adding a Tikhonov term to χ^2 :

$$\chi^{2}(x) = (x_{a} - x)^{t} S_{a}^{-1}(x_{a} - x) + (y - F(x))^{t} S_{y}^{-1}(y - F(x)) + (x_{s} - x)^{t} R_{\Lambda}(x_{s} - x),$$

where

- > x_s is an estimate of the solution,
- ► $R_{\Lambda} = L_i^t \Lambda L_i$ is such that:
 - ► L_i is a linear operator approximating the *i*-th derivative: $(L_i x_k)_j \simeq \frac{d'}{d_{i-j}} x_k(\omega_j)$,
 - Λ is a positive diagonal matrix such that $\Lambda_{jj} = \lambda(\omega_j)$.

IVS regularization

Let

- k be the iteration count at convergence for the minimization of χ² without the regularization term,
- $\triangleright x_{\mathsf{OE}} \equiv x_{k+1},$
- ► x_s = 0,

then the G-N minimizer x_{Λ} has the form:

$$\begin{aligned} x_{\Lambda} &= x_{k} + \left(\mathcal{K}_{k}^{t} \mathcal{S}_{y}^{-1} \mathcal{K}_{k} + \mathcal{S}_{a}^{-1} + \alpha_{k} \operatorname{diag}(\mathbf{K}_{k}^{t} \mathbf{S}_{y}^{-1} \mathbf{K}_{k}) + \mathbf{R}_{\Lambda} \right)^{-1} \cdot \\ & \cdot \left[\mathcal{K}_{k}^{t} \mathcal{S}_{y}^{-1} (y - \mathcal{F}(x_{k})) + \mathcal{S}_{a}^{-1} (x_{a} - x_{k}) - \mathcal{R}_{\Lambda} x_{k} \right]. \end{aligned}$$

IVS regularization

The procedure:

Starting with a large $\Lambda^{(0)} = \lambda^{(0)}I$, we decrease the profile until both the following conditions are fulfilled:

$$|x_{\Lambda}^{q}(\omega) - x_{\mathsf{OE}}^{q}(\omega)| \le w_{e}(\omega)\sqrt{S_{y}(\omega,\omega)},$$

 $\blacktriangleright \ \nu_{\Lambda}^{q}(\omega) \leq w_{r}(\omega)\nu_{\mathsf{OE}}^{q}(\omega),$

where q is the regularization step, $\nu_{\Lambda}(\omega)$ and $\nu_{OE}(\omega)$ are the spectral resolutions of the x_{Λ} and x_{OE} profiles respectively.

Decreasing the λ profile:

for each point ω_j such that the conditions are not satisfied we multiply by a triangular function $t_j(\omega)$:



with r = 0.99, h = 1 or h = 2.

The amplitude is set either with the independent variable, or in number of points (**ztri**).

Retrieval Qualifiers

- DOF: number of degrees of freedom of the solution;
- POQ (Profile oscillations quantifier, Ω₁): given a profile x_i = x(ω_i) it measures its oscillations:

$$\Omega_1 = \frac{1}{n-2} \sum_{i=2}^{n-1} \frac{\left|x_i - x_{i-1} - \frac{x_{i+1} - x_{i-1}}{\omega_{i+1} - \omega_{i-1}} (\omega_i - \omega_{i-1})\right|}{\sqrt{(x_{i+1} - x_{i-1})^2 + (\omega_{i+1} - \omega_{i-1})^2}}$$

Test scenarios

Sensitivity to emissivity in the FIR depends on the **PWV** of the atmosphere: total atmospheric water vapour contained in a vertical air column of unit area from the Earth's surface to the top of the atmosphere



- Water case: PWV = 36.33 mm → wet atmosphere → no sensitivity.
- Snow case: PWV = 3.31 mm → dry atmosphere → good sensitivity.
- ► Desert case: PWV = 23.14 mm → fairly dry atmosphere → some sensitivity.

WATER CASE PVW: 36.33 mm						
	BEFORE IVS	AFTER IVS ($\lambda_0 = 10^7$,	$\underline{w}_{e} = 1, \underline{w}_{L} = 5$			
	DEFOREINO	h = 1	h = 2			
DOF	29.167	9.524	11.048			
POQ	271E-6	97E-6	165E-6			
χ^2	1.0287	1.0365	1.0356			

Results - water case



FORUM - Water case (33.75,18.75) - $\lambda_0 = 10^7$ - $w_r = 5$

SNOW CASE PVW: 3.31 mm					
	BEFORE IVS	AFTER IVS ($\lambda_0 = 10^7$, $\underline{w}_e = 1$, $\underline{w}_L = 5$)			
	DEI ONE IVO	h = 1	h = 2		
DOF	45.343	10.920	14.809		
POQ	473E-6	34E-6	166E-6		
χ^2	1.0262	1.0376	1.0341		

Results - snow case



Results - desert case

DESERT CASE PVW: 23.14 mm					
	BEFORE IVS	AFTER IVS ($\lambda_0 = 10^7$, $\underline{w}_e = 1$, $\underline{w}_L = 5$)			
		h = 1	h = 2		
DOF	38.403	17.605	19.535		
POQ	422E-6	254E-6	283E-6		
χ^2	1.2046	1.2506	1.2409		

Results - desert case



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Conclusions, ongoing and future works

- the IVS for surface emissivity profile has been recently added to the official algorithm;
- in the optimal IVS setting it turned out to be crucial to start from a strong regularization and then softly reduce the λ profile in a quite large range of wave numbers;

Future work

- Optimization of the retrieval grid.
- Global map for the sensitivity to emissivity in the FIR and MIR.

Thank you!

References

Huang, X., Chen, X., Zhou, D. K., and Liu, X.: An Observationally Based Global Band-by-Band Surface Emissivity Dataset for Climate and Weather Simulations, J. Atmos. Sci., 73, 3541–3555, https://doi.org/10.1175/JAS-D-15-0355.1, 2016.

Hersbach, H., Bell, B., Berrisford, P., Hirahara, S., Horányi, A., Muñoz-Sabater, J., Nicolas, J., Peubey, C., Radu, R., Schepers, D., Simmons, A., Soci, C., Abdalla, S., Abellan, X., Balsamo, G., Bechtold, P., Biavati, G., Bidlot, J., Bonavita, M., De Chiara, G., Dahlgren, P., Dee, D., Diamantakis, M., Dragani, R., Flemming, J., Forbes, R., Fuentes, M., Geer, A., Haimberger, L., Healy, S., Hogan, R. J., Hólm, E., Janisková, M., Keeley, S., Laloyaux, P., Lopez, P., Lupu, C., Radnoti, G., de Rosnay, P., Rozum, I., Vamborg, F., Villaume, S., and Thépaut, J.-N.: The ERA5 global reanalysis, Q. J. Roy. Meteor. Soc., 146, 1999–2049, https://doi.org/10.1002/qj.3803, 2020.

Remedios, J. J., Leigh, R. J., Waterfall, A. M., Moore, D. P., Sembhi, H., Parkes, I., Greenhough, J., Chipperfield, M. P., and Hauglustaine, D.: MIPAS reference atmospheres and comparisons to V4.61/V4.62 MIPAS level 2 geophysical data sets, Atmos. Chem. Phys. Discuss., 7, 9973–10017, https://doi.org/10.5194/acpd-7-9973-2007, 2007.

References

Clough, S., Shephard, M., Mlawer, E., Delamere, J., Iacono, M., Cady-Pereira, K., Boukabara, S., and Brown, P.: Atmospheric radiative transfer modeling: a summary of the AER codes, J. Quant. Spectrosc. Ra., 91, 233–244, https://doi.org/10.1016/j.jqsrt.2004.05.058, 2005.

Sgheri L., Belotti C., Ben-Yami M., Bianchini G., Carnicero Dominguez B., Cortesi U., Cossich W., Del Bianco S., Di Natale G., Guardabrazo T., Lajas D., Maestri T., Magurno D., Oetjen H., Raspollini P., Sgattoni C.: The FORUM end-to-end simulator project: architecture and results, Atmospheric Measurement Techniques, 15 (3), 573-604, https://doi.org/ 10.5194/amt-15-573-2022 2022.



Ridolfi, M. and Sgheri, L.: Iterative approach to self- adapting and altitude-dependent regularization for atmospheric profile retrievals, Opt. Express, 19, 26696–26709, https://doi.org/10.1364/OE.19.026696, 2011.



Sgheri, L., Raspollini, P., and Ridolfi, M.: Auto-adaptive Tikhonov regularization of water vapor profiles: application to FORUM measurements, Appl. Anal., https://doi.org/10.1080/00036811.2020.1751825, 2020.

Retrieval grid: fine vs coarse

Fine grid

- Minimization of the smoothing error. Sharp features of the emissivity model are reproduced.
- Reduced precision, possible biases.

Coarse grid

- If the retrieval grid step is larger than the retrieval feature, the feature cannot be reproduced.
- Good precision. Each retrieval point is the average of a large number of measurements. Thus, the random error is smaller and there are no biases.

Retrieval grid: fine vs coarse

