1. Introduction

Although ground based MAX-DOAS measurements at different elevation angles have been used for several years to investigate the distribution of trace gases and aerosols, the retrieval of vertical profiles is still a difficult task and results of well-established algorithms differ strongly.

Here, we introduce IUP Bremen’s new profile retrieval algorithm BOREAS (Bremen Optimized estimation REtrieval for Aerosols and trace gases) and apply it to synthetic data computed with the radiative transfer model SCIATRAN and real data from the CINDI2 campaign (Cабау, 2016).

The results indicate that commonly used regularization tends to give not the proper weight to the measurement which results in oscillating profiles.

2. MAX-DOAS measurement vs. retrieval

- Azimuthal scans with different elevation angles allow retrieval of trace gases.
- Inverse problem is ill-posed! (\( \text{dSCD}_{\text{true}} = \text{BAMF} \cdot x \))
- Adding of known information on the atmosphere (a priori information)
- Maximum number of degrees of freedom (DOF)

3. SCIATRAN

Calculations within a full-spherical atmosphere including multiple scattering.

- Tracegas retrieval:
  Calculations of box air-mass factors for all geometries and altitude layers: \( \text{BAMF} = \text{dSCD/VCD} \)
- Aerosol retrieval:
  Minimization of \( \Omega \) optical depth of measurement and forward model by variation of the aerosol extinction profile via Tikhonov regularization.

4. Aerosol profile retrieval

Assumption: Variation of absorber is is equal to a scaled a-priori

The sun-normalized intensity can be written as Taylor series:

\[
\ln(I_{\text{true}}) = \ln(I_{\text{true}}) = \sum_i W_F \cdot y_i + \sum_i W_F \cdot y_i - \text{with retrieval parameter } y_i.
\]

\[
\ln(I_{\text{true}}) = \ln(I_{\text{true}}) + \ln(I_{\text{true}}) + \text{min} \ln(I_{\text{true}}) + \ln(I_{\text{true}}) + \text{min}
\]

This minimization problem is solved iteratively within a Tikhonov regularization.

\[
x_i = x_i + \frac{1}{\lambda_i} \cdot S_i \cdot (y_i - y_i - x_i)\]

with \( S_i = S_i + S_i + \text{Convergence/Invariance matrix} \)

5. Tikhonov regularization

Known problems:

- Profiles are underestimated when the a-priori is too small:
  scaling needed
- Weaker regularization leads to oscillations for scenarios close to the a-priori.
- Chosen settings might be good for pre retrieval of AODs but bad for bottom values (or vice versa)

Why is a-priori scaling important?

6. Trace gas retrieval

A-priori scaling for NO2:

\[
x_{i+1} = x_i + \frac{1}{\lambda_i} \cdot S_i \cdot (y_i - y_i - x_i)
\]

With different regularization factors for NO2 and without pre scaling, \( \text{BAMF} = \text{dSCD/VCD} \)

Pre scaled settings converge with a decreasing layer for 15:00 and 16:00h.

6.1. Aerosol retrieval

 Retrieval without a-priori on a coarser vertical and spectral grid

7. CINDI2 aerosol study

Case study on the example of the aerosol layer on the 12th of September 2016 in Cабау.

8. Summary

- The best regularization between a-priori and measurement weighing differs strongly for individual scenarios
- A-priori pre scaling improves the profiling results for days with a large variability in aerosol and trace gas concentrations.
- Even with best settings there might be stable solutions which improve either the bottom concentration or the integrated concentration but not both.
- An automatic regularization via derivative of norms might be a solution for optimized weighting.
- Different minima introduce a need for regularization factor limitations by the user.

9. Acknowledgement & Selected References

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References:

