

PROFFIT I: Inversion method

PROFFIT is the retrieval tool used at IMK to analyse the solar absorption spectra measured with high-resolution ground-based FTIR spectrometers. It uses the forward code KOPRA, also developed at IMK.

Various retrieval options are implemented, that can be chosen individually for each gas to be retrieved in a joint fit of several MWs:

- Scaling of a-priori profile
- Tikhonov-Phillips (TP) method*
- Optimal Estimation (OE) method*
- Scaling of a-priori profile in restricted height regime (used for evaluation of ClO)

To be implemented:

- Diabatic descent and tropopause shift

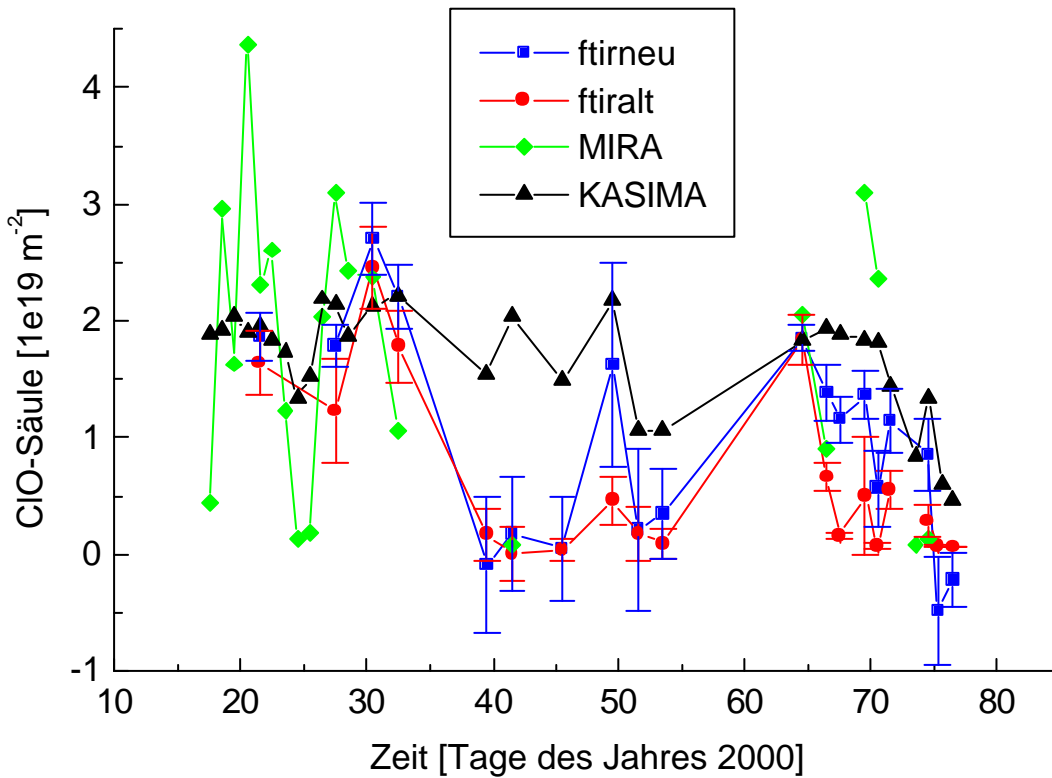
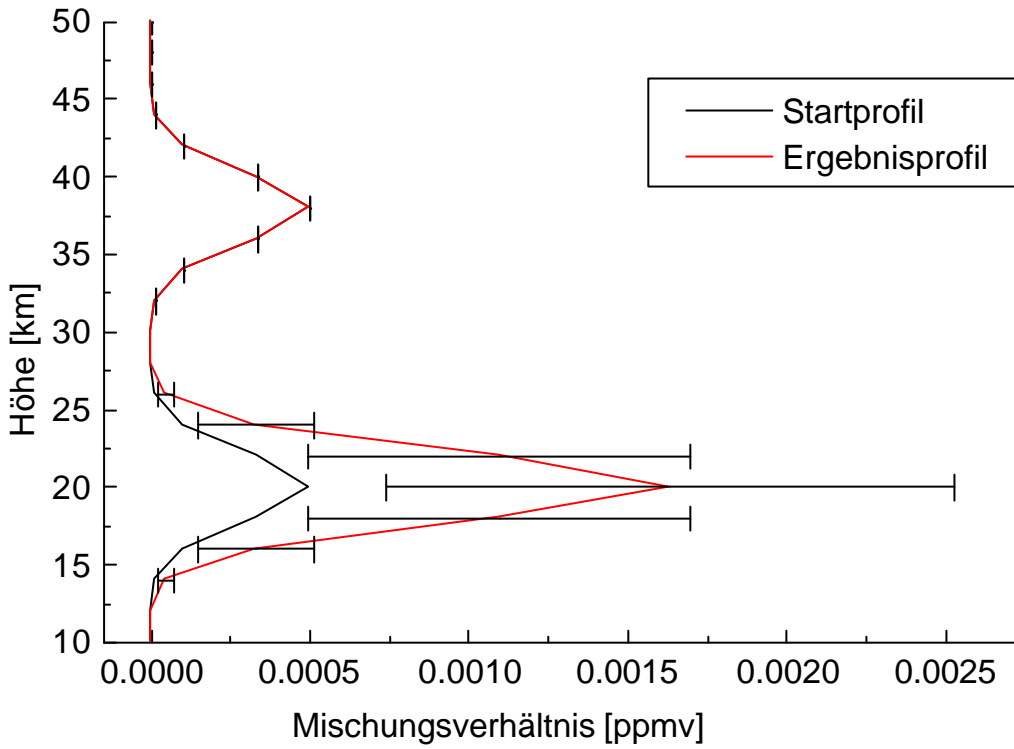
*: on linear or logarithmic VMR scale (the latter options excludes negative VMR values)

Note: TP and OE inversion methods are mathematically equivalent

$$\text{TP: } \bar{f}^{i+1} = (A^{iT} A^i + \mathbf{g}^2 B^T B)^{-1} [A^{iT} (\Delta \bar{L}^i + A^i \bar{f}^i) + \mathbf{g}^2 B^T B \bar{f}_{reg}]$$
$$\text{minimises } |A^i (\bar{f}^{i+1} - \bar{f}^i) - \Delta \bar{L}^i|^2 + \mathbf{g}^2 (B \bar{f}^{i+1} - \bar{f}_{reg})^T (B \bar{f}^{i+1} - \bar{f}_{reg})$$

$$\text{OE: } \bar{f}^{i+1} = (A^{iT} A^i + \mathbf{s}^2 S_f^{-1})^{-1} [A^{iT} (\Delta \bar{L}^i + A^i \bar{f}^i) + \mathbf{s}^2 S_f^{-1} \bar{f}_0]$$
$$\text{minimises } |A^i (\bar{f}^{i+1} - \bar{f}^i) - \Delta \bar{L}^i|^2 + \mathbf{s}^2 (\bar{f}^{i+1} - \bar{f}_0)^T S_f^{-1} (\bar{f}^{i+1} - \bar{f}_0)$$

PROFFIT II: Inversion of CIO



PROFFIT III: TP+OE – Non-standard features

Equivalence of TP and OE methods:

$$\mathbf{s}^2 S_f^{-1} \Leftrightarrow \mathbf{g}^2 B^T B \quad (\text{genauer: } \mathbf{s}^2 S_f^{-1} \Leftrightarrow \mathbf{g}_1^2 B_1^T B_1 + \mathbf{g}_2^2 B_2^T B_2 + \dots)$$
$$\tilde{f}_0 \Leftrightarrow \tilde{f}_{reg}$$

Idea:

Replacing in standard TP ansatz $\mathbf{g}^2 B^T B \Rightarrow \mathbf{s}^2 \tilde{\mathbf{g}}^2 B^T B$

results in “readjustment” of regularisation strength appropriate to noise level and scale in each individual measurement

Replacing in standard OE ansatz $\mathbf{s}^2 S_f^{-1} \Rightarrow \mathbf{s}^2 (\mathbf{g}_1^2 S_{1f}^{-1} + \mathbf{g}_2^2 S_{2f}^{-1})$

results in splitting of diagonal and non-diagonal contributions to S, allows simple “fine-tuning” of a-priori covariance matrix S

Question: Which variance to be used in the inversion ($\mathbf{s} = \mathbf{s}^i$)?

Idea:

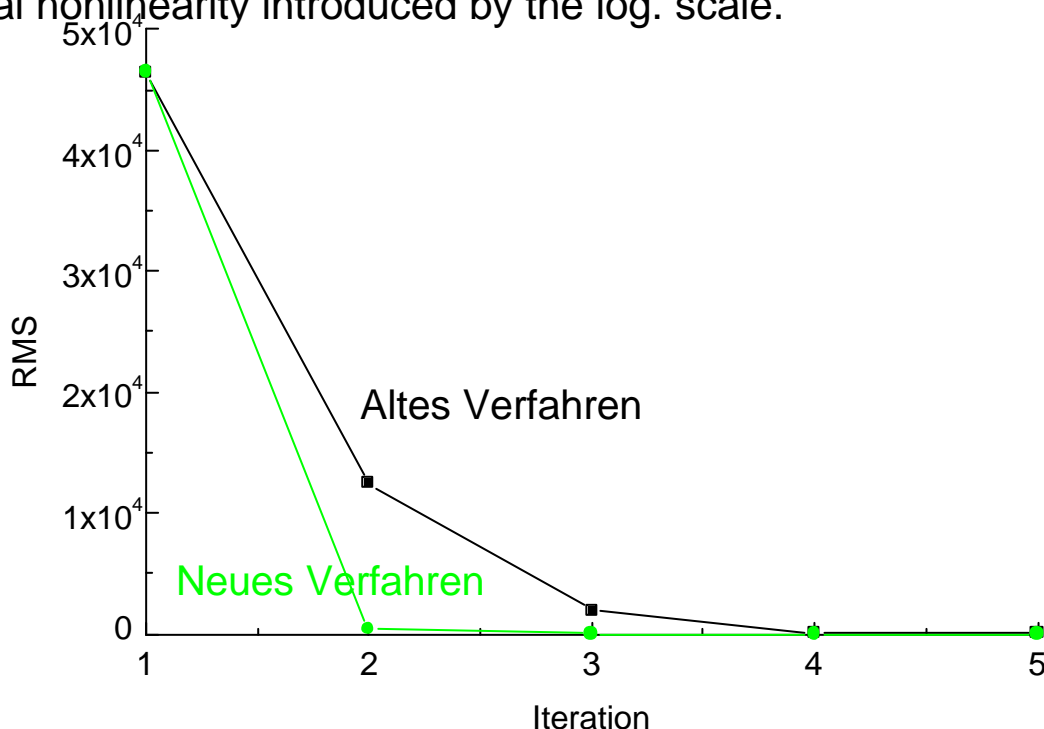
Use spectral variance according to the previous iteration.

Thereby modified convergence and (a kind of) “dynamical L-curve criterion“

PROFFIT IV: Superior convergence behaviour

Inversion on logarithmic VMR-scale can be advantageous since it avoids the occurrence of (highly improbable) negative mixing ratios. A major drawback of this trick is the additional nonlinearity introduced in the inversion problem, strongly deteriorating the convergence behaviour.

To eliminate these problems, PROFFIT uses a refined iteration scheme in case of the logarithmic option: Two iteration cycles are nested: The outer cycle calls the forward model and updates the Jacobian and the synthetic spectrum $A^i, \Delta \bar{L}_{calc}^i$. The inner cycle relies on the linearisation $\bar{L}(\bar{f}^i + \Delta \bar{f}) \approx L(\bar{f}^i) + A^i \Delta \bar{f}$ and is repeated several times, absorbing the additional nonlinearity introduced by the log. scale.



The iteration is stopped when convergence is reached. The convergence criterion used by PROFFIT is of the form

$$\max \left(\sum_j \left| \sum_k A_{jk}^{i+1} (f_k^{i+1} - f_k^i) \right| / \text{Mittelwert}(MW) \right) \leq \text{Schwellwert}(MW)$$

PROFFIT V: Supported file formats for spectra

PROFFIT supports OPUS *.dpt format, SFIT-format and our own binary *.bin format. This format is flexible due to its pointer structure, and uses a header format that enables the user to read the information given there with any editor. The header is followed by the spectrum in binary format. The software generating the binary files also interpolates the spectrum to $1/2 \cdot OPD_{\max}$ -grid, thereby minimising the amount of data and generating a diagonal spectral covariance matrix.

Location

Date

Time eff. UT [h,decimals]

Apparent elevation [deg]

\$

Kiruna

010121

11.15889

2.63790

Filter

OPDmax [cm]

semi FOV [rad]

\$

6

180.00

2.39E-03

ILS simple(1) or extended(2) modulation efficiency

\$

2

1.000E+00, 0.000E+00

1.000E+00, 0.000E+00

1.000E+00, 0.000E+00

.....

firstnue

lastnue

deltanue

Ngridpts

\$

650.1444444

1379.6694444

2.777777778E-03

262630

Comments

Forschungszentrum Karlsruhe

Technik und Umwelt

anne dezentriert fuer laengere Messzeit (+0.15 Grad)
977hPa, T=-11.5 C

\$
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Äó-• Äíµ™Ä@È©Ä0pdÄ%öÖ• Ä#AIÄíD,,BöfpCz• ÖC%ö<²D-HLÄóÖ'Äíä£Do™FÄ_RxB

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