Retrieval for emission limb sounders

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The forward and the inverse problem

The measured signal is determined for several values of the frequency $\sigma$ and of the limb angle $\Theta$:

$$S(\Theta, \sigma),$$

and depends on the properties of the atmosphere which, in the case of a stratified atmosphere, are only a function of the altitude $z$:

$$S(\Theta, \sigma) = F(p(z), T(z), VMR_i(z))$$

where $p(z)$ is the pressure, $T(z)$ is the temperature and $VMR_i(z)$ is the volume mixing ratio of the atmospheric species $i$. 
The forward and the inverse problem

In our case, the relationship:

\[ S(\omega, \sigma) = F(VMR_i(z), p(z), T(z)) \]

is the forward problem and its reciprocal

\[ p(z) = F_1(S(\omega, \sigma)) \]
\[ t(z) = F_2(S(\omega, \sigma)) \]
\[ VMR_i(z) = F_i(S(\omega, \sigma)) \]

is the inverse problem.

The forward and the inverse problem

The inverse problem does not always have an useful solution.

In particular it can be:

- ill posed (either impossible solution or infinite possible solutions). This occurs when either an error is made in the definition of the problem or the observations do not provide the required information.
- ill conditioned (the solution exists but small errors in the observations lead to large errors in the solution). This occurs when the observations contain insufficient information.
The mathematics of the retrieval

The inversion

In the forward problem

\[ S(\Theta, \sigma) = F(p, T, VMR) \]

\((\Theta, \sigma) = m\) are the observation variables that number the observations and \((p, T, VMR) = q\) are the atmospheric variables that become the unknowns in the inverse problem. Using these notations:

\[ S_m = F_m(q) \]

In general, this equation cannot be analytically inverted and does not have an exact solution.

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The mathematics of the retrieval

The least-squares solution

We can look for a least-squares solution. The least-square solution \(q'\) is the value of \(q\) which minimises the quantity:

\[ \chi^2 = y^T (V y)^{-1} y \]

where \(V y\) is the variance covariance matrix of the measurements and

\[ y = S_m - F(q_r) \]

is the difference between the measurements and the forward model calculated for \(q_r\).
The mathematics of the retrieval

The Gauss-Newton method

The least-square solution can be found using the Gauss-Newton method for the solution of the equation:

$$\frac{\delta \chi^2}{\delta q} = 0.$$

The Gauss-Newton method is an iterative procedure that starts from an initial guess $q_o$ of the unknown (assumed to be near enough to the solution $q_r$).

At each step of the iterative process a new estimate $q_n$ of $q$ is obtained:

$$q_n = (K^T (V^y)^{-1} K)^{-1} K^T (V^y)^{-1} (S_m - F(q_n-1))$$

where the quantity $K = \frac{\partial (S(q))}{\partial (q)}$ is the Jacobian of the measurements.

When convergence criteria are satisfied the iterative process is stopped and $q_r = q_n$.

The variance covariance matrix of the solution is equal to:

$$V^q = (K^T (V^y)^{-1} K)^{-1}$$
The mathematics of the retrieval
The Levenberg - Marquardt Method

The iterative process may be unstable (the values retrieved at each iteration oscillate around the solution). In order to limit this effect it is useful to introduce a damping in the variation of the unknown (Levenberg - Marquardt method). In this case the solution is equal to:

$$q_r = \left(K^T (V^y)^{-1} K + \lambda I \right)^{-1} K^T (V^y)^{-1} \left(S_m - F(q_{n-1})\right)$$

where $I$ is the unit matrix.

Optimised Retrieval Model (ORM)

- The Optimised Retrieval Model (ORM) is a scientific code that was developed, under an ESA contract, for the near real time (NRT) retrieval of geophysical parameter from MIPAS measurements.
- The ORM is the reference code used for the Level 2 operational analysis of MIPAS.
ORM Team

- IFAC-CNR - Italy
- University of Bologna - Italy
- ISAC-CNR - Italy
- IMK - Germany
- University of Oxford - U.K.
- University of Leicester - U.K.
- LPPM - France

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Operations of ORM and Level 2

Calibrated and geolocated spectra -> Level 2 -> Retrieved profiles

Retrieved vertical profiles of:
- altitude correction and temperature (p,T retrieval)
- VMR of minor constituent (H₂O, O₃, HNO₃, CH₄, N₂O and NO₂)
ORM approach

- Use of micro-windows

- Use of non-linear least-square fit
ORM approach

- Use of micro-windows
- Use of non-linear least-square fit
- Global fit of limb scanning sequence
ORM approach

- Use of micro-windows
- Use of non-linear least-square fit
- Global fit of limb scanning sequence
- Sequential fit of species

- p,T retrieval
- H₂O retrieval
- O₃ retrieval
- HNO₃ retrieval
- CH₄ retrieval
- N₂O retrieval
- NO₂ retrieval

ORM approach

- Use of micro-windows
- Use of non-linear least-square fit
- Global fit of limb scanning sequence
- Sequential fit of species
- Near real time operation
Diagram of the operations of each retrieval

Unknowns of each retrieval

- profile of the parameter (one value for each tangent altitude)
- profile of the atmospheric continuum for each micro-window at altitudes < 30 km
- altitude independent instrumental continuum for each micro-window
Numerical and physical choices in ORM

Use of complementary information

- In the case of an ill-conditioned retrieval a-priori information must be used (e.g., optimal estimation).
- MIPAS measurements provide enough information and a simple non-linear least-square solution can be used.
- However, the complementary information that is provided by the combination of LOS engineering measurements and hydrostatic equilibrium equation is also used in p, T retrieval.

Numerical and physical choices in ORM

Retrieval vertical grid

- The vertical profiles are retrieved at an altitude grid defined by the tangent altitude levels, since this provides the most accurate results
- The representation of the profile at an user defined vertical grid requires interpolation.
Numerical and physical choices in ORM

Atmospheric continuum

- All the sources that have a constant amplitude (far wings of the lines, broad bands, aerosols, etc.) in a micro-window (3 cm\(^{-1}\)) are not modelled in the radiative transfer, but are modelled as a fitted continuum.
- The continuum is considered to be an altitude dependent and micro-window dependent absorption coefficient present at altitudes < 30 km.

Jacobian

The calculation of the Jacobian is performed using as much as possible an analytical approach.
The terms of the analytical expression of the derivatives are calculated as part of the forward model calculation.

<table>
<thead>
<tr>
<th>Tangent pressure</th>
<th>Analytical</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>Optimised numerical</td>
</tr>
<tr>
<td>VMR</td>
<td>Analytical</td>
</tr>
<tr>
<td>Continuum</td>
<td>Analytical</td>
</tr>
</tbody>
</table>

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Data Products

- Tangent pressures
- temperature profile
- VMR profiles of five gasses
- continuum profiles of fitted micro-windows
- VCM of the above retrieved quantities
- instrument offset for each micro-window
- $\chi^2$ for each retrieval
- annotation data

Error budget

The error budget includes:
- measurement error (random)
- temperature errors (only VMR)
- line of sight error (only VMR)
- NLTE errors
- spectroscopic errors
- calibration errors (gain and offset)
- uncertainties of interfering gasses
Error budget

Temperature profile error budget

Water Vapour error budget
Averaging kernels

The Averaging Kernels are provided as tabulated data.

In the ideal case of absence of both random and systematic errors in the measurements and in the instrument’s forward model, for each state of the atmosphere $\mathbf{x}$ the observing system provides a retrieved profile $\hat{\mathbf{x}}_v$.

Expanding $\hat{\mathbf{x}}_v$ up to the first order about a generic atmospheric state $\mathbf{x}_0$, we obtain:

$$\hat{\mathbf{x}}_v - \mathbf{x}_0 = \left. \frac{\partial \hat{\mathbf{x}}_v}{\partial \mathbf{x}} \right|_{x_0} (\mathbf{x} - \mathbf{x}_0)$$

The quantity:

$$\mathbf{A} = \left. \frac{\partial \hat{\mathbf{x}}_v}{\partial \mathbf{x}} \right|_{x_0}$$

is called averaging kernel matrix and it is a function of the state $\mathbf{x}_0$. 
Averaging kernels

The AK describe how the real state of the atmosphere is distorted in the retrieved quantities.

This information is important whenever the retrieved quantities are used in a new context (data assimilation, comparison of different measurements).

Averaging kernels

Because AK depend on the state of the atmosphere calculations were repeated for four seasons (January, April, July and October) and six latitude bands:

- 90° South – 65° South
- 65° South – 20° South
- 20° South – 0°
- 0° – 20° North
- 20° North – 65° North
- 65° North – 90° North
Averaging kernels

Ozone, all latitudes (April only)

Averaging kernels

Ozone, all seasons (75° North only)
Cloud filtering

- In the radiative transfer of emission MIR measurements scattering effects can be neglected, and the occasional extinction of aerosols can be modelled as a continuum effect.
- However, thick clouds are opaque in the MIR and when present in the line of sight lead to measurements that are not correctly modelled in the retrieval.
- A cloud filtering algorithm is used in MIPAS Level 2 pre-processor. The algorithm detects the presence of clouds in the line of sights and excludes from the analysis the sweeps that are affected by clouds.
Altitude range of the retrieval

- A customised retrieval range is used for each retrieval
- Preliminary results and the use of cloud filtering have recently suggested the extension of the retrieval range.

<table>
<thead>
<tr>
<th></th>
<th>Nominal case (V3.1)</th>
<th>Extended case (V3.2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PT</td>
<td>12-68 km</td>
<td>9-68 km</td>
</tr>
<tr>
<td>H2O</td>
<td>12-60 km</td>
<td>9-68 km</td>
</tr>
<tr>
<td>O3</td>
<td>12-60 km</td>
<td>9-68 km</td>
</tr>
<tr>
<td>HNO3</td>
<td>12-42 km</td>
<td>9-42 km</td>
</tr>
<tr>
<td>CH4</td>
<td>12-60 km</td>
<td>9-68 km</td>
</tr>
<tr>
<td>N2O</td>
<td>12-47 km</td>
<td>9-60 km</td>
</tr>
<tr>
<td>NO2</td>
<td>24-47 km</td>
<td>24-68 km</td>
</tr>
</tbody>
</table>

Concluding remarks

- The ORM is presently used in the ground processor of MIPAS for the NRT retrieval of temperature and of the six target species.
- Comparison with field measurements is in progress for a full validation of MIPAS products.
- The ORM could also be used for the retrieval of other species and increase the NRT products.
Other species retrieved with ORM

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