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Iterative regularization methods for atmospheric remote sensing

Adrian Doicu*, Franz Schreier, Michael Hess

DLR—German Aerospace Center, Remote Sensing Technology Institute, Oberpfaffenhofen, 82234 Weß ling, Germany

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Abstract

In this paper we present different inversion algorithms for nonlinear ill-posed problems arising in atmosphere remote sensing. The proposed methods are Landweber's method (LwM), the iteratively regularized Gauss–Newton method, and the conventional and regularizing Levenberg–Marquardt method. In addition, some accelerated LwMs and a technique for smoothing the Levenberg–Marquardt solution are proposed. The numerical performance of the methods is studied by means of simulations. Results are presented for an inverse problem in atmospheric remote sensing, i.e., temperature sounding with an airborne uplooking high-resolution far-infrared spectrometer.

Keywords: Inverse problems; Nonlinear least squares; Regularization; Atmospheric spectroscopy; Remote sensing

1. Introduction

Optimal estimation, otherwise known as Bayesian inversion, is the dominating approach in atmospheric remote sensing [1]. In this approach a priori information about the atmospheric state is encapsulated in the form of probability distributions, which are independent of the observed data. When such distributions are combined with probabilistic information about data uncertainties (both random and theoretical) it is possible to derive a final (a posteriori) probability distribution assimilating both types of information. From a deterministic point of view optimal estimation is equivalent to Tikhonov regularization with a regularization term given by the a priori covariance matrix of the solution. However, the construction of the a priori probability distribution is a controversial matter

* Corresponding author. Tel.: +49-8153-28-3015; fax: +49-8153-28-1446.
E-mail address: adrian.doicu@dlr.de (A. Doicu).

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when the statistical information about the atmosphere variability is poor. In this case iterative regularization methods like Landweber's method (LwM), the Gauss–Newton method (GNM), or the Levenberg–Marquardt method (LMM) are pleasant alternatives.

A convergence theory for LwM for solving nonlinear ill-posed problem was first developed by Hanke et al. [2] and Binder et al. [3]. The iteratively regularized GNM was introduced by Bakushinskii [4] and its mathematical foundations were discussed by Blaschke et al. [5], Hohage [6], and Deuflhard et al. [7]. In atmospheric inversion this method was used by Tautenhahn [8] for temperature retrieval. Tautenhahn used the identity matrix as regularization matrix and a parameter choice method based on the noise level. The convergence of a so-called regularizing LMM for ill-posed problems has been proven by Hanke [9]. Hanke used the regularizing LMM for parameter identification problems arising in inverse groundwater hydrology. Note that the applicability of the conventional LMM [10] for ill-posed problems is still an open research topic.

In the present paper we analyze the performances of the above mentioned iterative regularization methods for the inversion problem of a vertical temperature profile from atmospheric spectroscopic measurements.

2. Formulation of the discrete problem

Atmospheric remote sensing in the microwave or infrared spectral regions utilizes measurements of the thermal emission of the atmosphere. From a computational point of view the basic problem is the inversion of the radiative transfer equation [11]. For an arbitrary slant path, the intensity (radiance) I at wavenumber v received by an instrument at position $\vec{r}$ is given by (neglecting scattering and assuming local thermodynamical equilibrium)

$$I(v) = I_{\mathrm{b}}(v)\mathscr{T}(v,\vec{r},\vec{r}_{\mathrm{b}}) + \int_{|\vec{r}-\vec{r}_{\mathrm{b}}|} \alpha(v,\vec{r}\,')B(v,T(\vec{r}\,'))\mathscr{T}(v,\vec{r},\vec{r}\,')\,\mathrm{d}s', \tag{1}$$

where B is the Planck function at temperature T, I_b is the background contribution at position $\vec{r}_{\mathrm{b}}$, and the integration is performed along the path segment between $\vec{r}$ and $\vec{r}_{\mathrm{b}}$. The monochromatic transmission $\mathscr{T}$ and the absorption coefficient α are related by Beer's law according to

$$\begin{aligned}\mathscr{T}(v,\vec{r},\vec{r}_0) &= \exp\left(-\int_{|\vec{r}-\vec{r}_0|} \alpha(v,\vec{r}\,')\,\mathrm{d}s'\right)\\ &= \exp\left[-\int_{|\vec{r}-\vec{r}_0|} \sum_g k_g(v,\, p(\vec{r}\,'), T(\vec{r}\,'))n_g(\vec{r}\,')\,\mathrm{d}s'\right],\end{aligned} \tag{2}$$

where p is the atmospheric pressure, n_g is the number density of molecule g and k_g is its absorption cross-section. In general, the absorption cross-section is obtained by summing over the contributions from many lines. For an individual line the spectral absorption cross section is the product of the temperature-dependent line strength and a normalized line shape function describing the broadening mechanism. For the infrared and under atmospheric conditions, the combined effect of pressure broadening (corresponding to a Lorentzian line shape) and Doppler broadening (corresponding to a Gaussian line shape) can be represented by a Voigt line profile. The instrumental response is taken into account by convolution of the monochromatic intensity spectrum (1) with an instrumental line shape function.

Spectroscopic instruments working in the infrared spectral region measure the intensity at a finite number m of typically equidistant wavenumbers v_i with $i=1,\ldots,m$. Therefore, a collocation method is used to discretize the integral equation (1). In addition, a quadrature approach is used to discretize the integrals in (1) and (2). As there is an unique relation between the path variable s and the altitude h, it is convenient to consider the temperature or the molecular density profiles at altitudes h_j, $j=1,\ldots,n$, as unknowns of the inverse problem.

The discretization process leads to the nonlinear system of equation

$$y = F(x), \tag{3}$$

where the mapping $F : R^n \rightarrow R^m$, $F = [f_i]_{i=1}^{m}$, representing the forward model is assumed to be continuously differentiable, $y \in R^m$ is the exact data vector and $x \in R^n$ is the state vector containing the atmospheric parameters (temperature and/or molecular density profiles) to be retrieved. Here R^n stands for the n-dimensional real Euclidian space with the usual inner product $\langle x, y \rangle = x^{\mathrm{T}} y$, while $\| \cdot \|$ denotes the l_2 vector norm and the subordinated l_2 matrix norm. In our analysis we assume that the exact data are attainable, i.e., that there exists the exact solution $\hat{x} \in D(F) \subseteq R^n$ such that $y = F(\hat{x})$. Measurements are made to a finite accuracy and in practice only the noise data vector y^δ, $y^\delta = y + \delta$, is available. In this context we consider a semi-stochastic data model in the sense that the exact solution $\hat{x}$ is deterministic but the measurement error δ is stochastic with zero mean and the covariance matrix S_δ, $S_\delta = \sigma^2 I$, where I is the identity matrix.

3. Iterative regularization methods for the discrete problem

The goal of our analysis is to find the state vector x^δ that is consistent with the data and whatever other deterministic information are available. An estimate x^δ can be found by approximately minimizing the so-called output least-squares function

$$\mathscr{F}(x) = \frac{1}{2} \| F(x) - y^\delta \|^2 \tag{4}$$

possibly by an iterative method. The Gauss–Newton method for the minimization of (4) is defined by the iterative solution

$$x_{k+1}^\delta = x_k^\delta - (F'(x_k^\delta)^{\mathrm{T}} F'(x_k^\delta))^{-1} [F'(x_k^\delta)^{\mathrm{T}} (F(x_k^\delta) - y^\delta)], \tag{5}$$

where $F'(x) \in R^{m \times n}$ denotes the Jacobian matrix $(\partial_j f_i(x))$ evaluated at x.

In an abstract Hilbert space setting the generalized inverse of $F'^* F'$ (where F'^* denotes the adjoint of F') is usually unbounded, so that each iteration would be unstable. Therefore, the term $F'^* F'$ has to be replaced by an operator with a bounded inverse. Due to the inherent instability of ill-posed problems, an iteration method has to be stopped appropriately to guarantee stability of the iterates. In this case the iterative method becomes a regularization method.

3.1. Landweber's method

In the finite-dimensional version of LwM the term $(F'(x_k^\delta)^{\mathrm{T}}F'(x_k^\delta))^{-1}$ in Eq. (5) is replaced by the identity matrix. This results in the method

$$x_{k+1}^\delta = x_k^\delta - \omega F'(x_k^\delta)^{\mathrm{T}}(F(x_k^\delta) - y^\delta), \tag{6}$$

where ω is a relaxation parameter. The Landweber iterates x_k^δ allow a stable and convergent approximation of the solution $\hat{x}$ provided the discrepancy principle is used as an a posteriori stopping rule, that is, the iteration is stopped at the first index $k_* = k_*(\Delta)$ for which

$$\|F(x_{k*}^\delta) - y^\delta\| \leqslant \tau\Delta < \|F(x_k^\delta) - y^\delta\|, \quad 0 \leqslant k < k_*, \tag{7}$$

where $\tau > 1$ and Δ is an upper bound for the error, $\|\delta\| \leqslant \Delta$. In practice, this bound can be choosen as the expected value of $\|\delta\|$, $\Delta = \sqrt{\mathscr{E}\{\|\delta\|^2\}} = \sigma\sqrt{m}$, where $\mathscr{E}$ is the expected value operator. In LwM the iteration index plays the role of the regularization parameter and the stopping criterion is the counterpart of the parameter choice rule in continuous regularization methods. For more details concerning the convergence of LwM for nonlinear problems we refer to Deuflhard et al. [7].

Often the number of iterative steps required to obtain useful approximations of the solution is too large. Several attempts have been made in the literature to speed up the iteration. The v-method (vM) of Brakhage (cf., e.g., [12]) is a two-step semi-iterative method for the linear equation $Kx = y$ and is given by

$$p_k = \lambda_k(x_k^\delta - x_{k-1}^\delta) - \omega_k K^{\mathrm{T}}(Kx_k^\delta - y^\delta), \tag{8}$$

$$x_{k+1}^\delta = x_k^\delta + p_k$$

for $k \geqslant 0$, where

$$\lambda_k = \frac{k(2k-1)(2k+2v+1)}{(k+2v)(2k+4v+1)(2k+2v-1)},$$

$$\omega_k = 4\frac{(2k+2v+1)(k+v)}{(k+2v)(2k+4v+1)}$$

for $k > 0$ and

$$\lambda_0 = 0, \quad \omega_0 = \frac{4v+2}{4v+1}.$$

Here v is a positive parameter which has to be chosen in advance. The vM in combination with the discrepancy principle as an a posteriori stopping rule is a regularization method in the sense of Engl et al. [12]. For a proof we refer to [13].

For moderately nonlinear problems we propose the following modified vM:

$$p_k = \lambda_k'(x_k^\delta - x_{k-1}^\delta) - \omega_k F'(x_k^\delta)^{\mathrm{T}}(F(x_k^\delta) - y^\delta),$$

$$x_{k+1}^\delta = x_k^\delta + a_k p_k. \tag{9}$$

The parameter λ'_k is choosen such that p_k is a descent direction, i.e., $g(x_k^\delta)^{\mathrm{T}} p_k < 0$, where $g(x_k^\delta) = F'(x_k^\delta)^{\mathrm{T}}(F(x_k^\delta) - y^\delta)$ is the gradient of $\mathscr{F}$ at x_k^δ. A possible scheme for parameter selection is

$$\lambda'_k = \begin{cases} \lambda_k & \text{if } g(x_k^\delta)^{\mathrm{T}} p_k < 0, \\ \varepsilon\omega_k \dfrac{g(x_k^\delta)^{\mathrm{T}} g(x_k^\delta)}{g(x_k^\delta)^{\mathrm{T}}(x_k^\delta - x_{k-1}^\delta)} & \text{else,} \end{cases}$$

where $0 < \varepsilon < 1$. Since p_k is a descent direction we determine the step length a_k so that the objective function (4) is sufficiently reduced. While this is a purely heuristic method, certain regularizing properties of the modified vM will be numerically verified.

Other schemes can be constructed in the same manner. For instance, the choice $\omega_k = \omega$ in (9) leads to

$$p_k = \lambda'_k(x_k^\delta - x_{k-1}^\delta) - \omega F'(x_k^\delta)^{\mathrm{T}}(F(x_k^\delta) - y^\delta), \tag{10}$$

while the use of stabilization term $\lambda'_k(x_k^\delta - x_0)$ gives

$$p_k = \lambda'_k(x_k^\delta - x_0) - \omega F'(x_k^\delta)^{\mathrm{T}}(F(x_k^\delta) - y^\delta). \tag{11}$$

The methods using the schemes (10) and (11) for search direction computation will be referred to as the modified LwM.

3.2. The regularized Gauss–Newton method

In the discrete case the regularized GNM uses the stabilization term

$$(\alpha_k L^{\mathrm{T}} L + F'(x_k^\delta)^{\mathrm{T}} F'(x_k^\delta))^{-1} \alpha_k L^{\mathrm{T}} L(x_k^\delta - x_a),$$

i.e.,

$$x_{k+1}^\delta = x_k^\delta - (\alpha_k L^{\mathrm{T}} L + F'(x_k^\delta)^{\mathrm{T}} F'(x_k^\delta))^{-1} \times [F'(x_k^\delta)^{\mathrm{T}}(F(x_k^\delta) - y^\delta) + \alpha_k L^{\mathrm{T}} L(x_k^\delta - x_a)], \tag{12}$$

where L is some regularization matrix, (α_k) is a monotonically decreasing sequence and x_a is the a priori state vector, the best beforehand estimate of $\hat{x}$. The iterative process is stopped according to the discrepancy principle (7). Note that x_{k+1}^δ has the variational characterization

$$\mathscr{F}_k^l(x) = \|F(x_k^\delta) - y^\delta + F'(x_k^\delta)(x - x_k^\delta)\|^2 + \alpha_k \|L(x - x_a)\|^2. \tag{13}$$

For a detailed analysis related to convergence results for different source conditions and nonlinearity assumptions on the mapping F we refer to [4–7]. A priori information like measures of solution magnitude and smoothness can be incorporated in the regularization matrix in order to stabilize the iterative process. The regularization matrix L is typically either the identity matrix ($L = L_0 = I$), a diagonal weighting matrix or a discrete approximation to the first ($L = L_1$) or second ($L = L_2$) derivative operator. Combining several derivative orders allows to take into account both types of information simultaneously. In this case the regularization matrix is determined by the Cholesky factorization $L^{\mathrm{T}} L = \sum_{k=0}^{2} w_k L_k^{\mathrm{T}} L_k$ with $w_k \geqslant 0$ and $\sum_{k=0}^{2} w_k = 1$. The weighting factors w_k are chosen in accordance with the peculiarities of the solution. The sequence of regularization parameters (α_k)

is constructed as suggested in [14,15],

$$\alpha_k = \beta\alpha_k^{LC} + (1-\beta)\alpha_{k-1}, \quad 0 \leqslant \beta \leqslant 1, \tag{14}$$

where α_k^{LC} is the regularization parameter for the linear subproblem (13) chosen by the L-curve criterion [16]. This parameter choice method allows enough regularization to be applied at the beginning of iterations and then to be gradually decreased. A numerical robust method for computing the new iterate x_{k+1}^δ and the regularization parameter α_k^{LC} relies on the use of the generalized singular value decomposition of the Jacobian and the regularization matrix [16].

3.3. The Levenberg–Marquardt Method

In the LMM the term $(F'(x_k^\delta)^{\mathrm{T}}F'(x_k^\delta))^{-1}$ in (5) is replaced by $(\alpha_k I + F'(x_k^\delta)^{\mathrm{T}}F'(x_k^\delta))^{-1}$, which results in the method

$$x_{k+1}^\delta = x_k^\delta - (\alpha_k I + F'(x_k^\delta)^{\mathrm{T}}F'(x_k^\delta))^{-1}F'(x_k^\delta)^{\mathrm{T}}(F(x_k^\delta) - y^\delta). \tag{15}$$

For comparison with the iteratively regularized GNM (13), we note that x_{k+1}^δ has the variational characterization

$$\mathscr{F}_k^l(x) = \|F(x_k^\delta) - y^\delta + F'(x_k^\delta)(x - x_k^\delta)\|^2 + \alpha_k\|x - x_k^\delta\|^2. \tag{16}$$

From (16) we see that the LMM does not take into account a priori information about the smoothness of the solution.

In conventional software packages (cf., e.g., [10]) the regularization parameter α_k is selected on the grounds of a trust region strategy. If the trust region (in which the linearized functional is minimized) is a sphere of radius ρ_k, and $x_{k,\alpha}^\delta$ denotes the minimizer of $\mathscr{F}_k^l(x)$ for a given parameter α, then the regularization parameter α_k is chosen as the solution of the secular equation

$$\|x_{k,\alpha}^\delta - x_k^\delta\| = \rho_k \tag{17}$$

and the new approximation is defined as $x_{k+1}^\delta = x_{k,\alpha_k}^\delta$. Note that among all x with $\|x - x_k^\delta\| \leqslant \rho_k, x_{k,\alpha_k}^\delta$ is the unique minimizer of $\|F(x_k^\delta) - y^\delta + F'(x_k^\delta)(x - x_k^\delta)\|$. The radius ρ_k of the trust region is modified so that the objective function decreases for each iteration and the linear model is accurate within the trust region. The difficulty of this approach is an appropriate strategy for choosing ρ_k which must rely on heuristic considerations. For the conventional implementation it is not clear what kind of stopping rule would be appropriate for ill-posed problems. In our implementation the convergence of iterates is used as stopping criteria. Note that the iterates of the Levenberg–Marquardt algorithm converges to a minimizer of (4) if the data $y = F(\hat{x})$ are given exactly but the sequence cannot converge if no solution of $y^\delta = F(x)$ exists.

The regularizing LMM copes with the ill-posedness of the problem and selects the regularization parameter α_k from a trust region approach for the error $\varepsilon_k = y^\delta - y + \mathscr{R}(x_k^\delta, \hat{x})$ rather some trust region around x_k^δ [9]. Here

$$\mathscr{R}(x_k^\delta, \hat{x}) = F(\hat{x}) - F(x_k^\delta) - F'(x_k^\delta)(\hat{x} - x_k^\delta)$$

denotes the Taylor remainder for the linearization around x_k^δ. With ς being a positive parameter, $\varsigma < 1$, the actual regularization parameter α_k will be determined from

$$\|F(x_k^\delta) - y^\delta + F'(x_k^\delta)(x_{k,\alpha}^\delta - x_k^\delta)\| = \varsigma\|F(x_k^\delta) - y^\delta\|. \tag{18}$$

Among all x with

$$\|F(x_k^\delta) - y^\delta + F'(x_k^\delta)(x - x_k^\delta)\| \leqslant \varsigma \|F(x_k^\delta) - y^\delta\|,$$

x_{k,α_k}^δ is the unique element of minimal norm. This choice of α_k leads to a stable approximation of $\hat{x}$, provided that the discrepancy principle (7) is choosen as stopping rule, and some nonlinearity assumptions on the mapping F are satisfied [9].

Because the regularizing LMM does not take into account a priori information about the smoothness of the solution, an a posteriori technique for improving the inversion performance can be given as follows:

(1) Let $x_{k_*}^\delta$ be the solution obtained by using the discrepancy principle. Smooth the solution by using Tikhonov regularization, that is, determine x_{smooth}^δ by minimizing the objective function

$$\mathscr{F}(x) = \|x - x_{k_*}^\delta\|^2 + \alpha \|L_2 x\|^2, \qquad (19)$$

where α is chosen according to the L-curve criterion [16].

(2) Choose x_{smooth}^δ as initial guess and restart the algorithm.

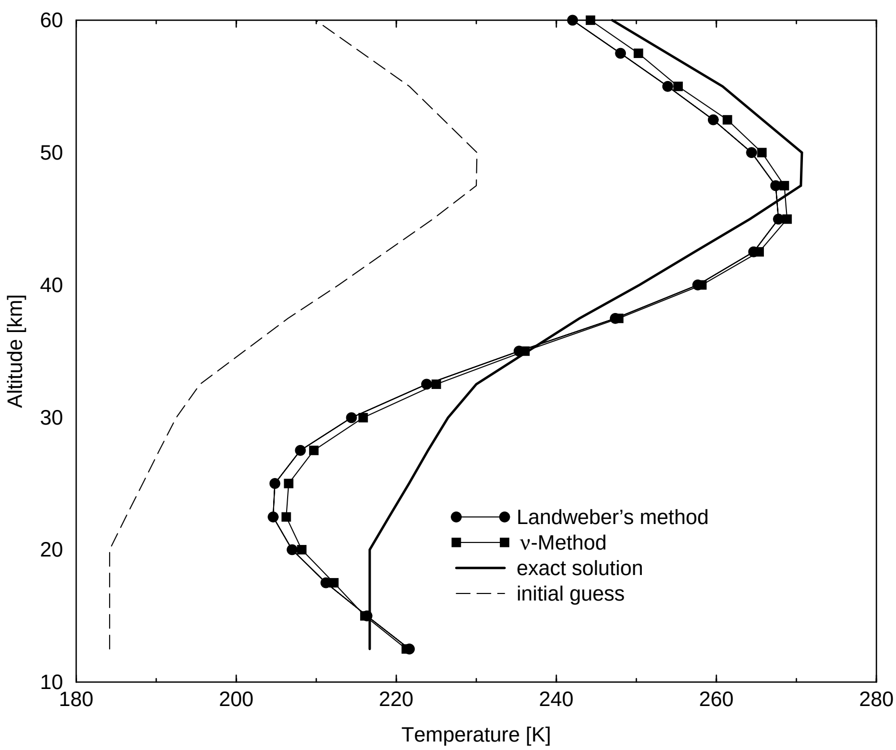

Fig. 1. Result of temperature retrieval using LwM and the νM for a signal-to-noise ratio of SNR = 100.

4. Numerical simulations

The background of our simulations is a study on the feasibility of (stratospheric) temperature retrievals from high-resolution far-infrared spectra observed by an airborne instrument. Far-infrared spectroscopy offers superior means to measure numerous stratospheric species from airborne, balloonborne, or spaceborne platforms (cf., e.g. [17]). The atmospheric spectrum is characterized by individual lines due to pure rotational transitions while the line profile is dominated by pressure broadening up to the stratosphere. Furthermore, aerosol scattering effects are negligible.

Ideally the (discretized) profile of the particular gas under investigation is the only unknown of the inverse problem. Unfortunately, as indicated by Eqs. (1) and (2) the atmospheric spectrum depends on pressure, temperature, and other gases with nonnegligible contributions in the selected spectral range, i.e., the state vector x comprises discretized representations of all these profiles. Thus, in order to keep the number of unknowns reasonably small (and hence the condition of the problem) assumptions have to be made on pressure, temperature and interfering species profiles. In practice these profiles are taken from climatological datasets, etc. Nevertheless, in view of the dominating role of temperature in the infrared, a better knowledge of the actual temperature profile would be advantageous for remote sensing of atmospheric composition.

Here the assessment of high-resolution far-infrared temperature soundings serves as an exemplary study to analyze the performance of iterative regularization methods. The synthetic

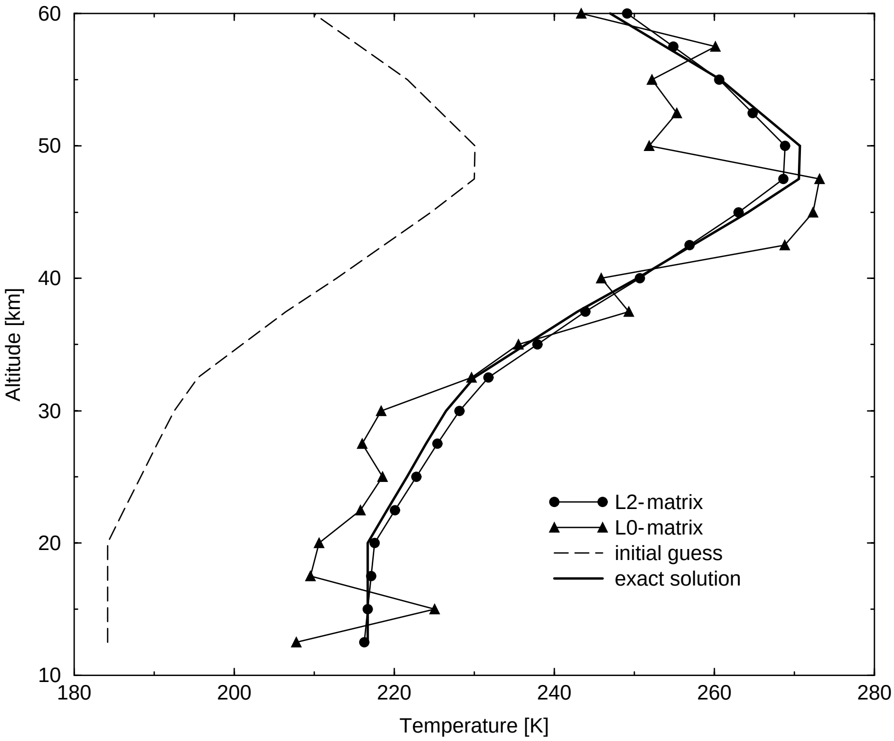

Fig. 2. Result of temperature retrieval using the iteratively regularized GNM with $L = L_0$ and $L = L_2$ (SNR = 100).

measurement spectrum used in this retrieval study largely resembled typical THOMAS observations made aboard the DLR research aircraft FALCON [18]. The 2.5 THz OH Measurement Airborne Sounder THOMAS is a high-resolution heterodyne spectrometer measuring the atmospheric thermal emission in the far-infrared. The dominant spectral signatures in the observed spectral region are due to the hydroxyl radical (a rotational line triplet at 83.869 cm^{-1}), water vapor (nb. the wing of a strong line at about 84.456 cm^{-1}), and ozone. An observer altitude of 12 km and a pointing angle of 80° from zenith has been assumed in these simulations. A radiance spectrum (1) of $m = 200$ data points between 83.84 and 83.88 cm^{-1} was simulated using a line-by-line atmospheric radiative transfer code [19]. Because water vapor, ozone, and the hydroxyl radical are dominant in the observed spectral region, no other gases were considered. Note that in the far-infrared highly altitude-dependent pressure broadening is dominant in the troposphere and stratosphere, whereas Doppler broadening is dominant in the upper atmosphere. The exact atmospheric temperature profile $\hat{x}$ as well as p, H_2O, O_3, and OH data were taken from the US standard atmosphere. For the exact temperature profile a noise contaminated spectrum with a signal-to-noise ratio of 100 and 1000 was generated. Here the signal-to-noise ratio is defined as $\mathrm{SNR} = \|y^\delta\|/(\sigma\sqrt{m})$.

The state vector x was selected as a discretized representation of the temperature profile assuming a vertical grid with 2.5 km spacing. The a priori and initial profile of temperature x_a and x_0^δ, respectively, were assumed to be identical and were choosen as a scaled version of the exact profile by a factor of 0.85, i.e., $x_a = x_0^\delta = 0.85\hat{x}$.

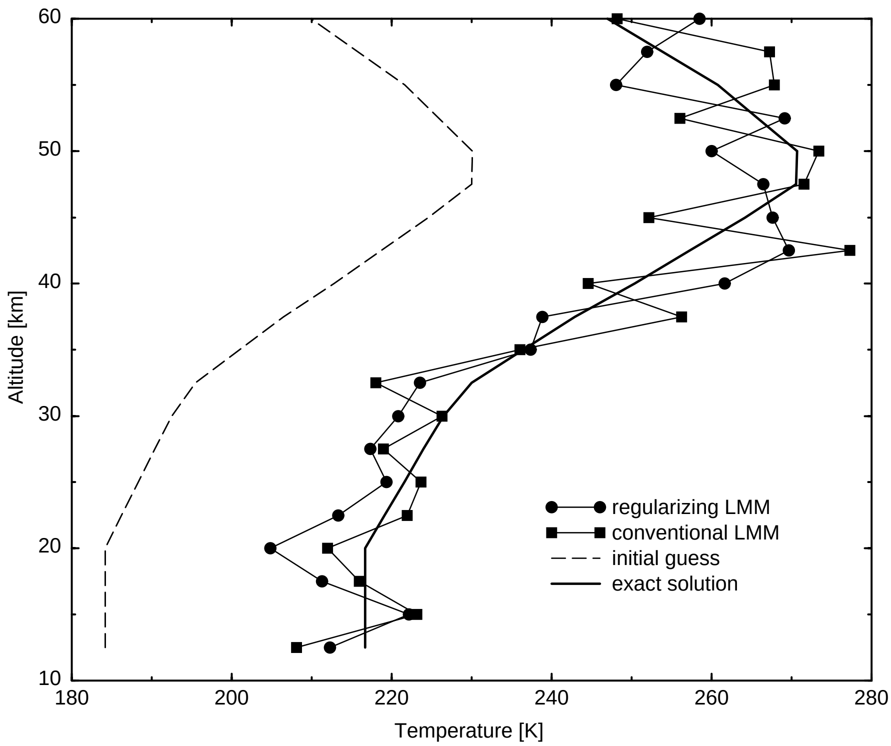

Fig. 3. Result of temperature retrieval using the LMM (SNR = 100).

Table 1
Relative errors $\varepsilon = \|\hat{x} - x_{k_*}^{\delta}\|/\|\hat{x}\|$ and iteration count n for Landweber's method (LwM), the modified ν-method (νM) the iteratively regularized Gauss–Newton method (GNM) with $L = L_0$, and $L = L_2$, and the conventional and regularizing Levenberg–Marquardt method (LMM)

	LwM	νM	GNM-L_0	GNM-L_2	LMM-conv.	LMM-reg.
ε (%)	3.48	3.09	3.21	0.5	3.48	3.10
n	97	53	5	3	10	6

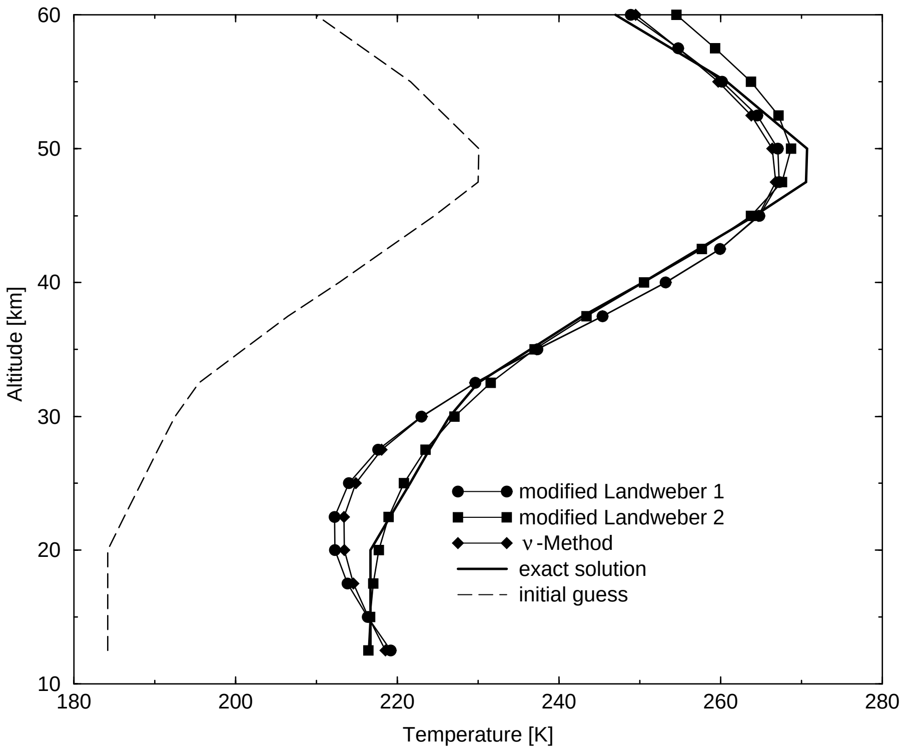

Fig. 4. Result of temperature retrieval using the modified LwMs and the νM (SNR = 1000).

The problem is moderately nonlinear. In order to indicate the nonlinearity of the problem we mention that the Euclidian norms of the Jacobian K at two different states, one of which corresponds to the exact solution $\hat{x}$ and the other to the initial guess x_0^{δ} are 351.15 and 420.26, respectively.

The retrieved profiles for a signal-to-noise ratio of 100 are plotted in Figs. 1–3. The relative errors $\varepsilon \equiv \|\hat{x} - x_{k_*}^{\delta}\|/\|\hat{x}\|$, and the iteration count are shown in Table 1. The parameter ν for the modified ν-method was choosen as 0.75, while the conventional Levenberg–Marquardt algorithm

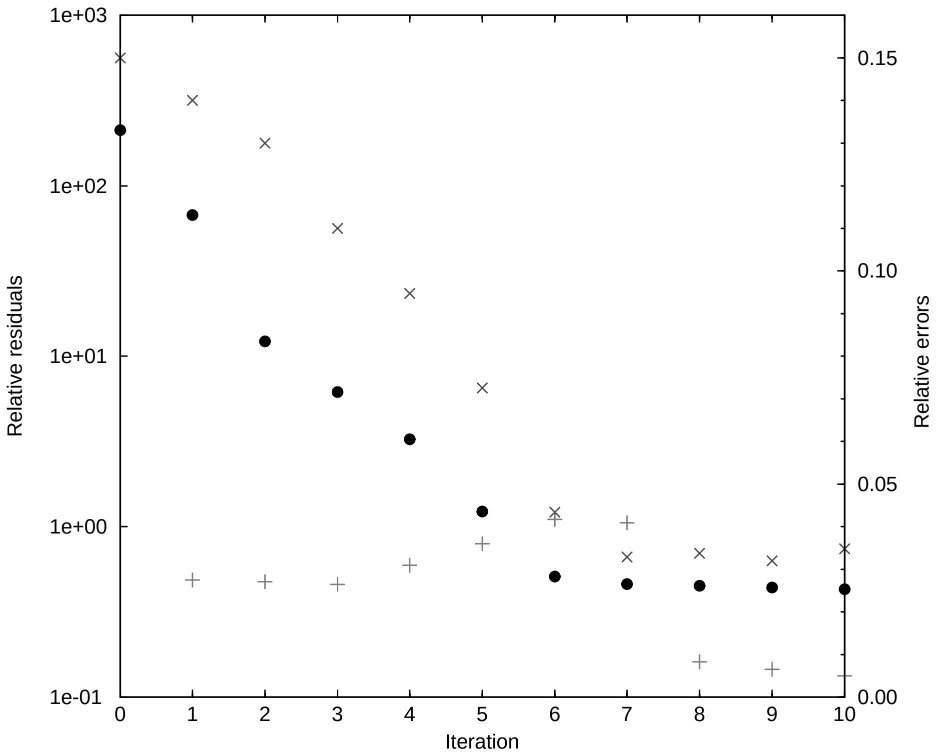

Fig. 5. History of the relative residuals $\mathscr{F}_{\rm r}=\mathscr{F}(x_k^\delta)/(m\sigma^2)$ (filled circles), the relative change of iterates $\varepsilon=\|x_k^\delta-x_{k-1}^\delta\|/\|x_k^\delta\|$ (+), and the relative errors $\varepsilon=\|\hat{x}-x_{k_*}^\delta\|/\|\hat{x}\|(\times)$ for the conventional LMM.

was stopped when the relative change of iterates $\varepsilon\equiv\|x_k^\delta-x_{k-1}^\delta\|/\|x_k^\delta\|$ was smaller than 0.5%. The modified ν-method gives comparable accuracy as Landweber's method but the speed of convergence is faster. The iteratively regularized Gauss–Newton solution with $L{=}L_0$ and the Levenberg–Marquardt solutions show pronounced oscillations. These results are a consequence of the algorithms' inability to account for the smoothness of the exact solution. In this context, the behavior of the exact solution can at best be reproduced by the iteratively regularized GNM with the L_2 regularization matrix. Note that oscillations in the upper atmosphere are also related to the reduced altitude information due to the dominant Doppler broadening.

The modified ν-method appears to be a regularization method for the nonlinear problem under examination. The relative error decreases from 3.09% to 1.34% if the signal-to-noise ratio increases from 100 to 1000. We mention that essentially the inversion performances of the modified Landweber methods are similar to that of the modified ν-method. The retrieved profiles for a signal-to-noise ratio 1000 are plotted in Fig. 4.

The conventional LMM gives comparable accuracy as the regularizing scheme. Because in the conventional implementation the choice of an appropriate stopping rule is an interesting open problem, we show in Figs. 5 and 6 the history of the relative residuals $\mathscr{F}_{\rm r}\equiv\mathscr{F}(x_k^\delta)/(m\sigma^2)$, the relative change of iterates ε and the relative errors ε. The conventional algorithm was stopped after 10

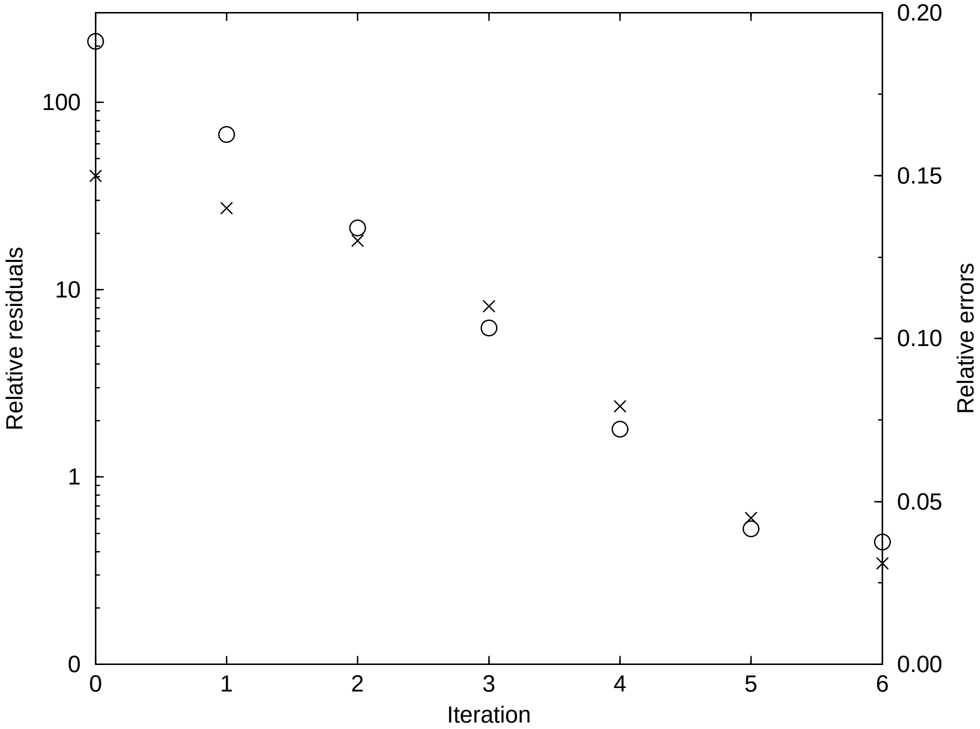

Fig. 6. History of the relative residuals $\mathscr{F}_{\mathrm{r}} = \mathscr{F}(x_k^\delta)/(m\sigma^2)$ (circles), and the relative errors $\varepsilon = \|\hat{x} - x_{k_*}^\delta\|/\|\hat{x}\|(\times)$ for the regularizing LMM.

iterations when $\varepsilon \leqslant 0.5\%$. In this case the relative error with respect to the exact solution was 3.48%. If the algorithm would be stopped according to the discrepancy principle (i.e., after 7 iterations when $\mathscr{F}_{\mathrm{r}} < 0.5$) the relative error would be about 3.29% and the computational effort would be substantially reduced.

In Fig. 7 we show the solutions that were obtained by smoothing the regularizing Levenberg–Marquardt solutions, cf. (19). The solutions correspond to two values of the signal-to-noise ratio, SNR = 100 and SNR = 1000. The relative errors decrease from 3.10% to 1.44% for SNR = 100 and from 1.87% to 0.75% for SNR = 1000.

5. Conclusions

The computational performance and accuracy of a variety of iterative regularization methods has been investigated numerically for an atmospheric retrieval problem.

Landweber's method (LwM) and its modified versions lead to smooth solution with comparable accuracy. The computer time of the modified ν-method is lower than that of LwM, but the speed of convergence is not significantly faster as in the linear case. We mention that in the linear case the number of iterations can be reduced to about the square root. The numerical analysis indicated

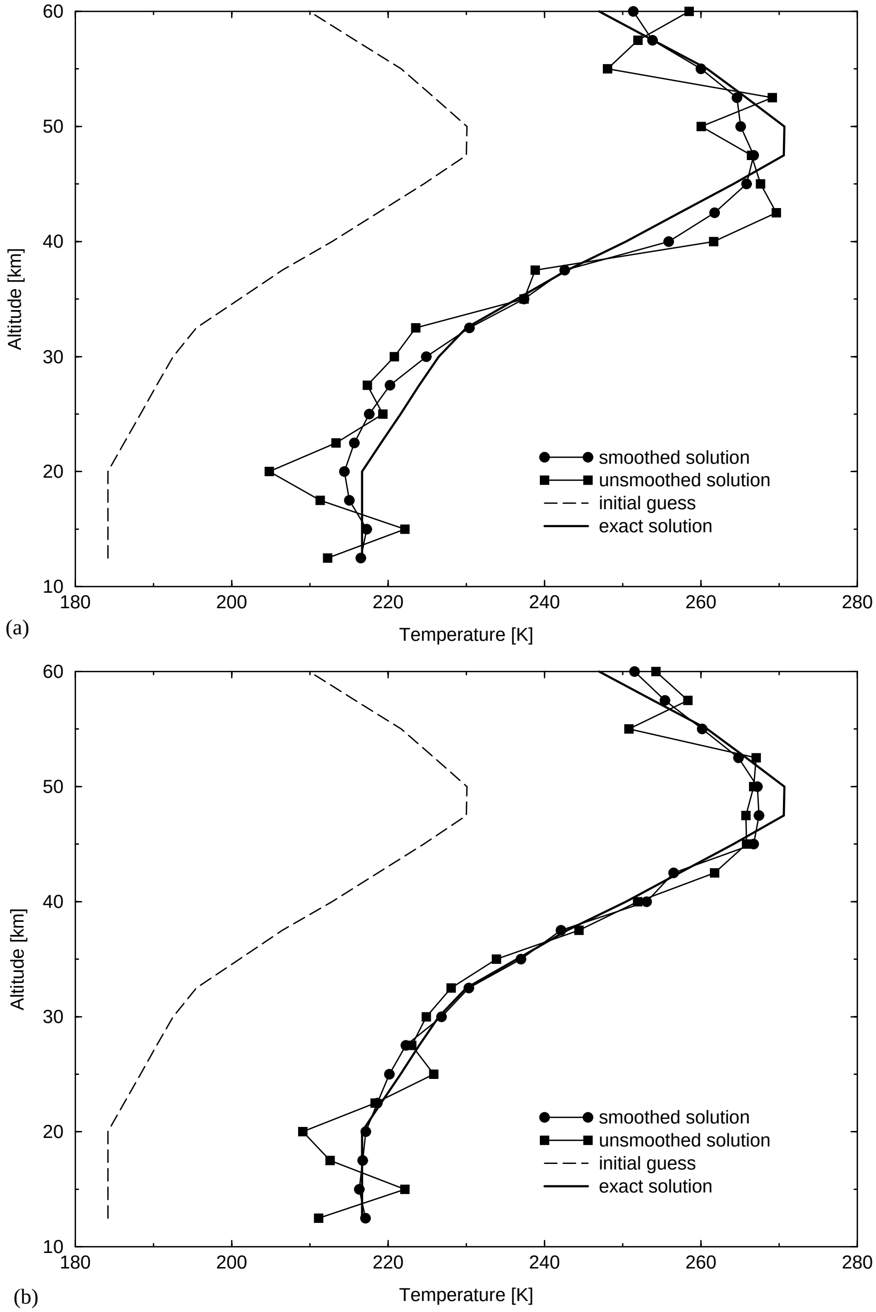

Fig. 7. Result of temperature retrieval using the regularizing LMM and the smoothing procedure: (a) SNR = 100 and (b) SNR = 1000.

that the modified ν-method combined with the discrepancy principle as an a posteriori stopping rule acts like a regularization method. Nevertheless, a rigorous proof of this result requires further investigations.

The iteratively regularized Gauss–Newton method (GNM) is the most efficient method due to its reduced computer time and high inversion performances. Various a priori information like magnitude and smoothness of the solution or 'incomplete' statistical information can be incorporated in the regularization matrix to obtain accurate results [15].

The numerical simulations demonstrated that the regularizing version of the Levenberg–Marquardt method (LMM) converges faster than the conventional approach. The explanation lies in the fact that the regularization parameter is chosen from two different adaptive strategies. However, the differences between the reconstruction performances are not significant, at least for the particular example consider in Section 4. The simulations indicate that the discrepancy principle can be used in the conventional implementation without any loss of solution accuracy. Whether the conventional LMM with the discrepancy principle as an a posteriori stopping rule is a regularization method remains to be clarified. A technique for improving the inversion performances of the regularizing LMM was also presented. This method relies on the use of Tikhonov regularization to smooth the solution.

The essential conclusion to be drawn is that the iteratively regularized GNM is an efficient candidate for regularizing ill-posed inverse problems in atmosphere remote sensing.

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