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Bayesian approach to retrieval of vertical ozone profile from radiometry data

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Abstract

A technique for retrieving vertical distributions (profiles) of atmospheric gas constituents from data of passive remote sensing of the atmosphere is proposed. The goal of the technique based on the statistical (Bayesian) approach to solution of inverse problems is construction of probability distribution for a sought quantity throughout the interval of the studied heights. It is assumed that initial data contain measurement noise, and a priori information about properties of the profile is used. It is proposed to approximate the sought profile by a function in the form of an artificial neural network. This approximation allows optimal inclusion of a priori information into retrieval procedure, thus ensuring the most effective regularization of the problem. Efficiency of the proposed technique is demonstrated on an example of retrieval of vertical ozone profile from data of ground-based sounding of the atmosphere in the millimeter wavelength range. Results of profile retrieval from model data and from spectra of radiation temperature of the atmosphere measured in the Apatity (67° N, 33° E) in the winter of 2002–2003 are presented.

Keywords: Remote sensing; Retrieval of atmospheric profiles; Incorrect inverse problem; Bayesian approach; Regularization

1. Introduction

Retrieval of vertical distributions (profiles) of atmospheric gas constituents by data of passive remote sensing of the atmosphere is known to be an incorrect inverse problem that requires solution of a nonlinear integral equation (Mocheneva et al., 1995). It is regarded to be incorrect as inaccuracy in specifying initial data due to their discreteness and presence of a noise component gives an infinite set of possible solutions, whereas there exists exact solution of the unperturbed problem and it is unique. Success and fidelity of retrieval depend on the following factors. First, it is a correct strategy of seeking solutions, i.e., physically justified formulation of likelihood test of one or another altitudinal distribution. The chosen strategy should ensure adequate evaluation of uncertainty (error) of retrieval without systematic bias. Second, it is correct allowance for various a priori information about the properties of the sought profile. This information has to be used for limitations of permissible properties of the sought solutions. As most restrictions of this kind inevitably lead to systematic error of retrieval, proper use of a priori information should minimize this error. Thus, development of a universal technique that would enable one to retrieve and, which is no less important, to represent correctly maximum complete information about a sought profile from data in combination with physically justified a priori information is a topical and important task.

The most frequently used methods of retrieval of atmospheric profiles are based on construction of a cost function, minimization of which solves the formulated problem. This function is usually a sum of squared errors and of a term setting a priori restrictions. The retrieval methods differ primarily by the type of regularization,

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i.e., by the form of the latter term. For example, in the technique (Phillips, 1962), which imposes the condition of a smoothness of retrieved profile (Tikhonov type regularization (Tikhonov, 1963)), the regularization term is proportional to average square of the first (or second) altitudinal derivative of solution, with rigidity of regularization chosen from the condition of equality of root mean square error to measurement noise that is regarded to be known. Such a noise-dependent choice of rigidity of a priori restrictions (referred to as "a posteriori choice" (Kuntz et al., 1999)) leads to uncontrolled systematic error that may be appreciable at sufficiently high noise. In other words, smoothness conditions are frequently too rigid, so that the algorithm is not sensitive to abrupt changes in the retrieved dependence. Another method, proposed and developed in the works (Strand and Westwater, 1968; Rodgers, 1976) uses for regularization *prior* statistics accumulated from previous measurements. This method gives unbiased solution and correct evaluation of retrieval error only if the statistics is sufficiently rich, i.e., it includes all physically possible variations of profile. Otherwise, "false" statistics "attracts" a solution "towards" a priori profile and thereby evokes systematic error which is especially weighty in the presence of various anomalies in the sought distribution, for example, when attempting to detect profile perturbations arising as a result of ozone hole formation. On the other hand, such statistics is far from always available for specific geographical location. Note also that in the greatest majority of available techniques piecewise-homogeneous (or piecewise-linear) approximation of the profile is employed, which strongly restricts usage of diverse a priori information.

Thus, the above methods are aimed at finding a unique optimal solution and have to be supplemented by analysis of retrieval errors that is a nontrivial task. This issue was addressed in ample detail in (Rodgers, 1990, 1998), where retrieval errors were analysed for linear and weakly nonlinear problems, i.e., when nonlinearity is insignificant within the error interval and equations may be linearized with respect to perturbations of the solution. However, in a number of cases nonlinearity is sufficiently strong, firstly, due to a high level of measurement noise in data obtained in experiments, which is typical of ground-based radiometric measurements and, secondly, because of nonlinear representation (approximation) of the solution. We will show below that such a representation is beneficial in terms of regularization.

We propose a retrieval method based on probabilistic representation of solution, that is most appropriate in the case of essentially nonlinear problem. The main idea of the underlying approach (Turchin et al., 1970) is that random error of experimental data should ensure random error of finding a sought profile, thus demanding statistical description of the solution. Within the framework of this approach noise distribution that is regarded to be known is recalculated to probabilistic distribution of the retrieved dependence (*posterior* distribution) in accord with the Bayes theorem, hence the approach is referred to as the Bayesian approach to solution of inverse problems (Turchin et al., 1970). Solution of the problem is, thus, a statistical ensemble of profiles distributed in compliance with the found *posterior* probability density function. Statistical analysis (we use the MCMC method (Gilks and Wild, 1992)) of this ensemble allows calculation of confidence intervals of the sought quantity with preset probability, hence giving an adequate representation of the solution (retrieval accuracy is evaluated automatically), provided that a priori restrictions are correct. In what will follow we will show to what the profiles retrieved by the above mentioned techniques (Phillips, 1962) and (Rodgers, 1976) correspond within the framework of the Bayesian approach (see expressions (4) and (5)). The descriptions of different techniques within the framework of the same (Bayesian) approach allow their direct comparison. An example of such comparison is presented in Section 3.

A priori restrictions dictated by incorrectness of the problem enter the resulting distribution as a separate co-factor – *prior* probability distribution function that specifies an ensemble of acceptable profiles. Besides these a priori restrictions, problem regularization depends also on the properties of the function used for profile approximation. As was noted above, the majority of traditional methods adopt piecewise approximations, with smoothness of the retrieved profiles determined by the number of layers used for altitudinal partitioning of the atmosphere.

We propose to approximate the function in the form of an artificial neural network (ANN) (Arbib, 1995) that is a superposition of a definite number of strongly nonlinear functions (neurons). It was demonstrated (Hornik et al., 1989) that such a function is a universal approximator, i.e., it approximates an arbitrary smooth dependence with preset accuracy. We will show on model examples that the ANN approximation is preferable to the piecewise approximations because it allows one to use in full measure available a priori information about the profile. The latter is especially significant when such information is scanty, for instance, when statistics of earlier measurements is not available.

The paper has the following architecture. In the first part we briefly describe the proposed technique for solution of inverse retrieval problems and detail the algorithm of constructing *posterior* probability density. The second part of the paper is concerned with methods of problem regularization and capabilities of the technique for retrieving vertical distribution of ozone from the self-radiation spectra of the atmosphere in the millimeter wavelength range. We present results of retrieval by both, model data and spectra measured in the Apatity (67° N, 33° E) in the winter of 2002–2003. To conclude we give a brief resume of the results obtained.

2. Bayesian approach

The used experimental data is the spectrum of atmosphere self-radiation $T_i(f_i)$, $i = 1,\ldots,n$, where f_i is the frequency of the ith frequency channel and n is the number of used frequencies. Retrieved function $N(z)$ (e.g., vertical distribution of ozone concentration) is related to the measured quantity by the known integral relationship J solving a direct problem:

$$T_i = J(N(z), f_i) + \xi_i, \tag{1}$$

where ξ is measurement error. According to the Bayesian approach (Turchin et al., 1970) we need to construct a likelihood function $P_{\mathrm{ps}}(.)$ of different $N(z)$, i.e., a probability density function of the sought dependence $N(z)$ under the condition of experimental data T_i (*posterior* probability density). Following the Bayes theorem this function is proportional to two co-factors:

$$P_{\mathrm{ps}}(N(z) \mid T_i(f_i)) \propto P(T_i(f_i) \mid N(z)) \times P_{\mathrm{pr}}(N(z)). \tag{2}$$

The first co-factor $P(T_i|N)$ is the conditional probability density of realization of experimental data T_i for the given profile $N(z)$. Clearly, this function is determined by probabilistic error distribution ξ that is usually assumed to be normal and uncorrelated (i.e. with diagonal covariance matrix), with known root-mean-square deviation σ_ξ corresponding to measurement error: $P_\xi(\xi) \propto \exp\left(-\frac{\sum_i \xi_i^2}{2\sigma_\xi^2}\right)$. Under this assumption, density function of conditional probability of the data on problem parametrization, i.e., after approximation of $N(z)$ by a function of a definite form with vector of the parameters $\boldsymbol{\mu}$, takes on the form

$$P(T_i(f_i) \mid N(z, \boldsymbol{\mu})) = P(T_i(f_i) \mid \boldsymbol{\mu}) \propto \exp\left(-\frac{\sum_i (T_i - J(\boldsymbol{\mu}, f_i))^2}{2\sigma_\xi^2}\right). \tag{3}$$

The used parametric representation of a profile introduces a priori constraints on a class of admissible solutions determined by the properties of approximation function $N(z,\boldsymbol{\mu})$ and described by *prior* probability density $P_{\mathrm{pr}}(\boldsymbol{\mu}) = P_{\mathrm{pr}}(N(z,\boldsymbol{\mu}))$. The sought *posterior* distribution then takes on the form

$$P_{\mathrm{ps}}(\boldsymbol{\mu} \mid T_i(f_i)) \propto P(T_i(f_i) \mid \boldsymbol{\mu}) \times P_{\mathrm{pr}}(\boldsymbol{\mu}). \tag{4}$$

Note that the optimal value of parameter vector $\boldsymbol{\mu}$ providing the maximum of distribution (3) corresponds to the minimum *nonlinear* least-squares error. There may arise a difficulty in using this distribution because the problem to be solved is ill-conditioned: a *set* of $\boldsymbol{\mu}$ corresponds to the maximum of function (3). Consequently, the class of the sought solution should be additionally defined making use of complementary a priori information about the profile features, for which the second co-factor in the expression (4) is responsible. This co-factor is probability density of *prior* distribution of profiles that selects an ensemble of possible solutions among the set of profiles (3). Both, using approximation $N(z,\boldsymbol{\mu})$ and introduction of such a priori ensemble provide problem regularization in the statistical formulation. In the section to follow we will describe a method of constructing *prior* distribution of parameters $P_{\mathrm{pr}}(\boldsymbol{\mu})$ for the parametrization using ANN.

Further analysis of the obtained *posterior* distribution (4) employing the proposed technique is the following. An ensemble of vector parameters $\boldsymbol{\mu}$ distributed in conformity with the constructed function (4) is generated using the MCMC method (Gilks and Wild, 1992). Apparently, this ensemble determines *posterior* distribution of possible profiles $N(z) = N(z,\boldsymbol{\mu})$. Further, by the ensembles of the sought dependence $N(z,\boldsymbol{\mu})$ at each height z we calculate boundaries of confidence intervals for N with a preset probability level.

Note that in constructing function (4) we did not take into consideration error of the parameters entering integral functional J from expression (1). When atmospheric profiles are retrieved from spectroscopic data, such parameters may be, for instance, atmospheric pressure and temperature profiles. We will show how inaccurate knowledge of parameters of functional J (we will call them $\mathbf{b}$) may be taken into account employing the Bayesian approach. For this we have to assume a priori statistics $P_b(\mathbf{b})$ that determines error distribution in determining $\mathbf{b}$. *Posterior* distribution (4) becomes conditional relative to $\mathbf{b}$: $P(\boldsymbol{\mu}|T_i(f_i)) \rightarrow P(\boldsymbol{\mu}|T_i(f_i),\mathbf{b})$. Then, the sought *posterior* distribution of parameters $\boldsymbol{\mu}$ may be written in the form

$$P(\boldsymbol{\mu} \mid T_i(f_i)) = \int_{-\infty}^{\infty} P(\boldsymbol{\mu} \mid T_i(f_i), \mathbf{b}) P_b(\mathbf{b})\, \mathrm{d}\mathbf{b}. \tag{5}$$

Depending on a specific problem, the integral in (5) may be calculated either analytically or numerically, for example by the Monte-Carlo method (the latter demands an ensemble of $\mathbf{b}$ distributed in accord with $P_b(\mathbf{b})$).

Let us consider the earlier techniques mentioned in the introduction in terms of the Bayesian approach. These techniques employ piecewise approximation of the profile; therefore, the parameter vector is a set of values N_j on a certain grid z_j.

Within the framework of Tikhonov's technique (Tikhonov, 1963) a profile corresponding to the minimum of cost function $\chi^2 = \sum_i (T_i - J(N, f_i))^2 + \alpha \sum_j (N'_{jz})^2$ is sought (here $(N'_{jz})^2$ is the square of the first derivative of $N(z)$ at point z_j). Parameter α is found from the condition of equality of r.m.s. error to noise dispersion σ_ξ^2. According to the Bayesian approach this cost function corresponds to the distribution

$$P(\mathbf{N} \mid T_i) \propto \exp\left(-\frac{\sum_i (T_i - J(\mathbf{N}, f_i))^2}{2\sigma_\xi^2}\right) \times \exp\left(-\alpha' \sum_j \left(N'_{jz}\right)^2\right), \tag{6}$$

i.e., *prior* distribution (the second co-factor) is a gaussian distribution of the first derivatives of the profile with dispersion determined by regularization parameter α' that is chosen a priori and must be physically justified. It should be emphasized that a posteriori choice of this parameter in Tikhonov's technique (Phillips, 1962) is incorrect from the point of view of the Bayesian approach.

In the technique proposed by Rodgers (1976) the cost function of the form $\chi^2 = \sum_i \frac{1}{\sigma_\xi^2}(T_i - J(\mathbf{N}, f_i))^2 + (\mathbf{N} - \mathbf{N_a})^{\mathbf{T}}\mathbf{C}^{-1}(\mathbf{N} - \mathbf{N_a})$ is optimized. Here, $\mathbf{N}_a$ is the vector corresponding to *prior* profile, $\mathbf{C}$ is *prior* covariance matrix of different layers N_j. Then, the probability density function is written in the form

$$P(\mathbf{N} \mid T_i) \propto \exp\left(-\sum_i \frac{1}{2\sigma_\xi^2}(T_i - J(\mathbf{N}, f_i))^2\right) \times \exp\left(-(\mathbf{N} - \mathbf{N_a})^{\mathbf{T}}\mathbf{C}^{-1}(\mathbf{N} - \mathbf{N_a})\right), \tag{7}$$

i.e., *prior* probability density is gaussian with mean vector $\mathbf{N}_a$ and covariance matrix $\mathbf{C}$. Analysis of expression (7) by the Monte-Carlo method may be useful when rich a priori statistics is available for $\mathbf{C}$ and function J is essentially nonlinear.

Solutions obtained by these techniques in traditional (not statistical) representation correspond to maxima of the distributions (6) and (7).

3. Retrieval of ozone profile from data of millimeter measurements

Consider the problem of retrieving vertical ozone profile from data of passive ground-based remote sensing of the atmosphere in the millimeter wavelength range. Experimental data for retrieval is a spectrum of atmospheric radiation temperature in the frequency band corresponding to one of the lines of ozone self-radiation. The data are first preprocessed, when the ozone radiation spectrum is separated from the background formed by radiation of oxygen and water vapor. The direct problem (calculation of ozone radiation spectrum by a known concentration profile) is solved by the following nonlinear integral equation

$$T_{\mathrm{r}}(f_i) = \int_0^\infty N(z)t(z)K(z, f_i) \times \exp\left\{-\int_0^z N(z')K(z', f_i)\,\mathrm{d}z'\right\}\mathrm{d}z. \tag{8}$$

This equation models the collision mechanism of line broadening (Mocheneva et al., 1995) that is valid for the heights up to approximately 70 km, while higher it is replaced by the Doppler mechanism. In (8), $N(z)$ is the dependence of ozone concentration on height, $t(z)$ is the altitude profile of the temperature, and $K(z,f)$ is the effective absorption cross-section of ozone molecule (Waters, 1976). The properties of kernel functions $K(z,f_i)$, as well as arrangement and number of frequency channels f_i determine sensitivity of the equation and, hence, of the retrieval procedure, to different variations of the profile. Altitude dependence of function K is plotted in Fig. 1 for different frequency detuning from the center of the line corresponding to rotational transition of ozone at 101 GHz. Positions of the K maxima demonstrate that solution of equation (8) is sensitive to profile perturbations at altitudes from 20 to 50 km. This means that successful retrieval can be expected within this range of heights.

For parametrization of the retrieved function $N(z)$ we employed the following ANN (Arbib, 1995; Hornik et al., 1989) function

$$N(z, \boldsymbol{\mu}) = \sum_{i=1}^{m} \alpha_i \sigma(w_i z + \gamma_i), \tag{9}$$

where $\boldsymbol{\mu} = \{\boldsymbol{\alpha}, \mathbf{w}, \boldsymbol{\gamma}\}$ is the vector of the parameters. Function $\sigma(.)$ in (9) referred to as activation function ("neuron") may have different forms, depending on the problem. In this work we used

$$\sigma(\cdot) = \tanh(\cdot). \tag{10}$$

Thus, we constructed *posterior* distribution for parameters $\boldsymbol{\mu}$ in compliance with the technique described above.

Let us consider in more detail how *prior* information can be used for retrieval under the approximation (9). Note that definite *prior* information is contained in

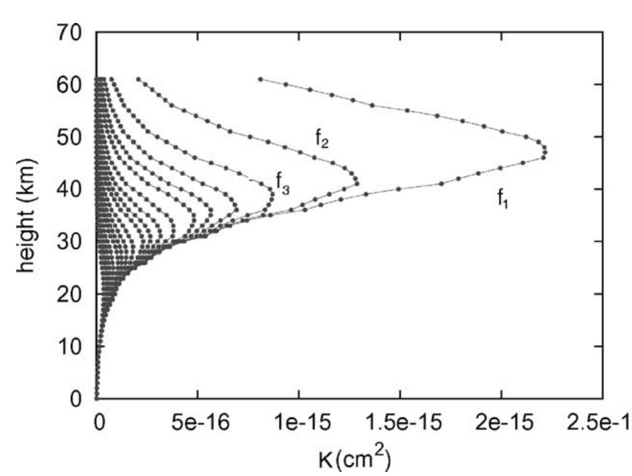

Fig. 1. Effective cross-section of ozone molecule absorption versus height for different frequency channels of the spectrometer.

the ANN function (9), namely, in parameter m that is the number of neurons. As follows from (10), this parameter limits the number of monotonic sections in the profile, thus effectively narrowing the range of admissible solutions. Value of this parameter can be chosen from the very general ideas about the vertical structure of ozone layer. Another kind of *prior* information such as restrictions imposed on the range of variation of concentration N, on profile smoothness and on altitudinal localization of the profile is introduced as *prior* distribution of parameters $\boldsymbol{\mu}$ of the neural network (9). We took gaussian distribution as we had no *prior* preferences for the form of distribution:

$$P_{\text{pr}} \propto \exp\left(-\frac{\|\boldsymbol{\alpha}\|^2}{2\sigma_\alpha^2} - \frac{\|\mathbf{w}\|^2}{2\sigma_w^2} - \frac{\|\gamma\|^2}{2\sigma_\gamma^2}\right). \tag{11}$$

By choosing in a definite manner values of dispersions σ^2 one can impose needed *prior* restrictions on the profile. For example, altitudinal profile localization depends on the $\mathbf{w}$ to γ ratio; altitudinal derivative determining smoothness is dependent on the product of $\mathbf{w}$ and $\boldsymbol{\alpha}$; the range of variation of N depends on $\boldsymbol{\alpha}$. As a result, diverse *prior* information in a convenient form may be used for retrieval, which makes regularization highly efficient.

For demonstration of advantages of the neural network over the piecewise approximations we solved a model retrieval problem. The ozone radiation spectrum calculated from a given profile containing rather sharp changes in ozone concentration (the dots connected by lines in Fig. 2)[1] was perturbed by gaussian white noise with standard deviation of 50% as compared to the signal magnitude "recorded" in the frequency channel farthest from the center of the line. The number and arrangement of frequency channels as well as the noise level in this spectrum corresponded to parameters of the measurements made in the 1998–2003 in the Apatity (67° N, 33° E) by the IAP RAS spectrometer (Kulikov et al., 2003, 2005). Further, from the "obtained" data we reconstructed the initial profile by the Bayes method using the likelihood corresponding to both, Tikhonov-type Philips technique (Phillips, 1962) (Fig. 2) and ANN parametrization (9), (11) (Fig. 3). The number of neurons m in (9) was equal to 7. The curves in Fig. 2 bound confidence intervals, with the probabilities of occurrence of the sought quantity within these intervals being 95% and 65%. Clearly, the use of ANN gives a less estimate bias, as well as better accuracy of retrieval. Specifically, by means of ANN we retrieved with good accuracy a sharp drop of concentration at the height of 28 km. It is worth noting that we used much

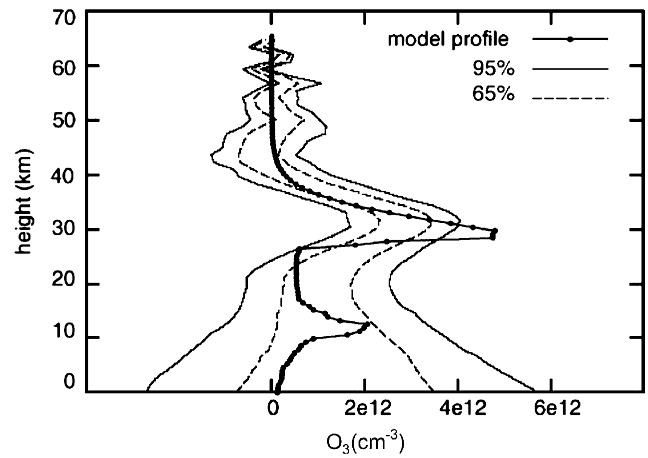

Fig. 2. Results of retrieval by model problem. The line with dots is the model profile; the dashed and solid curves show the boundaries of confidence intervals with probability 65% and 95%, respectively. The piecewise approximation and Tikhonov's regularization were used.

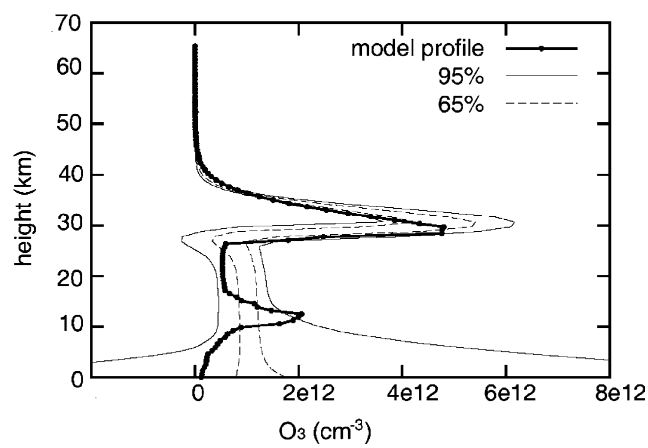

Fig. 3. The same as Fig. 2, but for ANN approximation and regularization (11).

weaker *prior* restrictions of the profile smoothness as compared to Tikhonov's technique.

For demonstration of the technique in application to a real experiment we used data of measurements in the 101 GHz ozone radiation band made in the Apatity in the winter of 2002–2003 by the spectrometer described in the work (Kulikov et al., 2005). The spectrum of ozone radiation temperature T_r shown in Fig. 4[2] was retrieved against the background of radiation of major atmospheric gases (O_2 and H_2O) by subtracting T_r of the atmosphere in the frequency channel that is farthest from the center of the line of all the radiation spectrum of the atmosphere.[3] The integral equation for the direct problem had the following form

[1] Such a profile is formed in the course of appearance of ozone hole in the Polar lower atmosphere (Nardi et al., 1999).

[2] This figure also illustrates arrangement of frequency channels in the spectrometer.

[3] For the considered frequency range (~101 GHz), the radiation spectrum of major constituents of the atmosphere can be regarded to be homogeneous.

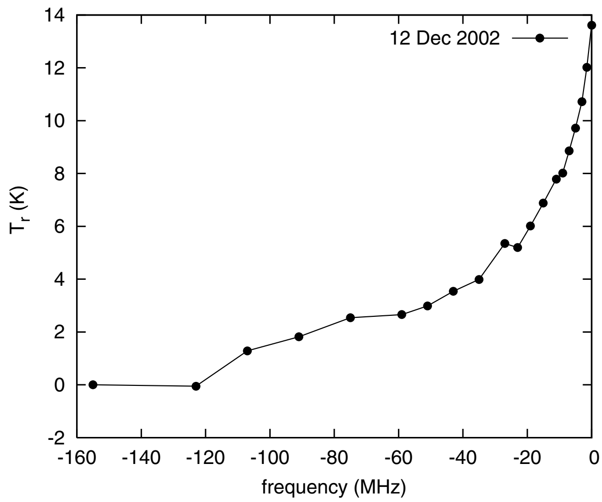

Fig. 4. Left wing of spectra of ozone radiation temperature measured in the Apatity. On the abscissa the frequency detuning from the center of spectral line is plotted.

$$T_i - T_n = J(N(z), f_i) - J(N(z), f_n),$$

where n is the number of the farthest frequency channel. Pressure and temperature profiles of the atmosphere for that day were taken from the MSISE90 model (Hedin, 1991). It was assumed that retrieval error due to inaccuracy of these profiles is negligibly small compared to error introduced by measurement noise and smoothing.

Boundaries of confidence intervals of ozone retrieval with 65% probability level, as well as the ozone profile corresponding to data of the ROSE model (WDC-RSA, 2004) are plotted in Fig. 5. It is clear from the figure that this profile lies within the mentioned boundaries of confidence intervals in a wide range of altitudes.

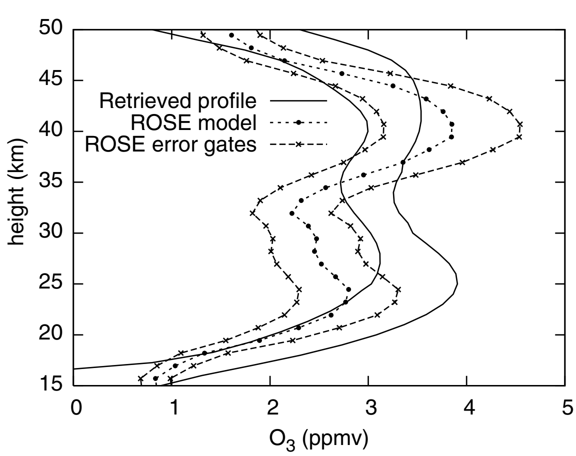

Fig. 5. Result of retrieval of ozone concentration profile from data of measurements in the Apatity in comparison with GOME/ROSE model profile. The boundaries of confidence intervals with probability 65% for suggested ozone concentration retrieval are plotted by solid lines; dashed lines are GOME/ROSE model profile with standard error gates for ROSE model (18% error (WDC-RSA, 2004)).

4. Conclusion

In this work we proposed a universal technique for solution of inverse problems of retrieval of minor atmospheric constituent profiles from ground-based remote sensing data. The technique is aimed at maximum complete retrieving of useful information about the profile by measured data. We adopted statistical (Bayesian) formulation of the problem. Consequently, a solution is *posterior* probability distribution of a sought quantity and is constructed on the basis of statistical properties of noise component in initial data. Analysis of retrieval errors is an integral part of the technique because within the framework of the proposed approach a solution is an error interval (confidence interval) of the sought quantity.

We proposed an original method for parametrization of the problem using approximation of the sought profile by an artificial neural network. The efficiencies of this and piecewise approximation were compared on a model example. It was shown that the proposed parametrization ensures more complete and effective usage of available *prior* information. It was demonstrated that the technique is capable of tracing rather sharp perturbations of the profile.

Finally, ozone profiles were retrieved from ground-based measurements of self-radiation of the atmosphere in the millimeter wavelength range in the Apatity (67° N, 33° E).

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