Retrieving the profiles of stratospheric ozone from lidar sensing data

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In this paper we discuss the application of well-known, mathematically simple smoothing procedures to retrieve vertical distribution of stratospheric ozone from lidar sensing data. The procedures include linear and exponential smoothing, linear approximation, and hybrid algorithms. The vertical ozone profiles, obtained using these techniques, are compared with the ozone profile retrieved using the method of spline approximation, mathematically justified for solving such tasks. Analysis is presented for the mean summer 1998 profiles and their interlevel correlations.

Introduction

Retrieving ozone concentration from differential absorption lidar (DIAL) data is an ill-posed inverse problem. Reference 1 formulates the ill-posed problems and gives general ways of their solution by use of regularization techniques. Applications of the regularization methods and techniques to laser sensing have been described quite thoroughly.[2] Also algorithms that use spline-approximation have been developed intensively to solve ill-posed inverse problems.[3–5] Both of these techniques (regularization and spline-approximation) involve solution of variational problem, in which the construction of functional is performed using the smoothing parameter α that is being chosen according to the accuracy of atmospheric lidar returns.

These methods provide obtaining mathematically reasonable results and they are very useful for reconstructing mean profiles of concentration in a certain altitude interval like in constructing models of vertical ozone distribution in which the key parameter is the accuracy of the initial data.

However, in studying interlevel correlations of the stratospheric ozone there is risk of overestimating the correlation coefficients and, hence, the correlations themselves. This overestimation is an inherent feature of the method of solving the variational problem because of introducing smoothing parameter that *a priori* sets a deterministic relationship in the entire altitude range studied to the extent that is difficult to estimate quantitatively.

These tasks can be solved most efficiently by the methods that can unambiguously identify spatial intervals with the algorithm-induced correlation without the loss of the acceptable solution stability. In these methods, for higher solution stability, the random error of lidar returns is reduced by uniting neighboring spatial intervals. This leads to signal enhancement at the expense of spatial resolution. Similar effect can be achieved by applying linear smoothing to lidar returns.[6,7]

In this paper, we consider some of the simple approaches to smoothing lidar returns used for ozone profile retrieval. The vertical ozone distributions obtained are compared with the ozone profile reconstructed using spline-approximation method, justified for solving problems of differentiation of empirical functions as well as ill-posed inverse problems.

Mathematical formalism and methods of calculation

Mathematically the retrieval of stratospheric ozone profiles $n(H)$ is expressed as follows[8]:

$$n(H) = \frac{1}{\sigma(H)} \left\{ \frac{\mathrm{d}}{\mathrm{d}H} [X(H) + Y(H)] \right\} - Z(H), \quad (1)$$

where

$$X(H) = \ln [\beta_\pi(H, \lambda_{\mathrm{on}})/\beta_\pi(H, \lambda_{\mathrm{off}})];$$

$$Y(H) = \ln [N(H, \lambda_{\mathrm{off}})/N(H, \lambda_{\mathrm{on}})];$$

$\sigma(H)$ is the differential absorption coefficient; $N(H, \lambda_{\mathrm{on}})$ and $N(H, \lambda_{\mathrm{off}})$ are "useful" (i.e., total minus background) lidar return signals at absorbing (λ_{on}) and reference (λ_{off}) wavelengths, respectively; $\beta_\pi(H, \lambda_{\mathrm{on}})$ and $\beta_\pi(H, \lambda_{\mathrm{off}})$ are the backscattering atmospheric properties including both molecular and aerosol components (total backscattering coefficient); and $Z(H) = \alpha(H, \lambda_{\mathrm{on}}) - \alpha(H, \lambda_{\mathrm{off}})$ is the difference between the total extinction coefficients at the corresponding wavelengths. If λ_{on} and λ_{off} differ only a little, the backscattering and extinction coefficient at these wavelengths almost coincide, so that both $X(H)$ and $Z(H)$ are zero. Otherwise, $X(H)$ and $Z(H)$ are nonzero and, hence, can be estimated. For simplicity, we restrict our consideration to the case when $X(H) = 0$ and $Z(H) = 0$.

The expression for estimating measurement error is too cumbersome.[8] However, in the present problem

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formulation, made assuming that the retrieval of ozone from DIAL signal is an ill-posed inverse problem, only components with random origin, i.e., lidar returns are of significance. The ill-posedness of the equation (1) lies in the need to evaluate the derivative $dY(H)/dH$, in which process a small variation of $Y(H)$, $\Delta Y(H)$, may cause large changes in the derivative itself.

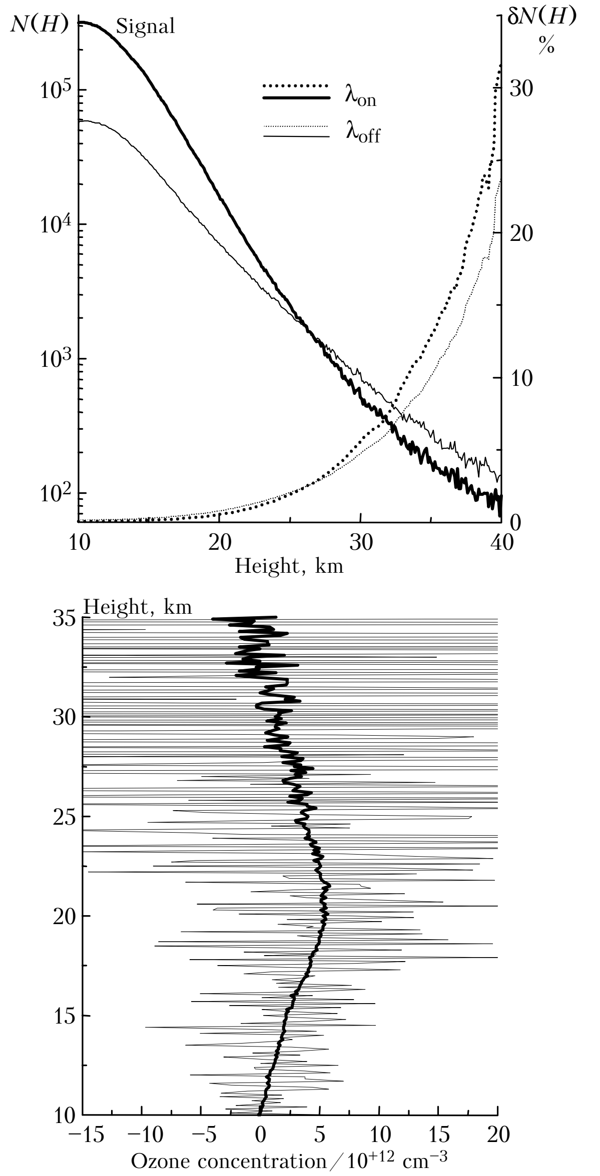


Fig. 1. Lidar return signals recorded on January 26, 2000, together with their relative errors (*a*), and stratospheric ozone profile, reconstructed from these signals, without (thin line) and after (thick line) linear smoothing over 50 points (*b*).

Therefore, a simplified expression for the square of the relative error in ozone retrieval can be written as

$$[\delta n(H)/n(H)]^2 = \sum_i [\delta N(H, \lambda_i)/N^2(H, \lambda_i)] =$$

$$= \sum_i \{\delta\tilde{N}(H, \lambda_i)/[\tilde{N}(H, \lambda_i) - N_b(\lambda_i)]^2, \qquad (2)$$

where λ_i stands for either λ_{on} or λ_{off}; while $\tilde{N}(H, \lambda_i)$ and $N_b(\lambda_i)$ denote the recorded lidar signal and the background interference at a corresponding wavelength. If the derivative is evaluated numerically, e.g., via $dY(H)/dH \approx \Delta Y/\Delta X = [Y(N_i) - Y(H_{i+1})]/\Delta X$ (finite-difference scheme), the sum in Eq. (2) must be doubled.

This problem is clearly illustrated by Fig. 1. Whereas Figure 1*a* presents statistically significant actual lidar returns with spatial resolution of 100 m, obtained at the Siberian Lidar Station in January 2000 at the wavelengths $\lambda_{on} = 308$ and $\lambda_{off} = 353$ nm, and used in the laser sensing of stratospheric ozone. Also shown are the relative errors of the "useful" signals $\delta N(H)/N(H)$.

Figure 1*b* shows vertical profile of the ozone concentration reconstructed from these return signals according to equation (1) using finite-difference scheme. As seen, $n(H)$ strongly varies from one gate interval to another, so it is very difficult to describe its vertical structure and use it in the subsequent interpretation. After linear smoothing, the laser sensing results become more suitable for analysis. As an example, Figure 1*b* shows the initial profile smoothed over 50 points. The smoothed profile has $\sqrt{50}$ times smaller relative error, estimated [from formula (2)] to be less than 2% at the height of 30 km and less than 9% at height 40 km; on the other hand, it has much lower spatial resolution. In the discussion that follows, we describe in a more detail the linear smoothing and other procedures with which the lidar sensing results can be reduced to the form that is more convenient for interpretation, and explain the meaning of spatial resolution after application of these procedures.

Linear smoothing

Linear smoothing (sliding mean) is a well-known procedure, which is widely used for processing experimental data in many natural science applications and is a particular case of digitally filtering signals by use of a rectangular-shaped window (with weighting coefficients all taken to be unity) in the presence of random error.[9] The smoothed values of experimental series $\overline{N}(H)$ (the vertical profile, in our case) and its variance $\overline{D}(H)$ are related to the initial data $N(H)$ and their variance $D(H)$ as follows[6,10]:

$$\overline{N}(H) = \frac{1}{2k+1}\left[\sum_{i=-k}^{k} N(H + i\Delta H)\right];$$

$$(3)$$

$$\overline{D}(H) = D(H)/(2k+1),$$

where ΔH is the spatial resolution of the initial series; k is the number of points of the series lying to the left and to the right of the smoothing point. In terms of digital filtering, $p = 2k + 1$ is the filter width.[9] Simultaneously with the decrease of the relative error due to linear smoothing, also decreases the spatial resolution of the series, by the same factor, i.e., $\Delta\overline{H} = p\,\Delta H$ (by the spatial resolution of the smoothed series, $\Delta\overline{H}$, we mean certain spatial interval outside of which there are the points currently not used in calculating the smoothed value of $\overline{N}(H)$).

Thus, the reduction of the variance is achieved at the expense of the spatial resolution. The trade-off between the profile's spatial resolution and the accuracy is determined by the laser sensing problem to be solved. When correlations between altitude levels 2.1 km apart are sought, a 21-point linear smoothing can safely be used. If vertical ozone distribution is reconstructed from lidar data with the spatial resolution of 0.1 km, this smoothing yields random error of less than 3% at 30 km and less than 14% at 40 km (all estimates are for lidar returns shown in Fig. 1). It is also worthy to note that all noise components contribute to the total variance $[\delta n(H)]^2$ additively (see equation (2)), so it does not depend on precisely what is to be smoothed (either $Y(H)$ in formula (1) or the final result $n(H)$ such as in Fig. 1).

The linear smoothing procedure applied twice (i.e., initial series → smoothed series → smoothing of smoothed series) is called the order II smoothing (Ref. 10) and, in terms of the components of the initial series, is expressed as:

– three-point smoothing (i.e., for $k = 1$ in formula (3))

$$\hat{a}_j = \frac{\overline{a}_{j-1} + \overline{a}_j + \overline{a}_{j+1}}{3} =$$

$$= \frac{1}{3}\left(\frac{a_{j-2} + a_{j-1} + a_j}{3} + \frac{a_{j-1} + a_j + a_{j+1}}{3} + \frac{a_j + a_{j+1} + a_{j+2}}{3}\right) =$$

$$= (a_{j-2} + 2a_{j-1} + 3a_j + 2a_{j+1} + a_{j+2})/9;$$

– five-point smoothing (i.e., in formulas

$$\hat{a}_j = (a_{j-4} + 2a_{j-3} + 3a_{j-2} + 4a_{j-1} +$$

$$+ 5a_j + 4a_{j+1} + 3a_{j+2} + 2a_{j+3} + a_{j+4})/25;$$

– $2k + 1$ - point smoothing (i.e., in the general form)

$$\hat{a}_j = \left\{\sum_{i=-2k}^{2k} [\underbrace{(2k + 1 - il)}_{M}\, a_{j-1}]\right\} / (2k + 1)^2, \quad (4)$$

where

$$l = -1 \text{ if } i < 0, \text{ and } l = 1 \text{ otherwise.}$$

Here $\{a_j\}$ is the initial series; $\overline{a}_j$ are the components of the smoothed series; $\hat{a}_j$ are the values after the order II smoothing is applied. In terms of the digital filtering, expression (4) defines a digital filter with the weighting coefficients M decreasing with the increase of distance from the smoothed point, the filter width being $p = 4k + 1$.

Therefore, upon applying this procedure, the initial resolution has now become $\Delta\hat{H} = p\,\Delta H$, i.e., $4k + 1$ times poorer. However, we note that the actual $\Delta\hat{H}$ value will be somewhat smaller than $\Delta\overline{H}$, the quantity introduced above for the filter with equal weights, i.e., for the case when all components $\{a_j\}$, falling within the filter, contribute equally to the calculated $\hat{a}_j$ value. As follows from equation (3), the variance of the smoothed series will be a factor of $(2k + 1)^2$ less than that of the initial one since

$$\hat{D}(H) = \overline{D}(H) / (2k + 1) =$$

$$= [D(H)] / (2k + 1) / (2k + 1). \quad (5)$$

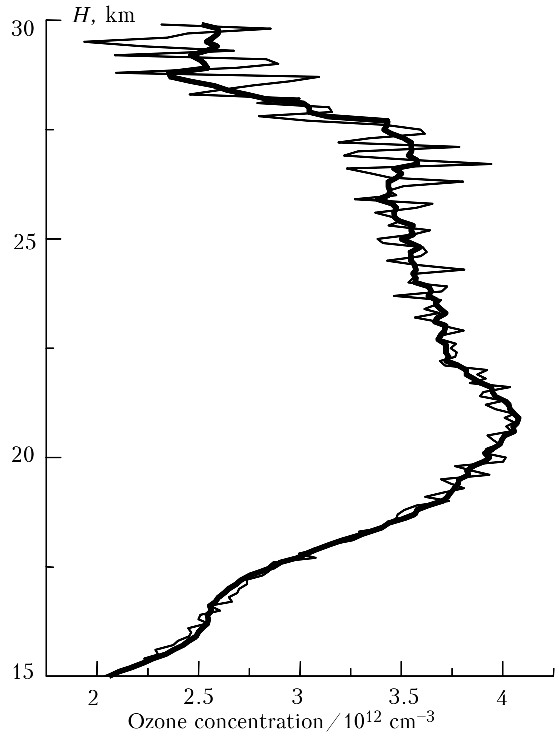


Fig. 2. Vertical ozone profiles reconstructed using 21-point order I linear smoothing (thin line) and 11-point order II linear smoothing (thick line).

Figure 2 shows profiles of the stratospheric ozone reconstructed from summer 1998 lidar sensing data using order I and II linear smoothing; the lidar returns have the same parameters as those used to plot Fig. 1. The 21-point ($k = 10$) order I smoothing was applied to the function $Y(H)$, which then was used to evaluate the derivative by the finite difference method and, thereby, to calculate $n(H)$ (see equation (1)). The 11-point ($k = 5$) order II linear smoothing first followed the same steps described above, and then the 11-point smoothing was applied to $n(H)$. Both profiles presented in Fig. 2 have the same spatial resolution equal to 2.1 km. In principle, one should not be confused that the order II smoothing is applied to different functions. Also, from Fig. 2 we see that the order II $n(H)$ profile has less error-induced altitude variations than its order I counterpart, primarily because of lower variance: 121 (i.e., $(2k + 1)^2$) versus 21 times less when compared to the initial series.

Linear approximation of derivative

The main idea of this procedure applied to lidar signals is that at each point j from the array $\{Y_j\}$ (see equation (1)) lying in the interval $2k + 1$, centered at the point j, a polynomial of the order I is constructed for each point, i.e., $y = Ax + B$. In this expression, the function y is a straight line obtained by the least squares method using specific values $Y_{j-k} - Y_{j+k}$; while the altitudes $H_{j-k} - H_{j+k}$ are taken as the variable x. Obviously, the slope A is the derivative dy/dx at a given point j, whose value is needed in formula (1). The A value can be calculated from the folrmula[9]:

$$A = \sum_{i=-k}^{k} (x_i - \bar{x})\,(y_i - \bar{y}) \Big/ \sum_{i=-k}^{k} (x_i - \bar{x})^2, \qquad (6)$$

with the error whose square is

$$(\delta A)^2 = W \Big/ \sum_{i=-k}^{k} (x_i - \bar{x})^2, \qquad (7)$$

where

$$W = \left[\sum_{i=-k}^{k} (y_i - \bar{y})^2 - A^2 \sum_{i=-k}^{k} (x_i - \bar{x})^2 \right] \Big/ (2k - 1).$$

In such an analytical method of evaluating the derivative, $(\delta A/A)^2$ enters formula (2) defining the retrieval error of the profile $n(H)$, while the spatial resolution is determined by the interval over which the derivative is taken. Further decrease of the error in $n(H)$ retrieval can be achieved by applying linear smoothing. Then, we obtain a hybrid (one might say, the order II) procedure involving elements of variational calculus and, as such, usable for analytical evaluation of the derivative $dY(H)/dH$ and linear smoothing.

With the retrieval methods outlined above, it is possible to identify unambiguously the spatial intervals along the sensing path where the used algorithms introduce correlations.

Exponential smoothing

Mathematically the procedure of exponential smoothing of experimental data can be expressed as[6,10]

$$\tilde{N}_i = (1 - \alpha)\, N_i + \alpha\, \tilde{N}_{i-1}, \quad i = 2 \ldots k,$$

$$\alpha < 1 \quad \text{for} \quad \tilde{N}_1 = N_1, \qquad (8)$$

where N_i is the component of the initial dataset; $\tilde{N}_i$ and $\tilde{N}_{i-1}$ are the components of the smoothed series; α is the smoothing parameter (proportional to the degree of smoothing); and k is the number of the last component in the series. In terms of the components of the initial series, formula (5) can be rewritten as

$$\tilde{N}_i = (1 - \alpha)\, N_i + (1 - \alpha)\, \alpha N_{i-1} + $$
$$+ (1 - \alpha)\, \alpha^2\, N_{i-2} + \ldots + (1 - \alpha)\, \alpha^{i-1}\, N_1. \qquad (9)$$

In terms of the digital filtering, expression (9) defines a digital filter in which successive components of the initial series contribute to the smoothed value of the ith component as follows: the component itself contributes the fraction $(1 - \alpha)$, and all preceding components contribute, respectively, $(1 - \alpha)\alpha$, $(1 - \alpha)\alpha^2$, etc. Thus, the greater the distance from the beginning of the series (or, in terms of the vertical profile, from its lowest point), the larger the number of points contributing to the smoothed value and, hence, the stronger the correlation between the components of the series processed.

The variance of the smoothed series is related to that of the initial series as[10]

$$\tilde{D}(H) = [\alpha/(2 - \alpha)]\, D(H). \qquad (10)$$

Since the smoothing parameter can be any real number, it can be varied to compensate for the increase of random error in the profile $n(H)$ with the increasing height. As an example, to ensure the quasi-constancy of the measurement error through introducing interlevel correlations, the smoothing parameter can be defined by the expression:

$$\alpha(H_i) = \alpha_0 + (0.95 - \alpha_0) \times$$
$$\times \exp\{0.25 \ln [(i - A)/(B - A + 5)]\}, \qquad (11)$$

where i is the gate interval number; A and B are the initial and final gate intervals of the retrieved profile, respectively. Expression (11), with the parameters $\alpha_0 = 0.4$, $i_0 = 150$, and $i_{end} = 350$, was used for exponential smoothing of vertical ozone profiles analyzed in this paper and reconstructed with this smoothing procedure. The latter was applied after derivative $dY(H)/dH$ was evaluated according to the finite-difference scheme.

Spline approximation

Splines are smooth (multiply differentiated) piecewise-polynomial functions used for data presentation over wide intervals. Here, we use a spline approximation based on the cubic splines as described in the monograph by K. De Bor.[3] For this, we construct the function $S(H)$ (spline) which, at a certain parameter ρ, minimizes the functional

$$\rho \sum_i (Y(H_i) - S(H_i))^2 + (1 - \rho) \int_A^B (S^{(2)})^2 \, dh \quad (12)$$

with respect to the function $S(H)$ and its second derivative $S^{(2)}$ (here, as before, A and B are the first and last points of a lidar return). The minimization of expression (12) is a sort of compromise between requirements to the spline to fit the empirical function $Y(H)$ and to be a smooth function, which is determined by the parameter ρ. The spline approximation reduces to linear data fit at $\rho = 0$ and to interpolation of (complete coincidence with) the data at $\rho = 1$.

Using spline approximation, the retrieval can be made accurate to within the mean measurement error over entire retrieved ozone profile, and the derivative $dY(H)/dH$ can be evaluated analytically.

Discussion of calculated results

The calculation techniques discussed above were used here to reconstruct the vertical profiles of stratospheric ozone. For an objective comparison of calculated results, the procedures were run for the parameters adjusted such that the retrieved profiles have nearly identical altitude variability and random error of less than 3% at the altitude of 30 km and less than 14% at 40 km. Specifically, in linear smoothing, the function $Y(H)$ (see formula (1)) was smoothed over 11 points, followed by 11-point smoothing of the derivative $Y(H)$, calculated using finite-difference scheme.

Thus, the order II linear smoothing was used. In linear approximation, the derivative was evaluated over 11 points, and the 11-point sliding mean was then applied to the result (hybrid procedure). The exponential smoothing was performed for the above presented parameters; and it was applied after the derivative was evaluated according to the finite-difference scheme. The spline-approximation was made for $\rho = 0.021$. According to the presented numerical results, the spatial resolution in the order II linear smoothing and in the hybrid procedure was 2.1 km. The interlevel correlations introduced by the exponential smoothing and by spline approximation are difficult to assess.

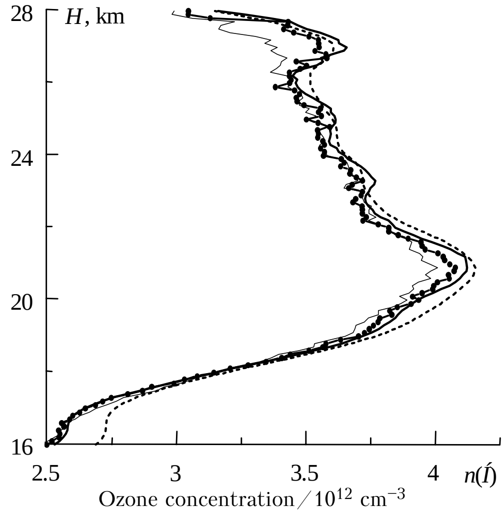
These procedures were used to calculate the mean vertical profiles of the stratospheric ozone for summer 1998; and the results are presented in Fig. 3*a*. As seen, the smoothest profile is the one obtained using the spline approximation. On the whole, the vertical ozone distributions reconstructed using different methods agree fairly well. However, the order II linear smoothing and exponential smoothing underestimate a little bit the ozone concentration throughout the altitude range studied. Probably, this is because in the finite-difference scheme the derivative is evaluated from

$$\frac{dY(H)}{dH} \equiv \frac{\Delta Y(H)}{\Delta H} = \frac{Y(H_i) - Y(H_{i+1})}{\Delta H},$$

where ΔH has finite value; whereas it would be more appropriate to take it in the limit

$$\frac{dY(H)}{dH} \equiv \lim_{\Delta H \to 0} \frac{\Delta Y(H)}{\Delta H}.$$

In two other cases, the derivative was evaluated analytically. In these, the profile reconstructed using spline approximation shows the largest differences around 16 km, probably because it was obtained without specifying boundary conditions in the form of zero second-order derivatives in the initial (16 km) and final (35 km) points.[3,9]



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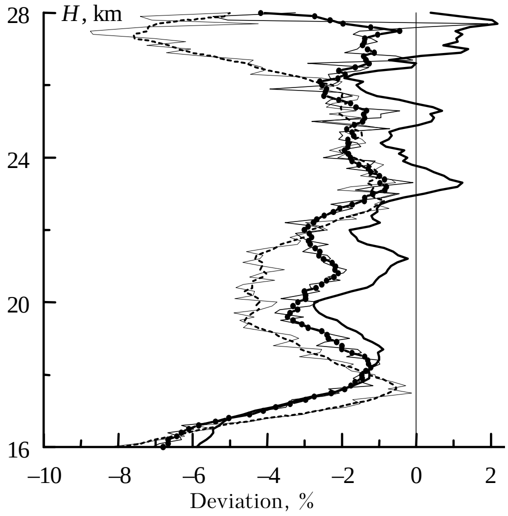

b

Fig. 3. The mean vertical profiles of the stratospheric ozone obtained using (*a*) hybrid procedure (curve *1*), spline-approximation (curve *2*), exponential smoothing (curve *3*), and linear smoothing (curve *4*); as well as (*b*) 5-point linear smoothing (curve *1*), 5-point exponential smoothing (curve *2*), hybrid procedure (curve *3*), exponential smoothing (curve *4*), and linear smoothing (curve *5*).

For better visualization of the inter-profile differences, Figure 3*b* shows deviations of the profiles from the one obtained using spline approximation: $[n_i(H) - n_{\rm spline}(H)]\ 100/n_{\rm spline}(H)$.

From Fig. 3*b* we see that the order II linear and exponential smoothing procedures give most diverse results which, for better comparison, were smoothed once more using 5-point sliding mean; hence, the two procedures are less efficient.

Moreover, when compared with the other procedures, the exponential smoothing procedure underestimates the ozone concentration in the ozone maximum and in the end of the studied interval. Most identical vertical profiles are obtained using the order II linear smoothing and the hybrid procedure. Moreover, the hybrid procedure provides for most close, in absolute value, results to those produced by the spline approximation.

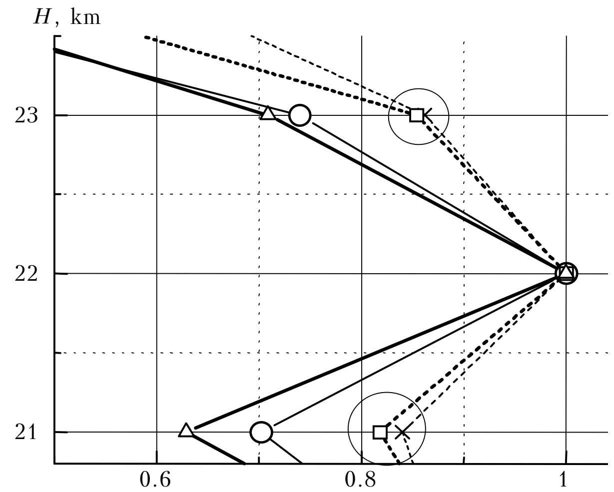

Fig. 4. Interlevel correlation functions of vertical ozone profiles obtained for the altitude 22 km using linear smoothing (○), exponential smoothing (×), spline approximation (□), and hybrid procedure (Δ).

Now we shall examine how these procedures influence interlevel correlations; the analysis will be made using statistical ensemble of 13 individual profiles of the ozone concentration, whose ensemble averages are shown in Fig. 3*a*. The level of stratospheric ozone maximum (22 km) is chosen as the initial one. The results of analysis are shown in Fig. 4. As seen, the spline approximation and the exponential smoothing lead to overestimation of the interlevel correlations by approximately 20% (in Fig. 4, these points are encircled), primarily because they introduce deterministic interlevel relationships.

Conclusion

Thus, the paper demonstrates that the vertical profiles of stratospheric ozone retrieved using different calculation methods and smoothing procedures differ only little. The spline approximation and the exponential smoothing, to a greater extent, introduce deterministic interlevel correlation and, hence, lead to overestimation of the correlation between different layers. Therefore, for solving this class of problems, most suitable are the order II linear smoothing and hybrid procedure, which can reliably identify the spatial intervals outside which the atmospheric layers are completely independent. At the same time, the hybrid procedure is more efficient than the order II linear smoothing; so it is more appropriate for retrieving vertical profiles of the stratospheric ozone, especially because it is capable of evaluating derivatives analytically.

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References

1. A.N. Tikhonov and V.Ya. Arsenin, *Methods of Solution of Ill-Posed Problems* (Nauka, Moscow, 1986), 288 pp.
2. V.E. Zuev and I.E. Naats, *Inverse Problems of Atmospheric Laser Sensing* (Nauka, Novosibirsk, 1982), 242 pp.
3. K.De Bor, *Practical Manual on Splines* (Radio i Svyaz, Moscow, 1985), 304 pp.
4. V.E. Zuev, V.V. Zuev, Yu.S. Makushkin, et al., Appl. Opt. **22**, No. 23, 3733–3741 (1983).
5. Yu.E. Voskoboinikov, M.Yu. Kataev, and A.A. Mitsel', Atm. Opt. **4**, No. 2, 151–158 (1991).
6. Yu.V. Chuev, Yu.B. Mikhailov, and V.I. Kuz'min, *Prediction of Quantitative Characteristics of Processes* (Sov. Radio, Moscow, 1975), 430 pp.
7. V.P. Diakonov, *User's Manual on Computer Algorithms and Programs in Basic Language* (Nauka, Moscow, 1987), 240 pp.
8. R.M. Measures, *Laser Remote Sensing* (John Wiley and Sons, New York, 1987).
9. R. Otnes and L. Enoknson, *Applied Analysis of Time Series* (Mir, Moscow, 1982), 428 pp.
10. V.A. Kolemaev, O.V. Staroverov, and V.B. Turundaevskii, *Probability Theory and Mathematical Statistics* (Vysshaya Shkola, Moscow, 1991), 400 pp.