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Ozone profile retrieval specially for the trend analysis: theoretical investigation of specialized retrieval algorithms

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Introduction

Atmospheric ozone measurements are performed for solving two main groups of problems [*WMO 1999*]. The former includes an analysis of the local atmospheric processes, such as radiative and photochemical simulation, and also local validation of other measurements. The latter includes a statistical analysis of long-term observational series with the main goal to reveal the ozone trends and long-term variability. Available algorithms for processing of remote observations are intended for solving the problems of the former group and, therefore, are optimized just for analyzing the local processes.

It is proposed a new kind of algorithms for ozone retrieval from remote sensing data - algorithms Specialized for Trend Analysis (STA). New STA retrieval algorithms could increase the current accuracy of trend estimation, because ozone data retrieved by a STA algorithm are intended for usage only for the trend analysis.. But if used for analysis of the local atmospheric processes the data could give worse results. It may be expected that the highest accuracy of estimation of the temporal variability will be achieved when the STA algorithms are applied to processing of data obtained with ozonometers characterized by averaging kernels differing significantly from the unit operator. For example, measurements can be performed with the SBUV and TOMS ozonometers or instruments based on the Umkehr method.

Direct determination of trends

An indirect remote measurement of the vertical ozone profile (VOP) $\boldsymbol{f}_t$ at the time point t can be described in the framework of the scheme

$$\xi_t = \boldsymbol{A}_t \boldsymbol{f}_t + \boldsymbol{\nu}_t , \qquad (1)$$

where ξ_t is the vector of directly measured parameters (for example, the spectrum of solar radiation); $\boldsymbol{\nu}_t$ is the random noise of the measurement with the mean $\mathrm{E}\boldsymbol{\nu}_t = 0$ and the covariance matrix $\boldsymbol{\Sigma}_i > 0$; $\boldsymbol{A}_t$ is the linear operator modeling the dependence of ξ_t on the VOP $\boldsymbol{f}_t$. When analyzing the temporal variability, we assume that VOP is related to the vector of predictors τ through the linear dependence

$$\boldsymbol{f}_t = \boldsymbol{K}_t \tau + \widetilde{\boldsymbol{f}}_t , \quad t=t_1,\ t_2,\ \ldots,\ t_n, \qquad (2)$$

distorted by the residual vector $\widetilde{\boldsymbol{f}}_t$; values of this vector are independent and random in time and are characterized by the mean value equal to zero and by the covariance matrix $\boldsymbol{H}$. We consider the problem of analyzing the temporal variability of VOP in a new formulation, namely, as a problem of determination of an unbiased linear estimate of a minimum variance $\sum_{i=1}^{n} \boldsymbol{R}_i \xi_i$ of predictors $\boldsymbol{U}\tau$

$$\mathrm{E}\left\| \sum_i^n \boldsymbol{R}_i \xi_i - \boldsymbol{U}\tau \right\|_2^2 = \min_{\boldsymbol{R}'_i} \left\{ \mathrm{E}\left\| \sum_i^n \boldsymbol{R}'_i \xi_i - \boldsymbol{U}\tau \right\|_2^2 \middle| \mathrm{E}\sum_i^n \boldsymbol{R}'_i \xi_i = \boldsymbol{U}\tau \right\} \qquad (3)$$

directly from a series of n indirect measurements $\xi_t = \boldsymbol{A}_t \boldsymbol{K}_t \tau + (\boldsymbol{A}_t \widetilde{\boldsymbol{f}}_t + \boldsymbol{\nu}_t)$, $t=t_1,\ t_2,\ \ldots,\ t_n$. It can be shown that, at $\boldsymbol{\Theta}_i = \boldsymbol{\Sigma}_i + \boldsymbol{A}_i \boldsymbol{H} \boldsymbol{A}_i^* > 0$ and $\sum_{i=1}^{n} \boldsymbol{K}_i^* \boldsymbol{A}_i^* \boldsymbol{\Theta}_i^{-1} \boldsymbol{A}_i \boldsymbol{K}_i > 0$, the optimum estimate (3) is given by the equality

$$\boldsymbol{R}_i = \boldsymbol{U}\left(\sum_{i=1}^{n} \boldsymbol{K}_i^* \boldsymbol{A}_i^* \boldsymbol{\Theta}_i^{-1} \boldsymbol{A}_i \boldsymbol{K}_i\right)^{-1} \boldsymbol{K}_i^* \boldsymbol{A}_i^* \boldsymbol{\Theta}_i^{-1} . \qquad (4)$$

Due to the fact that algorithm (4) allows estimation of the temporal variability of $\boldsymbol{U}\tau$ directly from observational data, an increase in the accuracy of estimation of $\boldsymbol{U}\tau$ is possible.

New algorithm (4) can be used with a database containing data on the operators $\boldsymbol{A}_i$ and $\boldsymbol{\Sigma}_i$ and also on the vectors ξ_t. Since, at present, such databases are not available openly, the usage of this algorithm is limited. Therefore, the possibility of improvement of available two-step schemes for trend analyses is still of interest.

Two-step determination of trends

As a rule, in the conventional two-step scheme of trend revealing for estimation of the temporal variability, the linear estimate of predictors, $\hat{\tau} = \sum_{i=1}^{n} \boldsymbol{L}_i \boldsymbol{U} \boldsymbol{f}_i$, is applied (linear operators $\boldsymbol{L}_i$ depend on $\boldsymbol{K}_i$ and $\boldsymbol{H}$). In reality, instead of a series of VODs, $\boldsymbol{U}\boldsymbol{f}_i$, their approximations, $\boldsymbol{R}_i \xi_i$, retrieved from a series of measurements (1) at $t=t_1$, $t_2,\ \ldots,\ t_n$ are used. Because of this fact, the estimate of predictors, $\widetilde{\tau} = \sum_{i=1}^{n} \boldsymbol{L}_i \boldsymbol{R}_i \xi_i$, that is factually used differs from the ideal estimate, $\hat{\tau}$, by the value

$$\widetilde{\tau} - \hat{\tau} = \sum_{i=1}^{n} \boldsymbol{L}_i \left[(\boldsymbol{R}_i \boldsymbol{A}_i - \boldsymbol{U}) \boldsymbol{f}_i + \boldsymbol{R}_i \boldsymbol{\nu}_i \right] . \qquad (5)$$

Let us consider two models allowing estimation of the arising hindrance $\widetilde{\tau} - \hat{\tau}$.

Model R (random). Suppose that $\boldsymbol{f}_t$ is a random vector with a known mean $\mathrm{E}\boldsymbol{f}_t = \boldsymbol{f}_0$ and a covariance matrix $\boldsymbol{F}$. Suppose also that ozone distributions at different time points are independent. (Further, for simplification of formulas, we take that $\boldsymbol{f}_0 = 0$ and that $\widetilde{\boldsymbol{f}}_t$ and $\boldsymbol{\nu}_t$ are uncorrelated.) Then, for the energy of hindrance we obtain the expression

$\mathrm{E}\|\tilde{\tau}-\hat{\tau}\|_2^2=\sum_{i=1}^{n}h_i^2(\boldsymbol{R}_i)$, where $h_i^2(\boldsymbol{R})=\left\|\boldsymbol{L}_i(\boldsymbol{R}\boldsymbol{A}_i-\boldsymbol{U})\boldsymbol{F}^{1/2}\right\|_2^2+\left\|\boldsymbol{L}_i\boldsymbol{R}\boldsymbol{\Sigma}_i^{1/2}\right\|_2^2$. It can be shown that, in this case, the operator $\hat{\boldsymbol{R}}_i=\boldsymbol{U}\boldsymbol{F}\boldsymbol{A}_i^*(\boldsymbol{A}_i\boldsymbol{F}\boldsymbol{A}_i^*+\boldsymbol{\Sigma}_i)^{-1}$ providing the nearest linear estimate $\boldsymbol{R}_i\xi_i$ of the vector $\boldsymbol{U}\boldsymbol{f}_i$ on the basis of measurement (1): $\mathrm{E}\left\|\hat{\boldsymbol{R}}_i\xi_i-\boldsymbol{U}\boldsymbol{f}_i\right\|_2^2=\min_{\boldsymbol{R}'}\mathrm{E}\left\|\boldsymbol{R}'\xi_i-\boldsymbol{U}\boldsymbol{f}_i\right\|_2^2$ [*Pyt'ev, Chulichkov, 1991*], provides the minimum $h_i^2(\boldsymbol{R})$. Consequently, for the model **R**, the locally optimum algorithm gives VOP retrieval that is optimum for trend estimation.

However, a basic assumption (used in the above consideration) of time-independence of ozone distribution is obviously not quite correct. A possible manifestation of underestimation of errors introduced by this assumption is a discrepancy in estimates of temporal variability obtained with direct and remote methods [*Miller et al., 1995*]. Therefore, at developing the STA algorithms and estimating the temporal variability, the following model should be preferred apparently.

Model MM (minimax). Let vector $\boldsymbol{f}_t$ belong to a range $\boldsymbol{f}_t\in\boldsymbol{\Psi}=\left\{\boldsymbol{f}:\left\|\boldsymbol{D}^{1/2}(\boldsymbol{f}-\boldsymbol{f}_0)\right\|_2^2\le 1\right\}$, $\boldsymbol{D}=\boldsymbol{D}^*>0$. (Hereafter, we take for simplification that $\boldsymbol{f}_0=0$.) Consider the majorant of hindrance energy,

$$\mathrm{E}\|\tilde{\tau}-\hat{\tau}\|_2^2=\sum_{i=1}^{n}\left\|\boldsymbol{L}_i\boldsymbol{R}_i\boldsymbol{\Sigma}_i^{1/2}\right\|_2^2+$$

$$+\sum_{i=1,j=1}^{i=n,j=n}(\boldsymbol{L}_i(\boldsymbol{R}_i\boldsymbol{A}_i-\boldsymbol{U})\boldsymbol{f}_i,\boldsymbol{L}_j(\boldsymbol{R}_j\boldsymbol{A}_j-\boldsymbol{U})\boldsymbol{f}_j)\le$$

$$\le\sum_{i,j}\left\|\boldsymbol{L}_i(\boldsymbol{R}_i\boldsymbol{A}_i-\boldsymbol{U})\boldsymbol{f}_i\right\|_2\left\|\boldsymbol{L}_j(\boldsymbol{R}_j\boldsymbol{A}_j-\boldsymbol{U})\boldsymbol{f}_j\right\|_2+$$

$$+\sum_{i}\left\|\boldsymbol{L}_i\boldsymbol{R}_i\boldsymbol{\Sigma}_i^{1/2}\right\|_2^2\le\sum_{i=1}^{n}\|\boldsymbol{L}_i\|^2\tilde{h}_i^2(\boldsymbol{R}_i),$$

where $\tilde{h}_i^2(\boldsymbol{R})=n\max_{\boldsymbol{f}\in\boldsymbol{\Psi}}\|(\boldsymbol{R}\boldsymbol{A}_i-\boldsymbol{U})\boldsymbol{f}\|_2^2+\left\|\boldsymbol{R}\boldsymbol{\Sigma}_i^{1/2}\right\|_2^2$. We develop the STA algorithms as algorithms $\overline{\boldsymbol{R}}_i$ minimizing each term of the majorant

$$\tilde{h}_i^2(\overline{\boldsymbol{R}}_i)=\min_{\boldsymbol{R}'}\tilde{h}_i^2(\boldsymbol{R}'). \qquad (6)$$

At $\mathrm{rang}\,\boldsymbol{U}=1$, the solution of problem (6) is the operator

$$\overline{\boldsymbol{R}}_i=\boldsymbol{U}(\boldsymbol{A}_i^*\boldsymbol{\Sigma}_i^{-1}\boldsymbol{A}_i+\tfrac{1}{n}\boldsymbol{D})^{-1}\boldsymbol{A}_i^*\boldsymbol{\Sigma}_i^{-1} \qquad (7)$$

For this operator, $\tilde{h}_i^2(\overline{\boldsymbol{R}}_i)=\mathrm{tr}\,\boldsymbol{U}(\boldsymbol{A}_i^*\boldsymbol{\Sigma}_i^{-1}\boldsymbol{A}_i+\frac{1}{n}\boldsymbol{D})^{-1}\boldsymbol{U}^*$ [*Lauter, 1975*]. Thus, for the model **MM**, the STA algorithm differs from the locally optimum algorithm

$$\tilde{\boldsymbol{R}}_i=\boldsymbol{U}(\boldsymbol{A}_i^*\boldsymbol{\Sigma}_i^{-1}\boldsymbol{A}_i+\boldsymbol{D})^{-1}\boldsymbol{A}_i^*\boldsymbol{\Sigma}_i^{-1}$$

minimizing a local retrieval error

$$\tilde{\boldsymbol{R}}_i=\arg\min_{\boldsymbol{R}'}\left\{\max_{\boldsymbol{f}\in\boldsymbol{\Psi}}\|(\boldsymbol{R}'\boldsymbol{A}_i-\boldsymbol{U})\boldsymbol{f}\|_2^2+\left\|\boldsymbol{R}'\boldsymbol{\Sigma}_i^{1/2}\right\|_2^2\right\}.$$

In simplified terms, the difference between STA algorithm $\overline{\boldsymbol{R}}_i$ and ordinary algorithm $\tilde{\boldsymbol{R}}_i$ can be illustrated as follows. The current retrieval algorithm $\tilde{\boldsymbol{R}}_i$ for analysis of the local atmospheric processes provide for a search of the optimum ratio between regular and random retrieval errors. A minimum of the sum of these errors is achieved. Regular errors can be described by bias of averaging kernel $\tilde{\boldsymbol{R}}_i\boldsymbol{A}_i$ from operator $\boldsymbol{U}$. A statistical analysis of observational series does not change the regular error and decreases the dispersion of random errors, since the latter obey the law of large numbers. Therefore, a statistical analysis destroys the optimum balance between regular and random errors, which is included in the current retrieval algorithms. Taking into account a decrease in the random error in the process of statistical analysis, a preventive decrease in the systematic error of ozone retrieval with the STA algorithm is necessary. However, this will result in some increase in the random error, but the total error could decrease if the data used for trend analysis. The detailed theoretical consideration of the problem gave the value of the acceptable increase in the random error, which leads to maximum decrease in the total error.

Conclusions

Method (4) is proposed for estimation of the temporal variability of the VOP directly from data of remote measurements without preliminary measurements of local VOPs. The composition of data of remote measurements to be archived for subsequent direct estimation of temporal VOP variability is determined.

It is shown that VOP retrieval algorithms optimized to study local processes are not necessarily optimum for creation of databases used for analyzes of temporal variability.

An approach is proposed for the VOP retrieval algorithms specialized for trend analysis (STA). Parameters of the optimum STA retrieval algorithm (7) depend on the observation period of the ozone data set, which will be used simultaneously with the results of retrieval. A priori information on ozone and experimental errors, which is used in the new STA algorithm, should be the same as information included into current algorithms.

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