ISSN 0001-4338, Izvestiya, Atmospheric and Oceanic Physics, 2014, Vol. 50, No. 3, pp. 330–336. © Pleiades Publishing, Ltd., 2014.
Original Russian Text © A.V. Polyakov, Yu.M. Timofeev, Ya.A. Virolainen, 2014, published in Izvestiya AN. Fizika Atmosfery i Okeana, 2014, Vol. 50, No. 3, pp. 373–380.

Using Artificial Neural Networks in the Temperature and Humidity Sounding of the Atmosphere

A. V. Polyakov, Yu. M. Timofeev, and Ya. A. Virolainen

St. Petersburg State University, ul. Ul'yanovskaya 3, Petrodvorets, St. Petersburg, 198504 Russia

e-mail: polyakov@troll.phys.spbu.ru

Received April 18, 2013; in final form, August 16, 2013

Abstract—The application of the radiative data inversion technique based on artificial neural networks (ANN) for the meteorological satellite sounding of the atmosphere is described. To increase the efficiency of solving inverse problems, the principal component method is used for the temperature and humidity profiles, as well as for IR radiation spectra, which allows the problem dimensionalities to be reduced substantially. Based on numerical experiments, errors of the temperature and humidity sounding are analyzed from the spectra of outgoing IR radiation (that were measured by the IKFS-2 instrument onboard the Meteor Russian satellite) using the iterative physical–mathematical (IPM) algorithm, multiple linear regression (MLR), and ANN-based methods. Appreciable advantages of the ANN-based method are revealed as compared to the MLR method. Therefore, in temperature sounding, the MLR method has a markedly large error at heights of 1–12 km (a difference of up to 1 K), while the IPM algorithm has almost the same error as the ANN method. The humidity determination error is about 10% when the ANN method is used at heights of 0–12 km. The IPM approach yields approximately the same error in the lower troposphere, but as the height increases the advantages of the ANN method grow.

Keywords: satellite sounding, neural networks, inverse problems, atmospheric optics

DOI: 10.1134/S0001433814030104

INTRODUCTION

Contemporary systems of atmosphere temperature and humidity sounding in the IR region of the spectrum (instruments of AIRS, IASI, CrIS, etc.) are characterized by a high rate of retrieval of large data amounts due to a great number of spectral measurements and spatial scanning. The need for processing a large amount of data makes it difficult to follow time requirements for the inversion of spectra measurement results when using the obtained data in a numerical weather forecast. To reduce time costs in an interpretation of satellite measurement results, different methods are used for increasing data-processing efficiency:

(i) the application of fast-acting procedures and algorithms to calculate the outgoing radiation, i.e., to solve a direct problem like [1];

(ii) compression of spectral data based on approximations using the empirical orthogonal functions (EOF) [2–4];

(iii) using the multiple linear regression (MLR) method at the first stage of analyzing measurement results [5].

The problem of effective software development faces also future satellite experiments with the IKFS-2 apparatus [6]. Earlier, ad hoc software was created for this instrument and its capabilities were analyzed [7–10]. While processing the measurement results, it is suggested in the initial approximation to use the fast MLR method for obtaining a solution and estimating its reliability by comparing the calculated and measured radiation spectra. If a difference is large, then a physical–mathematical approach is applied, e.g., the iterative process based on nonlinear generalization [11, 12] of the known method for optimal estimation in solving the integral equation of heat radiation transfer.

Numerical simulation has shown that the use of MLR at the first stage of satellite data analysis often requires solving the subsequent nonlinear inversion of the problem, especially in the retrieval of the atmosphere humidity profile, which leads to a substantial increase in time of processing of satellite measurement results. To use the methods based on artificial neural networks (ANN) instead of MLR is offered in a number of works [13–16]. In this work the possibilities of using ANN for interpreting the results of measurements by means of the Russian satellite Fourier spectrometer IKFS-2 [6] are considered.

CALCULATION TECHNIQUE

The construction of an inverse operator in the ANN method (like in the MLR method) requires using a vast ensemble of realizations of state parameters of the atmosphere and underlying surface (training set). Our databank of atmosphere models and

Table 1. Rms errors of expansion of profiles of temperature ($T(z)$) and relative humidity $RH(z)$, %, depending on the basis dimensionality (number of PCs)

PC number	1	5	10	11	12	13	14	15	16	17	18	19
$T(z)$, K	8.81	2.21	0.87	0.74	0.64	0.56	0.49	0.43	0.38	**0.34**	0.29	0.26
$RH(z)$, %	19.3	7.9	3.9	3.5	3.2	**2.8**	2.5	2.2	2.0	1.8	1.6	1.5

characteristics of surfaces is used for this purpose; it has been created previously on the basis of the known TIGR set of atmosphere models [17, 18] and added with parameters needed for the simulation of measurements in the spectral IR region (the surface temperature differing from the near-ground air temperature and emissivity of land and water surface). The statistical model constructed on the basis of a combination of data from different sources is a set of 2311 states of the atmosphere–surface system. It was applied in [8, 9].

The inverse problem can be solved in the space of the sought functions themselves of the atmospheric temperature and humidity or in the space of coefficients of expansion of sought functions with respect to one or another orthogonal basis (method of principal components (PCs)). In this work, to solve the inverse problem, we used the ANN method in combination with the PC method in respect of both sought functions and the outgoing radiation spectra measured by IKFS-2. This made it possible to substantially reduce the amount of data to be processed using the algorithm for solving the problem. In this case it is necessary to choose an optimal number of PCs (a basis dimensionality) for the parameterization of both sought vertical profiles and measured spectra. The number of PCs of parameterization of vertical profiles of temperature and humidity was chosen on the basis of comparing parameterization errors with potential errors of solving the inversion problem. Table 1 presents the errors of parameterization of vertical profiles of temperature ($T(z)$) and relative humidity ($RH(z)$) for several different values of the PC number.

Based on Table 1 analysis, it was decided to use PC values of 17 and 13 for the parameterization of vertical profiles of temperature and humidity, respectively. In this case a growth in the total error of remote measurements due to the parameterization of the temperature and humidity profiles is less than 10%.

While choosing the number of PCs of parameterization of the outgoing radiation spectra measured by the IKFS-2 instrument (the total number of spectrum measurements is 2701), the results of [4] were used, where it is shown that 40 PCs are enough for that. For ANN training and the simulation of the temperature and humidity sounding of the atmosphere, the radiation spectra (with the addition of the normally distributed model error of measurements) with their PCs for different random zenith angles of observations were calculated from data of measurements by IKFS-2. The sample was divided randomly into two parts: "training" and test sets in a ratio of 85 : 15. Following the overwhelming majority of publications on the application of ANN in inverse problems of atmospheric optics for solving the inverse problem, we chose a three-layer perceptron and hyperbolic tangent as a function of neuron activation. A technique for using the PC method in combination with ANN method is described in detail in [19].

An important issue of ANN organization is choosing the optimal number of network neurons. The number of input (n_x) and output (n_y) signals and, correspondingly, neuron "sensors" and output neurons is determined by sets of predictors and predictands, but the number of hidden-layer neurons (HLNs) n_h is an arbitrary value. It is easy to evaluate that the total number of coefficients (N) that is determined in the ANN training process is given by the formula

$$N = (n_x + 1)n_h + (n_h + 1)n_y. \tag{1}$$

For example, for $n_x = 40$, $n_h = 30$, and $n_y = 20$, the total number of coefficients is 1850. A large number of coefficients may lead to the excess determination of the network and an approximation implemented by this network will correspond to peculiarities of an individual set, including a random noise of measurements, rather than to physical regularities of the problem, because the number of determined parameters will be excessive with respect to the information conditionality of the problem. At the same time, a small number of HLNs limits the neural network capabilities with respect to the approximation of complicated nonlinear relationships, which may also lead to a growth in error of the inverse problem solution.

We have performed a series of computations to analyze the dependence of the error on the HLN number. For an ANN with 40 PCs of the spectrum at input and 17 PCs of the temperature profile at output, the HLN number was varied. Table 2 presents the rms errors of determining a temperature in a layer of 0–40 km using the training and test sets of atmosphere models. We shall clarify rows 3 and 4 of Table 2. Network training is conducted during 100 iterations; each of them includes performing 3000 steps of minimization. Upon completing iteration, the minimum error values are computed for this iteration on the training and test sets. The error of the training set can only decrease as the iteration number increases because it is just the object of minimization, but the error of test set behaves differently: its value for the last (100th) iteration is not

Table 2. Errors of temperature profile determination, K, with a different HLN number

HLN number		10	15	20	23	25	30	35
Training set		1.67	1.52	1.45	1.41	1.31	1.29	1.26
Test set	Optimum	1.76	1.75	1.74	1.67	1.53	1.52	2.06
	Final value	1.76	1.76	1.77	1.76	1.54	1.67	2.26

necessarily minimal or close to minimal (see Table 2 and Fig. 1). Therefore, for the test set we give two errors: optimal (minimal) and final (i.e., obtained for the last iteration) ones.

It can be seen from Table 2 that, with an increase in the HLN number, the error of training set, as should be expected, decreases monotonically. The optimal error of test set reduces as the HLN number increases to 25–30, while for 35 HLNs it sharply grows. The final error remains roughly unchanged as the HLN number increases to 23, which is evidence that the approximation accuracy of the ANN inverse-problem operator is almost constant. However, with 25 HLNs, a visible stepwise decrease in the final error occurs, which is likely caused by the accumulation of a “critical mass” of ANN complexity and, as a consequence, by the qualitative change in the solution approximation nonlinearity. However, by 30 HLNs, the final error markedly exceeds the optimal error, while for 35 HLNs the optimal error also stops declining. This is explained by the ANN redundancy at the HLN number exceeding 25.

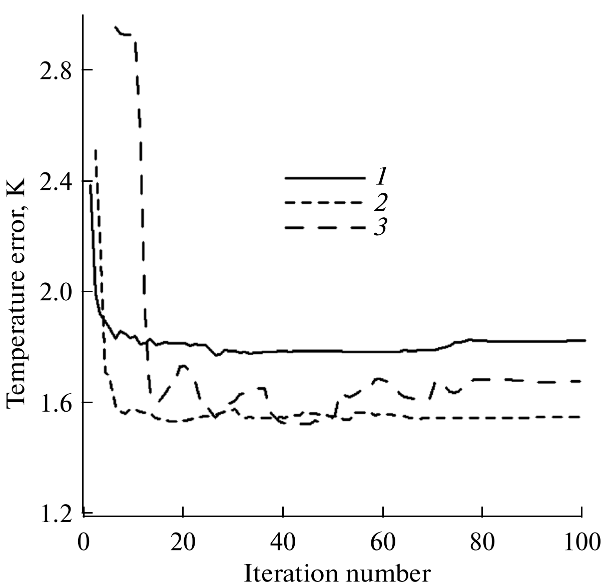

Fig. 1. The dependence of rms error of temperature determination using ANN upon the iteration number in training the network for 20 (*1*), 25 (*2*), and 30 (*3*) HLNs in case of the test set corresponding to nadir measurements over land.

Figure 1 demonstrates in more detail the error behavior depending on the iteration number for three values of the HLN number. It follows from Fig. 1 that, with 20 and 25 HLNs, the test set error decreases (as minimization occurs), reaching the asymptotic value with insignificant oscillations after 40–60 iterations. The oscillations are caused, in particular, by the random order of summation in parallel calculations. In this case the value obtained for 25 HLNs is approximately by 0.2 K less than for 20 HLNs. At the same time, the appreciable oscillations of this value are observed for 30 HLNs, while the asymptotic value reached after 80 iterations is by roughly 0.15 K larger than that for 25 HLNs. It shows that, with 30 HLNs, the test set approximation stops describing general regularities (independent of random noise) and allows 25 to be assumed as the optimal HLN number.

ATMOSPHERE TEMPERATURE AND HUMIDITY SOUNDING USING ANN

After ANN training, the retrieval of the temperature and humidity profiles for the test set was implemented and errors were analyzed on the basis of comparing the retrieved and initial profiles of temperature and humidity. In this case measurements under cloudless atmosphere conditions were simulated. Figure 2 presents examples of the mean (Fig. 2a) and rms (Fig. 2b) temperature errors for the global ensemble over the water surface with the application of the MLR and ANN methods and the iterative physical–mathematical (IPM) approach. The systematic-error analysis shows that it does not exceed 0.2 K for ANN and IPM, while for MLR, it is 0.4 K.

While analyzing the rms errors, we note first and foremost that the errors with ANN application are around 1 K for the free atmosphere at heights of 5–25 km. In the lower troposphere, the errors markedly grow and amount to around 3 K for the near-ground temperature. A growth in temperature-sounding errors is also observed at heights of over 25 km. From Fig. 2 it also follows that, for a layer of 1–12 km, the MLR method yields a visibly large error (a difference of up to 1 K!), while the IPM algorithm yields almost the same error as the ANN method. In the stratosphere, the IPM approach advantages can be noted, though all three methods used yield close errors within the limits of 1–2 K. We note that a priori temperature variations for the global ensemble of temperature real-

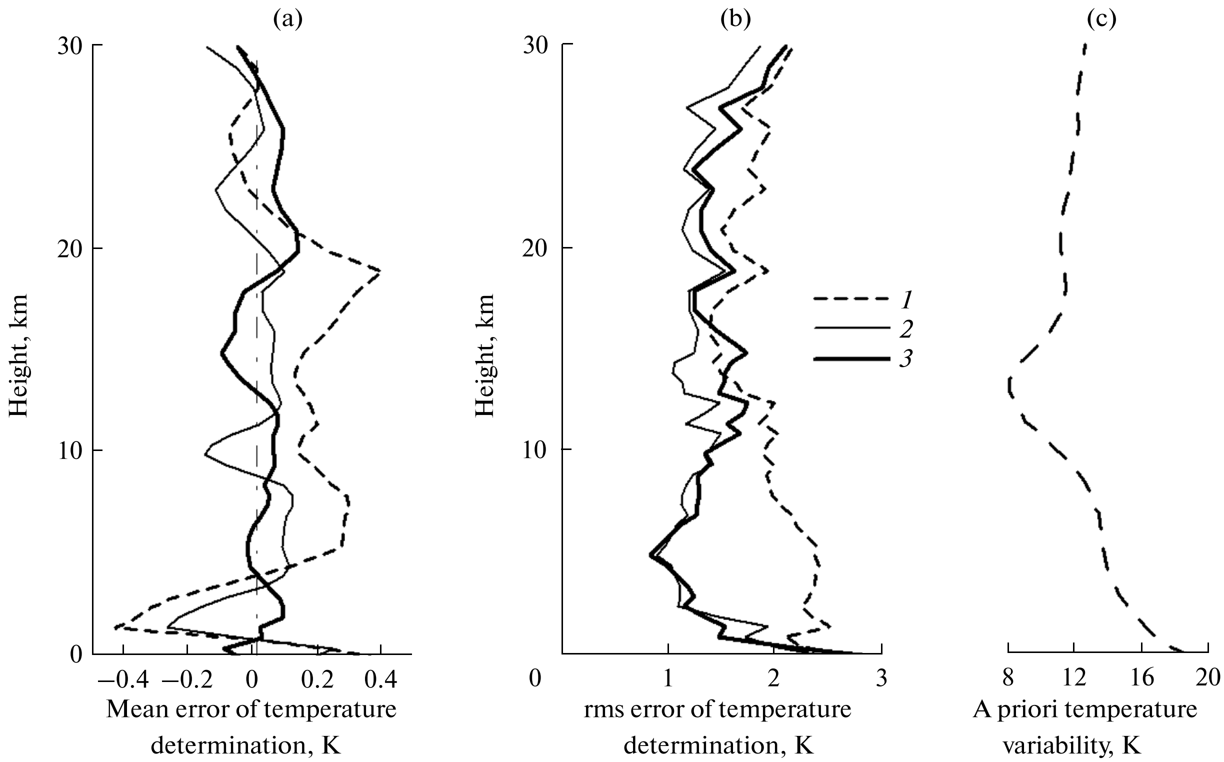

Fig. 2. (a) Mean and (b) rms errors of temperature profile determination from IKFS-2 measurements (obtained under cloudless atmosphere conditions using the global sample over a water surface with the application of linear regression (*1*), iterative algorithm (*2*), and ANN (*3*)) in comparison with (c) a priori variability.

izations used in these calculations oscillate depending on the height within the limits of 8–18 K (Fig. 2c).

The results of analogous numerical experiments from the results of experiments over land are given in Fig. 3. We note that, for the case of satellite sounding over land in solving the inverse problem, the spectral emissivity of the surface $\varepsilon(\nu)$ is not specified (like in the case of sounding over water surface) but is determined by finding coefficients of expansion with respect to the appropriate EOF basis [9]. This leads to five additional unknown parameters that are also determined from the outgoing IR radiation spectrum. This peculiarity yields the certain increase in errors of temperature sounding near the underlying surface.

An analysis of Fig. 3 points out the small advantage of the IPM approach in the troposphere when compared with the ANN method and the higher error of the MLR method (approximately by 1 K). In the stratosphere for the case of sounding over land, the advantage of the IPM approach is revealed (by 0.2–0.4 K), while the MLR and ANN methods have almost identical errors.

Errors of determining relative humidity in sounding over water surface and over land are given in Figs. 4 and 5. The mean errors for all retrieval methods, as a rule, do not exceed 2–3%. The rms errors for the water surface in the ANN method are around 10% at heights of 0–12 km. In the lower troposphere, approximately the same error is provided by the IPM approach, but as the height grows the ANN method advantages increase. At last, in the MLR method, errors of relative humidity retrieval in the low and middle troposphere are around 20% and substantially grow in the upper troposphere. This demonstrates the substantial nonlinearity of the inverse problem with respect to humidity profile. It is important to note that the approach with the IPM algorithm also has substantial errors in humidity retrieval in the upper troposphere.

Errors of relative humidity determination over land (Fig. 5), like temperature errors, also grow markedly in the lower troposphere. The advantage of the ANN method over the IPM algorithm (and especially MLR) is revealed, which is particularly significant at heights of over 6 km.

The analysis of applicability of the ANN method for different latitude zones has shown no substantial variations in errors of temperature sounding regardless of the variations in a priori latitude-to-latitude variability of temperature. The temperature errors while using the ANN method are 1–2 K at heights of 5–25 km. In this case the best accuracy of determining the temperature profile in the upper stratosphere is obtained for the tropical sample, in which a priori temperature variability is minimal (4–8 K). The similar pattern is also observed in retrieving the relative humidity profile

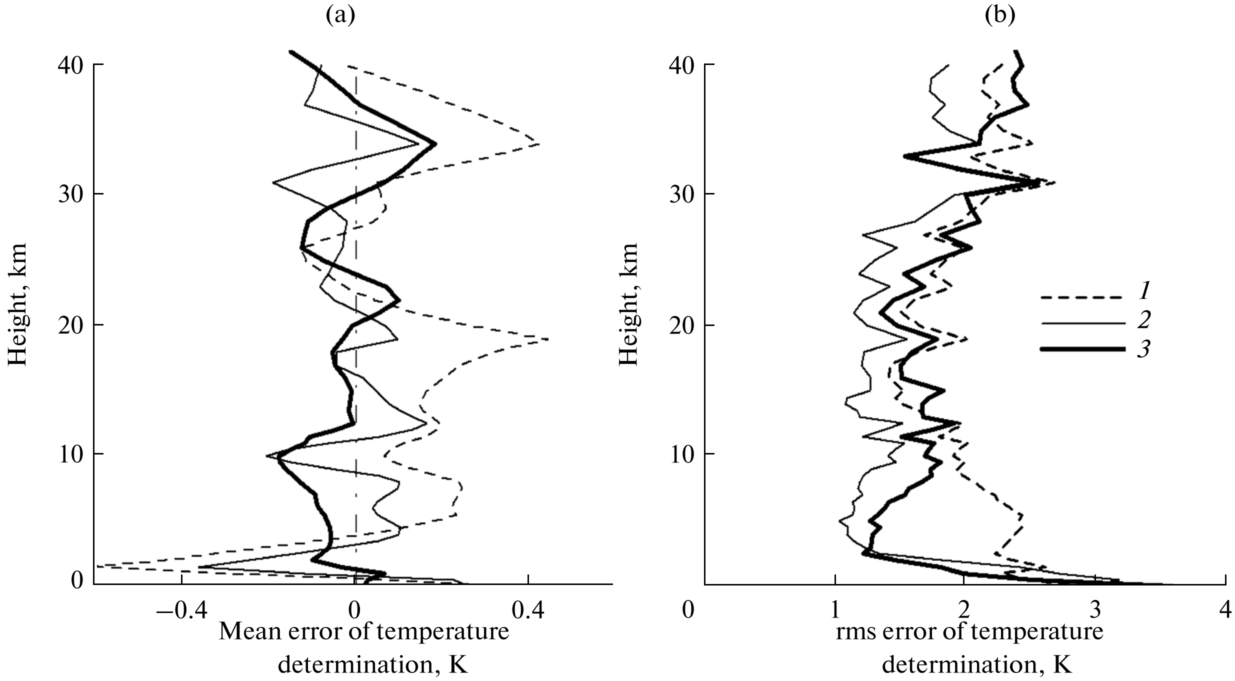

Fig. 3. (a) Mean and (b) rms errors of temperature profile determination from IKFS-2 measurements obtained under cloudless atmosphere conditions using the global sample over land with application of linear regression (*1*), iterative algorithm (*2*), and ANN (*3*).

using ANN. Errors at troposphere heights for different latitudinal zones are 10–20% on average.

MAIN CONCLUSIONS

Errors of the temperature and humidity sounding of a cloudless atmosphere are analyzed from spectra of outgoing IR radiation measured using the IKFS-2 instrument onboard the Meteor Russian satellite. Algorithms of satellite data interpretation are implemented that are based on using artificial neural networks. In this case, to increase the efficiency of solving inverse problems, the principal component method is used for temperature and humidity profiles, as well as for IR radiation spectra, which allows the problem dimensionalities to be substantially reduced.

Based on numerical analysis, optimal dimensionalities of parameterization are chosen. For temperature and humidity, 17 and 13, respectively, are used, while for outgoing radiation spectra in the spectral region of 660–2000 cm^{-1}, 40 principal components are selected. Based on numerical experiments with implementing the ANN method, the optimal number of hidden-layer neurons is chosen, amounting to 25 neurons for the inverse problem under consideration.

Numerical experiments to analyze errors of the temperature and humidity sounding of cloudless atmosphere with the use of different interpretation methods (MLR, ANN, and IPM) have shown the following:

(1) The ANN method error of temperature profile retrieval in a height range of 5–25 km over a water surface is around 1 K. In the lower troposphere, the error grows markedly and is around 3 K for the near-ground temperature. The error grows also at heights of more than 25 km. At heights of 1–12 km, the MLR method yields a noticeably large error (growth up to 1 K), while the IPM algorithm gives almost the same error as the ANN method. In the stratosphere, the IPM approach advantages are observed, though all the three methods give close results (within the limits of 1–2 K).

(2) When the vertical temperature profile is determined over land, additional unknown parameters arise (describing the land emissivities), which leads to a certain increase in errors of temperature sounding. In the troposphere, the IPM approach has small advantages when compared with the ANN method, while the MLR method yields a large error (approximately 1 K). In stratospheric sounding, for the case of sounding over land, the IPM approach has an advantage (by 0.2–0.4 K), while the MLR and ANN methods give roughly identical errors.

(3) The error of relative humidity determination using the ANN method for sounding over water surface is around 10% at heights of 0–12 km. In the lower troposphere, the IPM approach gives approximately the same error, but as height grows the ANN method advantage increases. The MLR method yields the markedly large error. The substantial nonlinearity of the inverse problem regarding the atmosphere humid-

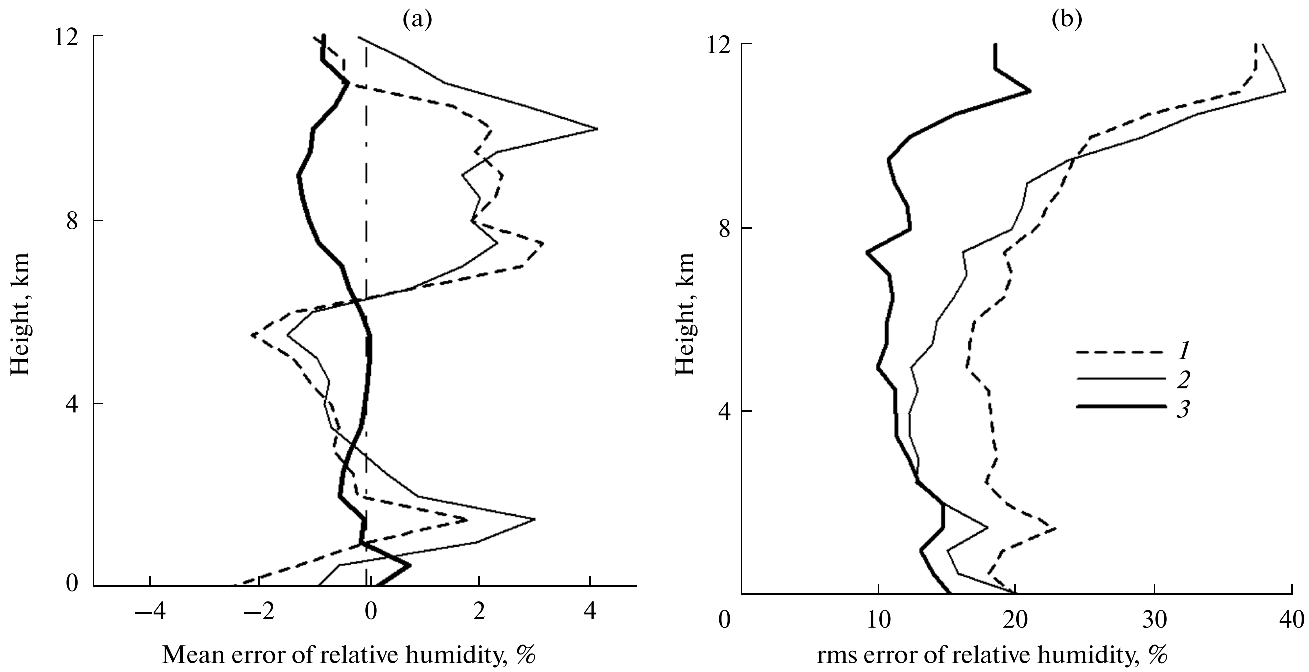

Fig. 4. (a) Mean and (b) rms errors of relative humidity profile determination from IKFS-2 measurements obtained for the global sample over water surface with the application of linear regression (*1*), iterative algorithm (*2*), and ANN (*3*).

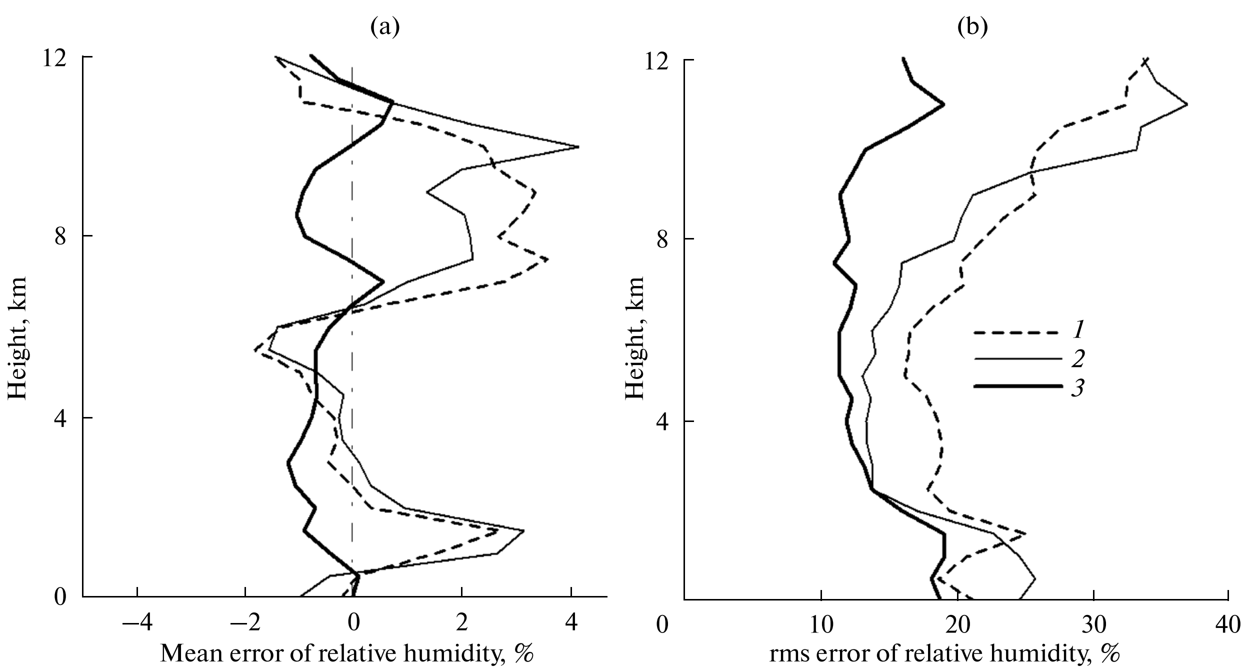

Fig. 5. (a) Mean and (b) rms errors of relative humidity profile determination from IKFS-2 measurements obtained for the global sample over land with the application of linear regression (*1*), iterative algorithm (*2*), and ANN (*3*).

ity profile is manifested by that. For the case of sounding over land, errors of relative humidity determination such as temperature errors grow noticeably in the lower troposphere. Here the ANN method has the advantage that is especially significant for heights above 6 km.

(4) The analysis of applicability of the ANN method for different latitudinal zones did not show any substantial variations in temperature-sounding errors despite the latitude-to-latitude variations in a priori temperature variability. The error of temperature determination using the ANN method is from 1 to

2 K at heights of 5–25 km. In this case the best accuracy of temperature profile determination in the upper stratosphere is characteristic of the tropical sample, for which a priori temperature variability is minimal (4–8 K). An analogous picture is also observed in retrieving the relative humidity profile by means of the ANN method. For different latitude zones, the errors are 10–20% on average at troposphere heights.

Thus, it is shown that the ANN method can successfully substitute for the MLR method at the first stage of the online system of the temperature and humidity satellite sounding, which will allow the time it takes to process large amounts of satellite data to be reduced significantly.

ACKNOWLEDGMENTS

This work was supported by the Russian Foundation for Basic Research (grant no. 12-05-00445-a) and the St. Petersburg State University (Research grants nos. 11.31.547.2010 and 11.37.28.2011).

REFERENCES

1. M. Matricardi, RTIASI-5 User's Guide, Report EUMETSAT, Contract EUM/CO/02/989/PS (ECMWF, Reading, 2004).
2. F. Aires, W. B. Rossow, N. A. Scott, and A. Chedin, "Remote sensing from the infrared atmospheric sounding interferometer instrument 1. Compression, denoising, and first-guess retrieval algorithms," J. Geophys. Res. **107** (D22) (2002). doi: 10.1029/2001JD000955
3. A. B. Uspenskii, S. V. Romanov, and A. N. Trotsenko, "The use of the method of main components for analyzing high-resolution IR-spectra measured from satellites," Issled. Zemli Kosmosa, No. 3, 26–33 (2003).
4. Ya. A. Virolainen, Yu. M. Timofeev, A. V. Polyakov, and A. B. Uspenskii, "Optimal parameterization of the spectra of outgoing thermal radiation with the data of the IKFS-2 spaceborne IR sensing device taken as an example," Atmos. Oceanic Opt. **23** (3), 215–221 (2010).
5. A. B. Uspenskii, A. N. Trotsenko, and A. N. Rublev, "Problems and perspectives of analysis and use of satellite IR-sensing data of high spectral resolution," Issled. Zemli Kosmosa, No. 5, 18–33 (2005).
6. F. S. Zavelevich, Yu. M. Golovin, A. V. Desyatov, et al., "Remote sensing of the earth using an IR Fourier-spectrometer," in *Abstracts of the International Symposium of CIS Countries "Atmospheric Radiation" (ISAR2006)* (SPbGU, St. Petersburg, 2006), pp. 113–114 [in Russian].
7. A. V. Polyakov, Yu. M. Timofeev, and A. B. Uspenskii, "Temperature–moisture sounding of the atmosphere by data of IKFS-2, a satellite IR sensing device with high spectral resolution," Issled. Zemli Kosmosa, No. 5, 3–10 (2009).
8. A. V. Polyakov, Yu. M. Timofeev, and A. B. Uspenskii, "Possibilities of determination of the content of ozone and other trace gases by data of IKFS-2, a satellite IR sensing device with high spectral resolution," Issled. Zemli Kosmosa, No. 3, 3–11 (2010).
9. A. V. Polyakov, Yu. M. Timofeev, and A. B. Uspenskii, "Possibilities of determination of temperature and surface reflectance by data of IKFS-2, a satellite IR sensing device with high spectral resolution," Issled. Zemli Kosmosa, No. 4, 85–90 (2010).
10. A. V. Polyakov, Yu. M. Timofeev, and V. S. Kostsov, "Satellite temperature sounding of the atmosphere in cloudy conditions," Issled. Zemli Kosmosa, No. 5, 37–42 (2010).
11. A. V. Polyakov and V. V. Rozanov, "An iterative technique for solving nonlinear inverse problems on the basis of a priori information," Tr. Gos. NITsIPR, No. 33, 99–103 (1989).
12. A. V. Polyakov, "On the problem of using a priori statistics to solve nonlinear inverse problems of atmospheric optics," Issled. Zemli Kosmosa, No. 3, 11–17 (1996).
13. H.-L. Huang and P. Antonelli, "Application of principal component analysis to high-resolution infrared measurement compression and retrieval," J. Clim. Appl. Meteorol. **40**, 365–388 (2001).
14. F. Aires, W. B. Rossow, N. A. Scott, and A. Chedin, "Remote sensing from the infrared atmospheric sounding interferometer instrument. 2. Simultaneous retrieval of temperature, water vapor, and ozone atmospheric profiles," J. Geophys. Res. **107** (D22), 4620 (2002). doi: 10.1029/2001JD001591
15. K. G. Gribanov and V. I. Zakharov, "Neural network solution for temperature profile retrieval from infrared spectra with high spectral resolution," Atmos. Sci. Lett. **5** (1–4), 1–11 (2004).
16. W. J. Blackwell and F. W. Chen, "Neural network applications in high-resolution atmospheric remote sensing," Lincoln Lab. J. **15** (2), 299–322 (2005).
17. A. Chedin, N. A. Scott, C. Wahiche, and P. Moulinier, "The improved initialization inversion method: a high resolution physical method for temperature retrievals from the TIROS-N series," J. Clim. Appl. Meteorol. **24**, 124–143 (1985).
18. F. Chevallier, F. Cheruy, N. A. Scott, and A. Chedin, "A neural network approach for a fast and accurate computation of a longwave radiative budget," J. Appl. Meteorol. **37**, 1385–1397 (1998).
19. A. V. Polyakov, "The use of the method of artificial neural networks in retrieving the vertical profiles of atmospheric parameters," Atmos. Oceanic Opt. (2014) (in press).

Translated by M. Samokhina