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OPTICAL INSTRUMENTATION

Optimal Parameterization of the Spectra of Outgoing Thermal Radiation with the Data of the IKFS-2 Spaceborne IR Sensing Device Taken as an Example

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Abstract—From the ensemble of the calculated spectra of the outgoing thermal radiation in the 660- to 2010-cm^{-1} range (2311 realizations) simulating global measurements by the IKFS-2 spaceborne device, the informativeness of the measurements of the outgoing thermal radiation has been analyzed in terms of Kozlov's data volume, the degrees of freedom, and the Shannon information gain. In the entire spectral range (660–2010 cm^{-1}), there are 106 independent parameters in the measurements of the outgoing radiation. The accuracy of the optimal parameterization of the spectral behavior of the radiation based on the radiation resolution into eigenvectors of the spectral covariance matrix has been analyzed. It is shown that to reach an rms error of the parameterization comparable with the random measurement noise for different spectral regions, it is sufficient to use from 20 to 50 first eigenvectors.

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INTRODUCTION

Currently, a promising field in the development of the satellite sensing of the atmosphere and the underlying surface in different spectral ranges is the use of devices with a rather high spectral resolution and a large number of measurement channels. Thus, in particular, AIRS and IASI infrared devices have a spectral resolution of ~0.5–2.0 cm^{-1} with a total number of channels of 2348 and 8461, respectively [1, 2]. The analysis of AIRS and IASI data has shown that they have a high informativeness and allow for the reconstruction of atmospheric and surface parameters with a high accuracy.

A large number of measurement channels creates certain problems in the online processing and analysis of data. The following approaches were proposed for the solution of these problems:

1. The use of relatively narrow "spectral windows" for the determination of particular atmosphere and surface parameters [3].

2. The separation of a limited set of "optimal" channels or "superchannels" with the maximal informativeness with respect to the studied parameters [4].

3. The optimal parameterization of the spectra of the outgoing radiation with the aid of the principal components analysis (PCA) or the resolution on the basis of the empirical orthogonal functions (EOFs) [5–8].

The optimal parameterization based on the application of PCA algorithms yields [9–12]

—the significant "compression" of the information for its storage,

—the decorrelation of the measurements in individual channels,

—the analysis of the informativeness of remote measurements,

—the optimization of the composition of the measurements as applied to some or another thematic problem of data "inversion,"

—the particular suppression of the filtering of the measurement noise, and

—the efficient data assimilation in the models of weather analysis and forecast.

In recent years, new applications of the optimal parameterization of high-resolution spectra appeared. They are connected with the detection of spectra "distorted" by cloudiness (see, for example, [13]), as well as with the development of ultrafast models of radiative calculations based on the use of PCA algorithms (Principal Component-based Radiative Transfer forward Model or PCRTM); see, for example, [14]. It should be noted that with the use of PCA algorithms, some spectra with "abnormal" features not included in the statistics used to construct the optimal parameterization are reconstructed poorly and are therefore excluded from the consideration (as noised ones). However, the use of the more representative statistics of atmospheric states can significantly minimize this negative effect. In addition, the PCA apparatus allows for the detection of spectra with abnormal features for the following analysis (see below).

In Russia, a new stage is occurring in the organization of the remote sensing of the atmosphere and the surface with increased accuracy and vertical resolution based on the construction of IFKS-2 IR Fourier transform spectrometers for the meteorological satellites of the Meteor-M series [15, 16]. This devices have a measurement spectral band of 660–2010 cm^{-1}, a resolution of 1200–4000, and a nadir spatial resolution of about 35 km (1 pixel). The total number of readings in the recorded spectrum is 5400. In [17–19], potential errors of the temperature–humidity sensing; the determination of the ozone, CH_4, and N_2O content; and the temperature and emissivity of the land surface were studied with the use of the multiple linear regression technique for the data inversion. This paper assesses the potential informativeness of the measurements of the outgoing thermal radiation by an IKFS-2 device with respect to the set of atmosphere and land surface parameters and analyzes the possibilities of using PCA algorithms for the optimal parametric representation of the spectra.

1. DETAILS OF THE CALCULATIONS

At the first stage of the study, using the original radiation code based on the direct calculation of the radiation of the inhomogeneous atmosphere (for details, see [17]), we have simulated the representative global sample of the $\{I_j(\nu_i)\}$ spectra recorded by the IKFS-2 device. Here, ν_i is the wavenumber of the ith channel, $i = 1, ..., 5400$, and j is the number of the realization, $j = 1, ..., 2311$. For the calculations of $I_j(\nu_i)$, we involved the atmospheric models of the well-known TIGR ensemble, which is described in [17, 20]. Then, every spectrum was considered as a vector of the dimension $(N \times 1)$, $N = 5400$. The random measurement error of the IKFS-2 device, according to [15, 16], has the following spectral dependence: for the 660- to 790-cm^{-1} range, the error (in terms of the standard deviation $\sigma(\nu)$) is equal to 0.1 $mW/(m^2\,sr\,cm^{-1})$, while at $\nu = 2000\,cm^{-1}$ it is 0.38 $mW/(m^2\,sr\,cm^{-1})$. To reduce to the common error level (0.1 $mW/(m^2\,sr\,cm^{-1})$), the signals in all channels were normalized $I'(\nu) = I(\nu)\dfrac{0.1}{\sigma(\nu)}$. For an ensemble of normalized spectra $\{I'(\nu)\}$, a sampling covariance matrix K was constructed, and the eigenvectors $\{f_\alpha(\nu)\}$ and eigennumbers $\{\lambda_\alpha\}$, $\alpha = 1, ..., N$, were determined.

Then, based on the known equations, we estimated the informativeness of the measurements by the IKFS-2 device in the whole spectrum and in some of its parts. In addition to the common indices of informativeness, we calculated the number of degrees of freedom for the signal and for the noise, which is popular in international published works [9]. The calculations were performed by the following equations:

(a) Kozlov's information amount [21],

$$V = \sqrt{\prod_{i=1}^{n}\lambda_i};$$

(b) degrees of freedom of a signal

$$d_S = \sum_{i=1}^{n}\lambda_i/(1+\lambda_i) \text{ and noise } d_N = \sum_{i=1}^{n}1/(1+\lambda_i);$$

(c) Shannon information gain [9]

$$\Delta I = \frac{1}{2}\log\prod_{i=1}^{n}(1+\lambda_i).$$

The value of n in the above equations is selected from the condition $n = \max\{\alpha: \lambda_\alpha \geq 1\}$, and, as a rule, $n \ll N$.

At the second stage of the study, we performed the optimal parameterization of all of the spectra of the ensemble with the use of a different number of vectors (EOFs) in the resolution. The optimal parametric representation of the signals in the channels or of the spectral dependence of the radiation $I(\nu)$ has the form [5]:

$$\tilde{I}_j(\nu) = \bar{I}'(\nu) + \sum_{p=1,n} a_p f_p(\nu).$$

Here, $\bar{I}'(\nu)$ is the sample-average spectrum; $f_p(\nu)$ are the eigenvectors of the covariance matrix K forming the EIF basis; and

$$a_p = \sum_{i=1,N}\delta I'_j(\nu_j) f_p(\nu_i),$$

where $\delta I'_j = I'_j - \bar{I}'$ are the corresponding coefficients of the resolution or principal components (PCs). It should be noted that the PCs are not correlated, in contrast to the signals I in different channels.

The condition of the selection of n has a clear interpretation [6, 8, 21]: the parameter λ_α is a ratio of the PC variance to the noise variance in the direction of the corresponding eigenvector f_α, in other words, it represents the signal-to-noise ratio. The boundary condition $\lambda_n = 1$ corresponds to the zero information contribution of the measurements. That is why in some papers the number n is referred to as the index of informativeness. It should be noted that the condition of the selection of n is heuristic. Its fulfillment for simulated data (with the known matrices K_f, K_e) actually allows for the useful signal to be separated against the background of noise, and for actual data (when only the sampled estimates of K_f, K_e are known) the additional analysis of the relation between the loss of informativeness and the noise level is required as the spectrum $I'(\nu)$ is replaced with its optimal parametric representation $\tilde{I}'(\nu)$. Additional details on the application of the PCA technique can be found in [6, 8, 21].

Table 1. Information characteristics of the determination of the atmospheric and surface parameters by the IKFS-2 device

Spectral region, cm^{-1}	Informativeness	Information volume	Degrees of freedom	Shannon information capacity, bit
660–2010	106	10^{90}	92.4	311
660–790	42	10^{40}	37.1	140
790–1260	70	10^{59}	61.5	203
1260–1650	22	10^{18}	19.2	63

Table 2. Number of terms of the resolution in the EOFs in the optimal parameterization and the number of spectra with the increased level of the rms deviation approximation

Spectral range, cm^{-1}	Determined parameter	Number of eigenvectors (EOFs)	Number of poorly approximated spectra, %
660–790	Temperature profile	50	1.9
790–970, 1120–1260	Surface temperature and reflection coefficient	40	4.8
970–1120	Ozone profile	40	1.2
1260–1330	Methane and N_2O profile	30	0.7 and 1.6
1330–1650	Water vapor profile	20	0

2. CHARACTERISTICS OF THE INFORMATIVENESS OF IKFS-2 MEASUREMENTS

Table 1 summarizes the different information characteristics of IKFS-2 measurements for the entire spectral band of 660–2010 cm^{-1} and for some of its subranges.

Column 2 presents the indices of informativeness, that is, the number of eigenvectors n for which the condition $\lambda_i \geq 1$ is true. The separation into spectral ranges was performed according to thematic inverse problems on the reconstruction of any of the parameters of the atmosphere and the surface (see Table 2). It should be noted, however, that the information about the parameters such as the water vapor and temperature profiles is contained in other spectral ranges as well. In particular, data of the ozone absorption band are used to reconstruct the stratospheric temperature.

IKFS-2 measurements of the outgoing radiation in the entire spectral region (660–2010 cm^{-1}) allow for the reconstruction of 106 independent parameters, and the number of distinguishable states of the atmosphere, which are determined by Kozlov's information volume, is 10^{90}, while the number of degrees of freedom corresponding to the measured signal is 92.4, and the Shannon information gain is 311 bits.

In the 660- to 790-cm^{-1} range, which is mostly used for the determination of the temperature profile, 42 independent parameters can be reconstructed (the number of degrees of freedom for the useful signal is 37.1). In addition to temperature, there is also some information about ozone and water vapor. The number of distinguishable atmospheric states is 10^{40}. The information gain is 140.

From the IKFS-2 measurements of the outgoing radiation in the 790- to 1260-cm^{-1} range, it is possible to determine 70 independent parameters, namely, to obtain information about the vertical thermal structure, water vapor, and ozone content in the atmosphere, as well as the temperature and emission properties of the surface. In this case, 10^{59} states of these parameters can be distinguished from the measurements. The analysis of the degrees of freedom shows that 61.5 of the 70 independent parameters correspond to a useful signal, while the others correspond to the random noise of the measurements. The information content (Shannon information gain) for this spectral range corresponds to 203 bits.

From the measurements of the radiation in the 1260- to 1650-cm^{-1} spectral range, it is possible to reconstruct only 22 parameters, namely, the vertical structure of the water vapor content and, additionally, the methane and nitrogen monoxide content, as well as some information about the temperature. The information volume of the measurements is 10^{18}, the number of degrees of freedom is 19.2, and the information gain is 63 bits.

3. OPTIMAL PARAMETERIZATION OF THE SIMULATED SPECTRA

The apparatus described above was used to construct parametric representations of each spectrum of the available ensemble with accounting for the different number of EOFs in the resolution. The errors of the parameterization were determined in order to

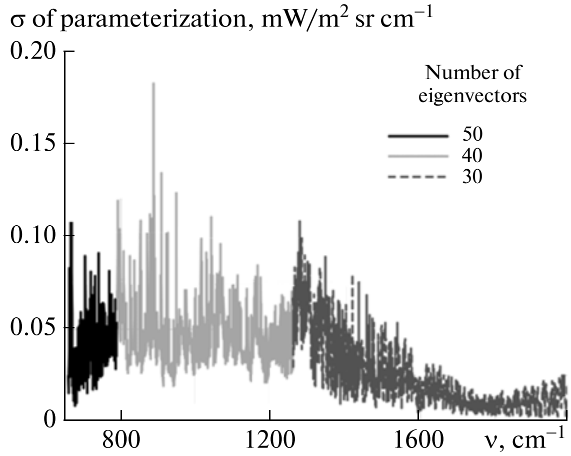

Fig. 1. Root-mean-square deviation of the optimal parameterization of the spectra of the outgoing thermal radiation with the use of a different number of EOFs (50 vectors for 660–790 cm^{-1}, 40 vectors for 790–1260 cm^{-1}, and 30 vectors for 1260–2010 cm^{-1}).

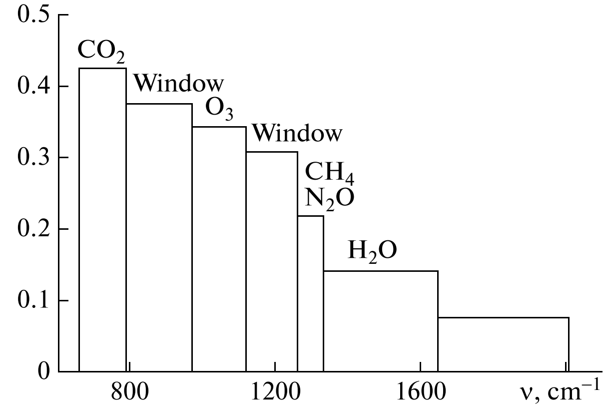

Fig. 2. Ratio of the optimal parameterization error to the random noise for different spectral ranges.

empirically estimate their optimal number. These estimates are only tentative, because they are not free from sampling effects, and, in addition, the actual characteristics of the IKFS-2 will be known only when it is launched into space. Thus, for simplicity and for better illustration, the number of EOFs was rounded to tens.

Figure 1 shows the spectral dependence of the root-mean-square deviation (rms) of the optimal parameterization for the whole ensemble of spectra with allowance for 30, 40, and 50 (depending on the spectral range) eigenvectors of the covariance matrix K in the resolution. The solid line shows the level of random noise in the measurements.

It should be noted that with 60 vectors taken into consideration, the rms error of the parameterization is distinctly lower than the random measurement noise for the entire spectral region. As can be seen from Fig. 1, with a smaller number of vectors taken into account, the rms deviation in some channels can somewhat exceed the noise level.

For a more detailed analysis of the error of the optimal parameterization, we considered the spectral intervals used for the reconstruction of some or another surface or atmospheric parameters. Figure 2 shows the ratio of the rms deviation of the parameterization to the random measurement noise for the spectral ranges in the absorption bands of carbon dioxide, ozone, methane, nitrogen monoxide, and water vapor.

In addition, parts of the spectral windows, the measurements in which are used to reconstruct the surface emissivity and temperature, as well as the edge of the IFKS-2 band (1650–2000 cm^{-1}), are separated. It can be seen from Fig. 2 that the parameterization errors are maximal in the carbon dioxide absorption band and decrease with the transition to the shorter wavelength part of the spectrum.

Carbon Dioxide Absorption Band at 15 μm

It can be seen from Fig. 1 that for the 15-μm band, which is used mostly in the temperature sensing of the atmosphere, the optimal parameterization is performed with allowance for the first 50 eigenvectors. Since the initial ensemble of spectra $\{I_j(\nu)\}$ is sufficiently large (2311 realizations), it is interesting to study the distribution of the errors over different realizations of the ensemble in order to estimate the percentage of the spectra in which the error exceeds the random measurement noise (due to abnormal features in the spectra). For this purpose, we have selected several characteristic channels in the carbon dioxide band: the channel of 666.75 cm^{-1}, in which the error of the optimal parameterization is maximal; the channel of 705.5 cm^{-1}, in which the error is also higher than the average over the range; and the channel of 692 cm^{-1}, in which the error of the optimal parameterization is typical for the entire interval. For the channel of 666.75 cm^{-1} and one realization of the spectrum, the error of the optimal parameterization exceeds the random measurement noise by more than an order of magnitude. In general, for this channel, in 43 of 2311 cases (1.9%) the parameterization error is higher than the measurement noise with the use of 50 eigenvectors. Figure 3 (top) shows the channel with a rather high parameterization error (705.5 cm^{-1}).

For this channel, the parameterization error exceeds the random measurement noise in seven cases (0.3%). For the channel of 692 cm^{-1}, the error of the optimal parameterization in all cases is distinctly lower than the measurement noise.

Ozone Absorption Band and Region of the Atmospheric Window

For the 790- to 1260-cm^{-1} range, the first 40 eigenvectors were used in the optimal resolution. In Fig. 1, we can see the rms error of the optimal parameterization for this spectral range. It follows from Fig. 1 that the rms deviation exceeds the measurement noise in a number of channels, in the atmospheric window, and in the ozone absorption band. Figure 3 (bottom) demonstrates the poor, from the viewpoint of the optimal parameterization, channel from the center of the ozone absorption band (1042.5 cm^{-1}). The analysis of the depicted histogram has shown that for the 1042.5-cm^{-1} channel with the use of 40 eigenvectors in the resolution, the number of realizations in which the parameterization error exceeds the random measurement noise is 29; that is, 1.2% of the total number of realizations in the ensemble. For the poorest channel in the atmospheric window (887.25 cm^{-1}), this number is 110 realizations (4.8%). In six cases, the parameterization error is an order of magnitude higher than the measurement noise. The error of the optimal parameterization in the most typical (mean) channels of the ozone band (1010 cm^{-1}) and the atmospheric window (1158.75 cm^{-1}) exceeds the random measurement noise in 4 and 14 cases, respectively.

Methane, Nitrogen Monoxide, and Water Vapor Absorption Bands

Figure 1 also shows the rms deviations of the optimal parameterization of the spectral dependence of radiation in methane, nitrogen monoxide, and water vapor absorption bands with the use of 30 eigenvectors. It should be noted that for the water vapor absorption band at 6.3 μm, it is sufficient to use the first 20 eigenvectors for the error of the optimal parameterization so that it does not exceed the level of the random measurement noise for any realization. In the 1283-cm^{-1} channel (in the N_2O absorption band), the parameterization error is maximal, and in 37 cases out of 2311 (1.6%) it exceeds the random measurement noise. For the methane absorption band, the poorest case is represented by the 1304.25-cm^{-1} channel. In this case, the error of the optimal parameterization in this channel exceeds the random measurement noise in 16 cases; that is, in 0.7% of all realizations of the considered ensemble.

Table 2 presents the spectral ranges used for the reconstruction of some or another parameter, the number of used vectors, and the maximal number (in %) of poor spectra, for which the parameterization error exceeds the random measurement noise.

As a general comment to the materials presented, we can note the following. The increase of the error during the parametric representation of some spectra is explained by the abnormal features of the spectral dependence in some bands, which, in turn, are induced by the features of the corresponding realizations of the atmospheric models of the TIGR ensemble. The independent analysis shows that, for example, the vertical temperature profiles over some regions of China have pronounced temperature inversions in the lower troposphere. This causes the abnormal behavior of the spectra in the atmospheric window and leads to the growth of the error of the approximation with the use of PCA algorithms. In such situations, the increase of the rms deviation can serve as an indicator of the out-of-order state of the atmosphere, and the corresponding spectra should be subjected to additional analysis.

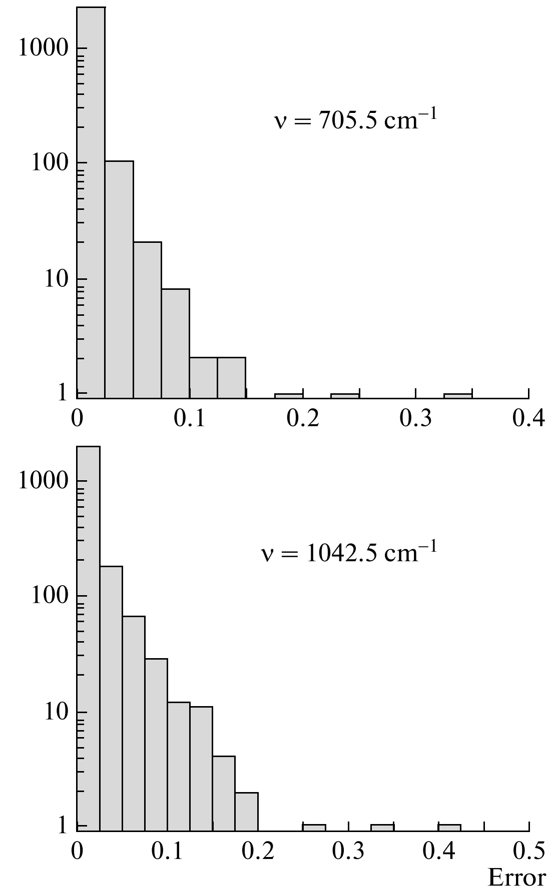

Fig. 3. Examples of the histograms of the optimal parameterization error for the whole ensemble of the spectra of the outgoing thermal radiation in some channels.

4. MAIN RESULTS AND CONCLUSIONS

The principal component analysis was used for the analysis of the ensemble of the calculated spectra of the outgoing thermal radiation in the 660- to 2010-cm^{-1} wavelength region (2311 realizations simulating global measurements by a spaceborne IKFS-2 device). The informativeness of the measurements of the outgoing thermal radiation has been analyzed in terms of Kozlov's information volume, the degrees of freedom, and the Shannon information gain. The calculations have been performed for the entire spectral range and some subranges used to reconstruct various surface and atmospheric parameters.

The atmospheric window of 790–1260 cm^{-1} is the most informative spectral range, from the measurements in which it is possible to determine up to 70 independent surface and atmospheric parameters. In the range of the carbon dioxide absorption band (660–790 cm^{-1}), it is possible to determine up to 40 parameters, and up to 22 parameters can be determined in the range of the methane, nitrogen monoxide, and water vapor absorption bands (1260–1650 cm^{-1}). In the entire spectral region (660–2010 cm^{-1}), 106 independent parameters are present in the measurements of the outgoing radiation.

The accuracy of the optimal parameterization of the spectral dependence of radiation based on the resolution of the radiation in eigenvectors of the spectral covariance matrix (EOFs) has been analyzed. It is shown that to achieve an accuracy comparable with the random measurement noise, in most cases it is sufficient to use the first 50 eigenvectors in the resolution. If the entire spectral range is divided into subranges, the number of eigenvectors in the resolution can be decreased. Thus, 50 eigenvectors should be used in the carbon dioxide absorption band, 40 eigenvectors are sufficient for the atmospheric window and the ozone absorption band, 30 eigenvectors are sufficient for the methane and nitrogen dioxide absorption bands, and 20 eigenvectors should be used in the water vapor absorption band.

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