A Three-Dimensional Satellite Retrieval Method for Atmospheric Temperature and Moisture Profiles

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ABSTRACT

A three-dimensional variational method is proposed to simultaneously retrieve the 3-D atmospheric temperature and moisture profiles from satellite radiance measurements. To include both vertical structure and the horizontal patterns of the atmospheric temperature and moisture, an EOF technique is used to decompose the temperature and moisture field in a 3-D space. A number of numerical simulations are conducted and they demonstrate that the 3-D method is less sensitive to the observation errors compared to the 1-D method. When the observation error is more than 2.0 K, to get the best results, the truncation number for the EOF's expansion have to be restricted to 2 in the 1-D method, while it can be set as large as 40 in a 3-D method. This results in the truncation error being reduced and the retrieval accuracy being improved in the 3-D method. Compared to the 1-D method, the rms errors of the 3-D method are reduced by 48% and 36% for the temperature and moisture retrievals, respectively. Using the real satellite measured brightness temperatures at 0557 UTC 31 July 2002, the temperature and moisture profiles are retrieved over a region $(20^\circ-45^\circ N, 100^\circ-125^\circ E)$ and compared with 37 collocated radiosonde observations. The results show that the retrieval accuracy with a 3-D method is significantly higher than those with the 1-D method.

Key words: atmospheric temperature and moisture profile, retrieval, EOF, three-dimensional method, satellite radiance

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1. Introduction

Since satellites can provide global coverage of observational data in the temporal and spatial scales, which can make up for the lack of radiosonde observations, the retrieval of atmospheric temperature and moisture profiles from satellite remote sensing data is an important research topic. In principle, the temperature and moisture retrievals are based on the atmospheric radiative transfer equation, which is a one-dimensional vertical integral equation. As a result, most of the existing approaches for the temperature and humidity retrievals, regardless of the statistical methods (e.g., Smith and Woolf, 1976; Thompson et al., 1985; Uddstrom, 1988; Lipton and Vonder Haar, 1987; Huang and Antonelli, 2001), or the physical methods (e.g., Smith, 1970, 1983; Smith et al., 1991; Hayden, 1988, 1994; Hayden and Schmit, 1994; Rodgers, 1976; Eyre, 1989, 1991; Eyre et al., 1993), as well as the statistical-physical methods (e.g., Li et al., 2000; Li and Huang, 2001; Wu et al., 2005; Ma et al., 1999), are regarded as a one-dimensional inversion problem, i.e., the radiances are processed independently of each other and the retrieval is made at a single location. However, the satellite radiance observations do not contain sufficient information to permit direct retrieval of some features of meteorological significance, therefore some additional information, in the form of the statistics of the atmospheric profiles, must be supplied to the retrieval equations. Smith and Woolf (1976) first employed EOF's decomposition method to the atmospheric temperature and moisture retrievals. By representing the temperature and moisture profiles in terms of the EOF's, the statistical

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information of the vertical structure of temperature and moisture profiles are introduced into the retrieval process and the number of the unknown variables is greatly reduced. There are many similar algorithms. To name a few, the pattern recognition techniques of Thompson et al. (1985, 1986) and Thompson (1992), the typical shape functions classification method of Uddstrom and Wark (1985) and Uddstrom (1988), and the principle component regression method of Huang and Antonelli (2001). In these methods the number of unknown variables is reduced efficiently and the system of equations to be solved is heavily overdetermined. Therefore, the effects of random errors of observations on the retrieval are greatly suppressed. In addition, by introducing statistical information into the retrieval, the retrieval procedure is constrained by the statistical structure determined from a priori sample dataset and the vertical structure, which is not directly measured by the satellite, will be introduced into the retrieval profiles.

Hoffman and Thomas (1989) first attempted to use the 3DVAR method to retrieve the temperature and cloud parameters by using simulated radiance data, which is one of the few three-dimensional retrieval approaches. The EOF's are used as the vertical basis functions, while the Fourier components are adopted as the horizontal basis functions. Their results indicate that the 3-D method properly guarantees the smoothness of the temperature field and reduces the impact of clouds on the retrieval process due to the use of the truncated Fourier basis functions (Hoffman and Thomas, 1989). In this paper, we propose a new 3-D retrieval method, which is based on the 3-D EOF's technique, to simultaneously retrieve the atmospheric temperature and moisture profiles. In this method, the EOF's are made in both the horizontal and vertical space so that information in both directions is included in the eigenvectors. In this case, more useful information is retained for temperature and moisture profile retrievals. The plan of this paper is as follows: The 3-D variational retrieval algorithm is discussed in section 2. The details of comparisons between 1-D and 3-D retrieval method with different observation errors are presented in section 3, and retrieval examples are shown in section 4.

2. Retrieval methodology

Deriving atmospheric temperature and moisture profiles from satellite observations is an inversion problem of resolving the initial condition of the radiative transfer equation (Smith and Woolf, 1976; Eyre, 1991). In general, the temperature and humidity inversion is regarded as a one-dimensional (vertical) problem. For most nonlinear physical retrieval algorithms (Barnett, 1969; Eyre, 1989; Eyre et al., 1993; Ma et al., 1999), the retrieval procedure is boiled down to find the optimal approximation to the actual atmospheric profile for the given satellite observation in the sense of least-squares estimation. Assuming that the atmospheric parameters containing L levels of atmospheric temperature and relative humidity profiles are denoted as $x = (T_1, \ldots, T_L, f_1, \ldots, f_L)$ and the satellite observed radiance is $\boldsymbol{y}_{\mathrm{o}}$. Here, the length of vector \boldsymbol{x} is $N_x = N_g \times N_v \times L$, where N_g is the number of satellite observations, and $N_{\rm v}$ is the number of retrieved variables. The length of the vector \boldsymbol{y}_{0} is $N_{y} = N_{g} \times N_{c}$, and $N_{\rm c}$ is the number of satellite channels used for retrievals. A general form of the optimum variance solution is to minimize the following cost function, which is similar to Eyre's method (Eyre, 1989)

$$J(\boldsymbol{x}) = (\boldsymbol{x} - \boldsymbol{x}_0)^{\mathrm{T}} \boldsymbol{B}^{-1} (\boldsymbol{x} - \boldsymbol{x}_0) + [H(\boldsymbol{x}) - \boldsymbol{y}_0]^{\mathrm{T}} \boldsymbol{O}^{-1} [H(\boldsymbol{x}) - \boldsymbol{y}_0] .$$
(1)

Here, \boldsymbol{x}_0 is the profile in the initial estimate, \boldsymbol{B} is the covariance matrix representing the expected errors in x_0, O is the observation error covariance matrix, and H denotes the forward model or radiative transfer model (RTM). At the minimum, the derivative of J with respect to \boldsymbol{x} is equal to zero. The minimum of Eq. (1) can be found by setting the derivative equal to zero and performing a large matrix inversion. The onedimensional variational inverse method (Eyre, 1989; Eyre et al., 1993; Ma et al., 1999) that employs the descent algorithm to seek the minimum is an effective method. Using the EOF's technique, the profile vector is presented as a linear combination of a series of eigenvectors of the temperature and moisture profile (Smith and Woolf, 1976; Ma et al., 1999). In this study, a method similar to Eyre's (or others) is used as follows:

$$\delta \boldsymbol{x} = \boldsymbol{x} - \boldsymbol{x}_0 = \sum \boldsymbol{v}_p f_p = \boldsymbol{V} \boldsymbol{f} , \qquad (2)$$

where \boldsymbol{v}_p is the *p*th eigenvector, the length of \boldsymbol{v}_p is N_x, f_p is the *p*th expansion coefficient, and *p* denotes the number of terms. $-\boldsymbol{V} = \boldsymbol{V}(\boldsymbol{v}_1, \boldsymbol{v}_2, \dots, \boldsymbol{v}_p)$ is the eigenvector matrix, \boldsymbol{f} is the expansion coefficient vector. The eigenvectors are derived from a statistical covariance matrix of a large sample of the observed or analytic temperature and moisture profiles. In our experiments the NCEP re-analysis temperature and moisture profiles are used to construct the sample dataset. The corresponding cost function to Eq. (1) can then be written as

$$J(\boldsymbol{f}) = \boldsymbol{f}^{\mathrm{T}} \boldsymbol{B}^{-1} \boldsymbol{f} + [H(\boldsymbol{f}) - \boldsymbol{y}_{\mathrm{o}}]^{\mathrm{T}} \boldsymbol{O}^{-1} [H(\boldsymbol{f}) - \boldsymbol{y}_{\mathrm{o}}] .$$
(3)

By doing this, the problem of retrieving atmospheric parameters becomes the problem of finding the optimal expansion coefficients and the computation is reduced greatly. The basic difference between the conventional 1-D retrieval method and the method

described here is that retrievals in this study are 3D instead of 1D. If $N_{\rm g}$ is set to $N_{\rm g} = 1$, then only a single profile will be retrieved in the 3-D retrieval, so the retrieval is equal to the 1-D retrieval.

The key stages of the proposed scheme in this paper are to simultaneously retrieve temperature-moisture profiles within an atmospheric column with multiple grid cells and to perform the EOF's in a threedimensional space instead of a one-dimensional space. In this way the eigenvectors not only represent the vertical structure of the atmospheric profiles but also include the horizontal characteristics. For simplification, the traditional retrieval method in which the atmospheric profiles are retrieved one-by-one is called the 1-D retrieval method; the method proposed here is called the 3-D retrieval method.

3. Numerical Experiments using simulated HIRS/3 data

A set of numerical experiments has been designed to compare the 3-D retrieval method with the 1-D retrieval method using simulated infrared brightness temperature data of 19 channels matching ATOVS HIRS/3 radiance observations. The retrieval is made at $1.0^{\circ} \times 1.0^{\circ}$ grids over a square area where the longitude is from 110° E to 120° E and the latitude is from 25° N to 35° N. The total number of the grid cells is 121. The simulated HIRS/3 (High Resolution Infrared Sounder) brightness temperatures are calculated from $1^{\circ} \times 1^{\circ}$ NCEP re-analysis temperature and humidity profiles by using RTM RTTOV7 which is developed by ECMWF. A total of 122 temperature and humidity profile samples are used in the study; they are

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taken from the NCEP re-analysis data in July from 2000 to 2003 over the retrieval region. The EOF's are calculated from the samples. For the 1-D method the EOF's are calculated grid-by-grid independently. However, they are calculated in the 3-D space for the 3-D retrieval method. As described in section 2, the atmospheric profile vectors can be expanded in terms of a few eigenvectors to capture the atmospheric spatial structure information contained in the radiance observations. The NCEP re-analysis data are considered as the "true" profiles, the average of the samples for each observation is adopted as the background profile. The "observations" are generated by adding random noises to the radiances calculated from the "true" profiles by RTM. The rmse of the brightness temperature observations for different experiments are set as 0.25 K, 0.5 K, 1.0 K, 2.0 K, and 4.0 K, respectively. The details of the comparisons between the 1-D and 3-D retrieval methods with different observation errors are presented in the following sections.

Figure 1 compares the rmse of the retrieved temperature (Fig. 1a) and relative humidity (Fig. 1b) profiles between the 3-D and 1-D methods over the whole retrieval region when the observation error is 0.25 K (the truncation number of the EOF expansion is set to p = 2 and p = 40 for the 1-D and 3-D retrieval methods, respectively). For the temperature retrieval (Fig. 1a), the 3-D method shows significant improvement compared to the 1-D method below 300 hPa. The retrieval error of the 3-D method is much smaller than that obtained from the 1-D method. But the 3-D method does not show good results at 100 hPa and the retrieval error is larger than that obtained from the 1-D method. For the relative humidity (Fig. 1b), although the retrieval results of these two methods are much closer below 400 hPa, the retrieval error from the 3-D retrieval is always smaller than that from the 1-D retrieval. Above 400 hPa, the retrieval results are very different between the two methods. In the 3-D retri-



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Fig. 1. The rmse of the (a) temperature and (b) relative humidity retrieval when the observation error is 0.25 K. Broken line denotes the background; thin solid and thick solid lines denote the 1-D and 3-D retrieval, respectively.



Fig. 2. Same as Fig. 1 except that the observation error is 2.0 K.



Fig. 3. The temperature increment field at 700 hPa for (a) true field, (b) retrieved field from 1-D method and (c) retrieved field from 3-D method, respectively. (units: K)

eval, the retrieved profiles corrected the backgrounds greatly, while in the 1-D retrieval, the retrieval error is even larger than the background error.

When the observation error increases to 2.0 K, the 3-D retrieval significantly improves the background temperature profiles for most levels and the retrieval error is much smaller than that obtained from the 1-D retrieval for temperature retrieval (see Fig. 2a). As for the relative humidity retrieval, the retrieval error of the 3-D method is always smaller than that of the 1-D method, although the background is improved to some extent below 300 hPa. Above 300 hPa the retrieval error of the 1-D method is larger than the background error. While in the 3-D retrieval the background can be improved obviously for all of the levels and the retrieval error is always smaller than the background error.

To assess the performance of the two methods, the increment fields, relative to the background, of the 1-D and 3-D methods are compared with the true increment field. As an example, the increments at 700 hPa are shown in Fig. 3a (true increment), Fig. 3b (for 1-D method) and Fig. 3c (for 3-D method), respectively. The temperature structure is nicely recovered by the 3-D method as shown in Fig. 3c, especially with respect to the relative position of the maximum and minimum centers in the increment field. However, the 1-D method cannot perform well. Similar results can be found for the relative humidity increment field from Fig. 4. The 3-D method can capture major features of the 3-D moisture field.

To compare the two retrieval methods further, a set of experiments is made with different observation errors and different truncation numbers. The statistical results of the averaged rms errors for the temperature and relative humidity retrieval over all grid cells are listed in Table 1 (for temperature) and Table 2 (for relative humidity), respectively. For the temperature retrieval, the rms errors of the 3-D method are smaller than those of the 1-D method in all of the experiments.

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		1-D				3-D		
Observation error (K)	Background error (K)	p=2	p = 3	p = 4	p = 5	p = 40	p = 60	p = 80
0.25	2.671	1.418	1.530	1.565	1.539	0.885	0.854	1.329
0.5	2.671	1.432	1.547	1.597	1.584	0.877	1.363	1.329
1.0	2.671	1.470	1.702	1.728	1.786	0.869	1.332	1.330
2.0	2.671	1.649	2.106	2.233	2.382	0.862	1.335	1.335
4.0	2.671	2.238	3.167	3.664	3.953	1.340	1.340	1.340

Table 1. Averaged retrieval errors for temperature of the two methods with different truncation number (p) and different observation errors. (Units: K)

Table 2. Averaged retrieval errors for relative humidity of the two methods with different truncation number (p) and different observation errors.

		1-D				3-D		
Observation error (K)	Background error (K)	p=2	p = 3	p = 4	p = 5	p = 40	p = 60	p = 80
0.25	0.196	0.129	0.140	0.142	0.152	0.087	0.081	0.114
0.5	0.196	0.130	0.141	0.141	0.152	0.087	0.110	0.114
1.0	0.196	0.126	0.145	0.144	0.162	0.0867	0.118	0.115
2.0	0.196	0.133	0.164	0.172	0.208	0.086	0.117	0.116
4.0	0.196	0.179	0.228	0.297	0.436	0.105	0.114	0.1226

When observation error is normalsize (≤ 0.5 K), there is no significant difference between the 1-D and 3-D retrieval; but when the observation error increases gradually (≥ 1.0 K), the 3-D method performs much better than the 1-D method. The results show that the larger the observation error is, the more obvious differences between the two retrieval methods can be found. For example, when the observation error increases to 4.0 K, the retrieval error of the 1-D method is even larger than the background error. But for the 3-D retrieval, a good retrieval result is still possible. The relative humidity retrieval is similar to the temperature retrieval (see Table 2). In addition, the results show that when the observation error is large, the 1-D method is sensitive to observation error and only very low truncation number is permitted. Whereas this situation will not appear in the 3-D retrieval and it is not sensitive to the truncation number in some range.

Why does the 3-D method perform better than the 1-D method for the same atmospheric parameter samples, observations and radiative transfer model? There are two factors that may cause the retrieval error differences between the 3-D and 1-D methods. These are the observation errors and the truncation errors, which come from the EOF expansion.

The statistical results listed by Table 1 and Table 2 show that the retrieval solution of the 1-D method is sensitive to the observation errors for larger truncation numbers. For example, when the truncation number is set to p = 5 the temperature retrieval error increases from 1.54 K to 3.95 K and the relative humidity retrieval error increases from 0.15 to 0.44 while

the observation errors increases from 0.25 K to 4.0 K. In order to depress the sensitivity to the observation errors we have to employ a very normalsize truncation number for EOF expansion for the 1-D method. This implies that there are larger truncation errors in the EOF expansion. In comparison to the 1-D retrieval method, the sensitivity of the 3-D retrieval to the observation errors is much weaker. For the 3-D retrieval, the retrieval error still remains normalsize even the truncation number is set to p = 80 since a lot of random observation errors are filtrated in the 3-D EOF expansion.

As depicted above, the 3-D method permits larger truncation numbers than the 1-D method in the EOF expansion. Nevertheless, the variables retrieved by the 3-D method are much larger than those in the 1-D method. Hence, it is not guaranteed that the truncation error for the 3-D method is smaller than that for 1-D method when the truncation number in the EOF expansion for the 3-D method is larger than that for 1-D method. We need further analysis of the truncation error in the two methods. Here, we set p = 2 for the 1-D retrieval and p = 60 for the 3-D retrieval. Following Eq. (2), the truncation error in the EOF expansion is $\boldsymbol{\varepsilon}_x = \delta \boldsymbol{x}_t - \Sigma \boldsymbol{v}_p f_p$. For the 1-D method, the expansion of EOF's is performed independently for each profile but it is performed in 3-D space for the 3-D method. Figure 5 is the rms truncation error for all the "true" atmospheric profiles over the retrieval area at different levels for the two expansion methods. With specified truncation numbers, the truncation errors in the 3-D expansion are always smaller than those in 1-D expan-



Fig. 4. The specific humidity increment field at 700 hPa for (a) true field, (b) retrieved field from 1-D method and (c) retrieved field from 3-D method, separately. (units: $g kg^{-1}$)

sion for both temperature (Fig. 5a) and relative humidity (Fig. 5b). This is the basic reason why the 3-D method performs better than the 1-D method.

4. Case study

In this section, the 1-D and 3-D retrieval methods are used to retrieve the temperature and relative humidity profiles from the real satellite measured brightness temperatures at 0557 UTC 31 July 2002. The retrieval is made over a region where the longitude is from 100° E to 125° E and the latitude is from 20°N to 45°N. The temperature and humidity samples used in the retrieval are the same as those in section 3. The NCEP re-analysis temperature and moisture profiles from 24 hours before the retrieval time are adopted as the background. In order to make the brightness temperatures computed by the radiative transfer model for the sample profiles match with the actual measured brightness temperatures, the bilinear interpolation method is used to interpolate sample data from grid points to the satellite observation locations. The retrieval is performed at the observation locations. The real radiosonde observations at 0600 UTC 31 July 2002 are taken as the true profiles to evaluate the retrieval accuracy. The distance between a retrieval sounding location and a radiosonde location is within 1.0° (i.e., approximately 110 km). The clear sky detection is made by following the procedure from Li et al. (2000); a simple quality control is made to reject the bad observations. The threshold for the quality control is that the averaged brightness temperature discrepancy over the 12 channels between the measured brightness temperatures and the computed background brightness temperatures is less than 5.0 K. After that, 37 profiles are selected for retrieval. Both the 1-D and 3-D retrieval methods are used to retrieve temperature and humidity profiles from the measured brightness temperatures at the clear sky observation locations, respectively.

The averaged rmse of the 37 profiles for the temperature and relative humidity retrieval with the 1-D and 3-D retrieval method over the whole retrieval region are given in Fig. 6. For the temperature, the retrieval error of 3-D method is significantly smaller than that of the 1-D method below 100 hPa (Fig. 6a). Above 100 hPa, although the difference between the two methods is not obvious, the 3-D retrieval still performs better than the 1-D retrieval. For the relative humidity (Fig. 6b), there is a good agreement between radiosondes and the 3-D retrievals, especially from 800 hPa to 300 hPa. The 3-D retrieval significantly improves the results when compared to the 1-D retrieval. For the relative humidity above 300 hPa, there is no absolute evaluation result for the two methods.

5. Summary and conclusions

In this study, a retrieval method based on the three-dimensional empirical orthogonal functions technique is proposed to retrieve the atmospheric temperature and moisture profiles from satellite radiance measurements. The eigenvectors of the 3-D EOF's, which are extracted from the sample dataset, not only represent the vertical structure of the atmospheric parameters, but also include the horizontal characteristics.



Fig. 5. The rms truncation error at different height levels in the two retrieval methods. Thin and thick lines denote the 1-D and 3-D retrieval method, respectively.



Fig. 6. The rmse of the (a) temperature and (b) relative humidity retrieval in the real retrieval. This solid and thick solid lines denote the 1-D and 3-D retrieval, respectively.

The advantages of this method are demonstrated by comparing results with the traditional 1-D method through several numerical experiments for simulated data and real radiance measurements. The results show that the new method is less sensitive to observation errors and it can filter out more observation errors. In this case, the retrieval accuracy of the 3-D method is significantly higher than that of the 1-D method for both temperature and humidity retrieval. When the observation error is more than 2.0 K, to get the best results, the truncation number for the EOF's expansion has to be restricted to 2 in the 1-D method, while it can be set as large as 40 in 3-D method. So, the truncation error is reduced and the retrieval accuracy is improved in the 3-D method. In addition, the 3-D approach can properly recover the three-dimensional temperature and moisture structures and accurately capture the major features of the background fields. The case study has similar results. A problem that needs to be pointed out is that this method requires a spatially dense observation network for the atmospheric temperature-humidity profiles to construct the historical ensemble samples for the EOF's. The radiosonde measurements are hardly sufficient to satisfy this requirement. Maybe the high-resolution numerical weather predication (NWP) model output or the assimilation data can be used to construct the ensemble sample. This is a topic for further study.

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