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Water vapor and air-temperature profile estimation with AIRS data based on Levenberg-Marquardt

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Abstract: A retrieval method for vertical profiles of air-temperature and relative humidity based on non-linear least square method of Levenberg-Marquardt is proposed. It is found that the proposed method is robust to the situation of which the solution does not exist or of which estimation accuracy is poor. In comparison to the estimation accuracy of the conventional method of Newton Rafson method, it is also found that the proposed method is superior to the conventional method for many cases.

Key words: non-linear square method, air-temperature profile, relative humidity profile

1. Introduction

There are two major methods for vertical profile retrievals of air-temperature, relative humidity with AIRS (Atmospheric Infrared Sounder) data. Those are regressive method and geophysical based method. The later is based on RTE (Radiative Transfer Equation). In accordance with AIRS/ATBD (Algorithm Theoretical Basis Document) by Aumann H. et al.[2001], AIRS RTE most closely follows Susskind et al. [1983] by parameterizing the optical depths rather than transmittances for channels where the influence of water vapor is small. Channels sensitive to water vapor are modeled using a variant of the Optical Path TRANsmittance (OPTRAN) algorithm developed by McMillin et al. [1979, 1995]. The AIRS infrared fast model is thus a hybrid of both Susskind's approach and OPTRAN. In accordance with AIRS/ATBD, a linearized RTE is used. Geophysical parameters are estimated as to minimize the difference between model derived radiance with geophysical parameters and actual AIRS radiance by solving the linearized RTE based on Newton method with Hessian. Air-temperature and relative humidity profile retrieval accuracy in troposphere is well reported in AIRS papers referenced in the American Geophysical Union's Journal of Geophysical Research, vol. 111, [2006]. That is 1K of air-temperature in 1km layer and 15% of relative humidity in 2km layer in troposphere. Meanwhile, that retrieval accuracy at around tropopause has not been well reported so far. This paper focuses on retrieval accuracy at 6-12km of altitude (80~200 hPa) where air-temperature is not changed so much. Earth's surface and the sharp variation of air temperature around tropopause, on the other hand, the retrieval accuracies of air temperature at the surface and around the tropopause are not so high (~4 K) in the previous works (Rodgers, 1996, Jeffrey et al., 2002) even using the high spectral resolution of sounder. Derivatives of air-temperature and relative humidity, accordingly, are not so large that it is not easy to achieve accurate retrievals (Arai, K.,et. al., 2008).

In order to solve RTE and to estimate vertical profiles of air-temperature and relative humidity, iteration method such as Newton method, etc., in general, is used. Starting from a given initial solution, solution is updated in accordance with gradient vector, Hessian of the surroundings of the current solution. It sometime occurs that elements of Hessian are too small so that it is not possible to reach optimum solution in such case. It is not so easy to determine Hessian analytically due to a strong non-linearity of relations between radiance and geophysical parameters. The proposed method uses numerical derivatives as elements of Hessian. Also it might be occurred a poor solution if Hessian contains a tiny element or elements as of air-temperature and relative humidity is not changed so much at round the boundary between troposphere and stratosphere. Moreover, rank of Hessian is decreased depending upon that elements of Hessian, derivatives are so small when relative humidity is increased at approximately the peak of weighting function which is situated at around 6 or 7 km above sea level. One of the non-linear least square methods of Levenberg-Marquardt (Press et al., 1988), meanwhile, is not so sensitive to such situation. However, it is not easy to determine analytical expression of Hessian so that numerical calculation of Hessian is proposed for Levenberg-Marquardt in this paper.

Experimental data shows relatively good accuracy

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for estimation of water vapor and air-temperature profiles derived from AIRS data in comparison to the corresponding the Global Data Assimilation Systems (GDAS) (GDAS site accessed in December 2007) of the National Centers for Environmental Prediction (NCEP) data.

2. Proposed method

In accordance with AIRS/ATBD, vertical profiles of air-temperature, water vapor, etc. are retrieved with AQUA/AIRS (Atmospheric Infrared Sounder) data. The transmittance of multiple layers is calculated by taking the product of the transmittances for each layer. This transmittance is then used in the radiative transfer equation to compute brightness temperature:

$$B_{TOA} = B_{direct} + \tau(0,Ps)\{B_s + B_{sky}(1 - \frac{B_s}{T_s})\} \qquad (1)$$

where B_{TOA} is the brightness temperature emitted from the top of the atmosphere, $\tau(0,P_S)$ is the one-way transmittance of the atmosphere, B_{direct} is the component of brightness temperature emitted from the atmosphere on a direct path to space, B_S is the surface brightness, B_{sky} is the sky brightness temperature (including the attenuated cosmic contribution) as it would be observed from the surface, and T_S is the physical surface temperature.

The monochromatic radiance leaving the top of a non-scattering atmosphere is:

$$R(\nu,\theta) = \varepsilon_s B(\nu,T_s)\tau(\nu,R_s,\theta) + \int_{\ln p_s}^{\ln p_0} B(\nu,T)\frac{\partial\tau(\nu,p,\theta)}{\partial \ln p}d\ln p$$
$$+\rho_s H_{sun}\tau(\nu,p_s,\theta)\tau(\nu,p_s,\theta_{sun})\cos(\theta_{sun}) + R_d \qquad (2)$$

where $B(\nu,T)$ is the Planck function emission at frequency n and temperature T, $\tau(\nu, p, \theta)$ is the transmittance between pressure p and the satellite at viewing angle θ, and T_s, ε_s, and R_s refer to the Earth's surface temperature, emissivity, and reflectivity respectively, and R_d is the reflected down welling thermal radiance. The solar radiance entering at the top of the atmosphere is represented by H_{sun}.

The derivation begins with linearizing the radiative transfer equations (RTE) for microwave and infrared about some *a priori* estimate. This is accomplished by expressing brightness temperature or radiance (R_c) in equations (1) and (2) as a function of the regression guess using a first order Taylor expansion such that:

$$R_c = R_0 + \sum_{k=1}^{N}\frac{\partial R}{\partial V_k}(V_k - V_0) \qquad (3)$$

where R_0 is the total integrated radiance for frequency computed from the regression solution and the RTE, V_k and V_0 are the k-th elements of the solution and regression first guess geophysical parameter vectors, $\partial R / \partial V_k$ is the incremental change of the radiance with respect to a incremental change in a particular geophysical parameter (e.g. V_k= temperature at 50 hPa), and N is the number of geophysical parameters. The value of $\partial R / \partial V_k$ is computed in a manner similar to Eyre [1989] by differentiating the numerical quadrate form of the RTE with respect to the geophysical parameters.

$$X - X_0 = (S_x^{-1} + A^T S_e^{-1} A)^{-1} A^T S_e^{-1}(R - R_0) \qquad (4)$$

X, X_0, S_x, A, S_e, R, R_0 are, respectively, geophysical parameter vector, designated geophysical parameter vector, variance and covariance matrix of air-temperature and relative humidity as a prior information at each layer, Jacobian of geophysical parameter and observation data, variance and covariance matrix of observation error as a prior information, observation data, and estimated data of X_0. The most appropriate geophysical parameter can be determined as to minimize estimation error. Staring from initially designated geophysical parameters derived from the regressive analysis, estimated geophysical parameter is updated in accordance with the following derivatives (first order derivatives for Jacobian):

$$\frac{\partial S}{\partial q_i} = -2\sum_{k=1}^{N}(R_k - R_{0k})\frac{\partial R_{0k}}{\partial q_i} \qquad (5)$$

where S is square of residual error, q_i denotes step size in the solution space and $\partial R_{0k}/\partial q_i$ is estimated with MODTRAN. Although the spectral resolution of MODTRAN is poor than that of AIRS, it also can be used for a rough sensitivity analysis with ~4 K error around tropopause.

$$S = \sum_{k=1}^{N}(R_k - R_{0k})^2 \qquad (6)$$

where R_k is derived from actual AIRS data and R_{0k} is derived from MODTRAN. Meanwhile, an element of second order derivatives for Hessian is calculated with the following equation:

$$\frac{\partial^2 S}{\partial q_i \partial q_j} = 2\sum_{k=1}^{N}\{\frac{\partial R_{0k}}{\partial q_i}\frac{\partial R_{0k}}{\partial q_j} - (R_k - R_{0k})\frac{\partial^2 R_{0k}}{\partial q_i \partial q_j}\} \qquad (7)$$

so that Jacobian can be calculated. Newton method can be expressed as follows,

$$X_{l+1} = X_l - H^{-1}J_l \qquad (8)$$

while Levenberg-Marquardt method is represented as follows,

$$X_{l+1} = X_l + (J_l^T J_l - \lambda I)^{-1} J_l^T (R_l - R_{0l}) \qquad (9)$$

where H and J denote Hessian and Jacobian, respectively, λ is convergence control parameter. Calculating elements of Hessian and Jacobian with equations (6) and (7) based on MODTRAN, together with updating the solution of geophysical parameters based on equations (8) and (9), then an optimum geophysical parameters are estimated.

The proposed method uses MODTRAN derived defalt air-temperature and relative humidity profiles as initial values for air-temperature and relative humidity profiles.

3. Experiments

We concentrate retrievals of air-temperature and relative humidity profiles at around tropopause, 6-12km because the retrieval accuracy at around such altitude is relatively poor due to the fact that air-temperature is not changed much at such altitude. So that from AIRS channels, the following channels of wave number are selected for air-temperature profile retrieval, 2388, 2386, 2253, 2255, 2285, 2268, 2382(cm^{-1}) while the following channels of wave number are selected for relative humidity profile retrieval for 6-12km of altitude, 1479, 1397, 1514, 1475, 1544, 1522, 1557(cm^{-1}). These show relatively greater weighting function at around the peak of weighting function.

An experiment with actual AIRS data is also conducted. AIRS level 1b of data of Atlantic Ocean area is selected. Fig.1 shows quick look browse image of the area. The data is acquired at 4:41:25 UTC on July 1 2006. Two AIRS datasets of Atlantic Ocean area for mid-latitude summer (July 1 2006) and winter (at 05:41:25 on December 30 2006) are selected. Relatively calm area of one degree mesh of 47-48 degree north as well as 47-48 degree west is extracted from the datasets. Examples of retrieved results of air-temperature and relative humidity profiles of Atlantic Ocean in the summer and the winter seasons are shown in Fig.2 while convergence processes are shown in Fig.3.

The proposed method is superior to the other two methods for almost all the cases. Retrieval error for relative humidity profile is greater than that for air-temperature profile. Also retrieval error for winter season is greater than that for summer season. Rank is dropped when the iteration number is greater than around 10 for Newton method then no solution is derived from Newton method after all. Meanwhile, bi-section method allows reach a stable solution for all the cases, error is greater than the other two methods though. In some cases, Newton method shows significant error when rank is dropped and when it reaches to one of local minima. As a conclusion, we may say that air-temperature profile retrieval error for the proposed method is within the rage of 10 K while relative humidity profile retrieval error is within the range of 25% and these errors are smaller than those for the conventional method of Newton method and bi-section method.

Residual error of relative humidity is greater than that of air-temperature profile. The proposed method uses MODTRAN derived default relative humidity and air-temperature as an initial value. In accordance with iteration number, retrieved air-temperature and relative humidity is getting closer to the GDAS derived air-temperature and relative humidity.

Convergence processes for air-temperature profile retrievals are faster than those for relative humidity profile retrievals. Also convergence processes for air-temperature and relative humidity profiles retrievals for summer dataset are faster than those for winter dataset. More importantly, convergence processes reach to a stable solution for summer dataset while those for winter dataset reach to an unstable solution.

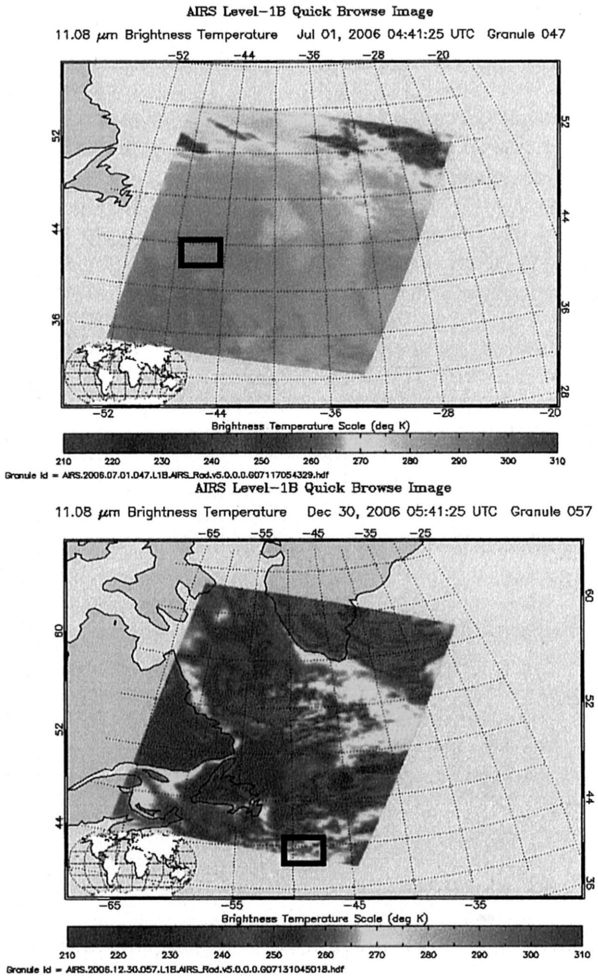
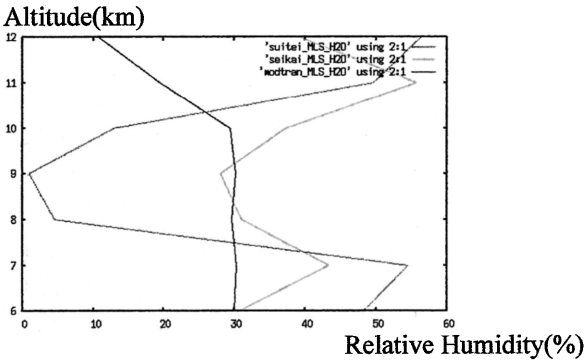
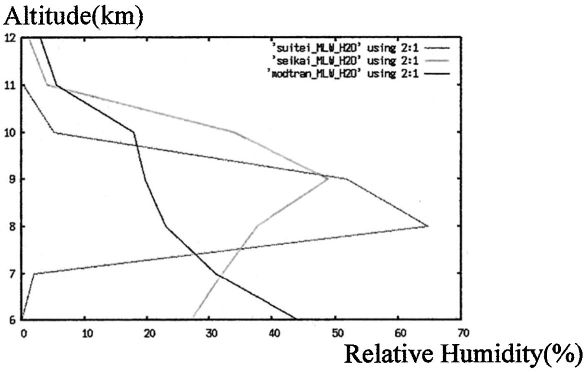


Fig.1 Browse image of AIRS data of Atlantic Ocean used.

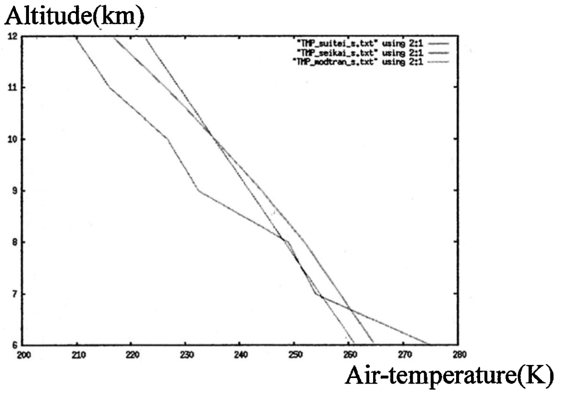
Retrieval accuracy and convergence processes of the proposed method are evaluated using MODTRAN. Firstly, AIRS data is estimated based on MODTRAN with the default parameters of mid-latitude summer and winter.



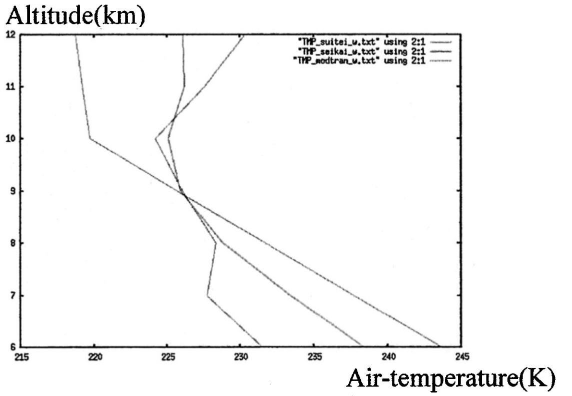
(a) Relative humidity profile in summer



(b) Relative humidity profile in winter

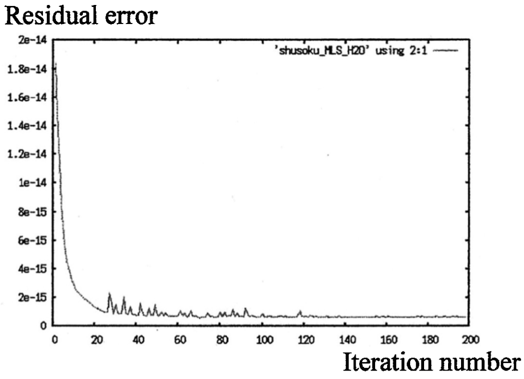


(c) Air-temperature profile in summer

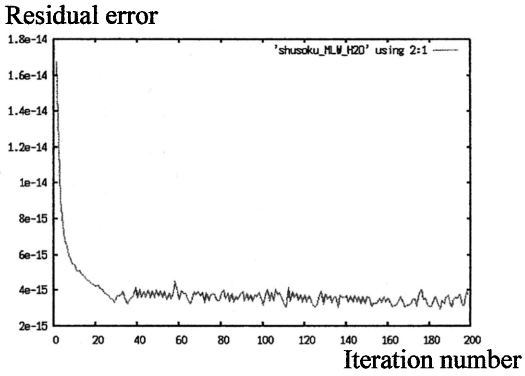


(d) Air-temperature profile in winter

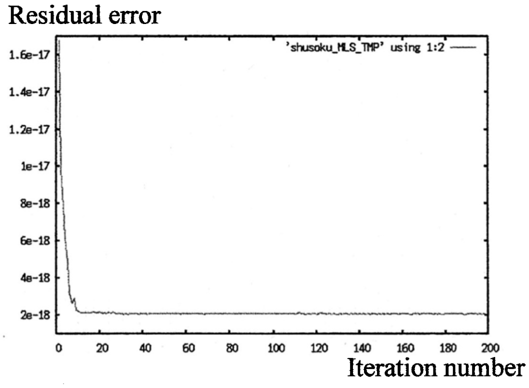
Fig.2 Comparison among retrieved (red), GDAS data derived (green) and MODTRAN based (blue) air-temperature ((c) and (d)) and relative humidity ((a) and (b)) profiles of Atlantic Ocean for summer ((a) and (c)) and winter ((b) and (d)) seasons.



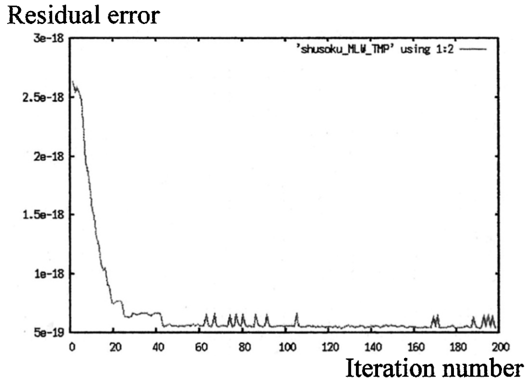
(a) Relative humidity in summer



(b) Relative humidity in winter

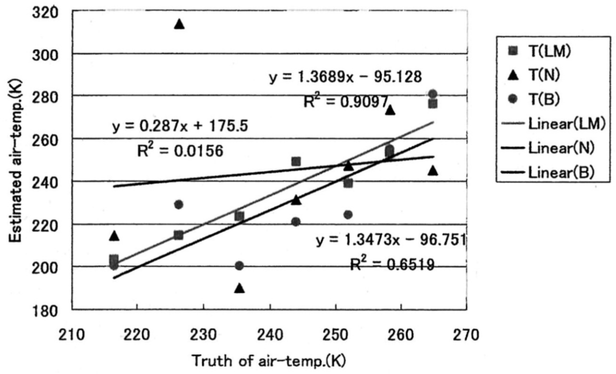


(c) Air-temperature in summer

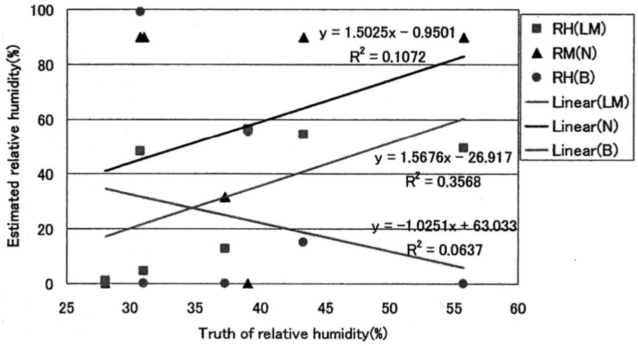


(d) Air-temperature in winter

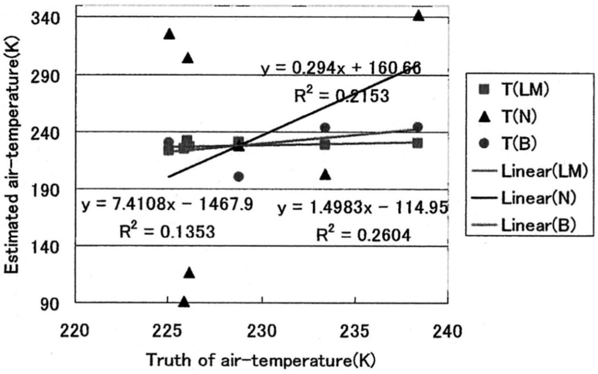
Fig.3 Convergence processes of Leavenberg Marquardt method for air-temperature ((c) and (d)) and relative humidity ((a) and (b)) profiles retrievals for summer ((a) and (c)) and winter ((b) and (d)) seasons.



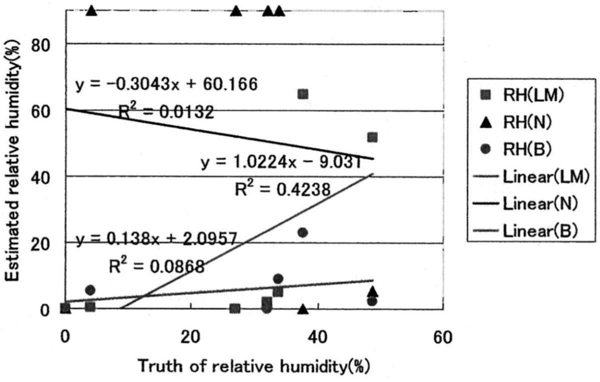
(a) Air-temperature for summer dataset



(b) Relative humidity for summer dataset



(c) Air-temperature for winter dataset



(d) Relative humidity for winter dataset

Fig.4 Relation between estimated and actual air-temperature and relative humidity profiles.

Air-temperature and relative humidity profiles are estimated with the proposed method and the conventional Newton method as well as Bi-section method for comparisons to minimize the square of difference between the estimated and actual AIRS data. To remove the influence due to the surface reflection, we only performed the sensitivity analysis for the ocean surface and assume the surface reflectance 0, i.e., the surface emissivity of 1.Step size q_i for $\partial R_{0k}/\partial q_i$ are set at 2% for relative humidity (it has to be ranged within 0 to 100%) and 0.5K for air-temperature. Convergence control parameter λ is set a relatively large when the residual error is large while that is set a comparatively small when the residual error is getting small.

After retrievals of air-temperature and relative humidity profiles with the proposed method, difference between retrieved and default profiles derived from MODTRAN is evaluated. Fig.4 and Table 1 shows the result from the evaluation. Experimental results show that the proposed method is superior to the conventional Newton method and bi-section method. Retrieval Root Mean Square Error (RMSE) of air-temperature for summer dataset is 4.08K while that for relative humidity is 7.56%. Meanwhile, RMSE of air-temperature for winter dataset is 1.62K while that for relative humidity is 14.11% as is shown in Table 1. Meanwhile, R^2 value of the proposed method shows 0.652, 0.260, 0.357, 0.424 for the dataset of air-temperature/summer and winter, as well as relative humidity/summer and winter, respectively as is indicated in Fig.4. These are the best R^2 values in comparison to the other two methods.

Table 1 Difference between GDAS derived truth of air-temperature (top 7 rows) and relative humidity (bottom 7 rows) and estimated those based on the conventional Newton (N), the proposed Leavenberg Marquardt (LM) and bi-section methods(B) as well as Root Mean Square Error (RMSE) for the summer (Sum.) and the winter (Win.) datasets.

h(km)	Sum,LM	Sum,N	Sum,B	Win,LM	Win,N	Win,B
6	-10.87	19.48	-15.8	8.21	-103.82	-5.35
7	5.2	-15.11	3.55	4.715	30.095	-10.125
8	13.05	4.5	27.75	-2.125	1.235	28.775
9	-5.17	12.79	23.15	1.185	135.285	0.175
10	12.215	45.475	35.425	1.765	-100.18	-4.625
11	12.03	-87.38	-2.5	-0.8	110.21	-0.55
12	13.42	1.75	16.4	-5.44	-78.03	-2.75
h(km)	Sum,LM	Sum,N	Sum,B	Win,LM	Win,N	Win,B
6	-17.49	30.35	-41.76	-35.28	-9.09	274.6
7	-11.24	-20.31	-35.51	18.66	74.85	247.7
8	26.48	-8.55	-85.48	23.25	90	216.1
9	27.13	17.96	0.87	10.36	0	211.8
10	24.31	33.26	-18.58	-10.05	31.52	190
11	6.16	-99.41	-40.41	84.88	90	217.8
12	-17.34	-11.67	56.34	14.65	-55.34	188

	RMSE(T)	RMSE(RH)
Sum.LM	4.08	7.56
Sum.N	14.64	16.2
Sum.B	7.95	17.77
Win.LM	1.62	14.11
Win.N	34.48	23.01
Win.B	4.49	84.18

4. Concluding remarks

Air-temperature and relative humidity profile retrieval accuracy at around tropopause is evaluated with the selected channels of AIRS data. It sometime occurs that no solution is reduced from the conventional Newton method due to the fact that elements of Hessian are too small results in inverse matrix of Hessian do not exist. Meanwhile, the proposed method based on Leavenberg Marquardt reaches a solution in such cases. Elements of Jacobian are calculated with numerical derivatives derived from MODTRAN based radiance at around the correct solution in solution space.

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