THE RETRIEVAL OF TEMPERATURE AND WATER VAPOR PROFILES
FROM ATOVS DATA: AN ADAPTATION OF THE 3I-SCHEME

M. Hervéou, N. A. Scott, A. Chédin
Laboratoire de Météorologie Dynamique
Palaiseau, France

INTRODUCTION: Studies of the earth climate and its variability require accurate long-term global observational datasets like the NOAA TOVS dataset started in 1979. However, in the near future, onboard the NOAA-next platform, the Microwave Sounding Unit with its four channels near 55 GHz will be replaced by an Advanced MSU, grouping the fifteen channels of AMSU-A and the five channels of MHS (or AMSU-B).

The AMSU-A instrument includes five window channels: four at lower frequencies (23.8, 31.4, 50.3 and 52.8 GHz) and a high-frequency one near 89 GHz, instead of the only MSU1 channel at 50.3 GHz. Replacing the MSU temperature-sounding channels 2, 3 and 4, sounding respectively at 700, 300 and 90 hPa, ten AMSU-A channels, five of them with weighting function peak located above 100 hPa, sound the atmospheric temperature from 700 to 2 hPa. The vertical resolution does not improve but, given the increased number of channels, temperature profile retrieval is expected to be more accurate. AMSU-B will measure radiation at higher frequencies: in two window channels at 89 and near 150 GHz and in three channels around the 183.3 GHz water-vapor strong absorption line (same channels as in SSM/T2). Both AMSU-A and AMSU-B instruments have a far better horizontal resolution: when MSU field-of-view (fov) intercepts a solid angle of 7.5°-110 km at nadir, AMSU-A fov ranges only 3.3° - 50 km and AMSU-B fov 1.1° - 15 km.

The adaptation of the current 3I algorithm to this new type of soundings is described in this paper. First a neural network approach has been derived to infer the first guess for the temperature inversion of ATOVS data as well as for the H_2O retrievals based on a coupling of MHS and AMSU-A. The line-by-line radiative transfer model STRANSAC has been used to extend the current TOVS TIGR climate data base to ATOVS data. This suite of algorithms is presently tested using the OSSE-ATOVS data base created at ECMWF.

1. 3I ADAPTATION TO ATOVS DATA

1.1. 3I main features

The 3I (Improved Initialization Inversion) algorithm has been designed to retrieve temperature and water vapor vertical profiles as well as cloud and surface characteristics from TOVS data at an intermediate horizontal resolution of about 100 × 100 km^2. An upstream routine maps MSU brightness temperatures to HIRS fovs, determines the cloud flag and the airmass type of each HIRS spot before building the 3I-box dataset.
The originality of the 3I procedure lies in the archival of the TIGR (Thermodynamic Initial Guess Retrieval) dataset: some 1800 atmospheric situations (temperature, water vapor and ozone profiles) issued from a large set of 150 000 radiosound measurements (Escobar, 1993) accounting for atmospheric variability and in the storage of the associated clear-column TOVS brightness temperatures, atmospheric transmissions and weighting functions that have been precalculated by the fast line-by-line radiative transfer model 4A (Automatized Atmospheric Absorption Atlas) (Scott et al, 1981). TIGR 1800 atmospheric profiles dataset is divided into five airmass types subsets: one tropical, two midlatitude and two polar classes. The associated TOVS radiative quantities are calculated for ten viewing angles, 19 surface pressures and two surface emissivities (land and water).

Once an initial guess of the atmospheric temperature profile has been obtained from the appropriate TIGR subset, the final atmospheric temperature profile is retrieved by solving the radiative transfer equation in order to minimize the difference between observed and calculated brightness temperatures associated with the guess.

The determination of an initial guess of the temperature profile is made using a linear pattern recognition in the space of TOVS brightness temperatures. There are two different paths in the algorithm, according to the cloud flag: In clear-sky situations, all temperature-sounding channels are used. In cloudy situations, a preliminary pattern recognition is done, using the only HIRS upper atmospheric and MSU channels, since they can be assumed not to be cloud-contaminated. Then a cloud-clearing routine is used to estimate clear-sky brightness temperatures in some of the HIRS channels sounding temperature in the low atmosphere.

Cloud parameters are then determined (Stubenrauch et al, 1997) and a cloud-clearing routine for HIRS water vapor and surface channels is applied. Water vapor inversion is currently performed using neural networks (Chaboureau et al, 1997).

1.2. Operational ATOVS data

Operational ATOVS data are to be provided at level1b. Flags for: rain, liquid water, cloudiness, surface emissivity, are determined at AMSU-A resolution and AMSU-B data mapped to AMSU-A resolution. After a mapping of AMSU A data to HIRS data, inversion should be performed at HIRS resolution. This implies an operational redefinition of the upstream part of 3I algorithm. Up to now, main attention has been put to the 3I scheme core: airmass-type classification, temperature and water vapor inversion.

1.3. A model for AMSU observations

An adaptation of 3I to ATOVS observations requires the extension of TIGR to AMSU. This has been
Moreover, for preliminary testing, an independent test dataset has also been built. ATOVS brightness temperatures and transmission profiles have been simulated for 861 atmospheric profiles belonging to a TIGR-like dataset (93 tropical type profiles, 388 temperate ones, 380 polar ones).

2. 3I-SCHEME ADAPTATION

2.1. Airmass-type classification

Airmass-type classification in the 3I-TOVS system uses observations of channels HIRS 3, MSU 2, 3 and 4, temperature-sounding channels not contaminated by cloud and which generate a partition of the TIGR atmospheric situations into the five airmass-type classes. Brightness temperature covariance matrix for this set of channels are computed on each of TIGR classes to help determine the weighted distances of a given observed situation to TIGR airmass-type gravity centers. A similar airmass-type classification has been built leading to the conclusion that MSU channels 2, 3 and 4 should be replaced by AMSU-A channels 5, 6 and 7.

2.2. Temperature inversion

AMSU-A temperature-sounding channels 5 to 14 are located in the oxygen absorption band around 60 GHz. In these channels, total atmospheric transmission is small enough to keep the noise created by the high variability of the surface microwave emissivity below an acceptable limit.

For measuring the impact of the instrument change, three sets of temperature-sounding channels have been built: a TOVS-set, coupling HIRS and MSU channels, an AMSU-set made of AMSU-A only channels and an ATOVS-set made of HIRS and AMSU-A channels. The so-called TOVS-set includes HIRS channels 2, 3 for upper atmospheric sounding, HIRS channels 4, 5, 6, 14 and 15 for tropospheric sounding and MSU channels 2, 3 and 4. The ten AMSU-A temperature-sounding channels -AMSU-A 5 to 14- makes up the AMSU-A-set. Finally, the ATOVS-set, comprising HIRS and AMSU-A channels, has been built by replacing in the TOVS-set the MSU channels by AMSU-A 5 to 14.

2.2.1. Temperature profile initial guess determination

In a first step, the pattern recognition method used in 3I has been adapted to the AMSU-A temperature-sounding channels. Results have shown a gain in accuracy in the upper atmosphere -from 100 hPa to 10 hPa and above- when AMSU-A sounding channels are involved. This was expected given the
number of AMSU-A channels sounding above 100 hPa. However, the increased weight given to upper atmospheric channels results in a loss of accuracy in the lower atmosphere.

These results have led to the development of a new method which estimates the initial guess of the temperature profile from the observed brightness temperatures using a neural network (NN) technique. As neural network design, a multilayer perceptron has been chosen: neurons -computation units- are put in layers and are connected individually to all the neurons of the contiguous layers. It has been chosen since this design may be associated to an efficient learning scheme known as the error gradient backpropagation. The learning is made by successively correcting, at each example presentation, the connexion -synaptic- weights to minimize the local quadratic error. With this learning paradigm, the multilayer perceptron has been proved to be an universal estimator: given the appropriate number of neuron layers and number of neurons on each layer, given an ideal learning set, an estimator of any function at any desired accuracy may be built (Rumelhart, 1986). Only the technical constraints on neural network architecture complexity and the related size of the learning dataset may restrain the neural estimator performance.

Each example of our learning set is made of a vertical temperature profile -the desired output- and the associated temperature-sounding brightness temperatures -the given input-. We use a neural network comprising as many input neurons as temperature-sounding channels and one hidden layer of 39 neurons. There are 40 output connections corresponding to the 40 levels used to describe the temperature profile from 1013 to 0.05 hPa. TIGR situations have been presented some 3000 times each. Results given in figure 2 are for the three sets of channels (TOVS, AMSU-A and ATOVS). On this figure, the classical pattern recognition method is compared to the neural network estimation technique, both applied to the 861 test situations.

For each set of channels, first guess accuracy of the NN inference which carries out an interpolation is greater than that of pattern recognition approach, which identifies a linear combination of TIGR elements. ATOVS set of channels gives a NN-inferred first guess temperature profile better than TOVS throughout the whole atmospheric column. Particularly, the rms error is kept around 1.5 K from 700 hPa to 10 hPa.

2.2.2. Brightness temperature first guess

The linear pattern recognition provides us with a linear combination of TIGR atmospheric situations and thus directly with the associated brightness temperatures and transmission profiles. The NN-inferred temperature profile does not, in principle, belong to the set of TIGR profile linear combinations. Thus ATOVS brightness temperatures and transmission profiles have to be associated to this temperature profile, before performing the inversion step. A fast radiative transfer model has thus to
be used to complete the guess.

The 3R - Rapid Radiance Recognition- model is a fast statistical radiative transfer model developed at LMD (Flobert, 1986). Starting from an input atmospheric situation -temperature and water vapor vertical profiles-, it performs a linear pattern recognition within the TIGR dataset. The TOVS brightness temperatures and transmission profiles associated to the nearest TIGR atmospheric situation are a first estimate of the desired radiative values. Once this recognition has been made, a linear correction of the brightness temperatures first estimate, corresponding to temperature and water vapor profiles departures between the atmospheric situation taken as input and the nearest situation in TIGR, is applied. For that purpose, temperature and water vapor jacobians, ie brightness temperatures partial derivatives, are computed from the transmission profiles.

Validation has been made with respect to the line-by-line radiative transfer models 4A and Stransac on our test dataset of 861 atmospheric profiles. Biases are not exceeding 0.1 K (except 0.16 K for channel AMSU-A 5) and standard deviations are kept below 0.2 K for most of the temperature-sounding channels except HIRS 5 (0.26 K), HIRS 6 (0.36 K) and AMSU-A 5 (0.38 K).

2.2.3. Temperature profile inversion

Concerning temperature retrievals using the ATOVS-set of channels, once obtained a complete initial guess, it has been noticed that the bayesian minimization inversion method did not decrease appreciably the rms error between the retrieved and the true vertical temperature profiles.

Consequently, the bayesian estimation step has not been maintained for temperature profile retrievals in clear-sky situations where the ATOVS-set of channels may be used. The NN initial guess is taken as the best retrieval.

2.2.4. $\Psi$ cloud-clearing routine for temperature-sounding channels

In cloudy situations, there is a need for a cloud-clearing routine for HIRS channels 4, 5, 15, 6 and 14 sounding the temperature of the lower atmosphere. Here, this routine relies on the microwave channels, not or weakly contaminated by the clouds, and on a-priori information extracted from TIGR. The so-called $\Psi$-method has been adapted to the AMSU channels with expected better performances than with MSU. The increased number of microwave channels sounding above 700 hPa allows more accurate predictions than with the only three MSU channels.

2.3. Water vapor inversion

An attempt has also been made to retrieve the vertical relative humidity profile from AMSU data using neural networks. Once again use has been made of a multilayer perceptron. Relative humidity profile on the 20 lower 4A-levels (from sea-level up to 130 hPa) is the desired output. The inputs include the brightness temperatures in AMSU-B water vapor channels, AMSU-A window channels
1, 2 and 15 and AMSU-A temperature-sounding channels 3 to 10 to account for AMSU-B channels
brightness temperature dependence on temperature profile. The architecture includes two hidden
layers of respectively 30 and 15 neurons (Cabrera-Mercader and Staelin, 1995).
Results on synthetic test data are encouraging : an rms accuracy of about 10 – 15 % is obtained
from sea-level up to 300 hPa (see figure 3). However, an application to real data goes through a
comprehensive analysis of the impact of surface emissivity on relative humidity profile inference.

3. THE ECMWF/OSSE DATABASE
Starting from the OSSE (Observation System Simulation Experiment) dataset designed for measuring
the impact of doppler wind lidar data assimilation on weather prediction, the ECMWF has built up
a database of one month simulated observations for several observing systems, including TOVS and
ATOVs (Stoffelen et al, Roquet et al, 1994).
The initial conditions have been taken from the operational analysis of 5 February 1993. Then IFS
-Integrated Forecasting System- has been run on an independant way : apart from the initial analysis,
only simulated data -both conventional and spatial- have been assimilated, so that OSSE runs differ
from real ones from day 7 onwards.
To simulate ATOVS data, IFS has been coupled with a fast radiative transfer model, RTATOV,
through an orbit simulator. Two systems of two quadrature satellites (3am, 3pm, 9am and 9pm
equator-crossing time) have been simulated, either for TOVS or for ATOVS data. NESDIS horizontal
scale (some 120 km) and sampling (one out of three) have been applied. The aim being to simulate
NESDIS cloud-cleared and surface-emissivity-decontaminated products, surface emissivity has been
put to 1 in all channels and only clear-column brightness temperatures have been computed. To assess
for the cloud-clearing route, a random noise depending on the situation cloudiness has been applied
to raw data.
The first task has been to compare the forward radiative transfer model Stransac and RTATOV prod-
ucts to correct for possible biases. Biases and standard deviations are presented, for each TIGR
airmass class (tropical, midlatitude 1, midlatitude 2, polar 1, polar 2), are presented on figures 4
and 5. Concerning AMSU-A channels, biases may reach 0.5 K or more for tropospheric channels
5, 6, 7 and 8 but standard deviations do not exceed 0.25 K and stay below 0.2 K for most of the
channels and airmass types. Larger standard deviations are observed for channels HIRS 4, 5, 6 and
15, reaching 0.48 K for HIRS 5. These methodological biases have been accounted for in the following.

4. TEST ON THE ECMWF/OSSE DATABASE
The database includes 4 daily analyses computed out of OSSE runs at UTC time 0:00, 6:00, 12:00
and 18:00 and displayed on a $1^\circ \times 1^\circ$ grid. 3-hours time colocations for most of the spots may then be obtained. Each global coverage means some 14 passes, which, with the application of a random sampling of one out of three, results in some 14000 points. Statistics have been calculated on a 3-hours time-colocation basis and with a 15 standard layers discretization for the four global coverages of February 8th (some 50000 grid-points). They are presented on figures 6 (over sea) and 7 (over land) for each airmass type. Polar type situations are not presented here: a few cases over elevated terrains of Antarctica.

Standard deviations generally stay in the range of 1.5 to 2 $K$ from surface up to 10 $hPa$ (near 1 $K$ for tropical situations over sea); biases appear mostly in tropospheric regions. The main problem appears over sea where positive biases may reach 2 $K$.

It might be caused by radiative transfer distortions observed between Stransac and RTATOV but also by atmospheric parameters not taken in account in our modelization, like surface skin temperature: ATOVS brightness temperatures associated to TIGR situations have been calculated with a surface skin temperature equal to the air temperature. AMSU-A 5 slightly larger atmospheric transmission than MSU2 may introduce some surface skin temperature impact and degrade somewhat the results. This is presently being investigated.

CONCLUSIONS

The use of neural networks appears to be an efficient way to deal with the increased amount of information provided by ATOVS data. In clear-sky situations, when all ATOVS channels may be used, temperature inversion has been reduced to a neural network temperature profile inference. Temperature inversion has been performed with a 1.5 $K$ rms accuracy from surface up to 10 $hPa$ on synthetic data. AMSU-B data lead to a with a clear-sky relative humidity vertical profile with a less than 15 % rms accuracy from the surface up to 250 $hPa$. When applied to independent data, biases appear in temperature profile retrievals, that might be related to surface emission. A surface emission noise has to be introduced for AMSU-A lower tropospheric channel 5.

Most of the codes have been run on the computers of the IDRIS (Institut du Développement et des Ressources en Informatique Scientifique du CNRS) center.

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Figure 1: AMSU-A temperature sounding channel weighting functions

Figure 2: First guess temperature profile rms error (861 items)
"classical" pattern recognition vs neural network inference
(left: TOVS, center: AMSU-A, right: ATOVS)
Figure 3: Relative humidity profile retrieval accuracy

Neural Network learned on TIGR 1761 situations

and applied to the 861 test situations (rms)
Figure 4: AMSU-A brightness temperature discrepancies between RTATOV and Stransac
Statistics computed on TIGR (1761 items): RTATOV minus Stransac Tb's
(left: mean, right: standard deviation - in K-)

Figure 5: HIRS brightness temperature discrepancies between RTATOV and 4A
Statistics computed on TIGR (1761 items): RTATOV minus 4A Tb's.
(left: mean, right: standard deviation - in K-)
Figure 6: Bias and Standard deviation over sea
Temperature profile retrieval from OSSE database
(left: Tropical, center: Temperate 1, right: Temperate 2)

Figure 7: Bias and Standard deviation over land
Temperature profile retrieval from OSSE database
(left: Tropical, center: Temperate 1, right: Temperate 2)
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