RESEARCH ON SATELLITE SOUNDINGS AT THE U.K. METEOROLOGICAL OFFICE

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1. INTRODUCTION

Recent research on TIROS Operational Vertical Sounder (TOVS) data at the Meteorological Office has been concerned mainly with more direct ways of applying radiance information in numerical weather prediction (NWP). Our motivation for pursuing this line of research has been strongly influenced by an improved understanding of the error characteristics and information content of conventional retrieved profiles, leading to an appreciation of the difficulties in using these data optimally in NWP. These ideas are discussed in section 2.

A theoretical approach to the direct use of radiances in NWP analysis is presented in section 3. The formulation is quite general and could be applied in 3- or 4-dimensional multi-variate data assimilation. However, at present it has only been explored in one-dimensional (vertical) schemes. Section 4 describes a linear method and demonstrates the correspondence between direct assimilation of radiance data and "forecast-background" retrievals. A scheme based on this method is currently applied to cloud-cleared brightness temperature in routine processing of TOVS data for use in operational NWP. Section 5 describes some aspects of current research on nonlinear schemes for inversion of raw, potentially cloud-affected TOVS radiances.

2. RETRIEVAL ERROR CHARACTERISTICS

Retrievals of vertical profiles of temperature and humidity have rather subtle error characteristics. This can be illustrated by considering a linear inversion scheme of the form:

$$\mathbf{x} = \mathbf{x}^b + \mathbf{W} \, . \, (\mathbf{y}^m - \mathbf{y}\{\mathbf{x}^b\}) \qquad (1)$$

where $\mathbf{x}$ is the retrieved atmospheric profile,

$\mathbf{x}^b$ is a "background" or "first guess" profile,

$\mathbf{y}^m$ is a vector of measured radiances or brightness temperatures,

$\mathbf{y}\{\mathbf{x}^b\}$ is the "forward model" giving the equivalent vector corresponding to the background profile,

and $\mathbf{W}$ is the inversion operator.

Most linear inversion schemes may be written in this form and vary only in the nature of the background profile and the method of calculating $\mathbf{W}$. In some schemes the background profile is not explicit but is nevertheless implied. In a regression scheme, for example, it is the mean of the sample of profiles from which the regression coefficients were calculated.

The linearised forward problem may be expressed as

$$\mathbf{y}^m - \mathbf{y}\{\mathbf{x}^b\} = \mathbf{K} \,.\, (\mathbf{x}^t - \mathbf{x}^b) + \mathcal{E}^m \tag{2}$$

where $\mathbf{x}^t$ is the true profile, $\mathcal{E}^m$ is the measurement error, and $\mathbf{K}$ is the "forward operator" representing the radiative transfer physics and is equivalent to the weighting functions for the linear case.

Substituting (2) into (1) leads to

$$\underbrace{\mathbf{x} - \mathbf{x}^t}_{\text{retrieval error}} = \underbrace{\mathbf{W} \,.\, \mathcal{E}^m}_{\text{measurement error}} + \underbrace{(\mathbf{I} - \mathbf{W} \,.\, \mathbf{K}) \,.\, (\mathbf{x}^b - \mathbf{x}^t)}_{\text{background error}} \tag{3}$$

where $\mathbf{I}$ is a unit matrix.

This equation shows that the retrieval error consists of two parts, one arising from the measurement error amplified by the inversion operator, and the second from the background error amplified by $(\mathbf{W.K} - \mathbf{I})$. Primarily because of the ill-posed nature of the inversion problem, $\mathbf{W.K} \neq \mathbf{I}$, and so the retrieval error inevitably contains a contribution from the background error.

Equation (3) has several important consequences related to the processing and application of satellite sounding data. Firstly it shows that, if the background information is locally biased with respect to the truth, then so also will be the retrievals. This is the major source of the horizontal correlation of error found in satellite retrievals; it is not a property of the radiance data themselves, but arises through the properties of the inversion process.

Secondly, it shows that satellite retrievals are not "pure" measurements; they contain "observed" information from the radiances and also "unobserved" information from the background profile and inversion constraints. When using data in NWP it is necessary to consider carefully the status of the unobserved part and to determine how it should be weighted (or excluded) in the data assimilation.

Thirdly it explains why much of the recent activity in satellite sounding research in many centres has been directed towards the improvement of the background or "first guess" information in the inversion. Obviously, an improved background will lead to an improved retrieval, but the problem of "background dependence" illustrated by equation (3) will still remain. If the nature of the background information is adequately understood, then it can be allowed for in the subsequent data assimilation process (see Lorenc *et al.* 1986). This applies in principle both to schemes which uses a forecast profile as an inversion background and to schemes in which it comes from other sources. It is interesting to note that some recent schemes (e.g. Uddstrom and Wark 1985, Chedin *et al.* 1985) achieve a skilful "first guess" (and subsequently improved retrieval) partly through use of the measured radiances, i.e. $\mathbf{x}^b$ is a function of $\mathbf{y}^m$. This further complicates the problem for the NWP system of determining what is truly "observed" information and what is additional, unobserved constraint.

The nature of retrieval errors for linear inversions is explored further by Eyre (1987). For nonlinear schemes, a simple analytical treatment is not possible, but the basic characteristics of retrieval error will be similar (see Rodgers 1987).

Equation (3) also illustrates the role of measurement error in the inversion process. In this context, "measurement" error means not only errors in $\mathbf{y}^m$ associated with the instrument (noise and errors in calibration) but also any errors in the forward model $\mathbf{y}\{\mathbf{x}^b\}$. In any physically-based retrieval scheme, this involves errors in the radiative transfer model, including those arising from uncertainties in the spectroscopic data. There are also potential sources of error in the treatment of other effects – scan angle, clouds, surface emissivity, etc. These may appear as errors in the pre-processed measurement or as errors in the forward model, depending on how the inversion problem is formulated. It is necessary to understand and control to a high degree all these potential sources of error if useful retrievals are to be provided. Indeed, in our experience, a scheme for monitoring and tuning biases between measured and calculated radiances is an essential component of a system for making effective use of satellite sounding data in NWP.

3. TOWARDS DIRECT USE OF RADIANCES IN NWP

The dependence of retrieved profiles on the background leads to error characteristics which are difficult to handle optimally in a conventional NWP analysis scheme. This has led us to look at more direct ways of using the radiances themselves.

The problem of providing the best analysis for NWP may be expressed in terms of the minimisation of a cost function measuring the departure of the analysis from the observations and the background plus other constraints (see Lorenc 1986). The cost function $J(\mathbf{x})$ for NWP analysis field $\mathbf{x}$ may be written as:

$$\begin{aligned} J(\mathbf{x}) &= (\mathbf{x}-\mathbf{x}^b)^T \,.\, \mathbf{C}^{-1} \,.\, (\mathbf{x}-\mathbf{x}^b) \\ &\quad + (\mathbf{y}^m - \mathbf{y}\{\mathbf{x}\})^T \,.\, \mathbf{E}^{-1}.(\mathbf{y}^m - \mathbf{y}\{\mathbf{x}\}) \\ &\quad + J_3\,(\mathbf{x}) \end{aligned} \qquad (4)$$

where $\mathbf{C}$ is the expected covariance of background error and $\mathbf{E}$ is the expected covariance of measurement error (including forward model error). $J_3(\mathbf{x})$ includes terms added to impose additional physical or dynamical constraints. $\mathbf{x}$ is a "field" which may, in general, represent a 3- or 4-dimensional NWP model state. However, if the vertical and horizontal parts of the analysis are separated, it may be applied in one dimension to the problem of the vertical analysis of a set of observations (such as satellite radiances) at a single horizontal location. In the short term, the operational data assimilation at the Meteorological Office will follow this approach (see below).

$J(\mathbf{x})$ is a minimum when its derivative with respect to $\mathbf{x}$ is zero:

$$J'(\mathbf{x}) = \mathbf{C}^{-1} \,.\, (\mathbf{x}-\mathbf{x}^b) - \mathbf{K}^T(\mathbf{x}) \,.\, \mathbf{E}^{-1} \,.\, (\mathbf{y}^m - \mathbf{y}\{\mathbf{x}\}) + J_3'\,(\mathbf{x}) = 0 \qquad (5)$$

where $\mathbf{K}(\mathbf{x}) = y'(\mathbf{x})$, the gradient of the radiative transfer model.

4. A LINEAR SCHEME

If $\mathbf{K}(x)$ can be taken as constant for all reasonable departures of $\mathbf{x}$ from $\mathbf{x}^b$, then the forward problem is linear:

$$\mathbf{y}\{\mathbf{x}\} = \mathbf{y}\{\mathbf{x}^b\} + \mathbf{K} \,.\, (\mathbf{x} - \mathbf{x}^b) \tag{6}$$

If in addition we ignore $J_3'(\mathbf{x})$, then (5) may be solved analytically:

$$\mathbf{x} = \mathbf{x}^b + \mathbf{C}.\mathbf{K}^T.\, (\mathbf{K}.\mathbf{C}.\mathbf{K}^T + \mathbf{E})^{-1}.\, (\mathbf{y}^m - \mathbf{y}\{\mathbf{x}^b\}) \tag{7}$$

This is equivalent to (1) where $\mathbf{W} = \mathbf{C}.\mathbf{K}^T.\, (\mathbf{K}.\mathbf{C}.\mathbf{K}^T + \mathbf{E})^{-1}$, and it is familiar as the minimum variance retrieval equation (see, for example, Rodgers 1976). Thus direct assimilation of radiances can be thought of as mathematically equivalent to a conventional minimum variance retrieval in which an NWP model field acts as the background for the inversion and its expected error covariance provides the constraint.

A one-dimensional (vertical) version of this approach is the basis of the current operational TOVS retrieval scheme run at the Meteorological Office. The Local Area Sounding System (LASS) described by Turner *et al.* (1985) has been running routinely since 1983. The "forecast background" inversion scheme was introduced in 1987 as a first step towards more direct use of radiance data.

In this scheme, the profile vector $\mathbf{x}$ includes the temperature and humidity profiles and the surface skin temperature, and the measurement vector $\mathbf{y}^m$ contains pre-processed, cloud-cleared TOVS brightness temperatures. $\mathbf{x}^b$ is a short-range (~12 hour) forecast interpolated in time and space to the location of the TOVS sounding. $\mathbf{y}\{\mathbf{x}^b\}$ is a forecast brightness temperature vector calculated in real time using a fast model based on the approach described by Weinreb *et al.* (1981). $\mathbf{W}$ is computed once per month using a $\mathbf{K}$ appropriate to a monthly mean profile for the European area. The effect on retrieval accuracy of errors in $\mathbf{C}, \mathbf{E}$ and $\mathbf{K}$ have been studied in detail (Watts and McNally 1988), and the values of $\mathbf{C}$ and $\mathbf{E}$ used in the inversion have been tuned through experiments with real data.

In addition to the development of the new inversion approach, it has been necessary to pay careful attention to many other aspects of the TOVS data processing. A new cloud-clearing scheme (Eyre and Watts 1987) was introduced into routine processing in 1987. Also considerable effort has gone into monitoring biases between retrievals, forecasts and collocated radiosondes and between the radiances calculated from them. On the basis of this monitoring, the biases applied to calculated radiances are tuned regularly.

Statistics of differences between operational retrievals and radiosonde profiles, collocated within 3 hours and 150 km, and between corresponding forecast profiles and the same radiosondes are monitored routinely. An example of these for May 1988 is shown in Figure 1. Retrieval biases are now generally small. Statistics for standard deviation and r.m.s. difference are somewhat disappointing; except for mid-upper tropospheric humidities, the retrievals appear to improve on the forecast very little. However the interpretation of these statistics is not straightforward. Firstly, they are statistics of "difference" and cannot be interpreted simply as "errors". They can be used as a measure of relative error only if radiosonde errors are uncorrelated with retrieval and forecast errors, and if errors introduced by the collocation process are well-behaved. It is possible that the collocation process penalises statistics for retrievals more heavily than those for forecasts, because the fields for the latter are smoother. Also the majority of collocations are over data-dense areas where the forecast accuracy should be highest. More sophisticated assessment methods are required to overcome these deficiencies.

Equation (7) may be considered as a conventional retrieval or as a vertical analysis at the observation point. The latter is consistent with the approach in the data assimilation scheme recently developed for operational use at the Meteorological Office (Lorenc *et al.* 1988), in which the horizontal and vertical aspects are separated. For all observation types, the datum is first interpolated to the vertical levels of the model at its own horizontal location, and then the information is spread in the horizontal to model grid points. For satellite radiances, the vertical stage is as described above. There is a problem of observational error correlation in the horizontal stage: because the background field is used in the inversion, retrieval errors are correlated with the background and hence with each other. However, since we can estimate this correlation through (3), we can allow for it in the horizontal analysis (see Lorenc *et al.* 1986). Thus, although our retrievals have correlated errors with the characteristics described in section 2, their conceptual equivalence to

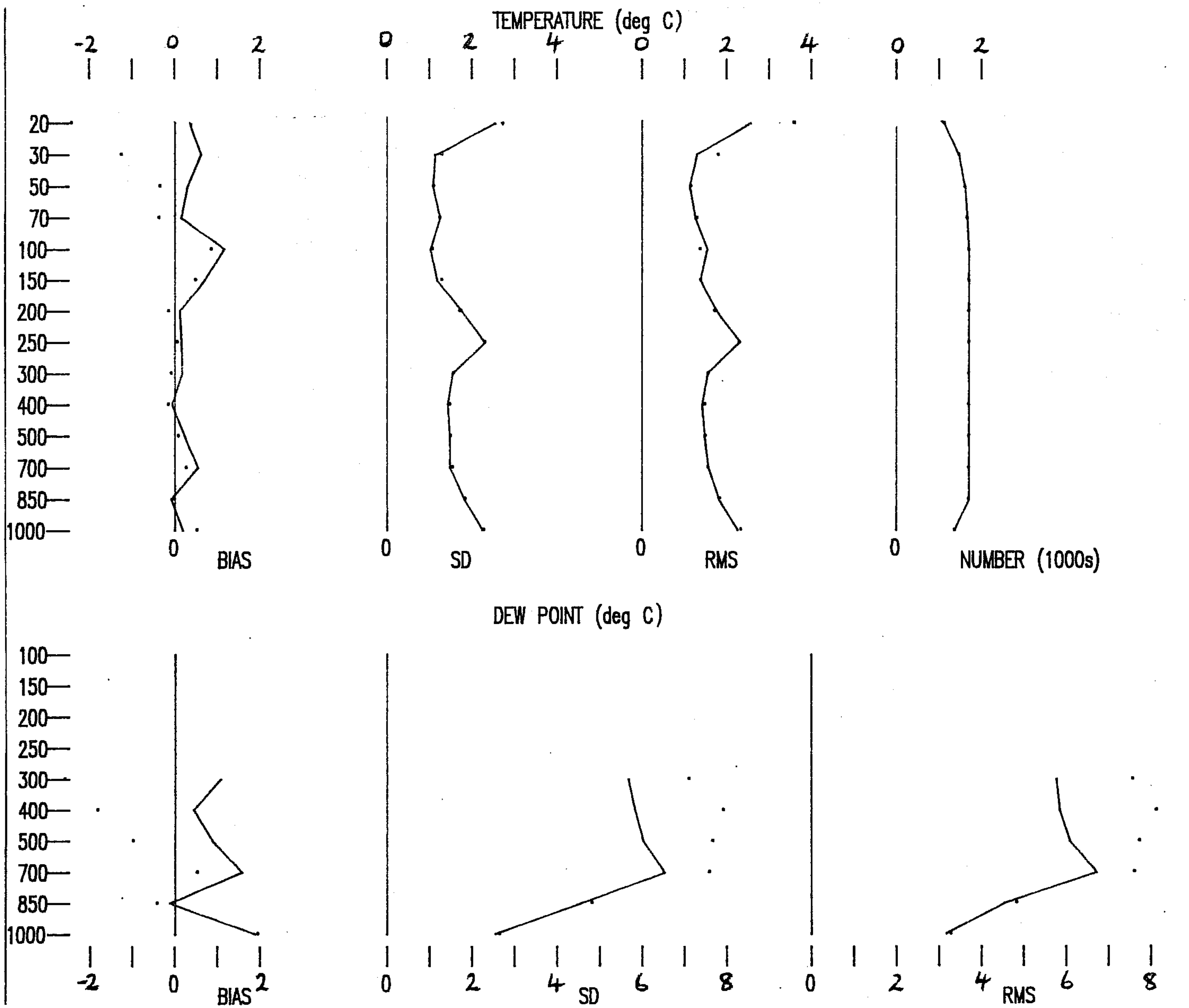

Figure 1

Collocation statistics showing differences from radiosondes for May 88.

\ retrieval-sonde

. forecast-sonde

the direct assimilation of radiance provides a theoretical framework for determining how the correlations of errors should be handled correctly within the horizontal stage of the assimilation.

5. NONLINEAR SCHEMES

The scheme described above assumes, a linear relationship between cloud-cleared brightness temperature and temperature/humidity profile. This is quite accurate for temperature but not really satisfactory for humidity. Also, in using pre-processed, cloud-cleared brightness temperatures, we are forced to tolerate errors in the radiances introduced by the cloud-clearing and pre-processing. In theory, it is preferable to use the raw, potentially cloud-affected radiances directly. This leads to a highly nonlinear problem, primarily because of the profound effect of clouds on infra-red weighting functions.

A nonlinear scheme for inverting raw radiances has been developed (Eyre 1987b). It is currently being refined and assessed. The profile vector $\mathbf{x}$ includes simultaneously the temperature and humidity profiles, the surface skin temperature and microwave emissivity, and the cloud top pressure and fractional coverage. Equation (3) is solved iteratively using Newton's method:

$$\mathbf{x}_{n+1} = \mathbf{x}_n - J''(\mathbf{x})_n^{-1} \,.\, J'(\mathbf{x}_n) \tag{8}$$

$$J''(\mathbf{x})_n = \mathbf{C}^{-1} + \mathbf{K}(\mathbf{x}_n)^T \,.\, \mathbf{E}^{-1} \,.\, \mathbf{K}(\mathbf{x}_n) \tag{9}$$

$$= \mathbf{C} - \mathbf{C} \,.\, \mathbf{K}(\mathbf{x}_n)^T \,.\, (\mathbf{K}(\mathbf{x}_n).\mathbf{C}.\mathbf{K}(\mathbf{x}_n)^T + \mathbf{E})^{-1} \,.\, \mathbf{K}(\mathbf{x}_n) \,.\, \mathbf{C} \tag{10}$$

A "damped" version of this approach has had to be adopted to overcome instability of the iteration (probably caused by the highly nonlinear nature of the problem). This involves, in the calculation of $J''(\mathbf{x})$, reducing the elements of $\mathbf{C}$ representing those variables which make the problem so nonlinear (i.e. the cloud parameters). When the iteration converges, a check is made on the fit of the measured to the calculated radiances in each channel. This is found to provide a powerful means of quality control. An important aspect for the practical implementation of this scheme has been the development of a fast method for computing $\mathbf{K}(\mathbf{x})$ in parallel with the calculation of $\mathbf{y}\{\mathbf{x}\}$.

The scheme has been applied successfully to real data (Eyre 1988). However it has not yet been shown to be consistently better than the linear scheme, and research continues. Also, the current version of the nonlinear scheme is rather expensive computationally. Although it converges in ~4 iterations, it involves at each step the computation of $J''(\mathbf{x}_n)$ and a full radiative transfer calculation of $\mathbf{y}\{\mathbf{x}_n\}$ and $\mathbf{K}(\mathbf{x}_n)$. A more efficient scheme should be possible through a different approach to the minimisation of (1) and more economical use of the full radiation transfer model. Such developments would be essential if the scheme were to be extended from its present one-dimensional (vertical) form to an application in a 3- or 4-dimensional data assimilation system.

6. CONCLUSIONS

The schemes described here represent the first steps along a path towards a closer integration between satellite data processing and NWP data assimilation systems. Through a more direct use of radiance data, we expect to exploit more fully the true strengths of satellite sounding data whilst allowing appropriately for their weaknesses. Present research is on TOVS data, but the approach should be equally applicable to the Advanced TOVS system on future NOAA satellites and to radiance data from other remote sounding systems.

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