1. WORKING GROUP 1: INVESTIGATING OBSERVATION TYPES AND RELATED PROBLEMS

1.1 GENERAL CONSIDERATIONS

1.1.1 Quality control

The presentation by Lorenc showed how non-Gaussian errors could be allowed for in a variational scheme, using a simple model of observation errors. The same model can also be used to derive rejection criteria in a quality control preprocessing step such as the current OI scheme.

Recommendation

The error model parameters (e.g. probability of gross error) should be introduced for each observation in the current system. The current OI quality control code should be adapted to use them or an independent pre-processing quality control module developed. This would provide an alternative to present OI quality control or to non-Gaussian variational methods.

A non-Gaussian observational error distribution adds significantly to the nonlinearity of the analysis and the likelihood of multiple minima in the penalty function. These effects are most serious in early iterations when the estimate is less good. Every effort should be made to get a good starting guess for the iteration, and it may be necessary to do early iterations with a modified (more nearly quadratic) penalty function.

The quality control of radiosonde data of heights and temperatures requires a complex algorithm properly to cover all eventualities. Consideration should be given to using a package developed by, or in collaboration with, other centres (e.g. NMC or UKMetO).

1.1.2 Observational error characteristics

Efforts to derive observation error statistics from routine monitoring should continue, and be extended to give a fuller description of the error distributions (e.g. probability of gross error, skewness of distribution, and bias).

Particular error characteristic problems to be mentioned are:

- Biases in radiosonde mass and humidity are significant.

- The TOVS radiance bias correction scheme has had a significant positive impact on assimilation of TOVS data. Efforts should continue.

- Representativeness errors exist in surface data and depend on e.g. surface subgridscale variations. Model output statistics techniques should be considered as potential observation operators.

For most of the observation types the observation error (which includes the representativeness error) may be correlated in the horizontal. Consequently experiments which assume a non-zero correlation are recommended.

1.1.3 Extension of the control variable

All the variational experiments performed so far have been updating model variables in spectral space. However, from the experience gained from these experiments with the surface and TOVS radiance operators, it is clear that not adjusting the surface (grid-point) variables may be a deficiency. They are currently treated as auxiliary variables.

It is felt that, in order to improve the use of such data, some of these auxiliary variables should be included in the control variable, with priority given to T_s (skin temperature) and W_s (soil wetness).

Furthermore, with a view to using 'raw' radiances, it may become necessary to have an additional part of the control variable defined only at the observation points. An example of this would be cloud cover parameters at TOVS locations.

1.1.4 Observation operators and their adjoints

The concept of an "observation operator", through which the model equivalent of an observation is calculated, is thought to be important for the optimal use of data. Also the use of exact adjoints of these operators allows the observations to be assimilated in a consistent manner. Significant effort is being directed towards the scientific formulation and coding of these operators for all observation types, but particularly those for satellite observations.

Recommendation

In order to reduce duplication of effort, it is recommended that the sharing and exchange of such code should be encouraged. The development of common interfaces for observation operators would assist this process.

1.1.5 Some remarks on the interface organisation

As a general statement we remark that the archives in relation to a data assimilation scheme should be:

a) Comprehensive - to allow monitoring of the history of the data through the scheme, to do statistics of data quality, observation errors etc.

b) In standard format (BUFR is a candidate).

c) Defined in cooperation with other institutes for maximum portability.

Recommendation

In addition to the development of common observation operators, we suggest a similar procedure for the development of pre-processing and quality control algorithms.

1.2 REVIEW OF THE OBSERVATIONS

Variational techniques facilitate the use of all types of data at full observational resolution. Efforts must be continued to obtain a more complete set of the observations potentially available. The Working Group reviewed the last statement in this area (ECMWF Tech Memo 15) and the following comments provide an update to it.

1.2.1 Surface observations (SYNOP, DRIBU, SHIP)

Surface pressure, 10m wind, 2m temperature and 2m RH observations have been used in current variational analysis. More work is required regarding the last 3 parameters. We especially need a better surface layer parametrization with coupling to suitable control variables: T_s, W_s (maybe more). Pressure tendency should be used but only when it provides independent information. [We expect this information to be more useful in the 4D context]. Variational techniques provide better possibilities to use cloud and present weather information which is in the SYNOP observations. Other parameters in the surface report should be checked for their usefulness (implying new observation operators!).

1.2.2 Aircraft reports

Temperature should be used as soon as possible. It was noted that many aircraft reports are not available on the GTS.

1.2.3 SATOBs

Observation errors increase with wind speed. Experiments should be done to use wind speed and direction rather than u and v, perhaps only wind direction when wind speed is thought unreliable. The application of bias correction or 1-sided PDFs should be investigated. Expected observation error characteristics or reliability should be assigned to the observational datum by the data producer, and used in analysis. 4DVAR is able to make use of the data at high frequency. ECMWF should press for hourly data.

1.2.4 Radiosondes

Experiments should be carried out to use the full temperature profile, instead of height. Interpolation should be done either before feeding the data into the scheme or as part of the observation operators, and similarly for wind. Position and time of observation change with height. This deserves special attention. Humidity is biased and lags. Bias correction and more sophisticated error statistics should be provided.

1.2.5 PAOBS and similar synthetic data (tropical cyclones)

4DVAR may provide the possibility for improved use of information contained in the temporal evolution of tropical cyclone positions. Similar information would be useful on the position of other cyclones.

1.2.6 Satellite sounding data

1.2.6.1 *TOVS*

An observation operator is already included in the IFS and is well tested. Short-term problems are:

- the absence from the control variable of some relevant fields (surface and stratospheric temperatures),

- appropriate observation error correlations, particularly between channels,

- sensitivity to the variances and vertical correlations of temperature error implied by J_g.

Current work is using cloud-cleared radiances. Attention is now turning to the potential use of raw (cloudy) radiances, initially for

- improved identification of clear radiances (through 1DVAR), and

- generation of cloud products, for diagnostics studies and for input to cloud analysis/assimilation procedures.

The main obstacle to direct use of cloudy radiances in 3D/4DVAR is the fact that the horizontal scales of cloud features, which affect the radiances dramatically, are not represented in the model. Inclusion of additional control variables at observation points seems the only way forward here.

1.2.6.2 *ATOVS*

These data raise only two new problems compared to TOVS:

- the effects of microwave surface emissivity over a large frequency range, demanding extensions to the treatment of surface fields,

- the enhanced effects of cloud liquid water.

1.2.7 SSM/I

An observation operator for SSM/I-derived total column water vapour has already been developed and tested. No major problems are expected here. An operator for surface wind speed is required. Although direct assimilation of radiances is possible here, the retrieval problems are sufficiently guess-independent that assimilation of radiances may have no significant advantages. However, processing radiances may be necessary to obtain useful information on cloud liquid water and precipitation.

1.2.8 Satellite imagery

These contain information on clouds which should be assimilated to improve the specification of model cloud and associated fields (humidity, rainfall, diabatic heating). Raw TOVS data treated as images are likely to provide the most convenient source of data in the short-term. AVHRR and geostationary image data may provide a useful supplement. Improvements in model parametrizations may be necessary before such information can be used effectively.

1.2.9 Scatterometer

An observation operator for $\sigma^o s$ is already present within IFS. The error characteristics of $\sigma^o s$ are known to be problematic; their specification as constant in $\ln\sigma^o$ may be preferred. Also the highly nonlinear nature of the observation operator could cause problems. An early experiment to study the significance of these effects is recommended. Horizontal correlations of observation error may be present but are not likely to need urgent treatment.

1.2.10 Altimeter

Use of surface wind speed should be investigated.

2. WORKING GROUP 2: USE OF A PRIORI INFORMATION, FIRST-GUESS, ATTRACTOR

ECMWF OI and ECMWF 3DVAR are both sub-optimal implementations of the general 3D estimation problem. It seems likely that the 3DVAR implementation will be closer to the ideal than OI, but it may not be superior in all aspects.

2.1 SHORT-TERM DEVELOPMENT OF THE J_g FORMULATION

We would wish to take advantage of the experience that has been built up with the OI implementation. It is not clear, however, how closely one should try to emulate OI. For example spatial variability of the standard deviation of the background errors may not be necessary in the first operational implementation and using horizontally uniform errors may actually help in the evaluation of other effects by not confusing the issue. However, some ideas might be evaluated within the OI framework and one should take advantage of this possibility.

Considerable flexibility has been introduced in the design of the J_g formulation. But not all of these features will be required in the first operational implementation. In addition to the spatial variability of the standard deviation of the background errors, it is not clear whether or not it is worthwhile insisting on the horizontal variability of the vertical error correlations. Sensitivity to these features should be investigated. Even if a horizontally uniform representation of the background errors is adopted for the first implementation, the exact fixed variances and vertical structure functions used should be reassessed.

The covariance matrix is currently considered to be diagonal with a constant value for each total wave number. This results in homogeneous and isotropic statistics. The inclusion of off diagonal terms (especially for larger scale) should be investigated. On the other hand, horizontal length scales which vary with the eigenvectors of the vertical structure functions and the use of appropriate equivalent depth for the separation Rossby-gravity may be more important. At the same time, analysing or diagnosing the kernel of the P to T, $\ln p_s$ transform is regarded as a serious problem at both ECMWF and NMC.

Another unknown area is the shape of the spectrum of the autocorrelation function to be used for the large scales.

Humidity analysis is currently formulated in a similar way as in OI being basically decoupled. It will soon be necessary to evaluate its behaviour.

2.2 POTENTIAL FOR FUTURE EVOLUTION

Evaluation of the system along the following lines should begin immediately.

2.2.1 Tropical analysis

In view of the potential for improvement, considerable effort should be spent on evaluating the performance of the variational analysis system in the tropical regions. In particular, just how far does one need to relax the current constraints in order to do a reasonable job at analysing Kelvin modes? One could also look at mixed Rossby-gravity modes, and even the 30-60 day wave. This would necessitate a small reformulation of the current scheme, as it currently lumps Kelvin waves together with the other gravity waves - a more flexible approach could be beneficial.

2.2.2 Dynamical balance

One could generalise the current approach by, for example carrying out the split of the increments into Rossby and gravity modes only for vertical modes 1 through 5 (or 6 or 7, ..) and treat the rest without separation in a univariate fashion. This has several potential benefits: the appropriate equivalent depths could be used; balance constraints are only applied as appropriate; one could use different vertical correlations for vorticity, divergence and P in the univariate regime. Also, one could think of doing something special for the highest vertical modes - those describing the boundary layer, perhaps reflecting Ekman balance.

The epsilon parameter which determines the relative weight given to Rossby and gravity modes should perhaps be made a function of wavenumber n or the rank of the EOF, but there is little observational evidence available to determine this relationship. A way of addressing this issue is to diagnose the relative importance within the model itself.

The current formulation allows one to take into account the nonlinear nature of the slow manifold solving the variational initialisation problem. Depending on the importance of this effect this could be a natural evolution of the system.

2.2.3 Boundary layer and surface

There are many complex relationships within the boundary layer. The introduction of these relationships into the analysis system should enhance the results. For example, imposition of a weak constraint in the form of an Ekman balance could substantially improve the near surface divergence. It was noted that the inclusion of this type of weak constraint could lead to a poorer convergence in the minimization algorithms.

Results shown in this workshop by *Andersson et al.* and *Vasiljevic et al.* indicate that a lack of a J_g for surface fields leads to near surface observations having an undesirably large impact on the analysis. Use of surface fields in the control variable is felt to be important in this regard.

A proper J_g formulation for the surface fields will have to be formulated. Difficulties might arise due to the grid-point nature of those fields.

2.2.4 Humidity

There is a lot of humidity data around which is currently not being used. Results from 1DVAR indicate that TOVS moisture channels can be successfully used to analyse moisture. However, models quite often diverge quite rapidly from the humidity analyses. Improvement in the humidity analyses is seen as important. Also, the possibility of implementing some kind of diabatic attractor information (weak constraint on the humidity) should be investigated. The work of Krishnamurti, Kasahara, Donner and others indicate techniques which could be adapted to the variational framework.

2.3 GENERAL RECOMMENDATIONS

There are many possibilities for research projects which could be studied by universities which would assist in our understanding of the behaviour of the system.

It is proposed that some analysis intercomparison exercise (with NMC and, perhaps, OI analysis systems) be conducted to assess the relative performance with real data. It might be more practical to begin this exercise with single isolated data, from the response to which one might learn a lot.

3. WORKING GROUP 3: TEMPORAL DIMENSION

3.1 GENERAL

There are strong connections between the 4D-VAR statement of the data assimilation problem and the statistical estimation-theoretic statement. The variational approach originally considered the dynamics to be non-linear but the model to be perfect, while in the statistical Kalman filter approach the model error statistics were considered, but within the framework of a linear model. One can say that these two approaches are trying to overcome different deficiencies.

The science of numerical weather prediction will be strengthened by recognizing and exploiting to the fullest extent possible the connections between the two approaches. Fruitful research cannot be pursued in one approach without exploring the other one. This is especially true for the determination of means and covariances of model and observation errors, which is required for both approaches.

3.2 4D-VAR AND SEQUENTIAL ASSIMILATION

Results presented at the workshop confirm that the potential for 4D variational assimilation is very promising. This is due in particular to the ability of variational assimilation to account exactly for the dynamics of the flow as represented by the model equations and to define implicit flow-dependent structure functions.

In the increment approach, as proposed at NMC, the increments from a basic trajectory are assumed to follow a simplified dynamical evolution. This approach, by allowing the cost and complexity of the algorithm to be varied at will, will significantly facilitate experimentation on, and implementation of 4D variational assimilation.

Variational assimilation and statistical assimilation are two similar approaches to solving similar problems. Intercomparisons between results produced by these two approaches will certainly prove to be instructive. Such intercomparisons should be made with the cooperation of other centres doing research in data assimilation.

Various approaches have been proposed to carry the forecast error covariances in time. It is not clear at present which of these is the most viable. In addition, connections have been demonstrated between optimal modes and the propagation of forecast error statistics over the assimilation period. These connections are fundamental for prediction of forecast skill. Experiments should be performed to establish the sensitivity of the assimilation product to background errors. The Centre should participate in collaborative research in this area.

3.3 THRESHOLD PROCESSES

Threshold processes, such as e.g. convection, formation of clouds, precipitation and change of snow cover, may cause problems in variational assimilation. For instance, the local gradient (local in phase space) obtained from observed rain will not generally convey the information to trigger convection in the case of no existing rain in the current model state. But the evidence so far of the importance of these problems in practice is not very conclusive. These problems are not specific to variational assimilation but also exist in Kalman filtering approaches, since both require linearization and hence differentiation of the model dynamics.

In the increment approach to variational assimilation the potential problem of threshold processes is avoided to some extent. This may be at the cost of a less accurate solution. Real experimentation at ECMWF and at NMC is needed. It will be necessary to develop the adjoints of physical processes (or approximations thereof) in order to perform these experiments and to decide which processes to include in operational practice.

Finally, the problem of threshold processes in 4D-VAR may be reduced by sufficient availability of observations. If a threshold process is triggered well before the end of the assimilation interval, and if observations of the process are available, then the inherent difficulty of defining a linearization at the trigger moment loses its relevance.

3.4 HOW TO DETERMINE AND TAKE INTO ACCOUNT MODEL ERROR IN 4D-VAR

Even though there is evidence of significant model errors, especially in the tropics, too little is known about their form to be practically useful in data assimilation. The first question that should be answered is whether model error is in fact a significant component of forecast error. This can be investigated in the context of 4D-VAR. It is possible, for example, to test the hypothesis that model error is insignificant by checking that the measure of fit of the model trajectory to the observations, as obtained by 4D-VAR, can indeed be explained by observational noise and initial error only.

Additional information about model error statistics can only be extracted from forecast-minus-observed residuals, since these contain the only available information about the relationship between model and truth. In order to estimate statistical model error parameters from these residuals , it is necessary to account for the propagation of initial error as well. Model error estimation is therefore intimately connected with forecast error covariance propagation, and the best way to achieve this is by means of adaptive Kalman filters or simplifications thereof.

There are several serious difficulties associated with the estimation of model error statistics. Model errors are not stationary, and are probably correlated in time. The number of parameters that describe model error statistics which can be estimated on the basis of available data is limited. Furthermore, the observed-minus-forecast residuals are affected by observational errors as well and the separation of observational error from model error may not always be possible.

In view of all these difficulties, it is clear that much theoretical work will need to be done before it is known what the important characteristics of model error are, and how they should be accounted for in 4D-VAR. The general approach should be to formulate hypotheses about the covariance structure of model errors, and then to test these hypotheses by means of parameter estimation techniques in the context of (simplified forms of) Kalman filters.

We also recommend that a theoretical study be made of the possible significance of Lagrange multipliers and adjoint trajectories obtained in 4D-VAR. There is a general feeling that these quantities should contain information about the nature of model error. This study should be performed in collaboration with more theoretically-oriented research groups elsewhere.

3.5 CONCLUDING REMARKS

The Centre has available the expertise and many of the tools for doing research in data assimilation of the highest quality. The Centre should continue to encourage scientists from other institutes to use these tools and expertise to carry out research of a theoretical nature.

The present OI scheme of the Centre has proven to be extremely efficient. Even if most of the Centre's effort in the coming years will be devoted to the development of 4D variational assimilation, it will be necessary not only to maintain but also to improve the ideas developed in the OI scheme in terms of its first guess error statistics and its propagation in time.