MONITORING AND QUALITY CONTROL OF THE OPERATIONAL OBSERVING SYSTEM

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1. INTRODUCTION

In this paper we discuss the study of differences between observations and short-range forecasts in a data assimilation context. Such differences are called 'departures' or sometimes 'innovations'. Their statistics are widely used to assess the quality of the observations, of the data assimilation system and of the short-range forecasts. We give examples of monitoring activities, and we describe the algorithms for data quality control within the operational four-dimensional variational (4D-Var) data assimilation system of ECMWF.

2. JUSTIFICATION

The reasons why the comparison of observations against short-range forecasts can provide such powerful diagnostic on the performance of the observation network and the assimilation were discussed by Hollingsworth *et al.* (1986).

- First, it was demonstrated that in areas where there is adequate radiosonde coverage the 6-hour forecast error is comparable with the observation error.
- Second, the forecast accounts for most of the evolution of the atmospheric state from one analysis to the next, so the analysis needs to make only a small correction to an accurate background field.
- Third, large variations of the departure statistics from station to station are indicative of problems in the data or in the assimilation system.

The forecast removes the large synoptic variations from the statistics. The high accuracy of the forecast enables useful comparison of departure statistic between stations and between observation types - the synoptic variations would otherwise render such comparison impossible.

3. MONITORING

Data monitoring has become an established and important part of the activities of most numerical weather prediction centres (Delsol 1984; Böttger *et al.* 1987; Kashiwagi and Baba 1989; Julian 1989; Uddström and Purnell 1989). In recent years the monitoring activities have been extended to incorporate an increasing number of space-based observing systems, such as cloud motion winds (Lalaurette *et al.* 1998; Butterworth 1998) and radiances from polar orbiting and geostationary satellites (McNally *et al.* 1999; Munro *et al.* 1999).

The data assimilation systems calculate differences (or departures) between the observations and their model equivalents computed from a short-range (typically 6-hour) forecast. From statistics of time series of these departures it is possible to make statements about the typical accuracy of the different types of observations. In many occasions it has also been possible to identify problems with individual stations, which after notification to the data producers have been corrected. Such examples were given by Hollingsworth *et al.* (1986; 1989), Radford (1987) and Strauss (1996). Monthly accumulations of monitoring statistics (stratified by type, station identifier, pressure ...) provide the basis for regular changes in the operational blacklist.

It is common practice that new types of observations are monitored for a time before they can be introduced actively into the data assimilation systems. Such pre-operational monitoring can be very effective in identifying problems with any new data. A good example is the validation of ERS-1 scatterometer data by Stoffelen and Anderson (1994). In this section we will show examples relating to profiler data, and in a later section dropsonde data, which are the two data types most recently introduced into operations at ECMWF.

3.1 Profiler data

The United States' network of profiler stations provides hourly wind profiles from approximately 25 sites. The high temporal resolution makes this data set particularly interesting for use in 4D-Var. The accuracy of the profiler data was compared with the accuracy of U.S. radiosondes, through comparison of their respective departures from the background (short-range forecasts). Studies revealed that most profilers were as accurate as radiosondes above 700 hPa and had larger errors below that level. It is unclear whether the larger departures in the lower parts of the profiles are due to inherent measurement problems, or to a lack of representativity as the profilers register boundary layer and small-scale orographic effects unresolved by the model. The monitoring statistics and the results from data assimilation experiments led to the decision to use most profiler data above 700 hPa, hourly. Only a handful of profiler stations required blacklisting. It was decided to assign the same observation error standard deviation for profiler data as for radiosondes wind profiles.

Examples of U-component profiler departure statistics are shown in Fig. 1. The figure shows that the data retained for use by the assimilation system has an r.m.s of between 3 and 4 m/s against the background (with largest departures at jet level) and small bias. These statistics compare favourably with radiosondes in the same geographical area (not shown). The histograms show symmetric near-Gaussian distributions, with almost zero mean.

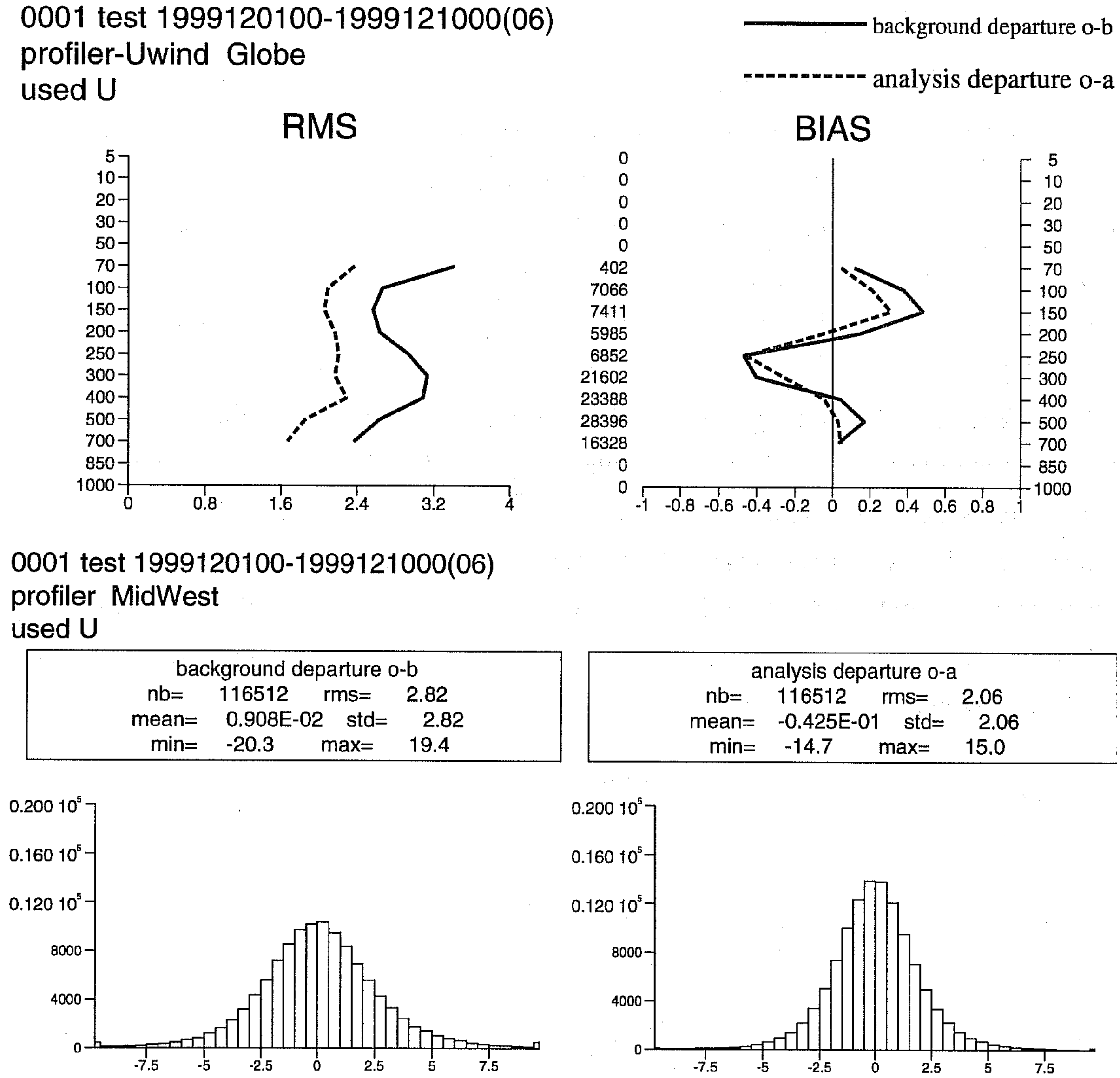

Figure 1: Statistics of U-wind component from profilers, 19990507-12 to 19990516-18. The top two panels show r.m.s. (left) and bias (right) for departures from the background (full lines) and the analysis (dashed). The histograms show departure from the background (left) and the analysis (right). The sample excludes blacklisted and otherwise rejected data.

4. PERFORMANCE OF DATA ASSIMILATION SYSTEMS

4.1 Error statistics

The departure statistics are used also to monitor the performance of the data assimilation system itself (Talagrand 1999, in this volume) and to charaterize the observation errors and background errors (Hollingsworth and Lönnberg 1986; Lönnberg and Hollingsworth 1986; Hall 1987; Järvinen 1999). Accurate estimates of these errors are required in order for the data assimilation system to assign the correct relative weights to the various data types, and to the background (Lorenc 1986). If the specified observation and background errors agree poorly with the actual errors, the performance of the data assimilation system will be poor. Evidence of significant correlation of observation error is of particular concern, as such correlations are neglected in many schemes currently, including ECMWF's 4D-Var.

4.2 Biases

The formulation of most data assimilation schemes assumes that both observation and background errors have zero mean, i.e. that they are unbiased. It is important to establish that this is indeed the case, as was done for profiler data in Fig. 1. Relative biases can reliably be detected through the study of monitoring statistics, but it may be more difficult to determine which component (background or observations) is the main contributor to the bias (Kållberg and Delsol 1986, Hollingsworth *et al.* 1988). Bias tuning algorithms based on monitoring statistics have been devised for radiosonde temperature data (correcting for solar radiation, Lalaurette 1999, personal comm.) and for TOVS radiance data (Eyre 1992; Harris and Kelly 2000). Bias correction of stratospheric TOVS radiance channels is a particularly delicate problem as there are few conventional data to compare against, and it cannot be assumed that the model's stratospheric temperatures are unbiased (McNally *et al.* 1999). Fig. 2 shows an example with a small overall bias but an excess of cold departures (caused, in this case, by residual cloud-contamination) results in a skewed distribution.

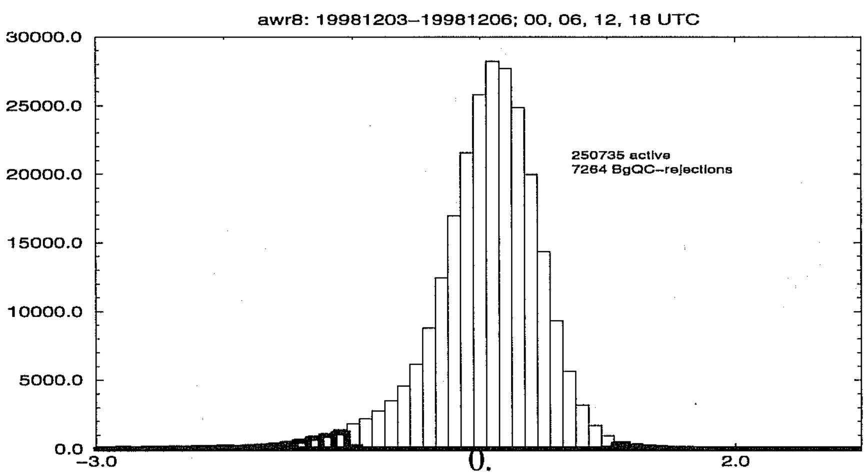

Figure 2: Histogram of radiance departures from the background, for HIRS channel 3, 19981203-00 to 19981206-18. The data highlighted in bold were rejected by quality control. The distribution is skewed with an excess of large negative departures.

5. QUALITY CONTROL

5.1 The Gaussian assumption

Histograms of departures represent the probability distribution of the sum of background and observation errors. Under the assumption of near-Gaussian background errors the histograms can give some indications of the main non-Gaussian characteristics of observation error. In all linear estimation problems Gaussian distributions of errors are assumed. In variational data assimilation the Gaussian assumption leads to a quadratic cost function (Lorenc 1986). In many cases the histograms of departures agree fairly well with the Gaussian assumption. In other cases there may be an excessive number of data with larger departures than would be expected from a purely Gaussian distribution of errors. Such data may need to be removed from assimilation as they are likely to be incorrect. Alternatively the Gaussian assumption can be relaxed, as will be shown in Section 6.1.

5.2 Quality control algorithms

There is a variety of different algorithms for quality control of meteorological data. Lorenc (1996) discusses the theoretical basis for three different approaches: 1) 'Buddy checking', 2) Optimum Interpolation quality control and 3) Variational quality control. Each of these algorithms may be applied prior to the main analysis, and their purpose is to remove incorrect data from further processing. Alternatively the variational quality control can be incorporated within the analysis itself through a generalization of the variational cost function. The quality control then takes place during the iterative search for the most probable analysis, while the costfunction is being minimized. This latter approach has been taken in ECMWF's 3D-Var and 4D-Var.

In the following sections two mechanism for quality control will be described: the background check (BgQC, Järvinen and Undén 1997) and the variational quality control (VarQC, Andersson and Järvinen 1999). BgQC and VarQC represent two fundamentally different approaches to quality control. The strategy of BgQC is to identify and remove those data that deviate significantly from the normal distribution, in order to make the subset of data presented to the analysis agree more closely to the Gaussian assumption. With the VarQC approach, on the other hand, the variational cost function is modified to account for non-Gaussian statistics, in an attempt to describe better the actual distribution of observation errors (Ingleby and Lorenc 1993; Schyberg and Tweiter 1999). The effect in data assimilation is that with VarQC the weight given to observations will vary with the magnitude of the departure, such that data far from the Gaussian distribution obtain reduced influence on the analysis. Effectively, a smooth and gradual rejection of severely deviating data can be achieved.

6. VARIATIONAL QUALITY CONTROL

6.1 The observation cost function of 3D and 4D-var

At ECMWF a four-dimensional variational scheme (4D-Var) became operational in November 1997 (Rabier *et al.* 1997), replacing the three-dimensional version (3D-Var) implemented in January 1996 (Courtier *et al.* 1998; Rabier *et al.* 1998; Andersson *et al.* 1998). The variational method for data assimilation, as described by e.g. Lorenc (1986), comprises minimizing a cost function made up of two terms, J_o and J_b, measuring the distance to the observations and to the background, respectively. Both cost functions are given a quadratic form, which assumes that the errors in both observations and background are Gaussian in nature. The expression for the observation cost function is thus

$$J_o = \frac{1}{2}(\mathbf{y} - H\mathbf{x})^{\mathrm{T}}\mathbf{O}^{-1}(\mathbf{y} - H\mathbf{x}), \tag{1}$$

where $\mathbf{y}$ is the array of observations, with error covariance matrix $\mathbf{O}$, $\mathbf{x}$ is the model state and H the observation operator. Eq. (1) degenerates in the case of uncorrelated data to a sum of individual J_o-contributions, i.e.

$$J_o = \sum\frac{1}{2}\left(\frac{y - H\mathbf{x}}{\sigma_o}\right)^2 \tag{2}$$

with σ_o the observation error standard deviation.

6.2 Incorporation of VarQC

The VarQC method is is based on Bayesian probability theory (Gelman *et al.* 1995, Lorenc and Hammon 1988). A modification of the observation cost function to take into account the non-Gaussian nature of gross errors has the effect of reducing the analysis weight given to data with large departures from the current iterand (or preliminary analysis). Data are not irrevocably rejected, but can regain influence on the analysis during later iterations if supported by surrounding data.

As in Dharssi *et al.* (1992) and Ingleby and Lorenc (1993) we generalize Eqs. (1) and (2) by assuming that an observation error belongs to either of two populations: one which follows the normal Gaussian distribution, representing random errors, and one which is modelled by a flat distribution, representing the population of data affected by gross errors. Other models to represent the probability density of incorrect data could also be used (e.g. Huber 1977; Gelman *et al.* 1995). The choice of a flat distribution is convenient since it corresponds to the assumption that those data provide no useful information to the analysis.

6.3 VarQC formulation

With a prior probability of gross error A and a probability of not having a gross error $1 - A$ we write the probability density function (pdf) p^{QC} for a single observation as a sum of two terms:

$$p^{QC} = (1 - A)N + AF \tag{3}$$

N and F are the Gaussian and the flat distributions, respectively:

$$N = \frac{1}{\sigma_o\sqrt{2\pi}}\exp\left[-\frac{1}{2}\left(\frac{y - \hat{y}}{\sigma_o}\right)^2\right] \tag{4}$$

$$F = \frac{1}{D} = \frac{1}{2d\sigma_o}, \text{ if } |y - \hat{y}| < D/2, \text{ zero otherwise} \tag{5}$$

where the observed value is y and the model equivalent, $\hat{y}$, of the observed quantity is the observation operator H applied to the model state $\mathbf{x}$, i.e. $\hat{y} = H\mathbf{x}$. The flat distribution is defined over an interval D (centred at zero) which in Eq. (5) for convenience has been written as a multiple d of the assumed observation error standard deviation σ_o. It is assumed in the following that absolute departures $|y - \hat{y}|$ greater than $D/2$ never occur or have been removed in a pre-analysis check against (for example) the background (see Section 7).

The observational cost function of the variational analysis (Lorenc 1986) is given by:

$$J_o = -\ln p + c \tag{6}$$

We obtain the normal quadratic cost function J_o^N by inserting in Eq. (6) the Gaussian pdf $p^N = N$, and arbitrarily choosing $c = -\ln(\sigma_o\sqrt{2\pi})$:

$$J_o^N = \frac{1}{2}\left(\frac{y - \hat{y}}{\sigma_o}\right)^2 \tag{7}$$

Its gradient ∇ with respect to the observed quantity $\hat{y}$ is:

$$\nabla_{\hat{y}} J_o^N = -\frac{1}{\sigma_o}\left(\frac{y - \hat{y}}{\sigma_o}\right) \tag{8}$$

Similarly substituting the modified pdf, Eqs. (3) to (5), into Eq. (6), we obtain after re–arranging the terms, an expression for the QC–modified cost function J_o^{QC} and its gradient $\nabla_{\hat{y}} J_o^{QC}$:

$$J_o^{QC} = -\ln\left[\frac{\gamma + \exp(-J_o^N)}{\gamma + 1}\right] \tag{9}$$

$$\nabla_{\hat{y}} J_o^{QC} = \nabla_{\hat{y}} J_o^N\left[1 - \frac{\gamma}{\gamma + \exp(-J_o^N)}\right] \tag{10}$$

(if $|y - \hat{y}| < D/2$, $\nabla_{\hat{y}} J_o^{QC} = \nabla_{\hat{y}} J_o^N$ otherwise), with γ defined as:

$$\gamma = \frac{A\sqrt{2\pi}}{(1 - A)2d}. \tag{11}$$

The term $\gamma/(\gamma + \exp(-J_o^N))$ modifying the gradient in Eq. (10) can be shown to be equal to the *a-posteriori* probability of gross error P, given $\mathbf{x}$, and assuming that $H\mathbf{x}$ is correct (see Ingleby and Lorenc, 1993, *section 2g*):

$$P = \frac{\gamma}{\gamma + \exp(-J_o^N)} \tag{12}$$

Note also that the VarQC modification of the cost function is a function of A, d and the normalized departure $(y-\hat{y})/\sigma_o$, only.

Following Eq. (10) we define a VarQC weight W^{QC} such that

$$\nabla_{\hat{y}} J_o^{QC} = \nabla_{\hat{y}} J_o^N \ W^{QC} \quad \text{, i.e. } W^{QC} = 1-P \tag{13}$$

Eq. (13) shows that data which are found likely to be incorrect ($P \approx 1$) are given reduced weight in the analysis. Conversely, data which are found likely to be correct ($P \approx 0$) are given the weight they would have had using purely Gaussian observation error pdf.

6.4 Application

An *a-priori* estimate A of the probability of gross error and the range of possible values d are assigned to each datum, based on study of historical data, such as departures from the background and from the analysis. Then, at each iteration of the variational scheme, an *a-posteriori* estimate of the probability of gross error P and the VarQC weight W^{QC} are calculated (using Eq. (13) etc.), given the current value of the iterand (the preliminary analysis). The calculated *a-posteriori* probability P depends on $\mathbf{x}$ and assumes that $H\mathbf{x}$ is correct, which means that it is important to have a preliminary analysis that is as good as possible at the start of the variational quality control. This is achieved in practice by performing the minimisation without quality control for a number of iterations (currently 40) before VarQC is switched on. VarQC then remains switched on until the end of the minimisation, i.e. during the remaining 30 iterations (Rabier *et al.* 2000). The most obviously wrong data do not influence the minimisation at all, as they have been removed in a pre-analysis check against the background (BgQC), to be described in Section 7.

The VarQC-modified cost function and its gradient are computed thereafter. The modified gradient becomes the input to the adjoint observation operators and provides the forcing for the adjoint integration in 4D-Var. This is a quality control algorithm without conditionals or threshold values. In the case of many observations, all with uncorrelated errors, J_o^{QC} is computed as a sum (over the observations i) of independent cost function contributions:

$$J_o^{QC} = -\ln \prod_i p_i + C = -\sum_i \ln p_i + C = \sum_i J_{oi}^{QC} \tag{14}$$

The global set of observational data includes a variety of observed quantities as used by the variational scheme through their respective observation operators. The application of VarQC is always in terms of the observed quantity.

6.5 Illustration

Eqs. (9) and (10) are illustrated for one single observation in Fig. 3. The figure show the normal and the VarQC cost functions (top), the VarQC gradient (middle) and the QC weight, W^{QC}, i.e. $1-P$ (lower panel), plotted against observation departure $y-\hat{y}$. The parameters are $A = 0.01$, $d = 5$ and $\sigma_o = 2$. The figure shows VarQC with a flat distribution for gross errors (as used in

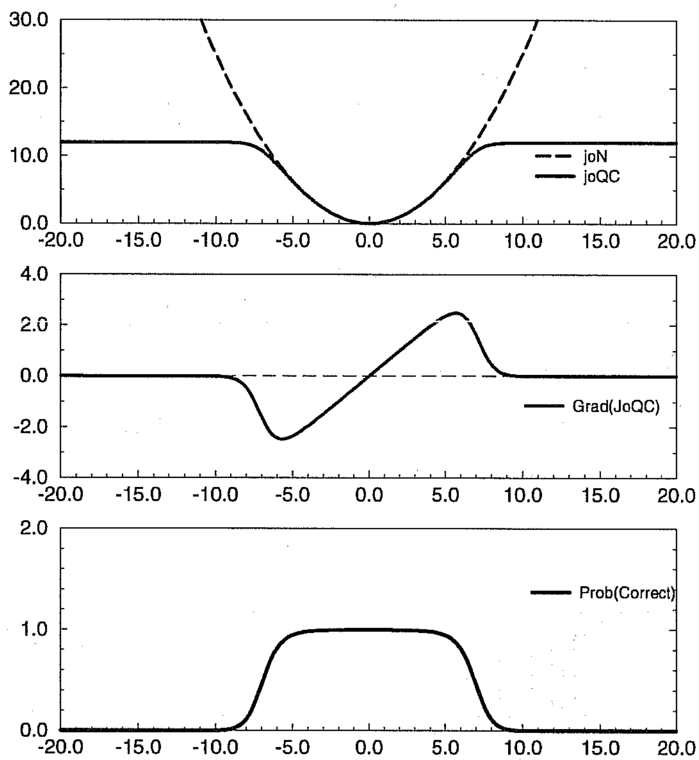

Figure 3: The top panel shows the observation cost function with (full) and without VarQC (dashed line). The middle panel shows the gradient of the VarQC cost function and the lower panel shows the *a posteriori* probability that the observation is correct $(1-P)$. A flat distribution has been used to represent the p.d.f. of incorrect data.

the ECMWF 3D/4D-Var). The cost function flattens out for large values of the departure, and its gradient goes towards zero, as the probability of the observation being correct also drops towards zero. The interval within which the observation is partly used/partly rejected is relatively narrow for this set of parameters.

7. BACKGROUND CHECK

VarQC relies on there being a pre-analysis screening of data, such as a check against the background fields. The BgQC (Järvinen and Undén 1997) has effectively remained unchanged during the transition from OI to 3D and 4D-Var. It checks that the normalized departure from the background $z_b = (y - H\mathbf{x}_b)/\sigma_b$ is less than a factor α times its estimated error variance, i.e.

$$z_b^2 \leq \alpha\ (1 + \sigma_o^2/\sigma_b^2) \tag{15}$$

The factor α may be different for different observation types and variables (Järvinen and Undén 1997). The values of σ_b in Eq. (15) are obtained from the background error standard deviations actually used in the background term of the variational analysis (Fisher and Courtier 1995), interpolated to the observation locations. For radiance observations the values of σ_b are estimated with the technique described by Andersson *et al.* (2000). Observations rejected by BgQC cannot currently be reinstated by VarQC.

8. DIFFICULTIES

The BgQC generally works well but problems can occur when the background itself is severely in error. In such cases there is a danger that valuable observation are rejected, not because the observations are wrong but because the background is wrong. Problems of this kind occur in the vicinity of rapid developments and intense systems. In a study of dropsonde data Cardinali (1999) found that valuable observations near the centre of tropical cyclones were systematically rejected by BgQC, as departures were frequently in excess of 20 m/s. As the intensity of the cyclone core is poorly resolved by the analysis, many data had large departures also against the analysis. Those with departures greater than 10 to 12 m/s (against the analysis) were rejected by VarQC (Fig. 4).

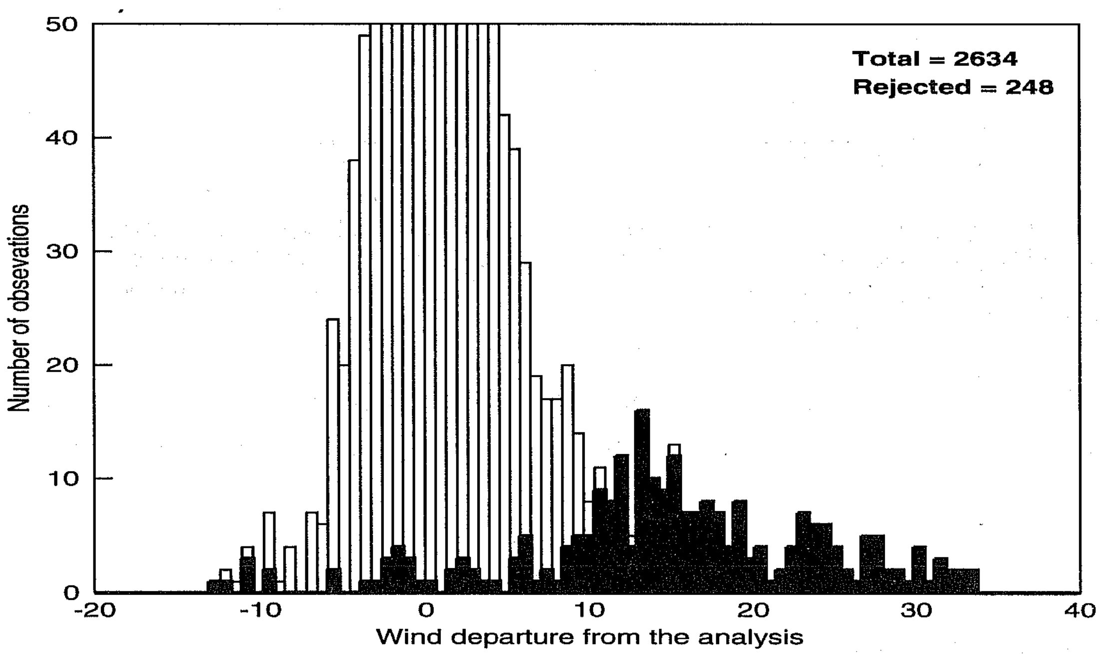

Figure 4: Histogram of departures from the analysis (19980830-00 to 19980901-18) for dropsonde wind data showing rejections by VarQC in bold. From Cardinali (1999).

It is hoped that the development of a Simplified Kalman Filter and flow dependent background errors will enable a more dynamic description of the variations of σ_b, so that more data can be retained in the most active areas.

9. SUMMARY AND CONCLUSION

Statistics of departures from the background (typically a 6-hour forecast) are used extensively for data monitoring, for assessing data assimilation performance and for specification of quality control parameters.

The two main mechanisms for quality control, the background check (BgQC) and the variational quality control (VarQC) were described and their application was discussed. VarQC is operational as an integral part of the ECMWF four-dimensional variational data assimilation scheme (4D-Var). The scheme provides an estimate of the probability that each observation is in error, given the observed value and the analysis. The weight given to the observation becomes smaller as the probability of gross error increases. The weight is recalculated at each iteration of the minimisation, which means that data can regain influence on the analysis if supported by surrounding data. The calculations are performed in terms of the observed quantities and all data from the global set of observations are used and quality controlled simultaneously.

The current BgQC is performed separately, prior to the analysis. It rejects observations for which the departure from the background is in excess of a certain multiple times its expectation, taking specified observation errors and background errors into account. This implementation, although found to perform satisfactorily in most cases, has a drawback. In extreme cases of rapid development the background itself can be so much in error that correct observations are mistakenly rejected. Currently, the BgQC rejections are irrevocable. It may be advantageous in the future to allow some of the data rejected by BgQC to have a second chance to influence the analysis during the iterations with active VarQC.

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