Progress towards better representation of observation and background errors in 4DVAR

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ABSTRACT

This paper reviews recent progress in the representation of observation and background errors for satellite data in 4DVAR. Current specifications of observation errors in assimilation systems are often rather simplistic, but more sophisticated approaches are emerging that better address the situation-dependent or correlated nature of contributions such as representativeness or forward model error. Significant gains in forecast skill have been obtained from more appropriate observation error specification. Various diagnostics are available that can guide this speciation, together with a better understanding of individual components of the error. Background errors, in contrast, have reached a high degree of sophistication, with ensemble methods being used increasingly to better account for flow-dependent aspects of the background error. These developments are leading to substantial improvements in forecast skill, and they have been shown to optimise the use of the available observations.

1 Introduction

Observation errors and background errors are essential components that have to be specified in any data assimilation system. Together, they determine the weight that an observation receives in an analysis. Specification of these errors is a core activity for any assimilation system. Particularly the representation of background error has progressed substantially in recent years.

This paper provides an overview and examples of current developments in the specification of observation and background errors, highlighting areas of particular relevance. It is beyond the scope of this paper to cover all aspects, and for more details, the reader is referred to the provided references.

2 Observation errors

2.1 Overview

Observation errors should describe the random component of any errors in the observations and the comparison between the observations and the model fields. Biases are assumed to be addressed separately in a bias correction step (e.g., Dee, 2004). In the standard notation used for data assimilation, the observation error covariance matrix is referred to as **R**, and sometimes conveniently described through the standard deviation of the error (σ_O) and an error correlation matrix.

There are a number of contributions that should be considered as part of the observation error covariance, and it is useful to categorise them broadly in the following way:

- **Measurement error:** for instance, the instrument noise for satellite radiances. If we are lucky, thiserror is globally constant and uncorrelated between different observations.
- **Forward model (observation operator) error:** for instance, radiative transfer error for satelliteradiances, arising through uncertainties in the spectroscopy, the assumed gas concentrations, spectral response functions, etc. This error is likely to be situation-dependent and correlated between different observations.

- **Representativeness errors:** these are errors arising through the mismatch of different scales being represented in the observations and the model fields, or, more generally, through the inability of the forecast model to represent atmospheric features present in the observations. These errors are highly situation-dependent and likely to be correlated between different observations.
- **Quality control error:** errors can arise when the observations are used that should have been eliminated by quality control, for instance, cloud-affected radiances assimilated under the assumption of clear-skies. Such errors are highly situation-dependent and likely to be correlated between different observations.

In most of today's assimilation systems, the *assumed* observation error specification for satellite data is relatively basic. For example, in the ECMWF system, radiances from all main sounding instruments (e.g., AMSU-A, AIRS, IASI) are assimilated assuming a globally constant, uncorrelated observation error. As highlighted above, this is a relatively crude assumption, as all observation error contributions other than measurement error are likely to be situation-dependent and will show some correlations either between channels or spatially. Some situation-dependence is taken into account, for instance, for the assimilation of data from microwave imagers in the all-sky system (larger errors are assigned in cloudy regions to address representativeness errors, see Geer and Bauer, 2011), or the assimilation of Atmospheric Motion Vectors (AMVs) (larger errors are assigned in regions of stronger shear, to address that height assignment error has a larger effect, see Forsythe and Saunders, 2008). Capturing such situation-dependence is an area of active research, highly specific to the observation in question.

2.2 Estimation of observation errors

An enhanced specification of observation errors requires a good estimate of this error. In the following, we will give an overview of some methods of how such an estimate can be obtained.

2.2.1 Error inventory

Ideally, an estimate for the observation error should be based on a physical understanding of all error contributions, also referred to as an "error inventory". For instance, for the assimilation of clear satellite radiances this would mean obtaining separate estimates of the instrument noise, the radiative transfer error, the error of representativeness, the cloud screening error, etc. An example of work in this direction can be found in Ventress and Dudhia (2013). A complete analysis of all contributions and their correlation structures is often challenging, especially for contributions such as the radiative transfer error or the representativeness error, and as a result this area has received only relatively little attention so far.

2.2.2 Departure-based diagnostics

Alternative methods have been developed that infer information on observation errors indirectly, either through evaluating collocated observations (e.g., Bormann et al., 2003), or by considering statistics based on an analysis of departures from assimilation systems. The latter have gained some popularity in recent years, mostly because such departure statistics are easily available from any assimilation system. We will therefore summarise these in more detail.

An illustrative qualitative and very basic measure of observation errors is the standard deviation of the background departures, i.e. the differences between observations and their background equivalent. Assuming that the background errors and observation errors are uncorrelated, the standard deviation of background departures gives an upper bound for the true observation error (σ_o). Figure 1 shows how standard deviations of background departures compare to the assumed observation errors for the ECMWF system for a selection of observing systems. We would expect the ratio shown to be greater than one, reflecting the contribution of background errors in addition to observation errors, whereas a value less than one suggests that the assumed observation error is too large. As can be seen, the assumed observation error is too large for many satellite observations, especially for some channels of the IASI instruments. The exception is GPS radio occultation data, which do not suggest such a clear over-estimation. The situation is quite different to, for instance, the assumed observation errors for radiosonde data. Related, more sophisticated diagnostics for assumed observation errors have been derived based on the cost function contribution of the analysis, see for instance Talagrand (1999) or Desroziers and Ivanov (2001) for further details.

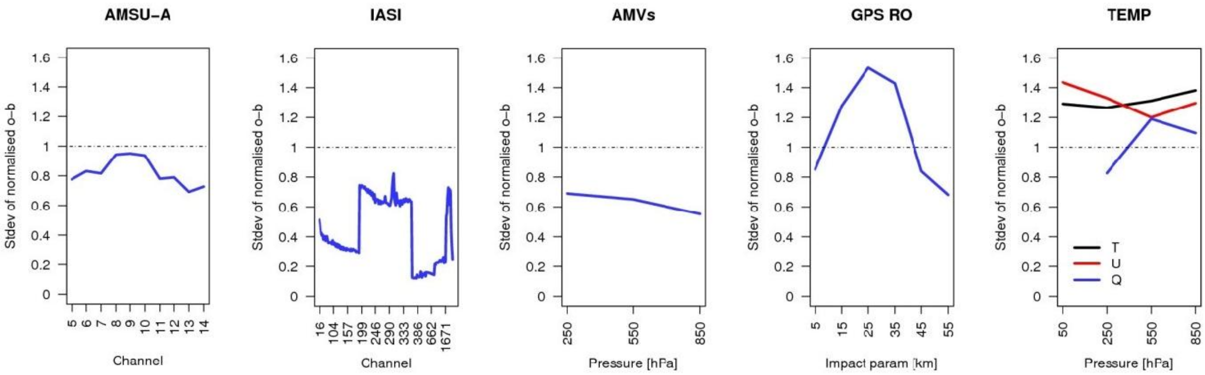

Figure 1: Standard deviation of background departures, normalised by the assumed observation error for the ECMWF operational system (August 2014) for 5 different observing systems: AMSU-A, IASI, Atmospheric Motion Vectors (AMVs), GPS radio occultation, and radiosondes.

Background departure covariances include a contribution from the background error, and over the years several methods have been developed aimed at partitioning this into observation and background error contributions. Two such methods shall be highlighted here:

- **Hollingsworth/Lönnberg:** This method assumes that background errors are spatially correlated, whereas observation errors are not. An estimate of observation error is therefore obtained from the spatially uncorrelated part of the background departure covariance calculated from a large database of pairs of observations, as described further in Hollingsworth and Lönnberg (1986).
- **Desroziers:** This method estimates an observation error covariance based on the relationship:

$$\tilde{\mathbf{R}} \quad = \quad Cov[\mathbf{d}_a, \mathbf{d}_b]$$

  where $\mathbf{d}_a$ and $\mathbf{d}_b$ are the analysis and background departures, respectively. The relationship has been derived with the assumption that the weights used in the assimilation system are consistent with the true weights, as discussed in Desroziers et al. (2005). Iterative application of the diagnostic has been suggested (e.g., Desroziers et al., 2009).

These diagnostics have been applied by numerous authors in recent years (e.g., Garand et al., 2007; Bormann and Bauer, 2010; Bormann et al., 2010; Stewart et al., 2014; Weston et al., 2014). Note that the diagnostics rely on a number of assumptions, and for a discussion of their relevance see, for instance, Bormann and Bauer (2010). In the following, we apply these diagnostics to the ECMWF system, and highlight how they can be used to provide guidance for the specification of observation errors.

2.2.3 Example: AMSU-A

The first example is that of the microwave temperature sounder AMSU-A, one of the most influential instruments currently assimilated. The above departure diagnostics were used to estimate observation errors (σ_O) as well as inter-channel and spatial error correlations (see Bormann and Bauer, 2010). The study found relatively good agreement between the estimates from several diagnostics, with σ_O values that were much lower than the observation errors assigned in the operational assimilation system at the time (Figure 2). At the same time, the diagnostics suggested little inter-channel error correlations, and the estimates for spatial error correlations were also small at the thinning scales used for this data. It appears that uncorrelated instrument noise completely dominates the true random observation error. The diagnostic provided little justification for the use of a very inflated observation error.

Assimilation trials were performed in which the assumed observation errors for AMSU-A were lowered from the previously assumed 0.35 K for tropospheric channels to 0.2 K (0.28 K for channel 5). This resulted in a very substantial improvement in forecast skill, as shown in Figure 3. It is apparent that AMSU-A data were previously under-weighted in the ECMWF system.

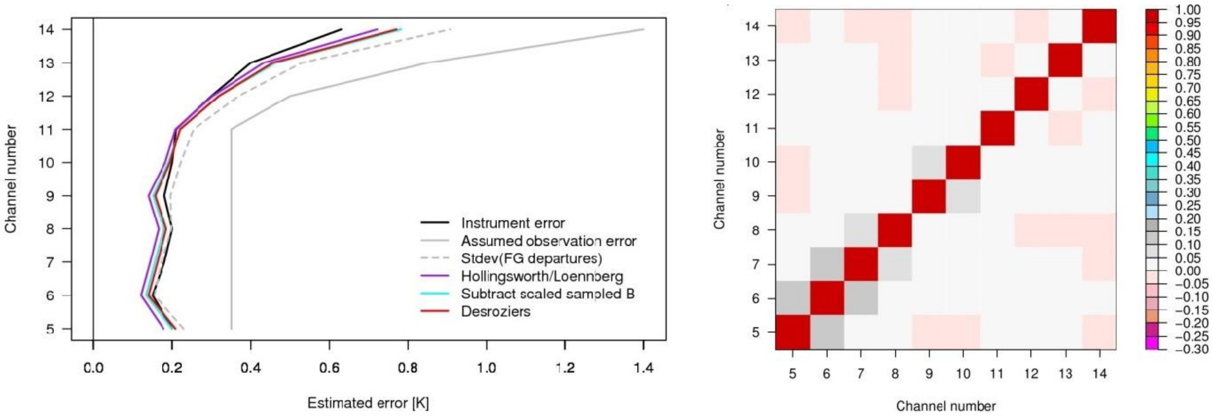

Figure 2: (left) Estimates of σ_o for AMSU-A on NOAA-18 from the Hollingsworth/Lönnberg (purple) and Desroziers (red) diagnostics, together with estimates of the instrument noise (black), the standard deviation of background departures (dashed grey), and the observation error assumed in 2008 (grey). (right) Estimates of observation error correlations obtained with the Desroziers diagnostic.

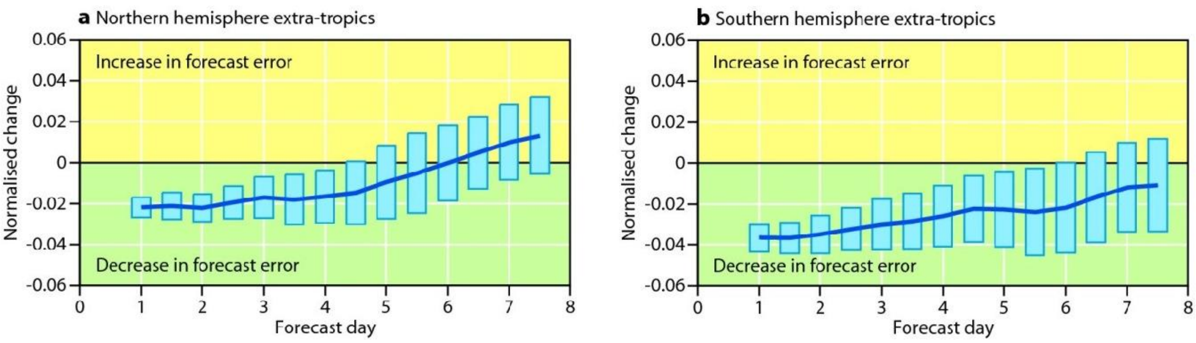

Figure 3: Forecast impact of reducing the AMSU-A observation errors in terms of the normalised difference in the root mean square error for the 500 hPa geopotential for the Northern Hemisphere (left) and Southern Hemisphere extra-tropics (right). Vertical bars indicate 95% significance intervals. The results are based on 120 forecasts obtained during December 2009–January 2010 and May–July 2010.

2.2.4 Example: IASI

The same diagnostics have been applied to IASI data, a hyperspectral infrared instrument and also a leading contributor to forecast skill. The estimates for observation error and inter-channel error correlations are shown in Figures 4 and 5. As for AMSU-A, the assumed observation errors are significantly larger than suggested by the diagnostics for many channels (consistent with Figure 1), but here we are finding significant inter-channel error correlations, especially for lower tropospheric/window channels (channels 312–921), ozone channels (1479–1658), and humidity channels (1671–5480). Similar results have been obtained by a number of authors using a variety ofdata assimilation systems (e.g., Garand et al., 2007; Bormann et al., 2010; Stewart et al., 2014). These diagnostics suggest that errors other than instrument noise (e.g., representativeness or cloud screening errors) are contributing considerably to the true observation error for hyperspectral infrared sensors.

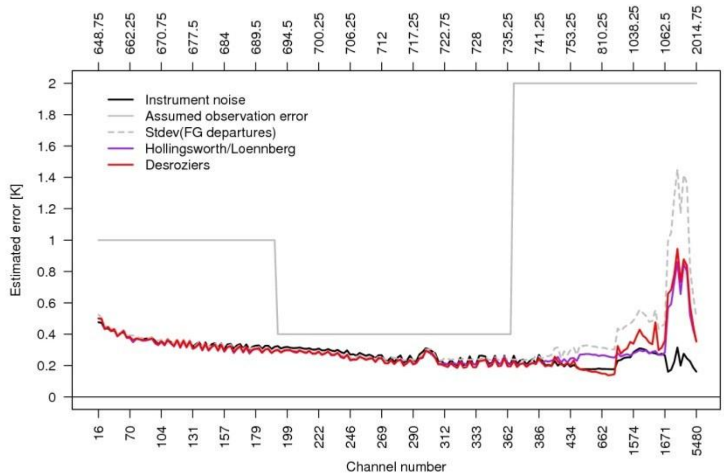

Figure 4: As Figure 2, but for METOP-A IASI.

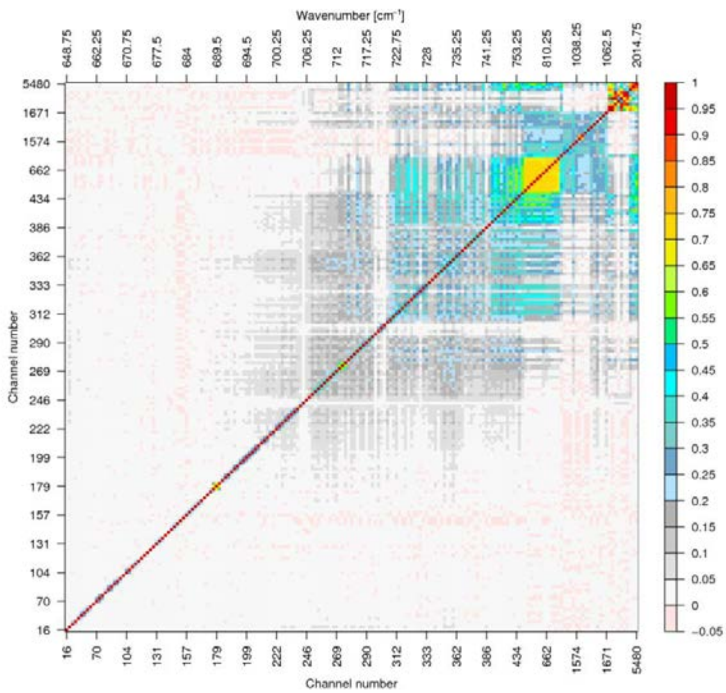

Figure 5: As Figure 3, but for METOP-A IASI and the Hollingsworth/Lönnberg diagnostic.

The question arises to what extent the error correlations affect what observation errors can be assigned to IASI data. One approach is to take the inter-channel error correlations into account during the assimilation, as efficient methods are available to do this. On the other hand, past experience has suggested that inflating the assigned observation errors, while still assuming uncorrelated observation errors, can be a useful way to circumvent the need to account for error correlations.

To investigate the inter-play between inflating observation errors and taking inter-channel error correlations into account, we performed two series of experiments: The first series uses a diagonal **R** matrix for AIRS and IASI, with σ_o specified from the observation error diagnostics, but multiplied with different scaling factors ranging from 1 to 4. The second series uses an **R** matrix for AIRS and IASI that includes the diagnosed inter-channel error correlations, with σ_o specified from the observation error diagnostics, but again multiplied with different scaling factors ranging from 1 to 3.

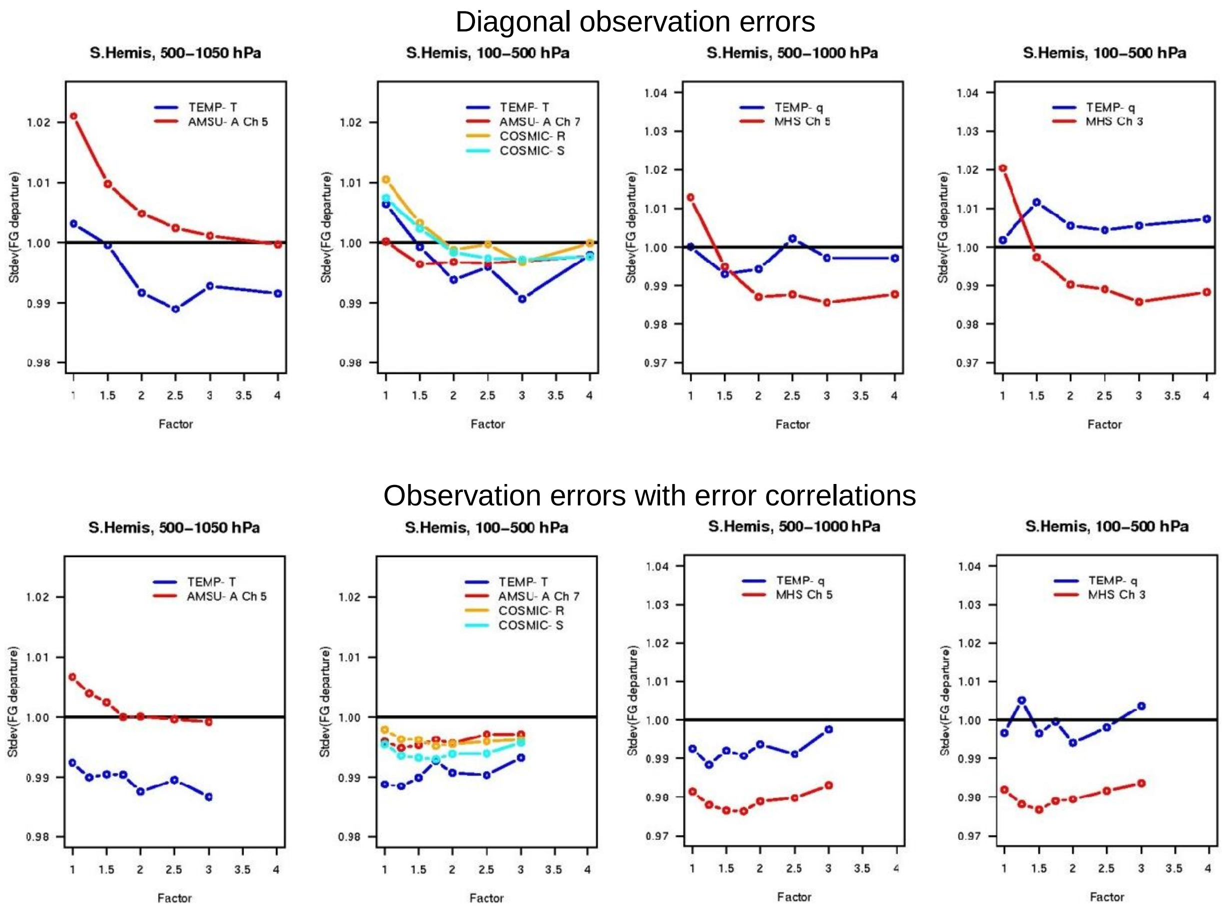

Figure 6: Standard deviations of background departures over the Southern Hemisphere for several observation types as a function of the scaling factor applied to the diagnosed observation errors for AIRS and IASI. The standard deviations are normalised to 1 for an experiment in which both AIRS and IASI are not assimilated. Data are for 15 December 2011 – 14 January 2012. Top row: diagonal observation errors are assumed; bottom row: error correlations are taken into account. For radiosondes (TEMP-T for temperature, TEMP-q for humidity) and GPS radio occultation bending angles (COSMIC-R, rising; COSMIC-S, setting), departure statistics have been combined in the approximate layers indicated above the three panels.

Figure 6 shows the evolution of the normalised standard deviation of background departures for several observing systems as a function of the scaling factor. These departure statistics are a useful and robust tool for evaluating the quality of the background, with values of less than one (i.e. standard deviations smaller than for a denial experiment) indicating an improvement and values larger than one indicating a degradation from assimilating AIRS and IASI.

The experiments with the diagonal observation error covariance show that there is a clear degradation from using AIRS and IASI when the unscaled diagnosed values are used. However, an improvement can be achieved when inflating the assumed observation error, with a minimum at a relatively large scaling factor of 2.5–3. This is consistent with the operational use of large observation errors for many channels.

For the series of experiments with full observation error covariance matrices, using the unscaled diagnosed matrix gives more reasonable results, but some scaling of the observation errors appears beneficial as well. The minimum standard deviations are achieved with a much smaller scaling factor of around 1.5–1.75. Comparing the experiments with optimised scaling factors, the fit for humidity-sensitive observations tends to be significantly better in the experiment with the full error covariance matrix, whereas for temperature-sensitive observations the difference is less clear. This may be related to the presence of particularly significant error correlations for the water vapour channels in the diagnosed error covariance matrices, so accounting for these shows clearer benefits.

For AIRS and IASI, where significant inter-channel error correlations have been diagnosed, it therefore appears to be beneficial to account for these, and it allows the use of an observation error (σ_o) more consistent with departure statistics. The use of inter-channel error correlations for IASI is used operationally at the Met Office since January 2013, leading to significant gains in forecast skill (Weston et al., 2014). Some reconditioning of the diagnosed matrix was found to be necessary, achieved by adding a significant uncorrelated component to the original matrix. This is thought to address the otherwise considerably larger condition number of the employed **R** matrix. Adjustments have been found necessary in some cases in the ECMWF system as well, but here they were traced back to the diagnosed matrices suggesting unrealistically small errors in the structures associated with the smallest eigenvalues of **R**. The experience hence suggests that some adjustments may be necessary when using the diagnosed matrices. Ideally, the diagnosed matrices should be backed up by guidance from an error inventory, to ensure physically meaningful robustness of the assumed matrices.

2.2.5 Adjoint-based diagnostics

With the advent of adjoint-based diagnostics, tools have been developed that estimate the sensitivity of the forecast error to the specification of the assumed observation error using adjoint methods (e.g., Daescu and Todling, 2010). These provide guidance where an inflation/deflation of the observation error or background error is likely to be beneficial. Extensions have also been developed that provide the sensitivity to specifying a correlation structure for the observation error, see Daescu and Langland (2013) for further details. It should be noted that these tools largely treat the assigned observation error as a tuning factor, and they currently rely on prior assumptions on the correlation structure of the errors. Care as to be taken that the suggested adjustments to the observation errors remain physically meaningful, either by consulting an error inventory or departure-based diagnostics.

3 Background errors

3.1 Overview and hybrid EDA 4DVAR

The background error describes the random component of the error in the background forecast used in the assimilation system and plays an important role in defining the structure of the analysis increments. A good specification of the background error is also crucial in successfully carrying forward in time the information analysed from past observations. As a result, enhancing the background error specification has received a large amount of attention since the development of modern assimilation systems. In fact, many of today's developments in data assimilation methodology are motivated by a better representation of background errors, and a more complete overview of those can be found in Lorenc et al. (2014).

A common theme of the improvements in the background errors in the ECMWF system and elsewhere is the better representation of flow-dependent aspects of the background error. This is achieved through an increasing use of ensemble-based methods. In the current operational configuration at ECMWF, the standard 12h 4DVAR is enhanced by providing a flow-dependent background errorfrom an Ensemble of Data Assimilations (EDA) (Isaksen et al., 2010). The EDA currently consists of 25 separate lower-resolution 4DVARs, that aim to represent the uncertainties involved in the assimilation system by using perturbed observations and perturbed versions of other input fields such as the sea surface temperatures, and also by employing stochastic physics to represent model error. The size of the perturbations applied to the observations is determined by the assumed observation errors, another note-worthy use of the assigned observation errors in the ECMWF system. The spread of the EDA can be related to the size and structure of the analysis and background errors, as outlined in Isaksen et al. (2010). The system developed at ECMWF is referred to as Hybrid EDA 4DVAR, and in the present configuration the EDA supplies a high-resolution 4DVAR with flow-dependent background error variances as well as flow-dependent structure functions (via a wavelet formulation, Fisher, 2003), derived over the last few days as described in more detail in Bonavita et al. (2014).

The use of a flow-dependent background error has led to a very substantial increase in forecast skill compared to the previously used static background error formulation (Figure 7).

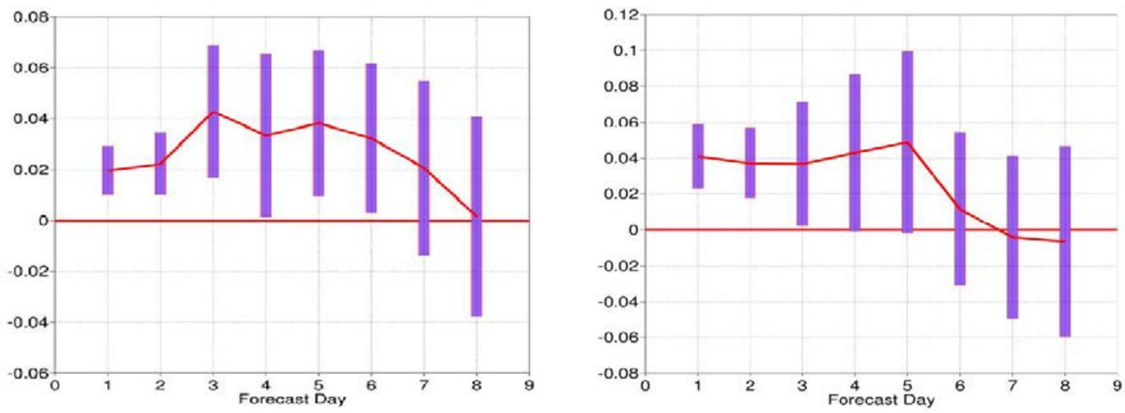

Figure 7: Forecast impact as in Figure 3 over the period June/July 2012. Here, positive values indicate a reduction in forecast errors, i.e. a positive forecast impact.

3.2 Case study: Hurricane Sandy

The role of adaptive and flow-dependent background errors on the use of satellite data has been highlighted based on the example of Hurricane Sandy that hit the east coast of the US on 30 October 2012 and caused wide-spread damage (McNally et al., 2013). The operational ECMWF forecast gave excellent guidance on the timing and positioning of Sandy's landfall about a week in advance, predicting accurately the unusual "left turn" of Sandy over the Atlantic. Three assimilation experiments highlight the role of satellite data and the background error specification: The *Control* experiment was the operational configuration. In a *Denial* experiment, all polar satellite data were withheld from the high-resolution 4DVAR (i.e. around 90% of the assimilated observations), but the EDA used for the background error specification continued to use all observations. In a *Denial+EDA* experiment, all polar satellite data were withheld from the 4DVAR as well as the EDA, hence allowing the background errors to adjust to the new observation coverage.

Figure 8 shows the track forecasts from these three experiments from two consecutive days, which can be compared to the observed track shown in Figure 9. The *Denial* experiment leads to a severely degraded forecast of the landfall position as a result of denying the polar satellite data. However, using background errors appropriate for the degraded observational coverage in the *Denial+EDA* experiment allows to recover some of the lost skill. While the forecasts are still clearly worse and less consistent without the polar satellite data compared to the *Control*, the more appropriate background error allowed a better use of the remaining observations. For instance, further investigations suggestethat the updated background errors affected quality control decisions for AMVs over the Pacific, and this contributed to better forecasts of Sandy's path.

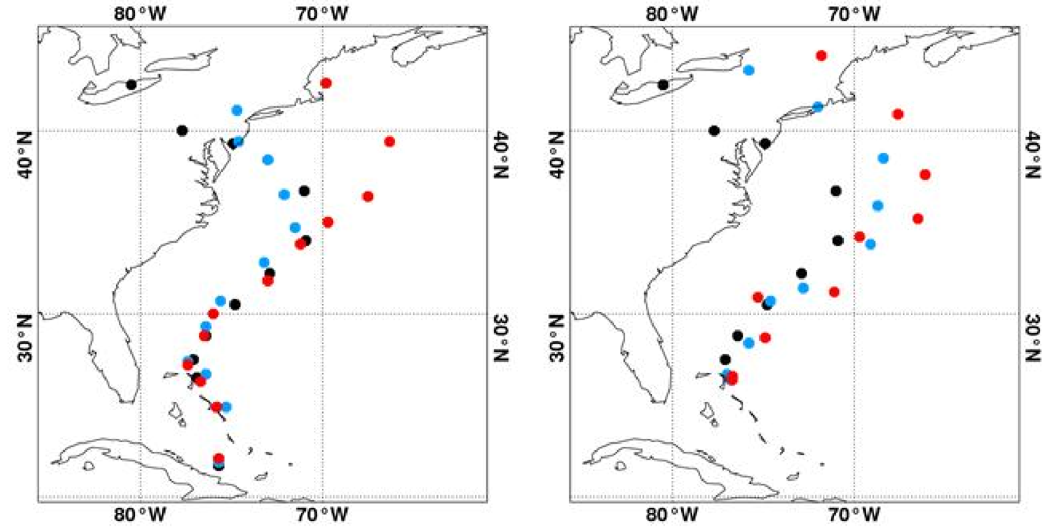

Figure 8: Forecast of Sandy's track (in 12 h intervals), starting from 25 October 2012 00UTC (left) and 26 October 2012 00UTC (right), respectively. Black dots are for the Control experiment, red dots for the Denial, and blue dots for the Denial+EDA experiment.

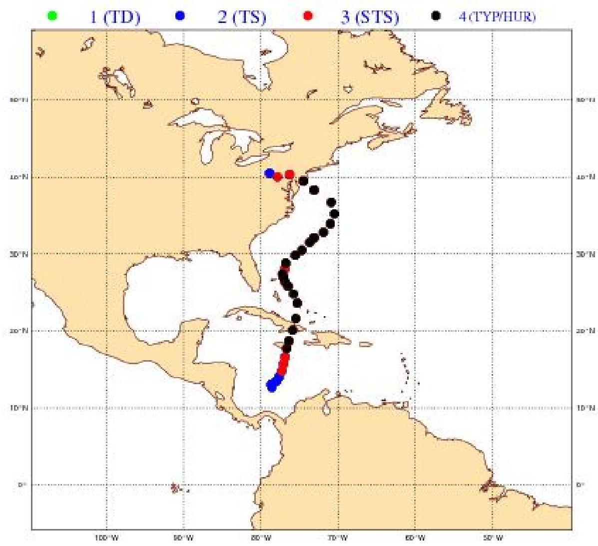

Figure 9: Sandy's observed track as given by the National Hurricane Centre, covering the period 20–31 October 2012.

3.3 Radiance diagnostics

With an increasing use of ensemble methods to specify flow-dependent background errors, there is an increasing need to critically assess and fine-tune the performance of the ensembles used. This can be done in a number of ways, but of particular interest in the context of this seminar is the use of satellite observations to do this, as in Flowerdew and Bowler (2011) or Bormann and Bonavita (2013).

Bormann and Bonavita (2013) performed an evaluation of the ECMWF EDA spread in radiance space for AMSU-A and MHS observations. To do so, the spread of the EDA in radiance space has been calculated by mapping each ensemble member to radiance space, and the resulting spread has been compared to background departure statistics from a high-resolution 4DVAR experiment. This leads to spread-skill diagrams as shown in Figure 10. These suggest that the EDA is underdispersive, for instance over the extra-tropics for AMSU-A channel 8. This is a common finding, also when evaluating the EDA spread using analyses. It is likely to be a result of suboptimalities in the applied perturbations, together with the lower spatial resolution used in the EDA. A calibration step is therefore applied before using the spread statistics for the specification of background errors, in addition to a spatial filtering step that addresses sampling errors as further described in Bonavita et al. (2012).

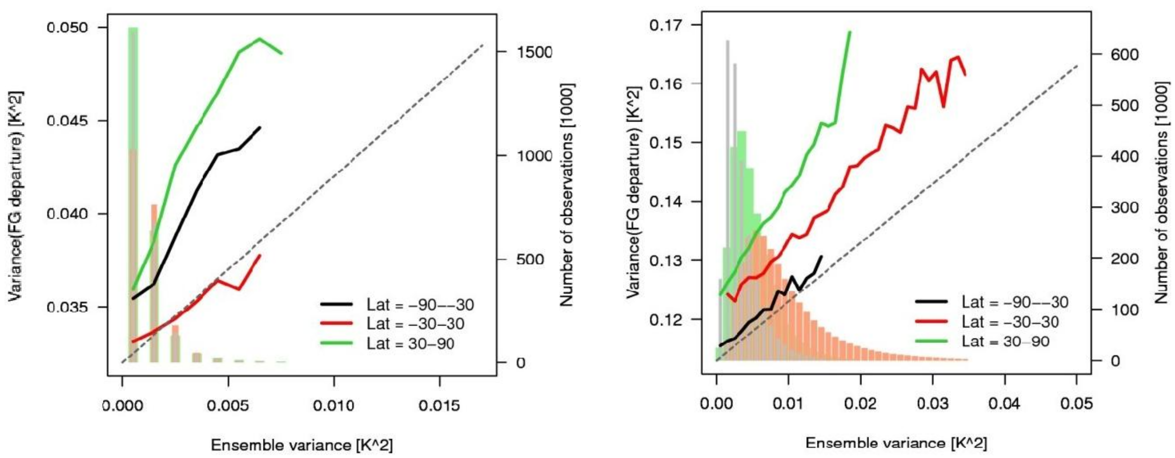

Figure 10: Variance of background departures for AMSU-A channels 8 (left) and 12 (right), binned by the ensemble variance in radiances space from the EDA, for the three latitude bands indicated in the legend. Histograms in lighter colours give the population for each variance bin (right y-axis). Also shown is a dashed line with the slope of one, indicating the slope of the departure/spread relationship for a perfectly calibrated ensemble. Statistics are derived for February 2012.

An estimate of flow-dependent background errors in radiance space, after calibration and spatial filtering, is provided in Figure 11. For AMSU-A channel 8, the estimate suggests that the random background error is well below 0.1 K for large parts of the globe, a result consistent with results from background departure statistics. Compare this to a typical noise figure of 0.2 K for currently available instruments. This highlights two aspects: firstly, a good description of the background error together with a careful use of observations is needed to preserve and improve the information already contained in the background. Secondly, lower instrument noise is likely to be needed for future instruments to achieve further gains in forecast accuracy.

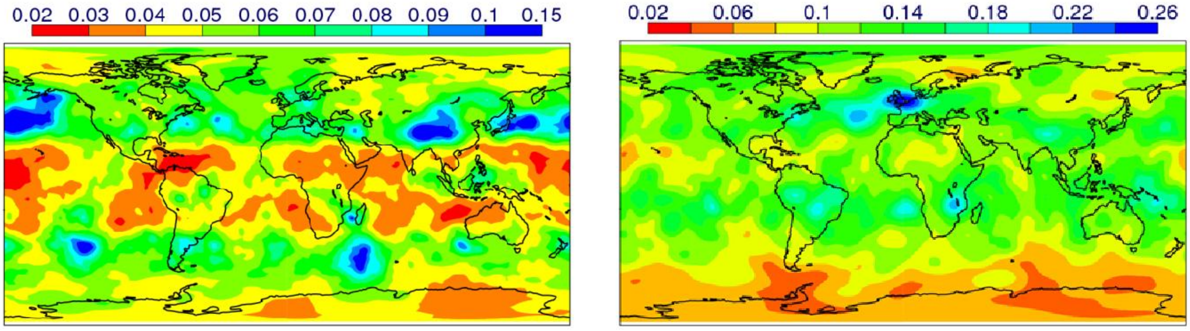

Figure 11: Estimates of background errors, as given by calibrated and filtered EDA spread values, for AMSU-A channel 8 (left) and channel 12 (right) for 15 February 2012 9Z.

4 Conclusions

This paper summarises the progress made in recent years in the area of observation error and background error representation in today's assimilation systems. For observation errors, current specifications are often fairly crude for satellite data, and inflated observation errors are frequently assumed, to compensate for observation error correlations (perceived or actual). However, more sophisticated representations of observation errors are emerging, taking into account the situation dependent or correlated nature of the representativeness or forward model error. Situation dependence has been particularly successful in the context of the assimilation of radiances in all-sky conditions and for AMVs. When error correlations are relatively large, current results suggest that taking these correlations into account and at the same time assuming observation errors closer to the true errors gives better results than assuming uncorrelated and inflated errors. The latter finding is likely to be particularly relevant for optimising the assimilation of new low-noise instruments such as CrIS, for which correlated contributions from errors other than instrument noise are more significant.

The representation of background errors has reached a high degree of sophistication, and ensemble methods are increasingly used to better capture the flow-dependent nature of background errors. Virtually all NWP centres are currently employing some form of ensemble data assimilation to better represent flow-dependent aspects.

Continuous monitoring of the evolution of the background and observation error representation is an important activity, aimed at optimising how new information from observations can complement the relatively high accuracy of the background. The paper has highlighted that the typical size of background errors for key variables such as temperature-sounding radiances is now rather small compared to the instrument noise of current data, posing new challenges to the design of future instruments, but also demanding novel ways to optimise the information content extracted from satellite observations.

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