Q. J. R. Meteorol. Soc. (2005), **131**, pp. 3385–3396 doi: 10.1256/qj.05.108

Diagnosis of observation, background and analysis-error statistics in observation space

By G. DESROZIERS†, L. BERRE, B. CHAPNIK and P. POLI
Météo-France, Centre National de Recherches Météorologiques, Toulouse, France

(Received 31 May 2005; revised 31 October 2005)

SUMMARY

Most operational assimilation schemes rely on linear estimation theory. Under this assumption, it is shown how simple consistency diagnostics can be obtained for the covariances of observation, background and estimation errors in observation space. Those diagnostics are shown to be nearly cost-free since they only combine quantities available after the analysis, i.e. observed values and their background and analysis counterparts in observation space. A first application of such diagnostics is presented on analyses provided by the French 4D-Var assimilation. A procedure to refine background and observation-error variances is also proposed and tested in a simple toy analysis problem. The possibility to diagnose cross-correlations between observation errors is also investigated in this same simple framework. A spectral interpretation of the diagnosed covariances is finally presented, which allows us to highlight the role of the scale separation between background and observation errors.

KEYWORDS: Estimation theory Optimality criterion Parameter estimation

1. INTRODUCTION

Most main operational assimilation systems are now based on the variational formalism (Lewis and Derber 1985; Courtier and Talagrand 1987, Rabier *et al.* 2000). Such a formalism allows the use of a large spectrum of observations and in particular satellite data that are not directly and linearly linked with model variables. However, those variational algorithms still rely on the theory of least-variance linear statistical estimation (Talagrand 1997). In the linear estimation theory, each set of information is given a weight proportional to the inverse of its specified error covariance. The pieces of information are classically given by observations and a background estimate of the state of the atmospheric flow. Analysis systems are then dependent on appropriate statistics for observation and background errors. Unfortunately those statistics are not perfectly known and their determination remains a major challenge in assimilation systems. One source of information on the observation and background errors is contained in the statistics of the innovations, that is the differences between observations and their background counterparts. Those statistics have for example been used by Hollingsworth and Lönnberg (1986), assuming that background errors carry cross-correlations while observation errors do not. From a slightly different point of view, Dee and da Silva (1999) have used a maximum likelihood method to estimate the information error statistics. Desroziers and Ivanov (2001) have proposed an approach based on a consistency criterion of the analysis relying on statistics of *observation-minus-analysis* differences to adapt observation-error statistics. The consistency criterion used in this method was defined by Talagrand (1999). Chapnik *et al.* (2004) investigated the properties of the algorithm and especially showed that it was equivalent to a maximum likelihood method, though less expensive to implement. Chapnik *et al.* (2006) also applied the same algorithm in an operational framework to tune observation-error variances.

This paper presents a set of diagnostics based on combinations of *observation-minus-background* (O–B), *observation-minus-analysis* (O–A) and *background-minus-analysis* (B–A) differences, which provide an additional consistency check of an analysis scheme.

† Corresponding author: Météo-France, CNRM, 42 av. G. Coriolis, 31057 Toulouse Cedex, France.
e-mail: gerald.desroziers@meteo.fr

In section 2 the general least-variance statistical estimation framework is introduced, as well as the consistency diagnostics. A geometrical interpretation of those diagnostics is given in section 3. An application of the computation of the diagnostics on operational analyses given by a four-dimensional variational (4D-Var) assimilation scheme is presented in section 4. Then, it is shown in section 5 how the diagnostics can be used to optimize observation and background errors, and an application of such a tuning algorithm in a simple assimilation toy problem is presented. It is shown in section 6 how such a method can also be used to determine cross-correlations between the errors corresponding to different observations. A spectral interpretation of the diagnosed covariances is proposed in section 7. Conclusions and perspectives are given in section 8.

2. Diagnostics in observation space

(*a*) *Consistency diagnostic on innovations*

In statistical linear estimation theory, the expression of the analysed state $\mathbf{x}^{\mathrm{a}}$ is given by

$$\mathbf{x}^{\mathrm{a}} = \mathbf{x}^{\mathrm{b}} + \delta\mathbf{x}^{\mathrm{a}} = \mathbf{x}^{\mathrm{b}} + \mathbf{K}\mathbf{d}^{\mathrm{o}}_{\mathrm{b}},$$

where $\mathbf{x}^{\mathrm{b}}$ is the background state, $\delta\mathbf{x}^{\mathrm{a}}$ the analysis increment,

$$\mathbf{K} = \mathbf{B}\mathbf{H}^{\mathrm{T}}(\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}} + \mathbf{R})^{-1}$$

the gain matrix in the analysis process and $\mathbf{d}^{\mathrm{o}}_{\mathrm{b}}$ the innovation vector (Talagrand 1997). The vector $\mathbf{d}^{\mathrm{o}}_{\mathrm{b}}$ is the difference between observations $\mathbf{y}^{\mathrm{o}}$ and their background counterparts $H(\mathbf{x}^{\mathrm{b}})$, where H is the possibly nonlinear observation operator and $\mathbf{H}$ the matrix corresponding to the linearized version of H. $\mathbf{B}$ is the background-error covariance matrix.

From the definition of the innovation vector, the following sequence of relations can be derived:

$$\mathbf{d}^{\mathrm{o}}_{\mathrm{b}} = \mathbf{y}^{\mathrm{o}} - H(\mathbf{x}^{\mathrm{b}}) = \mathbf{y}^{\mathrm{o}} - H(\mathbf{x}^{\mathrm{t}}) + H(\mathbf{x}^{\mathrm{t}}) - H(\mathbf{x}^{\mathrm{b}}) \simeq \boldsymbol{\epsilon}^{\mathrm{o}} - \mathbf{H}\boldsymbol{\epsilon}^{\mathrm{b}},$$

where $\mathbf{x}^{\mathrm{t}}$ is the unknown true state, $\boldsymbol{\epsilon}^{\mathrm{o}}$ the vector of observation errors and $\boldsymbol{\epsilon}^{\mathrm{b}}$ the vector of background errors. Then, the covariance of innovations is

$$E[\mathbf{d}^{\mathrm{o}}_{\mathrm{b}}(\mathbf{d}^{\mathrm{o}}_{\mathrm{b}})^{\mathrm{T}}] = E[\boldsymbol{\epsilon}^{\mathrm{o}}(\boldsymbol{\epsilon}^{\mathrm{o}})^{\mathrm{T}}] + \mathbf{H}E[\boldsymbol{\epsilon}^{\mathrm{b}}(\boldsymbol{\epsilon}^{\mathrm{b}})^{\mathrm{T}}]\mathbf{H}^{\mathrm{T}},$$

using the linearity of the statistical expectation operator E, and assuming that observation errors $\boldsymbol{\epsilon}^{\mathrm{o}}$ and background errors $\boldsymbol{\epsilon}^{\mathrm{b}}$ are uncorrelated.

As a consequence, it is easy to check that the relation

$$E[\mathbf{d}^{\mathrm{o}}_{\mathrm{b}}(\mathbf{d}^{\mathrm{o}}_{\mathrm{b}})^{\mathrm{T}}] = \mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}} \tag{1}$$

should be fulfilled, if the covariance of observation errors, $\mathbf{R}$, and the covariance of background errors in observation space, $\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}$, are correctly specified in the analysis. This is a classical result that provides a global check on the specification of those covariances (Andersson 2003).

It is shown below how additional relations can be obtained, which provide separate diagnostics on the background-, observation- and analysis-error statistics.

(*b*) *Consistency diagnostic on background errors*

From the previous expression for $\mathbf{x}^{\mathrm{a}}$, the $\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}$ (A–B) differences in observation space can be written

$$\mathbf{d}_{\mathrm{b}}^{\mathrm{a}} = H(\mathbf{x}^{\mathrm{a}}) - H(\mathbf{x}^{\mathrm{b}}) \simeq \mathbf{H}\delta\mathbf{x}^{\mathrm{a}} = \mathbf{HK}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}.$$

As a consequence, the cross-product between the $\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}$ (A–B) differences in observation space and the $\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}$ (O–B) differences is

$$\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}(\mathbf{d}_{\mathrm{b}}^{\mathrm{o}})^{\mathrm{T}} = \mathbf{HK}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}(\mathbf{d}_{\mathrm{b}}^{\mathrm{o}})^{\mathrm{T}}.$$

Matrix $\mathbf{HK}$ is given by $\mathbf{HBH}^{\mathrm{T}}(\mathbf{HBH}^{\mathrm{T}} + \mathbf{R})^{-1}$. Thus, the statistical expectation of this expression is given by

$$E[\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}(\mathbf{d}_{\mathrm{b}}^{\mathrm{o}})^{\mathrm{T}}] = \mathbf{HBH}^{\mathrm{T}}(\mathbf{HBH}^{\mathrm{T}} + \mathbf{R})^{-1}E[\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}(\mathbf{d}_{\mathrm{b}}^{\mathrm{o}})^{\mathrm{T}}],$$

using the linearity of the statistical expectation operator E. It is easy to check that this whole expression simplifies to

$$E[\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}(\mathbf{d}_{\mathrm{b}}^{\mathrm{o}})^{\mathrm{T}}] = \mathbf{HBH}^{\mathrm{T}}, \tag{2}$$

if matrix $\mathbf{HK} = \mathbf{HBH}^{\mathrm{T}}(\mathbf{HBH}^{\mathrm{T}} + \mathbf{R})^{-1}$ is in agreement with the true covariances for background and observation errors.

This is a first additional diagnostic to the diagnostic on innovations. It provides a separate consistency check on background-error covariances in observation space.

(*c*) *Consistency diagnostic on observation errors*

Similarly, the $\mathbf{d}_{\mathrm{a}}^{\mathrm{o}}$ (O–A) differences are given by

$$\begin{aligned}\mathbf{d}_{\mathrm{a}}^{\mathrm{o}} &= \mathbf{y}^{\mathrm{o}} - H(\mathbf{x}^{\mathrm{b}} + \delta\mathbf{x}^{\mathrm{a}})\\ &\simeq \mathbf{y}^{\mathrm{o}} - H(\mathbf{x}^{\mathrm{b}}) - \mathbf{HK}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}\\ &= (\mathbf{I} - \mathbf{HK})\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}\\ &= \mathbf{R}(\mathbf{HBH}^{\mathrm{T}} + \mathbf{R})^{-1}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}},\end{aligned}$$

then the statistical expectation of the cross-product between the $\mathbf{d}_{\mathrm{a}}^{\mathrm{o}}$ (O–A) differences and the $\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}$ (O–B) differences is

$$E[\mathbf{d}_{\mathrm{a}}^{\mathrm{o}}(\mathbf{d}_{\mathrm{b}}^{\mathrm{o}})^{\mathrm{T}}] = \mathbf{R}(\mathbf{HBH}^{\mathrm{T}} + \mathbf{R})^{-1}E[\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}(\mathbf{d}_{\mathrm{b}}^{\mathrm{o}})^{\mathrm{T}}],$$

which simplifies to

$$E[\mathbf{d}_{\mathrm{a}}^{\mathrm{o}}(\mathbf{d}_{\mathrm{b}}^{\mathrm{o}})^{\mathrm{T}}] = \mathbf{R}, \tag{3}$$

if matrix $\mathbf{HK} = \mathbf{HBH}^{\mathrm{T}}(\mathbf{HBH}^{\mathrm{T}} + \mathbf{R})^{-1}$ agrees with exact covariances for background and observation errors.

This is a second additional diagnostic providing a separate consistency check on observation-error covariances.

(*d*) *Diagnosis of analysis errors*

Finally, the cross-product between the $\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}$ (A–B) differences in observation space and the $\mathbf{d}_{\mathrm{a}}^{\mathrm{o}}$ (O–A) differences can also be derived:

$$\begin{aligned}\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}(\mathbf{d}_{\mathrm{a}}^{\mathrm{o}})^{\mathrm{T}} &= \mathbf{HK}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}(\mathbf{d}_{\mathrm{b}}^{\mathrm{o}})^{\mathrm{T}}(\mathbf{I} - \mathbf{HK})^{\mathrm{T}}\\ &= \mathbf{HBH}^{\mathrm{T}}(\mathbf{HBH}^{\mathrm{T}} + \mathbf{R})^{-1}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}(\mathbf{d}_{\mathrm{b}}^{\mathrm{o}})^{\mathrm{T}}(\mathbf{HBH}^{\mathrm{T}} + \mathbf{R})^{-1}\mathbf{R}.\end{aligned}$$

Again, the statistical expectation of this expression simplifies to

$$E[\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}(\mathbf{d}_{\mathrm{a}}^{\mathrm{o}})^{\mathrm{T}}] = \mathbf{HBH}^{\mathrm{T}}(\mathbf{HBH}^{\mathrm{T}} + \mathbf{R})^{-1}\mathbf{R},$$

if matrix $\mathbf{HK} = \mathbf{HBH}^{\mathrm{T}}(\mathbf{HBH}^{\mathrm{T}} + \mathbf{R})^{-1}$ is in agreement with the true covariances for background and observation errors.

It is easy to show that the right-hand side of the last relation is an expression for $\mathbf{HAH}^{\mathrm{T}}$ (where $\mathbf{A}$ is the analysis-error covariance matrix in model space), if $\mathbf{HBH}^{\mathrm{T}}$ and $\mathbf{R}$ are correctly specified in the analysis. Thus, in that case, the following relation should hold:

$$E[\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}(\mathbf{d}_{\mathrm{a}}^{\mathrm{o}})^{\mathrm{T}}] = \mathbf{HAH}^{\mathrm{T}}. \tag{4}$$

This is a third additional diagnostic providing information on analysis errors in observation space.

3. A GEOMETRICAL INTERPRETATION

From what has been shown in the previous section, relations (1) to (4) should be fulfilled in an optimal linear analysis, with linearized observation operators. They can be summarized as follows:

$$\begin{aligned} E[\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}(\mathbf{d}_{\mathrm{b}}^{\mathrm{o}})^{\mathrm{T}}] &= \mathbf{HBH}^{\mathrm{T}}, & E[\mathbf{d}_{\mathrm{a}}^{\mathrm{o}}(\mathbf{d}_{\mathrm{b}}^{\mathrm{o}})^{\mathrm{T}}] &= \mathbf{R}, \\ E[\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}(\mathbf{d}_{\mathrm{b}}^{\mathrm{o}})^{\mathrm{T}}] &= \mathbf{HBH}^{\mathrm{T}} + \mathbf{R}, & E[\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}(\mathbf{d}_{\mathrm{a}}^{\mathrm{o}})^{\mathrm{T}}] &= \mathbf{HAH}^{\mathrm{T}}. \end{aligned}$$

These relations are matricial, that is to say that they should be also true for cross-covariances between differences associated with different observations.

A geometrical interpretation of these relations can be proposed in the space of the eigenvectors $\mathbf{V}$ of matrix $\mathbf{HK}$, such as $\mathbf{HK} = \mathbf{V\Lambda V}^{\mathrm{T}}$, where $\mathbf{\Lambda}$ is the diagonal matrix of the eigenvalues of $\mathbf{HK}$. With this decomposition of matrix $\mathbf{HK}$, the vector $\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}$ of the differences between analysis and background in observation space can be rewritten: $\mathbf{d}_{\mathrm{b}}^{\mathrm{a}} = \mathbf{H}\delta\mathbf{x}^{\mathrm{a}} = \mathbf{HKd}_{\mathrm{b}}^{\mathrm{o}} = \mathbf{V\Lambda V}^{\mathrm{T}}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}$. Then, the projection of $\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}$ onto the eigenvectors of $\mathbf{HK}$ is given by $\mathbf{V}^{\mathrm{T}}\mathbf{d}_{\mathrm{b}}^{\mathrm{a}} = \mathbf{V}^{\mathrm{T}}\mathbf{V\Lambda V}^{\mathrm{T}}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}} = \mathbf{\Lambda V}^{\mathrm{T}}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}$. If $[\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}]_i$ and $[\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}]_i$ stand respectively for the projections of $\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}$ and $\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}$ onto a particular eigenvector $\mathbf{v}_i$ of $\mathbf{HK}$, it follows that $[\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}]_i = \lambda_i[\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}]_i$, where λ_i is the corresponding eigenvalue of $\mathbf{HK}$. (The notations $[\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}]_i$, $[\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}]_i$ are used here to specify that these two vectors are unidimensional vectors.)

In Figure 1, $H(\mathbf{x}^{\mathrm{t}})_i$, $\mathbf{y}^{\mathrm{o}}{}_i$ and $H(\mathbf{x}^{\mathrm{b}})_i$ respectively stand for the projections onto a particular eigenvector $\mathbf{v}_i$ of the true, observed and background equivalents of $\mathbf{x}$ at observation locations. The triangle $H(\mathbf{x}^{\mathrm{b}})_i$, $H(\mathbf{x}^{\mathrm{t}})_i$, $\mathbf{y}_i^{\mathrm{o}}$ is right in $H(\mathbf{x}^{\mathrm{t}})_i$ since the projections $[\boldsymbol{\epsilon}^{\mathrm{o}}]_i$ and $[\mathbf{H}\boldsymbol{\epsilon}^{\mathrm{b}}]_i$ of observation errors and background errors onto vector $\mathbf{v}_i$ are assumed to be uncorrelated and hence orthogonal. This orthogonality is defined for the particular scalar product $\langle[\boldsymbol{\epsilon}_1], [\boldsymbol{\epsilon}_2]\rangle = E(\epsilon_1\epsilon_2)$, where $[\boldsymbol{\epsilon}_1]$ and $[\boldsymbol{\epsilon}_2]$ are two vectors of random errors, with respective components ϵ_1 and ϵ_2 being two random variables. It means that the orthogonality of $[\boldsymbol{\epsilon}^{\mathrm{o}}]_i$ and $[\mathbf{H}\boldsymbol{\epsilon}^{\mathrm{b}}]_i$ is only true from a statistical point of view. With this definition of the scalar product, the angle between two random error vectors is also directly linked with the correlation of the errors; a zero angle and a right angle respectively correspond to perfect correlation and decorrelation and an angle between 0 and $\pi/2$ to an intermediate correlation.

It is a classical result that the analysis error $\mathbf{H}\boldsymbol{\epsilon}^{\mathrm{a}}$ is also orthogonal to the innovation vector $\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}$, again from a statistical point of view. Since Fig. 1 corresponds to a projection

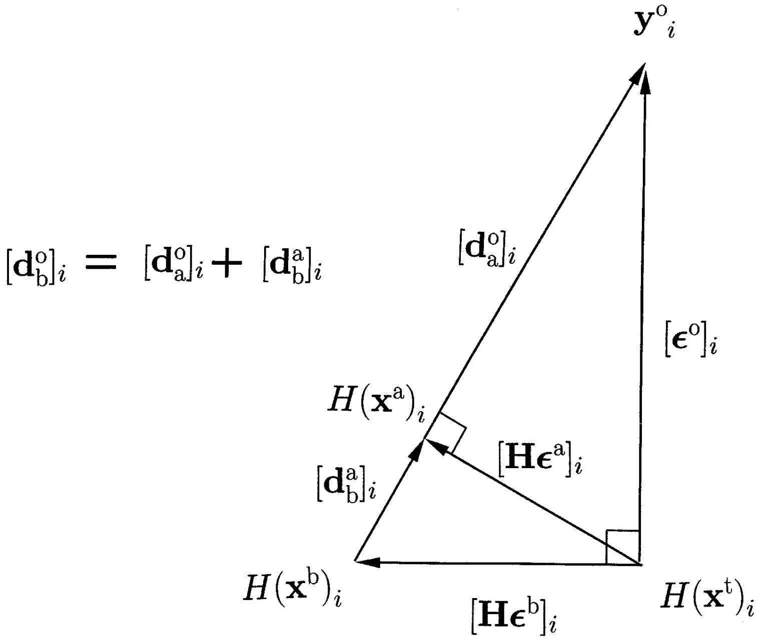

Figure 1. Geometrical representation of the analysis projected onto a particular eigenvector $\mathbf{v}_i$ of matrix **HK**.

onto a particular eigenvector $\mathbf{v}_i$, it follows that $[H(\mathbf{x}^{\mathrm{b}})_i H(\mathbf{x}^{\mathrm{a}})_i] = [\mathbf{d}^{\mathrm{a}}_{\mathrm{b}}]_i = \lambda_i [\mathbf{d}^{\mathrm{o}}_{\mathrm{b}}]_i$ and then $H(\mathbf{x}^{\mathrm{a}})_i$ is on the line defined by the point $H(\mathbf{x}^{\mathrm{b}})_i$ and the vector $[\mathbf{d}^{\mathrm{o}}_{\mathrm{b}}]_i$. The vector $[\mathbf{H}\epsilon^{\mathrm{a}}]_i$ is thus orthogonal to $[\mathbf{d}^{\mathrm{o}}_{\mathrm{b}}]_i$ in $H(\mathbf{x}^{\mathrm{a}})_i$.

Hence, the application of the Pythagoras theorem to this triangle implies that $\|[\mathbf{d}^{\mathrm{o}}_{\mathrm{b}}]_i\|^2 = \|[\mathbf{H}\epsilon^{\mathrm{b}}]_i\|^2 + \|[\epsilon^{\mathrm{o}}]_i\|^2$, where the norm $\|\ \|$ is associated with the previous scalar product. This relation corresponds to the first classical diagnostic on innovation covariances.

From the application of Euclid's theorems in a right triangle, the three additional relations can be written:

$$\langle [\mathbf{d}^{\mathrm{a}}_{\mathrm{b}}]_i, [\mathbf{d}^{\mathrm{o}}_{\mathrm{b}}]_i \rangle = \|[\mathbf{H}\epsilon^{\mathrm{b}}]_i\|^2,$$
$$\langle [\mathbf{d}^{\mathrm{o}}_{\mathrm{a}}]_i, [\mathbf{d}^{\mathrm{o}}_{\mathrm{b}}]_i \rangle = \|[\epsilon^{\mathrm{o}}]_i\|^2,$$
$$\langle [\mathbf{d}^{\mathrm{a}}_{\mathrm{b}}]_i, [\mathbf{d}^{\mathrm{o}}_{\mathrm{b}}]_i \rangle = \|[\mathbf{H}\epsilon^{\mathrm{a}}]_i\|^2,$$

corresponding to the diagnostics of background, observation and analysis-error variances, respectively.

In the case where background and observation-error covariances are homogeneous, and the data density is uniform, the eigenvectors of matrix **HK** are the spectral harmonics (Fourier on the plane, spherical harmonics on the sphere). Then, Fig. 1 shows a projection onto a particular spectral component. This case will be further developed in section 7.

4. Application of the diagnostics to ARPEGE 4D-Var analyses

The diagnostics shown in section 2 potentially provide information on the full covariances of observation, background and analysis errors in observation space.

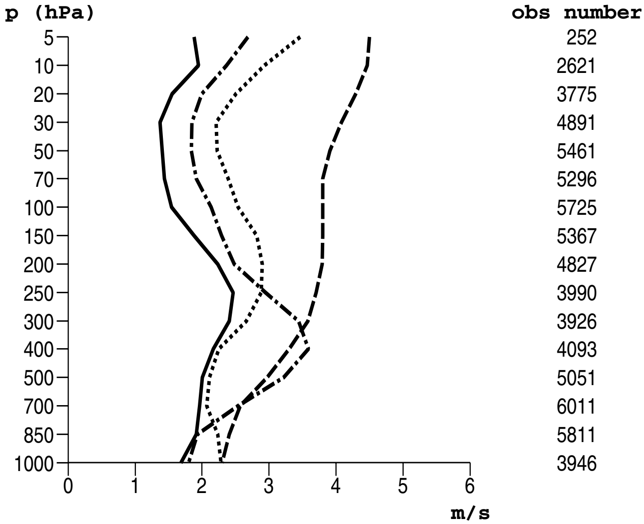

Figure 2. Vertical profiles of diagnosed square roots of background (solid) and observation (dotted) error variances for radiosonde wind observations in the northern hemisphere, compared with profiles for corresponding background (dash-dotted) and observation errors (dashed). All values are in m s^{-1}. The numbers of observations used to compute statistics are shown on the right.

One first application of these diagnostics is to diagnose observation and background-error variances. Thus for any subset of observations i with p_i observations, it is possible simply to compute the quantities

$$(\widetilde{\sigma_i^{\rm b}})^2 = (\mathbf{d}_{\rm b}^{\rm a})_i^{\rm T}(\mathbf{d}_{\rm b}^{\rm o})_i/p_i = \sum_{j=1}^{p_i}(y_j^{\rm a} - y_j^{\rm b})(y_j^{\rm o} - y_j^{\rm b})/p_i$$

$$(\widetilde{\sigma_i^{\rm o}})^2 = (\mathbf{d}_{\rm a}^{\rm o})_i^{\rm T}(\mathbf{d}_{\rm b}^{\rm o})_i/p_i = \sum_{j=1}^{p_i}(y_j^{\rm o} - y_j^{\rm a})(y_j^{\rm o} - y_j^{\rm b})/p_i,$$

where $y_j^{\rm o}$ is the value of observation j and $y_j^{\rm b}$, $y_j^{\rm a}$ respectively their background and analysis counterparts. The quantities $(\widetilde{\sigma_i^{\rm b}})^2$ and $(\widetilde{\sigma_i^{\rm o}})^2$ are the diagnosed values of background and observation errors that can be different from the specified values in the analysis. They correspond to the use of relations (2) and (3) respectively, but for mean diagonal elements of those matrices only. These computations are nearly cost-free and can be performed, a posteriori, using one or several analyses.

Such computations have been performed on analyses produced by the French operational ARPEGE† 4D-Var assimilation. This 4D-Var assimilation is based on an incremental formulation (Courtier *et al.* 1994) and shares many aspects with the 4D-Var analysis of the European Centre for Medium-range Weather Forecasts (Rabier *et al.* 2000). Figure 2 shows an example of diagnosed background and observation variances for wind observations given by radiosondes in the northern hemisphere. These statistics have been computed after ten 4D-Var analyses. They show that both background and observation errors seem to be overestimated in the analysis. This is consistent for observation errors with what has been found by Chapnik *et al.* (2006) using a different diagnostic. On the other hand, similar diagnosed profiles have been retrieved for the

† Action de Recherche Petite Echelle Grande Echelle.

TABLE 1. TRUE AND TUNED VALUES OF σ_o AND σ_b AFTER FIXED-POINT ITERATIONS

	True value	Initial value	Iteration 1	2	3	4	5
σ_o	2	1	1.73	1.89	1.95	1.97	1.98
σ_b	1	2	1.41	1.19	1.10	1.07	1.03

southern hemisphere (not shown), thus giving some confidence in those diagnostics. The same kind of diagnostics have been produced for all observations taken into account in the ARPEGE 4D-Var. Results (not presented here) confirm the overestimation of background and observation error for most of the observations.

5. TUNING OF ERROR VARIANCES

Since background and observation errors are expected to be incorrectly specified in an operational analysis, a method can be envisaged to tune them. The rationale of such a tuning procedure is to find the values of the σ_i^b and σ_i^o, for the different subsets i of observations such that those values fulfil the relations $(\sigma_i^b)^2 = (\mathbf{d}_b^a)_i^T(\mathbf{d}_b^o)_i/p_i$ and $(\sigma_i^o)^2 = (\mathbf{d}_a^o)_i^T(\mathbf{d}_b^o)_i/p_i$. This is a nonlinear problem since the $(\mathbf{d}_b^a)_i$ and $(\mathbf{d}_a^o)_i$ depend themselves on the σ_i^b and σ_i^o values. However the form of those nonlinear equations suggests the use of an iterative fixed-point method to solve this tuning problem.

This iterative procedure is similar to the procedure proposed by Desroziers and Ivanov (2001) to solve the same kind of problem but with a different optimality criterion.

A preliminary test of the previous tuning algorithm has been made in a toy problem given by a spectral analysis on a circular domain (say on an earth meridian) and also used by Desroziers and Ivanov (2001). The length of the domain is set to 40 000 km and the truncation to 200 corresponding to $n = 401$ spectral coefficients. The background-error covariance matrix **B** is built in spectral space from a Gaussian structure function in physical space. Assuming homogeneity on the domain makes the **B** matrix diagonal, so that the diagonal of **B** is given by the Fourier transform of the Gaussian correlation in physical space. Here the length-scale of the Gaussian correlation is set to 300 km. The analysis problem is solved with $p = 401$ observations and a diagonal observation-error covariance matrix **R**, assuming that error observations are uncorrelated. Observations have the same nature as the state variable **x**. Thus the observation operator **H** only involves interpolation of **x** at observation locations. Both background and observations are simulated in agreement with the corresponding **B** and **R** covariance matrices with homogeneous values $\sigma^b = 1$ and $\sigma^o = 2$.

Table 1 shows that, starting from erroneous values $\sigma^b = 2$ and $\sigma^o = 1$, the fixed-point iterative algorithm allows us to recover a good approximation of the true values with only a few iterations.

6. DIAGNOSIS OF OBSERVATION ERROR CROSS-COVARIANCES

The diagnostic $E[\mathbf{d}_a^o(\mathbf{d}_b^o)^T] = \mathbf{R}$ on observation errors, introduced in section 2, can potentially provide some information on cross-correlations between two different sets of observations, for instance observations issued from different channels of the same satellite instrument. The capability of such a diagnostic to recover observation error cross-correlations is investigated here with the same previous analysis toy problem but

TABLE 2. TRUE, INITIAL AND DIAGNOSED VALUES OF OBSERVATION ERROR CROSS-COVARIANCES FOR THREE SIMULATED OBSERVATION SETS

	1			2			3		
Set	True	Init.	Diag.	True	Init.	Diag.	True	Init.	Diag.
1	1.00	1.00	1.00	1.00	0.00	1.01	0.10	0.00	0.10
2				4.00	1.00	3.73	−0.20	0.00	−0.18
3							0.25	1.00	0.25

with the addition of a vertical dimension. The analysis domain is now a periodic vertical plane with three levels with 5 km separation. All parameters are the same as previously, and the additional vertical length-scale of background errors is set to 3 km. At each horizontal observation location, a set of three simulated observations y_1^{o}, y_2^{o} and y_3^{o} are defined as simple combinations of the state variable at the three levels:

$$y_1^{\mathrm{o}} = 0.75x_1 + 0.25x_2, \quad y_2^{\mathrm{o}} = 0.10x_1 + 0.80x_2 + 0.10x_3, \quad y_3^{\mathrm{o}} = 0.30x_2 + 0.70x_3,$$

where x_1, x_2 and x_3 are the state variable values at the three levels. This is done to mimic, in a rough way, satellite observations integrated within the vertical. These observations are simulated with correlated observation errors as given in Table 2.

The diagnosed values of observation error cross-covariances (Table 2) show that such a simple diagnostic is able to recover most of the information on observation-error covariances starting from a mis-specified representation of those covariances (with no cross-correlations and homogeneous error variance).

7. A SPECTRAL INTERPRETATION OF THE DIAGNOSED COVARIANCES

(*a*) *The adjustment equations of the spectral variances*

The diagnosed covariance matrices in Eqs. (2) and (3) may be seen as some adjusted covariance estimates, noted $\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^{\mathrm{T}}$ and $\widetilde{\mathbf{R}}$ respectively:

$$\begin{aligned} E[\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}(\mathbf{d}_{\mathrm{b}}^{\mathrm{o}})^{\mathrm{T}}] &= \mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^{\mathrm{T}} = \mathbf{HBH}^{\mathrm{T}}(\mathbf{HBH}^{\mathrm{T}} + \mathbf{R})^{-1}(\mathbf{HB}^*\mathbf{H}^{\mathrm{T}} + \mathbf{R}^*) \\ E[\mathbf{d}_{\mathrm{a}}^{\mathrm{o}}(d_{\mathrm{b}}^{\mathrm{o}})^{\mathrm{T}}] &= \widetilde{\mathbf{R}} \qquad = \mathbf{R}(\mathbf{HBH}^{\mathrm{T}} + \mathbf{R})^{-1}(\mathbf{HB}^*\mathbf{H}^{\mathrm{T}} + \mathbf{R}^*), \end{aligned}$$

where $\mathbf{B}^*$, $\mathbf{R}^*$ are the true covariance matrices.

Following Hollingsworth (1987) and Daley (1991, pp. 125–128), one may consider for example the 1D or 2D case where the background and observation-error covariances are homogeneous, and the data density is uniform.

In this case, the different covariance matrices have common eigenvectors, which are the spectral modes: $\mathbf{HBH}^{\mathrm{T}} = \mathbf{S}\Lambda^{\mathrm{b}}\mathbf{S}^{\mathrm{T}}$, $\mathbf{R} = \mathbf{S}\Lambda^{\mathrm{o}}\mathbf{S}^{\mathrm{T}}$, where $\mathbf{S}$ is an orthogonal matrix whose columns are the common eigenvectors of $\mathbf{HBH}^{\mathrm{T}}$ and $\mathbf{R}$, and Λ^{b}, Λ^{o} are diagonal matrices which contain the corresponding eigenvalues. The eigenvectors are the spectral harmonics (Fourier on the plane, spherical harmonics on the sphere), and $\mathbf{S}$ is the inverse spectral transform. Moreover, the eigenvalues correspond to the variances of the spectral components.

Similar equations hold for the diagnosed and true covariance matrices respectively. The equation of the diagnosed background-error covariance matrix can thus be written as follows:

$$\begin{aligned} \mathbf{S}\widetilde{\mathbf{\Lambda}}^{\mathrm{b}}\mathbf{S}^{\mathrm{T}} &= \mathbf{S}\mathbf{\Lambda}^{\mathrm{b}}\mathbf{S}^{\mathrm{T}}(\mathbf{S}\mathbf{\Lambda}^{\mathrm{b}}\mathbf{S}^{\mathrm{T}} + \mathbf{S}\mathbf{\Lambda}^{\mathrm{o}}\mathbf{S}^{\mathrm{T}})^{-1}(\mathbf{S}\mathbf{\Lambda}^{\mathrm{b}*}\mathbf{S}^{\mathrm{T}} + \mathbf{S}\mathbf{\Lambda}^{\mathrm{o}*}\mathbf{S}^{\mathrm{T}}) \\ &= \mathbf{S}\mathbf{\Lambda}^{\mathrm{b}}\mathbf{S}^{\mathrm{T}}\mathbf{S}^{\mathrm{T}^{-1}}(\mathbf{\Lambda}^{\mathrm{b}} + \mathbf{\Lambda}^{\mathrm{o}})^{-1}\mathbf{S}^{-1}\mathbf{S}(\mathbf{\Lambda}^{\mathrm{b}*} + \mathbf{\Lambda}^{\mathrm{o}*})\mathbf{S}^{\mathrm{T}} \\ &= \mathbf{S}\mathbf{\Lambda}^{\mathrm{b}}(\mathbf{\Lambda}^{\mathrm{b}} + \mathbf{\Lambda}^{\mathrm{o}})^{-1}(\mathbf{\Lambda}^{\mathrm{b}*} + \mathbf{\Lambda}^{\mathrm{o}*})\mathbf{S}^{\mathrm{T}}. \end{aligned}$$

The same kind of relations can be written for the diagnosed observation-error covariance matrix. This provides the final eigenvalue relations:

$$\begin{aligned}\widetilde{\mathbf{\Lambda}}^{\mathrm{b}} &= \mathbf{\Lambda}^{\mathrm{b}}(\mathbf{\Lambda}^{\mathrm{b}} + \mathbf{\Lambda}^{\mathrm{o}})^{-1}(\mathbf{\Lambda}^{\mathrm{b}*} + \mathbf{\Lambda}^{\mathrm{o}*}) \\ \widetilde{\mathbf{\Lambda}}^{\mathrm{o}} &= \mathbf{\Lambda}^{\mathrm{o}}(\mathbf{\Lambda}^{\mathrm{b}} + \mathbf{\Lambda}^{\mathrm{o}})^{-1}(\mathbf{\Lambda}^{\mathrm{b}*} + \mathbf{\Lambda}^{\mathrm{o}*}),\end{aligned}$$

where $\{\mathbf{\Lambda}^{\mathrm{b}*}, \mathbf{\Lambda}^{\mathrm{o}*}\}$, $\{\mathbf{\Lambda}^{\mathrm{b}}, \mathbf{\Lambda}^{\mathrm{o}}\}$ and $\{\widetilde{\mathbf{\Lambda}}^{\mathrm{b}}, \widetilde{\mathbf{\Lambda}}^{\mathrm{o}}\}$ respectively stand for the eigenvalues of the true, specified and diagnosed covariance matrices for background and observation errors.

(*b*) *Two visions of the adjustment equations*

A first insight into the previous relations is to note that the true innovation variance spectrum $\mathbf{\Lambda}^{\mathrm{b}*} + \mathbf{\Lambda}^{\mathrm{o}*}$ is multiplied by two filtering ratios

$$\mathbf{F}^{\mathrm{b}} = \frac{\mathbf{\Lambda}^{\mathrm{b}}}{\mathbf{\Lambda}^{\mathrm{b}} + \mathbf{\Lambda}^{\mathrm{o}}}, \quad \mathbf{F}^{\mathrm{o}} = \frac{\mathbf{\Lambda}^{\mathrm{o}}}{\mathbf{\Lambda}^{\mathrm{b}} + \mathbf{\Lambda}^{\mathrm{o}}}$$

to provide the respective (adjusted) variance spectra of $\boldsymbol{\epsilon}^{\mathrm{b}}$ and $\boldsymbol{\epsilon}^{\mathrm{o}}$:

$$\widetilde{\mathbf{\Lambda}}^{\mathrm{b}} = \frac{\mathbf{\Lambda}^{\mathrm{b}}}{\mathbf{\Lambda}^{\mathrm{b}} + \mathbf{\Lambda}^{\mathrm{o}}}(\mathbf{\Lambda}^{\mathrm{b}*} + \mathbf{\Lambda}^{\mathrm{o}*}), \quad \widetilde{\mathbf{\Lambda}}^{\mathrm{o}} = \frac{\mathbf{\Lambda}^{\mathrm{o}}}{\mathbf{\Lambda}^{\mathrm{b}} + \mathbf{\Lambda}^{\mathrm{o}}}(\mathbf{\Lambda}^{\mathrm{b}*} + \mathbf{\Lambda}^{\mathrm{o}*}).$$

These two filters are represented in Fig. 3(a) for the example evoked in section 5. Due to the shape of the two kinds of error correlation, $\mathbf{F}^{\mathrm{b}}$ and $\mathbf{F}^{\mathrm{o}}$ are respectively low-pass and high-pass filters. Figures 3(c) and (d) illustrate that applying $\mathbf{F}^{\mathrm{b}}$, $\mathbf{F}^{\mathrm{o}}$ to $(\mathbf{\Lambda}^{\mathrm{b}*} + \mathbf{\Lambda}^{\mathrm{o}*})$ allows us to extract its large-scale and small-scale components respectively. They correspond to the (estimated) contributions of the background and observation errors, respectively. These provide some adjusted variance spectra, which are closer to the true spectra than the specified ones. This is also consistent with the fact that the equations indicate, in particular, that if the analysis is optimal, then these two filtering steps will provide the two exact error variance spectra.

Another complementary insight is to notice that the adjustments amount to scaling each specified information error spectral variance by the ratio between the exact and specified innovation variances:

$$\widetilde{\mathbf{\Lambda}}^{\mathrm{b}} = \mathbf{\Lambda}^{\mathrm{b}}\frac{\mathbf{\Lambda}^{\mathrm{b}*} + \mathbf{\Lambda}^{\mathrm{o}*}}{\mathbf{\Lambda}^{\mathrm{b}} + \mathbf{\Lambda}^{\mathrm{o}}}, \quad \widetilde{\mathbf{\Lambda}}^{\mathrm{o}} = \mathbf{\Lambda}^{\mathrm{o}}\frac{\mathbf{\Lambda}^{\mathrm{b}*} + \mathbf{\Lambda}^{\mathrm{o}*}}{\mathbf{\Lambda}^{\mathrm{b}} + \mathbf{\Lambda}^{\mathrm{o}}}.$$

The perfect adjustment ratios would instead be $(\mathbf{\Lambda}^{\mathrm{b}*}/\mathbf{\Lambda}^{\mathrm{b}})$ and $(\mathbf{\Lambda}^{\mathrm{o}*}/\mathbf{\Lambda}^{\mathrm{o}})$ respectively. However, as illustrated in Fig. 3(b), the innovation misfit ratio $N = (\mathbf{\Lambda}^{\mathrm{b}*} + \mathbf{\Lambda}^{\mathrm{o}*})/(\mathbf{\Lambda}^{\mathrm{b}} + \mathbf{\Lambda}^{\mathrm{o}})$ is close to $(\mathbf{\Lambda}^{\mathrm{b}*}/\mathbf{\Lambda}^{\mathrm{b}})$ at the large scales (i.e. where the background errors have their largest amplitudes), and it is close to $(\mathbf{\Lambda}^{\mathrm{o}*}/\mathbf{\Lambda}^{\mathrm{o}})$ over a wide range of small scales (i.e. where the observation errors predominate). In other words, the close links between N and $(\mathbf{\Lambda}^{\mathrm{b}*}/\mathbf{\Lambda}^{\mathrm{b}})$ or $(\mathbf{\Lambda}^{\mathrm{o}*}/\mathbf{\Lambda}^{\mathrm{o}})$, as a function of scale, indicate that the adjustments are done in a relevant scale-dependent way.

The two visions are consistent, in the sense that they both indicate that the adjustments are particularly relevant when the background errors and the observation errors tend to predominate in different scales. This is summarized by the fact that

$$\frac{\mathbf{\Lambda}^{\mathrm{b}*} + \mathbf{\Lambda}^{\mathrm{o}*}}{\mathbf{\Lambda}^{\mathrm{b}} + \mathbf{\Lambda}^{\mathrm{o}}} \simeq \frac{\mathbf{\Lambda}^{\mathrm{b}*}}{\mathbf{\Lambda}^{\mathrm{b}}}$$

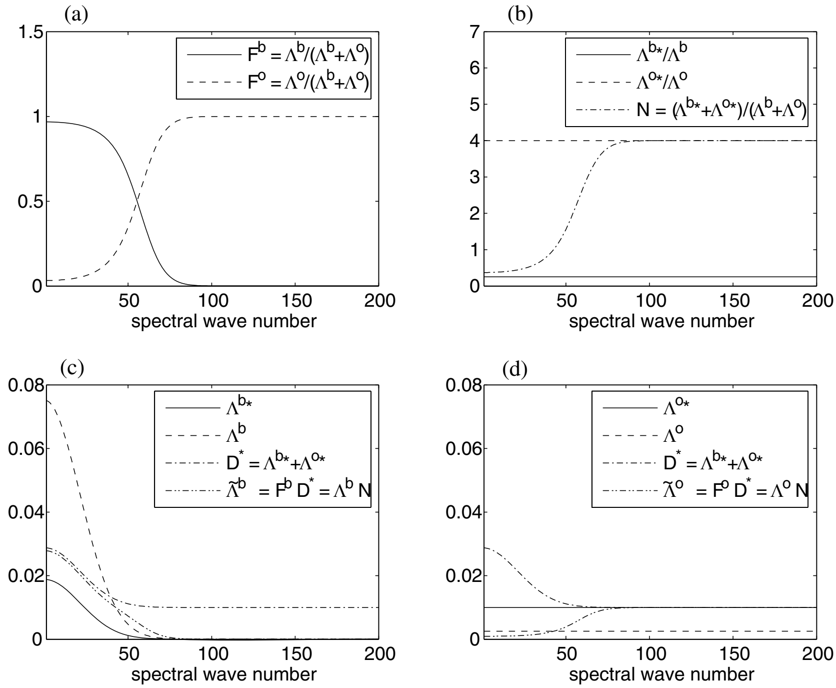

Figure 3. Spectral interpretation of diagnosed covariances: (a) filtering functions, (b) misfit ratios, (c) background error, and (d) observation error. See text for definitions.

in the large scales if both $\mathbf{\Lambda}^{\mathrm{b}*} \gg \mathbf{\Lambda}^{\mathrm{o}*}$ and $\mathbf{\Lambda}^{\mathrm{b}} \gg \mathbf{\Lambda}^{\mathrm{o}}$ and

$$\frac{\mathbf{\Lambda}^{\mathrm{b}*} + \mathbf{\Lambda}^{\mathrm{o}*}}{\mathbf{\Lambda}^{\mathrm{b}} + \mathbf{\Lambda}^{\mathrm{o}}} \simeq \frac{\mathbf{\Lambda}^{\mathrm{o}*}}{\mathbf{\Lambda}^{\mathrm{o}}}$$

in the small scales if both $\mathbf{\Lambda}^{\mathrm{b}*} \ll \mathbf{\Lambda}^{\mathrm{o}*}$ and $\mathbf{\Lambda}^{\mathrm{b}} \ll \mathbf{\Lambda}^{\mathrm{o}}$.

The adjusted standard deviations that were presented in section 5 are simply the square root of the sum of the different (adjusted) spectral variances. The relevance of the standard deviation adjustments is therefore consistent with the adjustments of the spectral variances.

From the previous discussion, it also appears that the adjustment of background and observation-error variances is only relevant if those errors have different structures. Hence, the application of such an adjustment will not work in the case where the two spectra (either $\mathbf{\Lambda}^{\mathrm{b}*}$ and $\mathbf{\Lambda}^{\mathrm{o}*}$ or $\mathbf{\Lambda}^{\mathrm{b}}$ and $\mathbf{\Lambda}^{\mathrm{o}}$) are proportional.

However, if the background and observation-error spectra are sufficiently different (both in the exact and specified statistics), the adjustment will be able to modify the variances in a correct way even if the correlations are not perfectly specified.

8. Conclusion

On the basis of linear estimation theory, simple consistency diagnostics should be fulfilled in an optimal analysis. These diagnostics can potentially provide information on imperfectly known observation and background-error statistics. Another advantage of these diagnostics is that they are nearly cost-free and can be applied to any analysis scheme.

The application of the computation of the diagnostics to analyses issued from the operational French 4D-Var system shows likely diagnosed values for observation and background errors. Even if the values of background errors cannot be directly used in a model-space assimilation scheme, the study of these errors can be quite useful to understand the relative impact in the analysis of observations that are not directly related to the state variables. This is particularly the case for satellite data, for which the diagnosed errors can also be compared to randomized estimates of $\mathbf{HBH}^{\mathrm{T}}$, where $\mathbf{B}$ is the specified covariance background-error matrix in the analysis, as proposed by Andersson *et al.* (2000). Since the observation operator $\mathbf{H}$ includes the model integration in a 4D-Var scheme, the proposed diagnostic can be similarly used to diagnose the implicit evolution of background errors in 4D-Var.

Furthermore, it has been shown that it is possible to adapt the values specified in an analysis scheme by an iterative method. This can be useful to adapt observation errors but also background errors in observation space that are classically used in first-guess quality control of observations.

The use of such consistency diagnostics also seems to be a promising way to tackle the problem of the estimation of correlation between observation errors.

Another domain of interest is the use of the diagnostic of estimation error in observation space, which will have to be investigated in the future.

Nevertheless, such diagnostics also have to be understood from theoretical and practical points of view. In particular it has been shown that a spectral vision can be helpful in this perspective, by highlighting the role of scale separation between background and observation errors.

REFERENCES

Andersson, E. 2003 'Modelling of innovation statistics'. Pp. 153–164 of Proceedings of Workshop on recent developments in data assimilation for atmosphere and ocean, ECMWF, Reading, UK

Andersson, E., Fisher, M., Munro, R. and McNally, A. 2000 Diagnosis of background errors for radiances and other observable quantities in a variational data assimilation scheme, and the explanation of a case of poor convergence. *Q. J. R. Meteorol. Soc.*, **126,** 1455–1472

Chapnik, B., Desroziers, G., Rabier, F. and Talagrand, O. 2004 Properties and first application of an error statistics tuning method in variational assimilation. *Q. J. R. Meteorol. Soc.*, **130,** 2253–2275

2006 Diagnosis and tuning of observational error statistics in a quasi-operational data assimilation setting. *Q. J. R. Meteorol. Soc.*, **132,** 543–565

Courtier, P. and Talagrand, O. 1987 Variational assimilation of meteorological observations with the adjoint vorticity equation. II: Numerical results. *Q. J. R. Meteorol. Soc.*, **113,** 1329–1347

Courtier, P., Thépaut, J.-N. and Hollingsworth, A. 1994 A strategy for operational implementation of 4D-Var, using an incremental approach. *Q. J. R. Meteorol. Soc.*, **120,** 1367–1387

Daley, R. 1991 *Atmospheric data analysis*. Cambridge atmospheric and space series. Cambridge University Press, UK

Dee, D. P. and da Silva, A. 1999 Maximum-likelihood estimation of forecast and observation error covariance parameters. Part I: Methodology. *Mon. Weather Rev.*, **127,** 1822–1834

Desroziers, G. and Ivanov, S. 2001 Diagnosis and adaptive tuning of observation-error parameters in a variational assimilation. *Q. J. R. Meteorol. Soc.*, **127,** 1433–1452

Hollingsworth, A. 1987 'Objective analysis for numerical weather prediction'. Pp. 11–59 in Proceedings of WMO/IUGG Symposium on short- and medium-range numerical weather prediction, Tokyo, 4–8 August 1986, Ed. T. Matsuno. *J. Meteorol. Soc. Japan*, special volume

Hollingsworth, A. and Lönnberg, P. 1986 The statistical structure of short-range forecast errors as determined from radiosonde data. Part I: The wind field. *Tellus*, **38A,** 111–136

Lewis, J. M. and Derber, J. C. 1985 The use of adjoint equations to solve a variational adjustment problem with advective constraints. *Tellus*, **37A,** 309–322

Rabier, F., Järvinen, H., Klinker, E., Mahfouf, J.-F. and Simmons, A. 2000 The ECMWF operational implementation of four-dimensional variational assimilation. I: Experimental results with simplified physics. *Q. J. R. Meteorol. Soc.*, **126,** 1143–1170

Talagrand, O. 1997 Assimilation of observations; an introduction. *J. Meteorol. Soc. Japan*, **75,** 191–209

1999 'A posteriori verification of analysis and assimilation algorithms'. Pp. 17–28 in Proceedings of Workshop on diagnosis of data assimilation systems, 2–4 November 1998, ECMWF, Reading, UK