Sensitivity analysis in variational data assimilation and applications

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ABSTRACT

Mathematical aspects of sensitivity analysis in unconstrained optimization are reviewed and the sensitivity equations of a variational data assimilation system (VDAS) to observations, background estimate, and to the specification of the associated error-variances are derived from the first order optimality condition. The error-variance sensitivity is introduced as a feasible approach to provide guidance for tuning procedures and a priori estimates of the analysis and forecast impact due to variations in the specification of the input error statistics. Applications of the sensitivity analysis methods are discussed including adjoint-based estimation of the observation impact and diagnosis and tuning of the observation-error and background-error variances. Numerical results from idealized data assimilation experiments are used to illustrate the theoretical concepts.

1 Introduction

The development of efficient methodologies to optimize the use of observational data in improving the analyses and forecasts of a specific data assimilation system (DAS) is a practical necessity and focus of research at numerical weather prediction (NWP) centers worldwide. Studies on quantification of the observation impact (OBSI) through observing system experiments (OSEs) and adjoint-DAS techniques may be found in the work of Atlas (1997), Bouttier and Kelly (2001), Langland and Baker (2004), Kelly et al. (2007), Gelaro and Zhu (2009), Cardinali (2009), and the references therein. An optimal use of the information provided by the observing system may be achieved only through an optimal data weighting in the analysis scheme and it is unanimously accepted that a major source of uncertainty in the analyses and forecasts is due to the practical difficulty of providing accurate information on the input-error statistics (Lorenc 2003). A significant amount of research in NWP is focused on modeling the observation and background error covariance matrices **R** and **B**, respectively (Janjić and Cohn 2006, Frehlich 2006, Hamill and Snyder 2002). Diagnosis and tuning of error variances used in variational data assimilation is discussed in the work of Desroziers and Ivanov (2001) and Chapnik et al. (2006). Novel sensitivity techniques are needed to provide guidance to the error-variance tuning procedures and *a priori* estimates of the analysis and forecast impact due to the variations in the specification of the input error statistics.

A proper understanding of how uncertainties in the specification of the input error covariances will impact the analysis and forecasts may be achieved by performing a sensitivity analysis with respect to the extended DAS input $[\mathbf{y},\mathbf{R},\mathbf{x}_b,\mathbf{B}]$ (Daescu 2008). The present work provides a brief review of the mathematical aspects and recent developments in the formulation of sensitivity analysis methods in a variational data assimilation system (VDAS). Results from idealized data assimilation experiments are used to illustrate some of the theoretical concepts and further research directions for practical applications are discussed.

2 Sensitivity analysis in a VDAS

Variational data assimilation methods (3DVAR, 4DVAR) provide an optimal initial state (analysis) $\mathbf{x}_a$ to a forecast model by minimizing the cost functional

$$\begin{aligned} J(\mathbf{x}) &= \frac{1}{2}(\mathbf{x}-\mathbf{x}_b)^{\mathrm{T}}\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_b)+\frac{1}{2}\left[\mathbf{h}(\mathbf{x})-\mathbf{y}\right]^{\mathrm{T}}\mathbf{R}^{-1}\left[\mathbf{h}(\mathbf{x})-\mathbf{y}\right] \\ \mathbf{x}_a &= \mathrm{Arg}\ \min J \end{aligned} \tag{1}$$

where $\mathbf{x}_b$ is a prior (background) state estimate, $\mathbf{B}$ and $\mathbf{R}$ are the background and observation error covariance matrices respectively, and $\mathbf{h}$ is the observation operator that maps the state into observations. In a 4DVAR DAS the operator $\mathbf{h}$ incorporates the nonlinear model to properly account for time-distributed data (Talagrand and Courtier 1987, Kalnay 2002).

A theoretical framework to sensitivity analysis in VDA is presented by Le Dimet et al. (1997) in the context of optimal control. As explained by Daescu (2008), the implicit function theorem applied to the first-order optimality condition

$$\nabla_{\mathbf{x}}J(\mathbf{x}_a)=0 \Leftrightarrow \mathbf{B}^{-1}(\mathbf{x}_a-\mathbf{x}_b)+\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}[\mathbf{h}(\mathbf{x}_a)-\mathbf{y}]=\mathbf{0} \tag{2}$$

where $\mathbf{H}=\partial\mathbf{h}/\partial\mathbf{x}$ is the linearized observation operator evaluated at $\mathbf{x}_a$, allows a succinct derivation of the analysis and forecast sensitivity equations with respect to any of the DAS input components $\mathbf{u}=\mathbf{y},\mathbf{R},\mathbf{x}_b,\mathbf{B}$

$$\nabla_{\mathbf{x}}J(\mathbf{x}_a,\mathbf{u})=0 \Rightarrow \nabla_{\mathbf{u}}\mathbf{x}_a=-\left[\nabla^2_{\mathbf{ux}}J(\mathbf{x}_a)\right]\mathbf{A}, \quad \nabla_{\mathbf{u}}e(\mathbf{x}_a)=-\left[\nabla^2_{\mathbf{ux}}J(\mathbf{x}_a)\right]\mathbf{A}\nabla_{\mathbf{x}}e(\mathbf{x}_a) \tag{3}$$

where

$$\mathbf{A}=\left[\nabla^2_{\mathbf{xx}}J(\mathbf{x}_a)\right]^{-1} \tag{4}$$

denotes the inverse of the Hessian matrix $\nabla^2_{\mathbf{xx}}J(\mathbf{x}_a)$ of the cost functional (1) which is assumed to be a nonsingular matrix, $\nabla^2_{\mathbf{ux}}J(\mathbf{x}_a)=\nabla_{\mathbf{u}}[\nabla_{\mathbf{x}}J(\mathbf{x}_a)]$, and $e(\mathbf{x})$ is a model functional aspect of interest e.g., a measure of the error in the forecast initiated from $\mathbf{x}$. From (3) it is noticed that the evaluation of the vector

$$\mu=\mathbf{A}\nabla_{\mathbf{x}}e(\mathbf{x}_a) \tag{5}$$

is necessary to estimate the sensitivity with respect to any of the DAS input components. From (2), (3), and (5), the sensitivities to $\mathbf{x}_b$ and $\mathbf{y}$ are expressed as

$$\nabla_{\mathbf{x}_b}e(\mathbf{x}_a)=\mathbf{B}^{-1}\mu, \quad \nabla_{\mathbf{y}}e(\mathbf{x}_a)=\mathbf{R}^{-1}\mathbf{H}\mu \tag{6}$$

The forecast sensitivities to the specification of the background error variance vector σ_b^2 and to the observation error variance vector σ_o^2 are obtained at a modest computational effort, once the sensitivities to background and observations are available (Daescu 2008):

$$\nabla_{\sigma_b^2}e(\mathbf{x}_a)=\left[\mathbf{B}^{-1}(\mathbf{x}_a-\mathbf{x}_b)\right]\circ\nabla_{\mathbf{x}_b}e(\mathbf{x}_a) \tag{7}$$

$$\nabla_{\sigma_o^2}e(\mathbf{x}_a)=\left[\mathbf{R}^{-1}(\mathbf{h}(\mathbf{x}_a)-\mathbf{y})\right]\circ\nabla_{\mathbf{y}}e(\mathbf{x}_a) \tag{8}$$

where $\circ$ denotes the Hadamard (componentwise) product. From the optimality condition (2) it follows that

$$\mathbf{B}^{-1}(\mathbf{x}_a-\mathbf{x}_b)=\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}[\mathbf{y}-\mathbf{h}(\mathbf{x}_a)] \tag{9}$$

and after replacing (9) into (7) the sensitivity to the background error variance is expressed as

$$\nabla_{\sigma_b^2}e(\mathbf{x}_a)=\left\{\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}[\mathbf{y}-\mathbf{h}(\mathbf{x}_a)]\right\}\circ\nabla_{\mathbf{x}_b}e(\mathbf{x}_a) \tag{10}$$

Since in practice the observation errors are often assumed to be uncorrelated, $\mathbf{R} = diag(\sigma_o^2)$, the computational overhead to estimate (8) and (10) once (6) is available is thus modest.

A sensitivity analysis fully consistent to the nonlinear optimization problem (1) requires an exact solution to the first-order optimality condition (2) and the ability to solve the linear system (4-5) involving the Hessian of the cost function. Current VDASs implement an incremental approach based on successive quadratic approximations to (1) (Courtier et al. 1994) and additional simplifying assumptions are necessary to alleviate the need for second order derivative information in the sensitivity computations when multiple outer loop iterations are performed. Trémolet (2008) provides a study on the observation sensitivity and observation impact calculations in a VDAS implementing multiple outer loop iterations.

3 Adjoint-DAS observation impact estimation

Adjoint-DAS techniques are currently implemented as an effective approach (all-at-once) to estimate the impact of *any data subset* in the DAS on a *specific forecast* aspect and to monitor the observation performance on short-range forecasts. Implementation was mainly considered for a linear analysis scheme

$$\mathbf{x}_a = \mathbf{x}_b + \mathbf{K}[\mathbf{y} - \mathbf{h}(\mathbf{x}_b)] \tag{11}$$

where

$$\mathbf{K} = \mathbf{B}\mathbf{H}^{\mathrm{T}}\left[\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}} + \mathbf{R}\right]^{-1} = \left[\mathbf{B}^{-1} + \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\right]^{-1}\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1} \tag{12}$$

is the optimal gain (Kalman) matrix. The adjoint-DAS OBSI estimation relies on the observation-space evaluation of the forecast impact due to assimilation of all data in the DAS

$$\delta e = e(\mathbf{x}_a) - e(\mathbf{x}_b) \approx (\delta\mathbf{y})^{\mathrm{T}}\mathbf{g} \tag{13}$$

in terms of the innovation vector $\delta\mathbf{y} = \mathbf{y} - \mathbf{h}(\mathbf{x}_b)$ and a properly defined weight vector $\mathbf{g}$ that is expressed in terms of the adjoint-DAS operator $\mathbf{K}^{\mathrm{T}}$ and the forecast sensitivity to initial conditions (Gelaro et al. 2007). A measure of the contribution of individual data components in the assimilation scheme to forecast error reduction, per observation type, instrument type, and data location, is obtained by taking the inner product between the innovation vector component and the corresponding $\delta\mathbf{y}$-amplification factor in (13)

$$I(\mathbf{y}_i) = (\delta\mathbf{y}_i)^{\mathrm{T}}\mathbf{g}_i \tag{14}$$

where $\mathbf{y}_i$ is the data component whose impact is being evaluated. Data components for which $I(\mathbf{y}_i) < 0$ contribute to the forecast error reduction (improve the forecast), whereas data components with $I(\mathbf{y}_i) > 0$ will increase the forecast error (degrade the forecast). As explained by Daescu and Todling (2009), to avoid the need for high-order derivative information required by a Taylor series approximation, the current implementation of high-order adjoint-DAS OBSI measures relies on the fundamental theorem of line integrals

$$\delta e = e(\mathbf{x}_a) - e(\mathbf{x}_b) = \int_{[\mathbf{x}_b,\mathbf{x}_a]} \nabla_{\mathbf{x}} e(\mathbf{x}) \cdot d\,\mathbf{x} = \int_0^1 (\delta\mathbf{x}_a)^{\mathrm{T}} \nabla_{\mathbf{x}} e(\mathbf{x}_\tau)\, d\tau = \int_0^1 (\delta\mathbf{y})^{\mathrm{T}}\mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}} e(\mathbf{x}_\tau)\, d\tau \tag{15}$$

where

$$\delta\mathbf{x}_a = \mathbf{x}_a - \mathbf{x}_b = \mathbf{K}\delta\mathbf{y} \tag{16}$$

is the analysis increment and

$$\mathbf{x}_\tau = \mathbf{x}_b + \tau\delta\mathbf{x}_a, \quad 0 \le \tau \le 1 \tag{17}$$

is the parametric initial state that describes the line segment from $\mathbf{x}_b$ to $\mathbf{x}_a$. Quadrature approximations to the integral (15) are then used to derive OBSI measures. For example, the second-order accurate δe-approximation provided by the trapezoidal rule

$$\delta e \approx (\delta\mathbf{y})^{\mathrm{T}}\mathbf{K}^{\mathrm{T}}\left[\frac{1}{2}\nabla_{\mathbf{x}} e(\mathbf{x}_b) + \frac{1}{2}\nabla_{\mathbf{x}} e(\mathbf{x}_a)\right] \tag{18}$$

has been first considered in the work of Langland and Baker (2004) and in recent adjoint-based OBSI studies (Cardinali 2009, Gelaro and Zhu 2009). Efficient alternatives to (18) such as the midpoint rule are discussed by Daescu and Todling (2009).

Derivation of high-order OBSI measures to fully account for nonlinear analysis schemes is an unresolved issue in observation impact studies and formulation of observation-sensitivity to properly account for incremental schemes implementing a multi-loop outer iteration is discussed by Trémolet (2008).

4 Illustrative numerical experiments

Numerical experiments are provided to illustrate some of the sensitivity analysis applications including observation impact estimation and diagnosis and tuning of the observation-error and background-error variances, using the Lorenz 40-variable model (Lorenz and Emanuel 1998)

$$\frac{\mathrm{d}x_j}{\mathrm{d}t} = (x_{j+1} - x_{j-2})x_{j-1} - x_j + F, \quad j = 1, 2, \ldots, n \tag{19}$$

where $n = 40, x_{-1} = x_{n-1}, x_0 = x_n, x_{n+1} = x_1$, The system (19) is integrated with a fourth-order Runge-Kutta method and a constant time step $\Delta t = 0.05$ that in the data assimilation experiments is identified to a 6-hour time period. The time evolution of the true state $\mathbf{x}^t$ is obtained by taking the external forcing to be $F = 8$ and a model error is considered in the forecast model by taking $F = 7.6$. An initial state $\mathbf{x}_0^t$ is obtained by a 90-days (360 time-steps) integration started from $x_j = 8$ for $j \neq n/2$ and $x_{n/2} = 8.008$; a background estimate $\mathbf{x}_b$ to $\mathbf{x}_0^t$ is prescribed by introducing random perturbations in $\mathbf{x}_0^t$ taken from the standard normal distribution $N(0,1)$. To simulate various observing system components, it is assumed that the DAS incorporates four data types $\mathbf{y}^{(1)}, \mathbf{y}^{(2)}, \mathbf{y}^{(3)}, \mathbf{y}^{(4)}$, each being a 10-dimensional vector, and that data type $\mathbf{y}^{(i)}$ is taken at locations $4k + i, k = 0, 1, \ldots, 9$. Data $\mathbf{y}^{(1)}$ is thus located at sites $1, 5, \ldots, 37$. Observational data is generated at each time step and the observation errors are normally distributed $N(0, \sigma_o^{(i)})$ with the standard deviations $\sigma_o^{(1)} = 0.1, \sigma_o^{(2)} = 0.2, \sigma_o^{(3)} = 0.6, \sigma_o^{(4)} = 0.8$ such that data of type $\mathbf{y}^{(1)}$ and $\mathbf{y}^{(2)}$ is of increased accuracy as compared to the data of type $\mathbf{y}^{(3)}$ and $\mathbf{y}^{(4)}$. The DAS implements a linear analysis scheme (11-12) and to simulate an optimal DAS the background estimate at time t_{i+1} and the associated background error covariance matrix are propagated using the Extended Kalman filter equations

$$\mathbf{x}_b(t_{i+1}) = \mathscr{M}_{t_i \to t_{i+1}}(\mathbf{x}_a(t_i)) \tag{20}$$

$$\mathbf{B}(t_{i+1}) = \mathbf{M}(t_i)\mathbf{A}(t_i)\mathbf{M}^{\mathrm{T}}(t_i) + \mathbf{Q}(t_i) \tag{21}$$

where $\mathbf{x}_a(t_i)$ is the analysis (11) at time t_i,

$$\mathbf{A}(t_i) = \left[\mathbf{B}^{-1}(t_i) + \mathbf{H}^{\mathrm{T}}(t_i)\mathbf{R}^{-1}\mathbf{H}(t_i)\right]^{-1} = [\mathbf{I} - \mathbf{K}(t_i)\mathbf{H}(t_i)]\mathbf{B}(t_i) \tag{22}$$

is the inverse Hessian matrix (analysis error covariance matrix) associated to a quadratic cost (1), and $\mathbf{M}(t_i)$ is the state dependent Jacobian matrix of the numerical model $\mathscr{M}_{t_i \to t_{i+1}}$ from t_i to t_{i+1}. The model error covariance matrix $\mathbf{Q}$ is taken to be time invariant, diagonal and with constant entries, $\mathbf{Q} = diag(\sigma_q^2)$ and by trial and error the specification $\sigma_q^2 = 0.01$ was found to provide improved analyses as compared to several other selections. This configuration, hereafter referred to as DAS-1, attempts to simulate an optimal DAS, although some deficiencies are still present. In particular, fine tuning of the model error variance vector σ_q^2 is addressed later in this section. DAS-1 is run for 3240 analysis cycles and the observation impact on the initial-condition error and on the 24-hour forecast error $e(\mathbf{x}(t_i)) = \|\mathbf{x}(t_i) - \mathbf{x}^t(t_i)\|^2$ and $e(\mathbf{x}(t_i)) = \|\mathbf{x}(t_{i+4}) - \mathbf{x}^t(t_{i+4})\|^2$ respectively, is estimated using the adjoint-DAS measure (18). Time-averaged OBSI estimates over the last N=2880 analysis cycles (a 2-years time period) are displayed at each observing site in Fig. 1 (left). It is noticed that the adjoint-DAS approach properly identifies at each observing site data of high accuracy ($\mathbf{y}^{(1)}$ followed by $\mathbf{y}^{(2)}$) as the most benefic data and that the OBSI on the forecast-error is of larger magnitude as compared to the impact on the initial-condition error. Negative OBSI values at all observing sites indicate that statistically, each data component is of benefit.

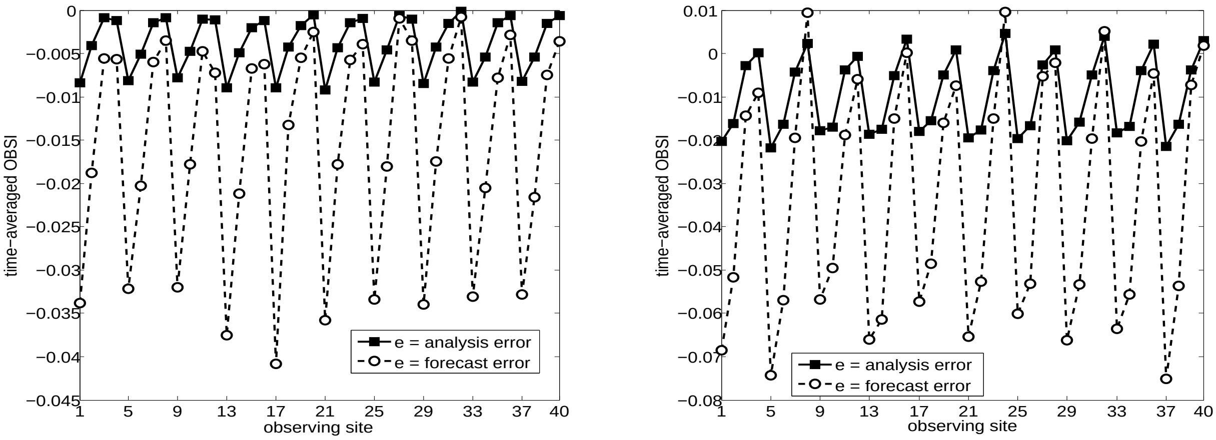

Figure 1: Time-averaged observation impact estimation at each observing site in DAS-1 (left) and in DAS-2 (right) for a functional e defined as a measure of the initial-condition error and as a measure of the 24-hour forecast error.

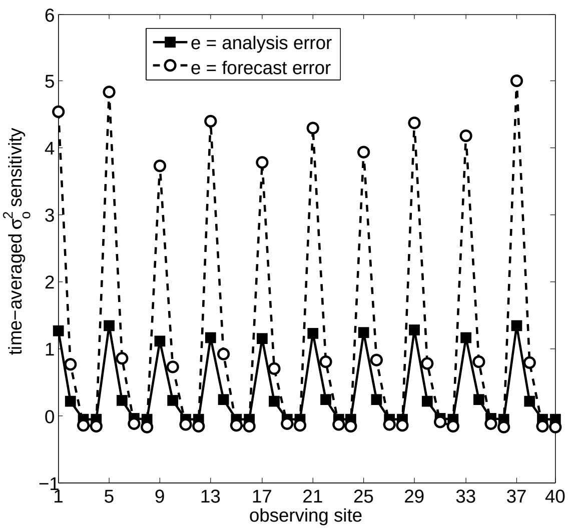

Figure 2: Time-averaged sensitivity to the observation-error variances in DAS-2.

4.1 Diagnosis and observation-error variance tuning

A suboptimal DAS is considered (DAS-2) where observational data is generated as described above however, in the DAS-2 an observation-error standard deviation $\sigma_o = 0.4$ is prescribed for all observations. In DAS-2 the errors in the data types $\mathbf{y}^{(1)}$ and $\mathbf{y}^{(2)}$ are thus overestimated, whereas the errors in the data types $\mathbf{y}^{(3)}$ and $\mathbf{y}^{(4)}$ are underestimated. Time-averaged adjoint-based OBSI estimates in DAS-2 are displayed at each observing site in Fig. 1 (right). Positive OBSI values at several observing sites of data type $\mathbf{y}^{(4)}$ indicate that assimilation of this data degrades the analyses and forecasts in DAS-2 due to the large underestimation of the observation-error variance.

While the OBSI estimation provides valuable information on the contribution of individual data sets to the forecast error reduction, as used in the existing DAS, additional information is necessary to optimize the use of the observational data through proper specification of the error-statistics. Such information may be obtained from the observation-error variance sensitivity analysis displayed in Figure 2.

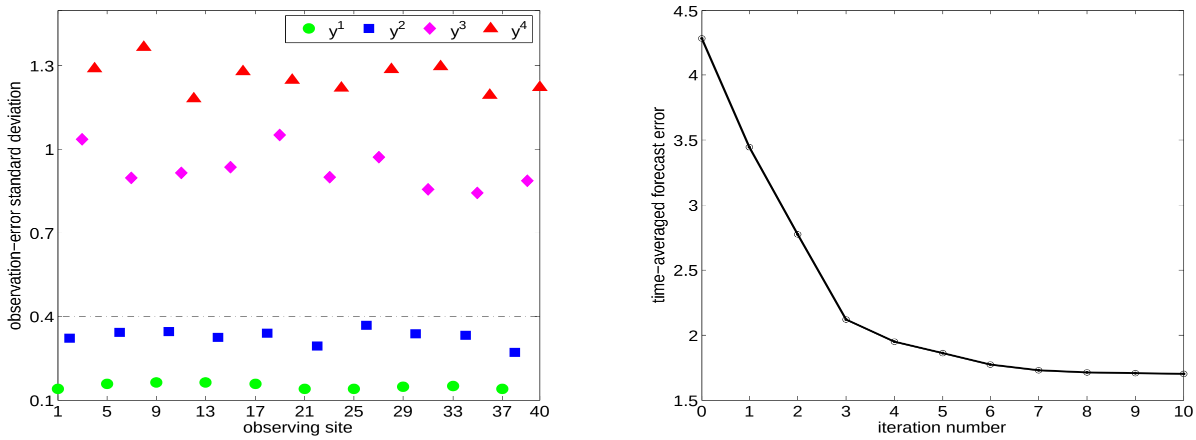

Figure 3: Left: estimated observation-error standard deviation $\sigma_{o,\star}$ at each observing site through the solution of the optimization problem (23). The dashed line indicates the initial guess setting in DAS-2. Right: the evolution of the forecast error functional during the iterative optimization process.

The steepest descent direction $-\nabla_{\sigma_o^2} e(\mathbf{x}_a)$ identifies the direction in the observation error-variance space where small variations in the specification of the error-variances, from the current DAS configuration, will be of largest analysis/forecast benefit.

It is noticed that at each observing site the observation-error variance sensitivity analysis properly identifies data types $\mathbf{y}^{(1)}$ and $\mathbf{y}^{(2)}$ as data where decreasing the error-variance input in the DAS will reduce the analysis/forecast error (positive derivative values indicate that locally the functional aspect is an increasing function of the corresponding parameter) and data types $\mathbf{y}^{(3)}$ and $\mathbf{y}^{(4)}$ as data where increasing the error-variance input in the DAS will reduce the analysis/forecast error (negative derivative values indicate that locally the functional aspect is a decreasing function of the corresponding parameter). The magnitude of the σ_o^2-sensitivity indicates that variations in the specification of the error-variances associated to data $\mathbf{y}^{(1)}$ and $\mathbf{y}^{(2)}$ will have a much larger impact on the forecast aspect as compared to the impact from variations in the specification of the error-variances associated to data $\mathbf{y}^{(3)}$ and $\mathbf{y}^{(4)}$.

The availability of the gradient $\nabla_{\sigma_o^2} e(\mathbf{x}_a)$ provides grounds for optimizing the observation error-variance input using a gradient-based iterative algorithm to approximate the solution to the optimization problem

$$\min_{\sigma_o^2} e(\mathbf{x}_a) \tag{23}$$

Bound constraints $\sigma_{o,min}^2 \leq \sigma_o^2 \leq \sigma_{o,max}^2$ may be associated to (23) based on a priori estimates to min/max observation error-variances. To achieve statistical significance, in our experiments the functional (23) is defined as the time-averaged forecast error. This formulation involves a simplifying assumption in the gradient estimation namely, it neglects the time propagation of the observation-error variance impact through various data assimilation cycles and this is also an unresolved issue in current adjoint-based OBSI estimates. The use of an ensemble of forecasts to define the functional aspect may be considered in practical applications as a feasible alternative (Torn and Hakim 2008).

Estimates $\sigma_{o,\star}$ to the observation error standard deviation obtained by solving the minimization problem (23) are displayed at each observing site in Fig. 3 together with the evolution of the forecast error during the iterative process. The optimization algorithm benefits from the gradient information and exhibits fast convergence.

In DAS-1 the time-averaged 24-hour forecast error was found to be $e(\mathbf{x}_a) \approx 1.73$ and as a result of the error-variance tuning, the time-averaged 24-hour forecast error in DAS-2 is reduced from an initial value of $e(\mathbf{x}_a) \approx 4.3$ at $\sigma_o = 0.4$ to $e(\mathbf{x}_a) \approx 1.78$ at $\sigma_{o,\star}$. It is noticed that significantly improved estimates are obtained for the error-variances associated to data of large forecast impact $\mathbf{y}^{(1)}$ and $\mathbf{y}^{(2)}$. The error-variances associated to the low-impact data components are largely overestimated by the optimization process. Several factors impair the quality of the error-variance estimates including statistical inconsistencies in the specification of the model error covariance and nonlinear error propagation. In this context, the estimates $\sigma_{o,\star}$ derived from the optimality condition

$$\nabla_{\sigma_o^2} e(\mathbf{x}_a)\Big|_{\sigma_o=\sigma_{o,\star}} = \mathbf{0} \tag{24}$$

are impaired by the suboptimal specification of other DAS components and by the simplifying assumptions that are necessary to make the implementation feasible.

For practical applications, a feasible approach to the observation-error variance tuning may be achieved by reducing the dimensionality of the problem (23) and formulating an optimization problem for tuning coefficients α_i, $\sigma_{o,\star}^{(i)} = \alpha_i \sigma_o^{(i)}$ associated to each data type $\mathbf{y}^{(i)}$. Experiments using this approach entailed a reduction in the dimension of the problem (23) from 40 to 4 and the observation-error standard deviations for each data set were estimated to $\sigma_{0,\star}^{(1)} \approx 0.13$, $\sigma_{0,\star}^{(2)} \approx 0.32$, $\sigma_{0,\star}^{(3)} \approx 0.89$, $\sigma_{0,\star}^{(4)} \approx 1.11$. The time-averaged 24-hour forecast error associated to these estimates was found to be $e(\mathbf{x}_a) \approx 1.87$.

4.2 Sensitivity to the background-error variance and model-error variance tuning

The sensitivity to the background-error variance is used as a diagnostic tool and to improve the performance of the DAS-1 through an improved specification of the model error variance. Time-averaged sensitivities to the background error variance in DAS-1 are displayed for each state component in Fig. 4 (left) for the analysis error and for the 24-hour forecast error. Positive sensitivity values show that the functional aspect is locally increasing with respect to the σ_b^2 thus indicating that in DAS-1 the background error variances are overestimated. As a result, although in the DAS-1 the specification of the observation-error variances is statistically consistent to the actual observation errors, the analysis error σ_o^2-sensitivities have negative values, as shown in Fig. 4 (right).

The steepest descent direction $-\nabla_{\sigma_b^2} e(\mathbf{x}_a)$ identifies the direction in the background error-variance space where small variations in the specification of the error-variances, from the current DAS configuration, will be of largest analysis/forecast benefit.

From (21)

$$\nabla_{\sigma_q^2(t_i)} \sigma_b^2(t_{i+1}) = \mathbf{I}_{n\times n} \tag{25}$$

and the availability of the gradient $\nabla_{\sigma_b^2} e(\mathbf{x}_a)$ provides grounds for improving the σ_b^2 specification in DAS-1 through an improved estimation to the model error variance σ_q^2 as the solution to the optimization problem

$$\min_{\sigma_q^2} e(\mathbf{x}_a) \tag{26}$$

The functional (26) is defined as the time-averaged 24-hour forecast error and this formulation neglects the time propagation of the model-error variance impact through various data assimilation cycles. Estimates $\sigma_{q,\star}^2$ to the model error variance obtained by solving the minimization problem (26) are displayed in Fig. 5 together with the evolution of the forecast error during the iterative process. It is noticed that a reduction of $\sim 5\%$ in the time-averaged forecast error was achieved as the result of the σ_q^2 tuning.

5 Conclusions

Recent advances in the software developments and theoretical foundations make feasible the implementation of sensitivity analysis in data assimilation to optimize the use of observational data. The necessary tools for observation impact estimation are in place or are being developed at NWP centers and in this work it is explained

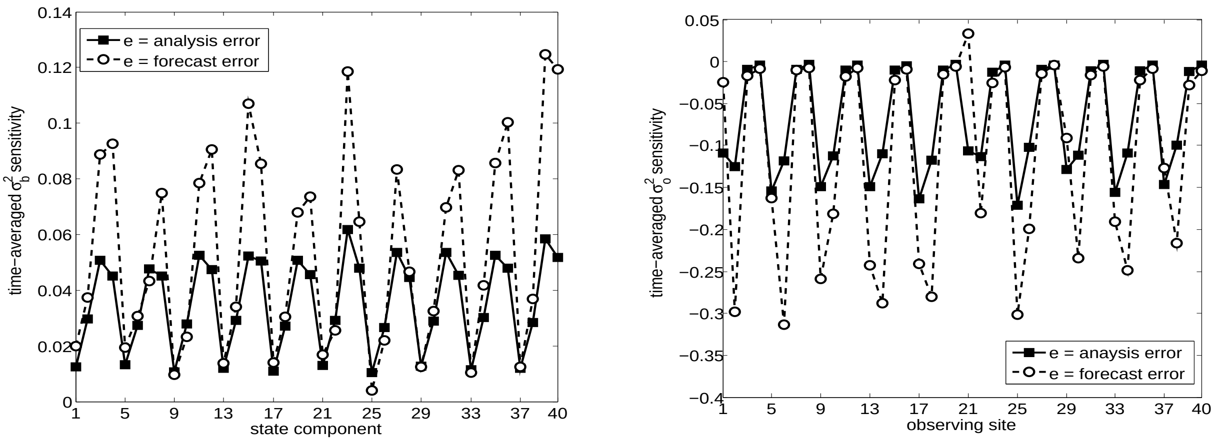

Figure 4: Time-averaged sensitivity to the background-error variance (left) and to the observation-error variance (right) in DAS-1.

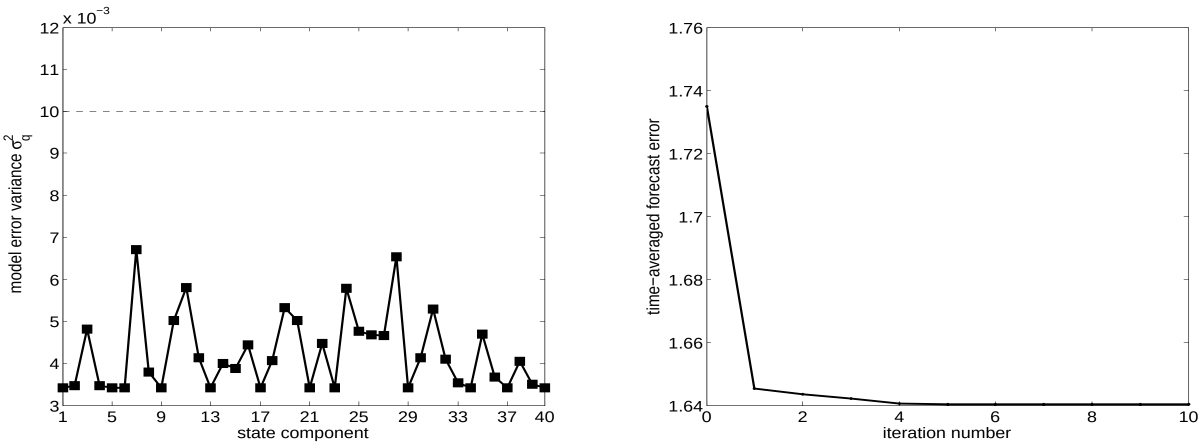

Figure 5: Left: estimated model error variance $\sigma^2_{q,\star}$ through the solution of the optimization problem (26). The dashed line indicates the initial guess setting in DAS-1. Right: the evolution of the forecast error functional during the iterative optimization process.

that error-variance sensitivities may be obtained at a modest additional computational effort. By extending the sensitivity analysis to the DAS error-variance input valuable information may be obtained for DAS diagnosis and design of efficient algorithms for tuning the input error-variances. These methodologies may be applied to both variational and Kalman filter based data assimilation systems. Applications of the adjoint-DAS sensitivity to a priori estimation of data removal in OSEs are discussed by Daescu (2009a). The adjoint-DAS approach provides sensitivities to all input parameters and the sensitivity to model error and model error-variance tuning in a weak-constraint 4DVAR DAS may be considered. An objective observing system assessment relies on the ability to provide verification states whose errors are unbiased and are statistically independent from the errors in the forecasts produced by the DAS. In practice, the difficulty of providing an accurate representation of the true atmospheric state in the forecast error measure may lead to an increased uncertainty in estimations derived from deterministic forecast error measures, in particular when suboptimal input error statistics are specified in the DAS (Daescu 2009b). A probabilistic framework may be considered by using an ensemble of verification states and/or an ensemble of data assimilation systems.

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References

Atlas, R. (1997). Atmospheric observations and experiments to assess their usefulness in data assimilation. *J. Meteorol. Soc. Japan*, **75**, No. 1B, 111–130.

Bouttier, F. and G. Kelly (2001). Observing-system experiments in the ECMWF 4D-Var data assimilation system. *Q.J.R. Meteorol. Soc.*, **127**, 1469–1488.

Cardinali, C. (2009). Monitoring the observation impact on the short-range forecast. *Q.J.R. Meteorol. Soc.*, **135**, 239–250.

Chapnik, B., G. Desroziers, F. Rabier, and O. Talagrand (2006). Diagnosis and tuning of observational error in a quasi-operational data assimilation setting. *Q.J.R. Meteorol. Soc.*, **132**, 543–565.

Courtier P., Thépaut J.N., and A. Hollingsworth (1994). A strategy of operational implementation of 4D-Var using an incremental approach. *Q.J.R. Meteorol. Soc.*, **120**, p.1367–1388.

Daescu, D.N. (2008). On the sensitivity equations of four-dimensional variational (4D-Var) data assimilation. *Mon. Wea. Rev.*, **136** (8), 3050–3065.

Daescu, D.N. (2009a). Adjoint estimation to observing system experiments outcomes. *The Eight International Workshop on Adjoint Model Applications in Dynamical Meteorology*, Tannersville, PA, USA, May 18-22, 2009. Available on-line at *http://gmao.gsfc.nasa.gov/events/adjoint_workshop-8/present/presentations.html*.

Daescu, D.N. (2009b). On the deterministic observation impact guidance: a geometrical perspective. *Mon. Wea. Rev.*, DOI: 10.1175/2009MWR2954.1, in press.

Daescu, D.N., and R. Todling (2009). Adjoint estimation of the variation in model functional output due to the assimilation of data. *Mon. Wea. Rev.*, **137**, 1705–1716.

Desroziers, G., and S. Ivanov (2001). Diagnosis and adaptive tuning of observation-error parameters in a variational assimilation. *Q.J.R. Meteorol. Soc.*, **127** (574), 1433–1452.

Frehlich, R. (2006). Adaptive data assimilation including the effect of spatial variations in observation error. *Q.J.R. Meteorol. Soc.* **132**, 1225–1257.

Gelaro, R., Zhu, Y., and R.M. Errico (2007). Examination of various-order adjoint-based approximations of observation impact. *Meteorologische Zeitschrift*, **16**, No. 6, 685–692.

Gelaro, R., and Y. Zhu (2009). Examination of observation impacts derived from observing system experiments (OSEs) and adjoint models. *Tellus*, **61A**, 179–193.

Hamill, T.M., and C. Snyder (2002). Using improved background-error covariances from an ensemble Kalman filter for adaptive observations. *Mon. Wea. Rev.*, **130**, 1552–1572.

Janjić, T., and S.E. Cohn (2006). Treatment of observation error due to unresolved scales in atmospheric data assimilation. *Mon. Wea. Rev.*, **134** (10), 2900–2915.

Kalnay, E. (2002). *Atmospheric Modeling, Data Assimilation and Predictability*. Cambridge University Press.

Kelly, G., Thépaut, J.N., Buizza, R., and C. Cardinali (2007). The value of observations. I: Data denial experiments for the Atlantic and the Pacific. *Q.J.R. Meteorol. Soc.*, **133**, 1803–1815.

Langland, R.H., and N.L. Baker (2004). Estimation of observation impact using the NRL atmospheric variational data assimilation adjoint system. *Tellus*, **56A**, 189–201.

Le Dimet, F.X., H.E. Ngodock, B. Luong, and J. Verron (1997). Sensitivity analysis in variational data assimilation. *J. Meteor. Soc. Japan*, **75**, 245–255.

Lorenc, A.C. (2003). Modelling of error covariances by 4D-Var data assimilation. *Q.J.R. Meteorol. Soc.*, **129**, 3167–3182.

Lorenz, E.N., and K.A. Emanuel (1998). Optimal sites for supplementary weather observations: simulation with a small model. *J. Atmos. Sci.*, **55**, 399–414.

Talagrand, O., and P. Courtier (1987). Variational assimilation of meteorological observations with the adjoint of the vorticity equations. I-Theory. *Q.J.R. Meteorol. Soc.*, **113**, 1311–1328.

Torn, R.D., and G.J. Hakim (2008). Ensemble-based sensitivity analysis. *Mon. Wea. Rev.*, **136**, 663–677.

Trémolet, Y. (2008). Computation of observation sensitivity and observation impact in incremental variational data assimilation. *Tellus* **A**, **60**, No. 5, 964–978.