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Forecast sensitivity to the observation error covariance in variational data assimilation

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Abstract

The development of the adjoint of the forecast model and of the adjoint of the data assimilation system (adjoint-DAS) make feasible the evaluation of the derivative-based forecast sensitivity to DAS input parameters in numerical weather prediction (NWP). The adjoint estimation of the forecast sensitivity to the observation error covariance in the DAS is considered as a practical approach to provide all-at-once first order estimates to the forecast impact as a result of variations in the specification of the observation error statistics and guidance for tuning of error covariance parameters. The proposed methodology extends the capabilities of the adjoint modeling tools currently in place at major NWP centers for observation sensitivity and observation impact analysis. Illustrative numerical results are presented with the fifth-generation NASA Goddard Earth Observing System (GEOS-5) atmospheric DAS and its adjoint.

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1. Introduction

Numerical modeling of the atmospheric dynamics and assimilation of observational data into large-scale atmospheric models are well-recognized as being among the most challenging and computationally intensive problems in applied sciences. Data assimilation techniques combine information from a model of atmospheric dynamics, observational data, and error statistics to produce an analysis of the state of the atmosphere (Bennett [1], Daley [2], Kalnay [3], Lewis et al. [4]). In practice, simplifying assumptions are necessary to achieve a feasible implementation and an increased amount of research in numerical weather prediction (NWP) is dedicated to the development of effective techniques for diagnosis and tuning of unknown error covariance parameters in both variational and Kalman filter-based assimilation systems [5], [6], [7], [8]. As

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the number of observations available has grown almost exponentially over the recent years, an optimal use of the information provided by the Earth Observing System requires the development of efficient techniques to identify the data components where uncertainties in the observation error statistics have a potentially large impact in determining the forecast uncertainties.

Valuable insight on the relative importance and contribution of various data assimilation system (DAS) components to reduce the forecast error uncertainties may be obtained by performing sensitivity studies to provide an assessment of the forecast impact as a result of variations in the DAS input. The development of the adjoint of the forecast model and of the adjoint of the data assimilation system (adjoint-DAS) allow an *all-at-once* evaluation of the derivative-based local sensitivity [9] of a scalar forecast aspect with respect to a large number of DAS input parameters. Baker and Daley [10] have shown the adjoint-DAS ability to provide observation and background sensitivity for applications to targeted observations. Recently, NWP centers have engaged in the effort of developing the adjoint-DAS as a tool to monitor the observation impact on reducing short-term forecast errors, to provide data quality diagnostics, and guidance for optimal satellite channel selection [11], [12], [13], [14].

To date, studies on the forecast impact as a result of variations in the specification of the observation error variance in the DAS have been performed only through additional assimilation experiments (Joiner and Coauthors [15]) and the increased amount and multitude of data types provided by conventional measurements and by the satellite network prevents a comprehensive observing system analysis. A study on derivative-based error covariance sensitivity analysis in variational data assimilation was provided by Daescu [16] using a simple shallow-water model.

The current work presents novel theoretical developments and capabilities of the adjoint-DAS approach that may be achieved by extending the forecast sensitivity to the space of input error covariances. Section 2 provides a brief review of the mathematical aspects of sensitivity analysis in VDA. All-at-once evaluation of sensitivity to observation error covariance parameters and forecast impact estimation is discussed in section 3. Sensitivity to multiplicative error covariance tuning coefficients is derived as a particular case of the error covariance perturbation analysis. In section 4, numerical results obtained with the fifth-generation NASA Goddard Earth Observing System (GEOS-5) atmospheric DAS and its adjoint developed at NASA Global Modeling and Assimilation Office (GMAO) are used to illustrate the practical applicability of the theoretical concepts. Summary and concluding remarks are in section 5.

2. Sensitivity analysis in VDA

Variational data assimilation (VDA) provides an analysis $\mathbf{x}^a \in \mathbb{R}^n$ to the true state $\mathbf{x}^t$ of the atmosphere by minimizing the cost functional

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

where $\mathbf{x}^b \in \mathbb{R}^n$ is a prior (background) state estimate, $\mathbf{y} \in \mathbb{R}^p$ is the vector of observational data, and $\mathbf{h}$ is the observation operator that maps the state into observations. In practice, statistical information on the background error $\boldsymbol{\epsilon}^b = \mathbf{x}^b - \mathbf{x}^t$ and observational error $\boldsymbol{\epsilon}^o = \mathbf{y} - \mathbf{h}(\mathbf{x}^t)$ is used to specify symmetric and positive definite weighting matrices $\mathbf{B} \in \mathbb{R}^{n\times n}$ and $\mathbf{R} \in \mathbb{R}^{p\times p}$ that are representations in the DAS of the background and observation error covariances $\mathbf{B}_t = E(\boldsymbol{\epsilon}^b {\boldsymbol{\epsilon}^b}^{\mathrm{T}})$

and $\mathbf{R}_t = E(\boldsymbol{\epsilon}^o \boldsymbol{\epsilon}^{o\mathrm{T}})$ respectively, where $E(\cdot)$ is the statistical expectation operator. In operational systems, the dimensionality of the state vector is in the range of $n \sim 10^7 - 10^8$ and data sets in the range of $p \sim 10^6 - 10^7$ are ingested in each data assimilation cycle (typically at a 6 to 12 hour time interval) such that simplifying assumptions are necessary to achieve a feasible implementation [17]. If the observation operator is assumed to be linear, $\mathbf{h}(\mathbf{x}) = \mathbf{H}\mathbf{x}$, the analysis (2) is expressed as

$$\mathbf{x}^a = \mathbf{x}^b + \mathbf{K}[\mathbf{y} - \mathbf{H}\mathbf{x}^b] \tag{3}$$

where the gain matrix $\mathbf{K}$ is defined as

$$\mathbf{K} = \left[\mathbf{B}^{-1} + \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\right]^{-1} \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1} \tag{4}$$

In four-dimensional VDA the operator $\mathbf{h}$ incorporates the nonlinear model to properly account for time-distributed data and an outer-loop iteration is used to approximate the solution to the nonlinear problem (1)-(2), as discussed in references [18], [19].

2.1. Error covariance sensitivity analysis

Baker and Daley [10] derived the equations of the sensitivity (gradient) of a scalar forecast aspect $e(\mathbf{x}^a)$ to observations and background for a linear analysis scheme (3)-(4):

$$\nabla_{\mathbf{y}} e(\mathbf{x}^a) = \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}} e(\mathbf{x}^a) \in \mathbb{R}^p \tag{5}$$

$$\nabla_{\mathbf{x}^b} e(\mathbf{x}^a) = [\mathbf{I} - \mathbf{H}^{\mathrm{T}}\mathbf{K}^{\mathrm{T}}] \nabla_{\mathbf{x}} e(\mathbf{x}^a) \in \mathbb{R}^n \tag{6}$$

Typically, the forecast score is defined as a short-range forecast error measure

$$e(\mathbf{x}^a) = (\mathbf{x}^a_f - \mathbf{x}^v_f)^{\mathrm{T}} \mathbf{C} (\mathbf{x}^a_f - \mathbf{x}^v_f) \tag{7}$$

where $\mathbf{x}^a_f = M_{t_0 \to t_f}(\mathbf{x}^a)$ is the nonlinear model forecast at verification time t_f, $\mathbf{x}^v_f$ is the verifying analysis at t_f which serves as a proxy to the true state $\mathbf{x}^t_f$, and $\mathbf{C}$ is an appropriate symmetric and positive definite matrix that defines the metric in the state space e.g., the total energy norm. Evaluation of the sensitivities (5-6) is performed by applying the *adjoint-DAS* operator $\mathbf{K}^{\mathrm{T}}$ to the vector $\nabla_{\mathbf{x}} e(\mathbf{x}^a)$ of forecast sensitivity to initial conditions that is obtained using the adjoint $\mathbf{M}^{\mathrm{T}}$ of the forecast model along the trajectory initiated from $\mathbf{x}^a$:

$$\nabla_{\mathbf{x}} e(\mathbf{x}^a) = 2[\mathbf{M}_{t_0 \to t_f}(\mathbf{x}^a)]^{\mathrm{T}} \mathbf{C} (\mathbf{x}^a_f - \mathbf{x}^v_f) \tag{8}$$

Additional simplifying assumptions are necessary to alleviate the need for higher order derivative information in the sensitivity computations when multiple outer loop iterations are used to provide an approximation to the solution to (1), as explained by Trémolet [20].

As shown by Daescu [16], implicit differentiation applied to the first-order optimality condition to (1)

$$\nabla_{\mathbf{x}} J(\mathbf{x}^a; \mathbf{x}^b, \mathbf{B}, \mathbf{y}, \mathbf{R}) = \mathbf{0} \tag{9}$$

allows to establish close relationships between the sensitivities to observations/background and to the associated error covariances. If $\{\mathbf{y}_i\}, i \in I$, denotes a partition of the observational data set

$\mathbf{y}$ such that for any $i_1, i_2 \in I, i_1 \neq i_2$ the observational errors in data $\mathbf{y}_{i_1}$ are uncorrelated to the observational errors in data $\mathbf{y}_{i_2}$, then the following identities hold [16]:

$$\frac{\partial e(\mathbf{x}^a)}{\partial \mathbf{R}_i} = \nabla_{\mathbf{y}_i} e(\mathbf{x}^a) \left[\mathbf{h}_i(\mathbf{x}^a) - \mathbf{y}_i\right]^{\mathrm{T}} \mathbf{R}_i^{-1} \in \mathbb{R}^{p_i \times p_i} \tag{10}$$

$$\frac{\partial e(\mathbf{x}^a)}{\partial \mathbf{B}} = \nabla_{\mathbf{x}^b} e(\mathbf{x}^a) \left[\mathbf{x}^a - \mathbf{x}^b\right]^{\mathrm{T}} \mathbf{B}^{-1} \in \mathbb{R}^{n \times n} \tag{11}$$

Modeling of the observation and background error correlations in the DAS is an area of active research in NWP [21], [22], [23], [24]. In practice the matrix $\mathbf{R}$ is often prescribed as diagonal with entries provided by statistical information on the observation errors variances, $\mathbf{R}_i = diag(\boldsymbol{\sigma}_i^2)$, where $\boldsymbol{\sigma}_i^2 \in \mathbb{R}^{p_i}$ is the vector of observation errors variances associated to the data subset $\mathbf{y}_i$. In this context the sensitivity to individual observation error variances $\sigma_{i,j}^2, j = 1, 2, \ldots, p_i$ is expressed as

$$\frac{\partial e(\mathbf{x}^a)}{\partial \sigma_{i,j}^2} = \frac{\partial e(\mathbf{x}^a)}{\partial y_{i,j}} \frac{\left[\mathbf{h}_i(\mathbf{x}^a) - \mathbf{y}_i\right]_j}{\sigma_{i,j}^2} \tag{12}$$

While the explicit evaluation and storage of the error covariance sensitivity matrices (10)-(11) is not feasible in an operational system, in particular for the background error covariance sensitivity, their use in an operator format may be considered and of significant importance is the practical ability to provide *directional derivatives* in the error covariance space and sensitivities to key parameters used to model the error covariances. For the purpose of this work, the mathematical formalism to exploit these novel adjoint-DAS capabilities is presented for the observation error covariance perturbation analysis and parametric sensitivity.

3. Forecast impact of observation error covariance perturbations

The forecast aspect $e(\mathbf{x}^a)$ is implicitly a function of the specification of the observation error covariances in the DAS, $e(\mathbf{R}) = e[\mathbf{x}^a(\mathbf{R})]$, and a first order approximation to the forecast impact as a result of variations $\delta\mathbf{R}$ in the observation error covariance may be expressed using the error covariance gradients

$$\delta e = e(\mathbf{R} + \delta\mathbf{R}) - e(\mathbf{R}) \approx \left\langle \frac{\partial e}{\partial \mathbf{R}}, \delta\mathbf{R} \right\rangle \tag{13}$$

where

$$\langle \mathbf{X}, \mathbf{Y} \rangle = Tr\left(\mathbf{X}\mathbf{Y}^T\right) \tag{14}$$

denotes the inner product associated to the Frobenius norm on the vector space of matrices of the same order and is expressed in terms of the matrix trace operator Tr. The right side of (13) is the $\delta\mathbf{R}$-directional derivative in the observation error covariance space of e evaluated at $\mathbf{R}$. The observation error covariance matrix has a block diagonal structure associated to data sets with uncorrelated observation errors $\mathbf{R} = diag(\mathbf{R}_i)$, $i \in I$, and for practical purposes the perturbations $\delta\mathbf{R}$ are assumed to be symmetric

$$\delta\mathbf{R}_i = (\delta\mathbf{R}_i)^{\mathrm{T}}, \; i \in I \tag{15}$$

The linear approximation (13) is thus the sum of the first order impacts of individual error covariance perturbations $\delta\mathbf{R}_i$

$$\delta e \approx \sum_i Tr\left(\frac{\partial e}{\partial \mathbf{R}_i} \delta\mathbf{R}_i\right) \tag{16}$$

Evaluation of the right side terms in (16) is computationally feasible by properly exploiting the outer vector product structure of the error covariance sensitivities (10) and properties of the matrix trace operator. For example, evaluation of the first order approximation to the impact δe_i associated to the observation error covariance perturbation $\delta \mathbf{R}_i$ proceeds as follows:

$$\begin{aligned}
\delta e_i &\approx Tr\left(\frac{\partial e}{\partial \mathbf{R}_i}\delta \mathbf{R}_i\right) \\
&= Tr\left(\nabla_{\mathbf{y}_i} e(\mathbf{x}^a)\left[\mathbf{h}_i(\mathbf{x}^a) - \mathbf{y}_i\right]^{\mathrm{T}} \mathbf{R}_i^{-1}\delta \mathbf{R}_i\right) \\
&= Tr\left(\delta \mathbf{R}_i \nabla_{\mathbf{y}_i} e(\mathbf{x}^a)\left[\mathbf{h}_i(\mathbf{x}^a) - \mathbf{y}_i\right]^{\mathrm{T}} \mathbf{R}_i^{-1}\right) \\
&= Tr\left\{\left[\delta \mathbf{R}_i \nabla_{\mathbf{y}_i} e(\mathbf{x}^a)\right]\left[\mathbf{R}_i^{-1}(\mathbf{h}_i(\mathbf{x}^a) - \mathbf{y}_i)\right]^{\mathrm{T}}\right\}
\end{aligned} \tag{17}$$

For column vectors of the same order, the trace operator property $Tr(\mathbf{a}\mathbf{b}^{\mathrm{T}}) = \mathbf{b}^{\mathrm{T}}\mathbf{a}$ allows to express (17) as

$$\delta e_i \approx \left[\mathbf{R}_i^{-1}(\mathbf{h}_i(\mathbf{x}^a) - \mathbf{y}_i)\right]^{\mathrm{T}}\left[\delta \mathbf{R}_i \nabla_{\mathbf{y}_i} e(\mathbf{x}^a)\right] \tag{18}$$

which is the equation of the first order approximation to the impact δe_i associated to the observation error covariance perturbation $\delta \mathbf{R}_i$. From (18) it is noticed that, having available the adjoint-DAS tools developed for observation sensitivity analysis, the evaluation of the linear approximation to the forecast impact δe_i requires only the additional ability to provide the product between the error covariance perturbation matrix and the associated vector of forecast sensitivity to observations.

3.1. Sensitivity to error covariance parameters

Forecast sensitivity to a parameter s_i in the observation error covariance representation $\mathbf{R}_i(s_i)$ is obtained by relating to a first order the error covariance variation $\delta \mathbf{R}_i$ to the parameter variation δs_i:

$$\delta \mathbf{R}_i \approx \frac{\partial \mathbf{R}_i(s_i)}{\partial s_i}\delta s_i \tag{19}$$

From (18) and (19) the first order approximation to the forecast impact is expressed as

$$\delta e_i \approx \left[\mathbf{R}_i^{-1}(s_i)(\mathbf{h}_i(\mathbf{x}^a) - \mathbf{y}_i)\right]^{\mathrm{T}}\left[\frac{\partial \mathbf{R}_i(s_i)}{\partial s_i}\nabla_{\mathbf{y}_i} e(\mathbf{x}^a)\right]\delta s_i \tag{20}$$

and the forecast sensitivity to the observation error covariance parameter s_i is

$$\frac{\partial e(\mathbf{x}^a)}{\partial s_i} = \left[\mathbf{R}_i^{-1}(s_i)(\mathbf{h}_i(\mathbf{x}^a) - \mathbf{y}_i)\right]^{\mathrm{T}}\left[\frac{\partial \mathbf{R}_i(s_i)}{\partial s_i}\nabla_{\mathbf{y}_i} e(\mathbf{x}^a)\right] \tag{21}$$

A particular case of practical significance is given by the specification

$$\mathbf{R}_i(s_i) = s_i \mathbf{R}_i \tag{22}$$

that is a common parametric representation used to design and implement error covariance tuning procedures [5], [6], [7]. From (21) and (22) the sensitivity to multiplicative error covariance coefficients is expressed as

$$\frac{\partial e(\mathbf{x}^a)}{\partial s_i} = \frac{1}{s_i}\left[\mathbf{h}_i(\mathbf{x}^a) - \mathbf{y}_i\right]^{\mathrm{T}}\nabla_{\mathbf{y}_i} e(\mathbf{x}^a) \tag{23}$$

and the parameter value $s_i = 1$ corresponds to the observation error covariance specification $\mathbf{R}_i$ in the DAS. Once the observation sensitivity $\nabla_{\mathbf{y}_i} e(\mathbf{x}^a)$ is available, all-at-once evaluation of the sensitivities to error covariance weight coefficients for all observing system components is obtained at a modest additional computational effort by taking the inner product between the observation sensitivity and the associated vector of analysis-minus-observed.

4. Numerical experiments

The adjoint-DAS capability to provide observation error covariance sensitivity analysis per data type and observing instrument is illustrated in numerical experiments with the NASA GEOS-5 atmospheric DAS and its adjoint developed at NASA GMAO. A complete documentation to GEOS-5 DAS is provided in the work of Rienecker and Coauthors [25]. GEOS-5 DAS assimilates conventional observations such as radiosondes, aircraft, and surface land data, and radiance observations from the satellite network such as data provided by the Advanced Microwave Sounding Unit-A (AMSU-A) from the National Oceanic and Atmospheric Administration (NOAA) satellites NOAA-15, NOAA-16, and NOAA-18, High Resolution Infrared Radiation Sounder-3 (HIRS-3) from NOAA-16 and NOAA-17, and the Atmospheric InfraRed Sounder (AIRS) and AMSU-A on the NASA's Aqua satellite.

Data assimilation and sensitivity experiments are performed at a horizontal resolution of $2.5° \times 2°$ with 72 hybrid levels in the vertical. The model functional aspect (7) is specified as the 24-hour average global forecast error between the model vertical grid levels 40 to 72 (from the surface to approximately 128 hPa) in a total (dry) energy norm. The analysis state $\mathbf{x}^a$ is obtained by assimilation of data valid at 0000 UTC 28 July 2007 and the verifying state $\mathbf{x}_f^v$ is provided at 0000 UTC 29 July 2007 by performing 6-hour analysis cycles. The computational overhead in the evaluation of the forecast sensitivity to observation error variances (12) and multiplicative parameters (18) consists on the integration of the adjoint of the GEOS-5 general circulation model to obtain the forecast sensitivity to initial conditions (8), evaluation of the observation sensitivity (5) by applying the adjoint-DAS operator, and followed by the observation-space product with the vector of analysis-minus-observed. The necessary software tools have been developed at NASA GMAO and other major NWP centers for observation sensitivity and impact assessment and the additional capability of performing all-at-once sensitivity to the specification of the observation error statistics is illustrated here.

Comparative maps of observation sensitivity and observation error variance sensitivity are displayed in Fig. 1 for the 500hPa radiosondes wind data and in Fig. 2 for the NOAA-15 AMSU-A channel 4 and for the NOAA-16 AMSU-A channel 6 brightness temperature data. The observation sensitivity was initially considered as an observation targeting tool and provides information necessary to assess the forecast impact as a result of changes in the observing system components, for a given specification of the observation error statistics in the DAS; the error-covariance sensitivity provides guidance on how uncertainties in the specification of the error statistics will impact the forecasts, for a given configuration of the existing observing system. The combined use of this information is necessary to optimize the use of data in reducing the forecast errors.

The observation error covariance sensitivity analysis is particularly valuable for satellite data where accurate estimations of the observational errors (including measurement and representation errors) are difficult to provide, as compared to conventional measurements. Sensitivity to observation error covariance weighting coefficients (23) are displayed in Fig. 3 per instrument channel number for NOAA-15 AMSU-A, NOAA-16 AMSU-A, and NOAA-17 HIRS-3 radiance

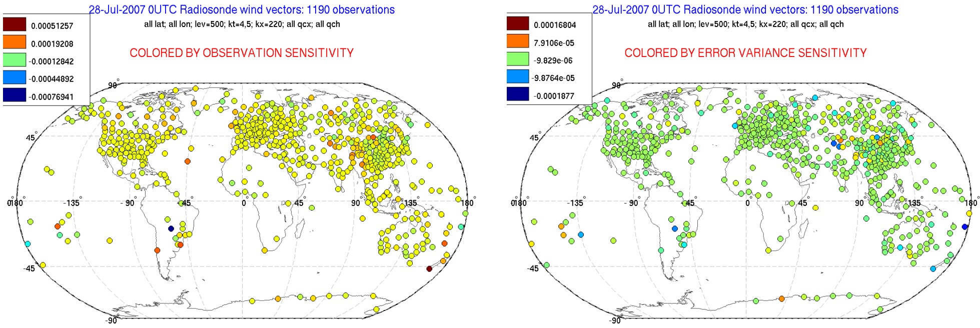

Figure 1: Forecast sensitivity to 500hPa radiosonde wind data (left) and to the associated observation error variances (right).

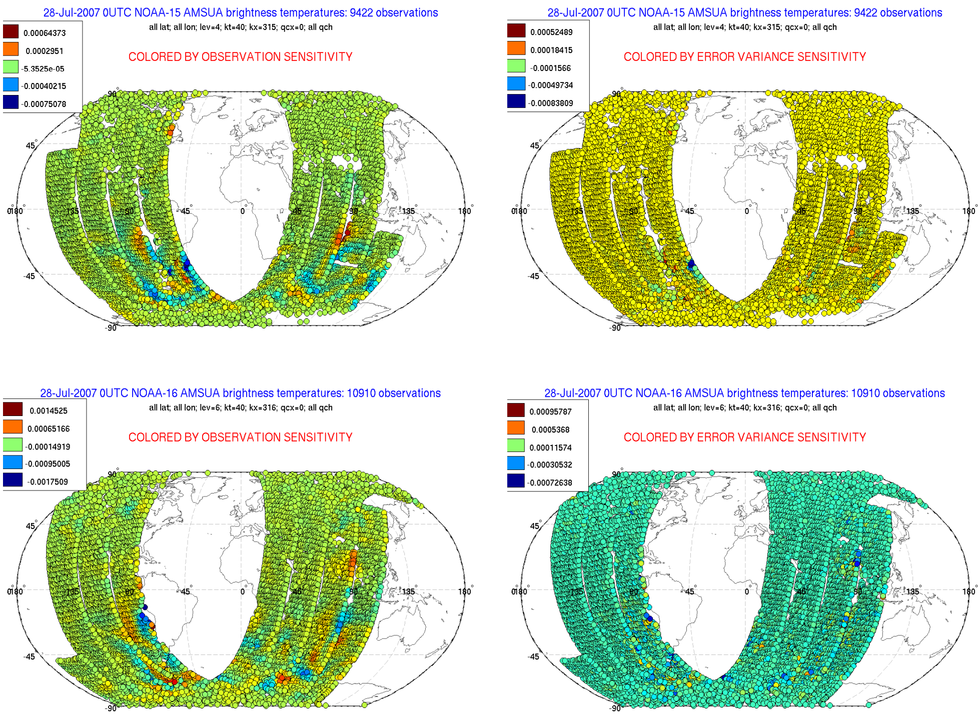

Figure 2: Same as Fig. 1 for NOAA-15 AMSU-A channel 4 radiance data (top row) and for NOAA-16 AMSU-A channel 6 radiance data (bottom row).

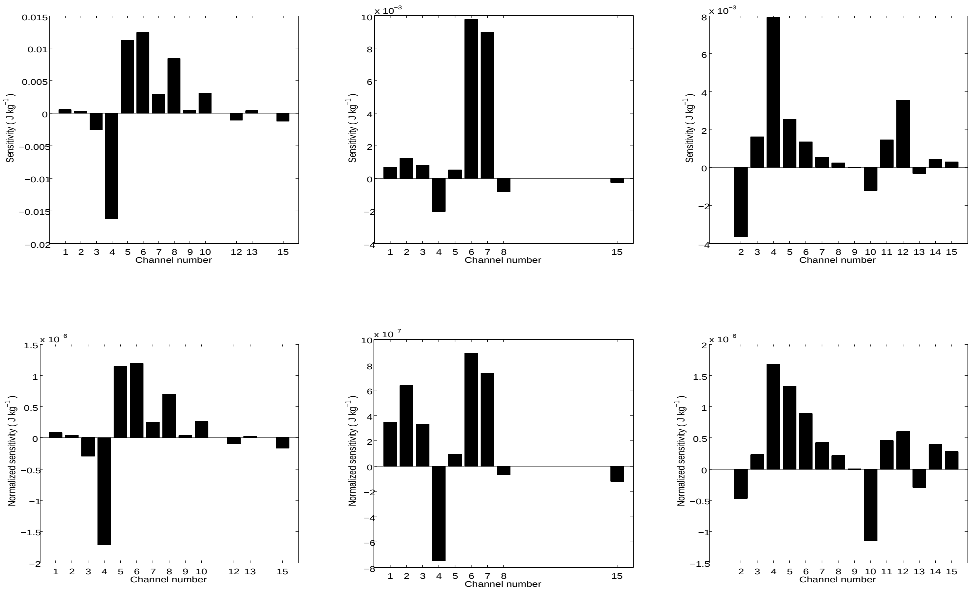

Figure 3: Sensitivity to observation error covariance weighting coefficients per instrument channel for satellite brightness temperature data from NOAA-15 AMSU-A, NOAA-16 AMSU-A, and NOAA-17 HIRS-3 instruments displayed left-to-right, respectively. The bottom row displays the sensitivities normalized by the number of observations per each instrument channel.

data that was incorporated in the assimilation cycle of interest. Radiance data provided by a subset of 281 channels of Aqua AIRS was selected for NWP centers [25] and sensitivity results for data from 152 channels incorporated in the assimilation cycle of interest are provided in Fig. 4. This information may be used to assess the forecast impact as a result of uncertainties in the specification of the error covariances and to provide guidance to error covariance tuning procedures. Deficiencies in the DAS specification of the observation error covariances may be identified by systematically monitoring the forecast sensitivity to error covariance parameters over an increased number of analysis cycles to achieve statistical significance. Large positive (negative) sensitivity values indicate that locally the forecast error aspect is an increasing (decreasing) function of the covariance weighting parameter and outcomes from long-term sensitivity studies may be used to identify the data components where the observation error covariance is overestimated (underestimated). It is emphasized that in the adjoint approach sensitivity information is obtained through a single application of the adjoint-DAS operator at a computational cost roughly equivalent to the cost of performing the analysis and that this information will be difficult to be obtained by other means in VDA. At the same time, the relevance of the adjoint sensitivity is closely determined by the specification of the forecast aspect of interest.

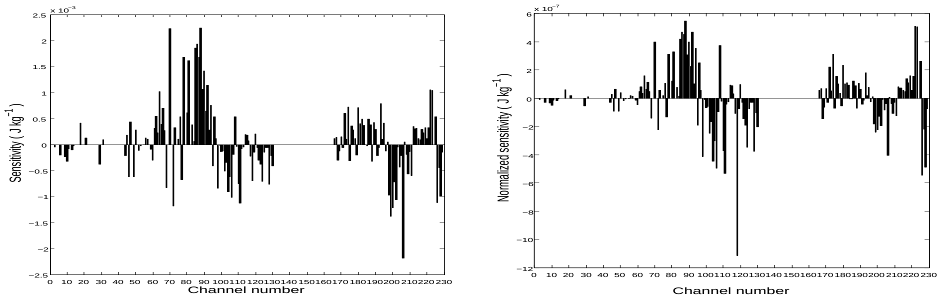

Figure 4: Sensitivity to observation error covariance weighting coefficients per assimilation channel for Aqua AIRS radiance data. The graphic on the right shows sensitivities normalized by the number of observations per each channel.

5. Conclusions and further research

The combined information derived from the adjoint of the forecast model and the adjoint of the data assimilation system make feasible all-at-once estimation of the forecast sensitivity to DAS input parameters. Observation sensitivity techniques are currently used at NWP centers to monitor the short-range forecast performance of observations and this study provided the theoretical aspects and a first illustration of the adjoint-DAS capability to perform sensitivity analysis in the space of input error covariances. A systematic monitoring of the forecast sensitivity to DAS error covariances parameters may be used to identify the observing system components and geographical regions where improved statistical information would be of most benefit to the analysis and forecasts and to provide guidance to parameter tuning procedures.

Modeling background error covariances is an area of intensive research in NWP and the adjoint-DAS approach may be extended to obtain sensitivity information on background error covariance parameters. Proper weighting between the information content of the prior state estimate and of the observational data is necessary to optimize the DAS performance and this is an area where further research is much needed.

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