NOTES AND CORRESPONDENCE

Adjoint Estimation of the Variation in Model Functional Output due to the Assimilation of Data

DACIAN N. DAESCU

Portland State University, Portland, Oregon

RICARDO TODLING*

Global Modeling and Assimilation Office, NASA GSFC, Greenbelt, Maryland

(Manuscript received 20 May 2008, in final form 5 October 2008)

ABSTRACT

A parametric approach to the adjoint estimation of the variation in model functional output due to the assimilation of data is considered as a tool to analyze and develop observation impact measures. The parametric approach is specialized to a linear analysis scheme and it is used to derive various high-order approximation equations. This framework includes the Kalman filter and incremental three-and four-dimensional variational data assimilation schemes implementing a single outer loop iteration. Distinction is made between Taylor series methods and numerical quadrature methods. The novel quadrature approximations require minimal additional software development and are suitable for testing and implementation at operational numerical weather prediction centers where a data assimilation system (DAS) and the associated adjoint DAS are in place. Their potential use as tools for observation impact estimates needs to be further investigated. Preliminary numerical experiments are provided using the fifth-generation NASA Goddard Earth Observing System (GEOS-5) atmospheric DAS.

1. Introduction

An optimal use of the increasing amounts of atmospheric data in numerical weather prediction (NWP) applications and the design of future observing networks require the development of efficient data analysis tools to quantify the value added by observations to a specific data assimilation system (DAS) and model forecast. A judicious assessment of the observation value must account for the data location in the time–space domain, observation type, instrument type, as well as data interaction in the presence of multiple observing systems. Estimation of the observation impact on the short-range model forecast may be performed through observing

DOI: 10.1175/2008MWR2659.1

system experiments (OSEs; Atlas 1997) where selected datasets are systematically added or removed from the assimilation procedure (Kelly et al. 2007). This approach is suitable when the impact of a few data subsets is investigated and becomes computationally prohibitive when the impact of a large number of data subsets or of all individual measurements is considered.

Adjoint-based observation sensitivity, initially developed in NWP as an observation-targeting tool (Baker and Daley 2000; Doerenbecher and Bergot 2001), provides a feasible (all at once) approach to the observation impact estimation for a large variety of datasets and individual observations. Techniques based on observation sensitivity are currently used to monitor the impact of observations provided by the routine observing systems on a selected short-range forecast aspect and to assess the efficiency of various observation-targeting strategies (Fourrié et al. 2002; Langland and Baker 2004; Langland 2005; Gelaro et al. 2007; Zhu and Gelaro 2008). Estimation of observation impact in an ensemble Kalman filter data assimilation scheme is discussed by Liu and Kalnay (2008).

^{*} Additional affiliation: Science Applications International Corporation, Beltsville, Maryland.

Corresponding author address: Dr. Dacian N. Daescu, Department of Mathematics and Statistics, Portland State University, P.O. Box 751, Portland, OR 97207. E-mail: daescu@pdx.edu

The observation impact estimation relies on the chain rule relationship: the change in a scalar forecast measure e (e.g., forecast error) is due to the changes in the initial conditions as a result of the data assimilation procedure. The analyzed forecast is implicitly a function of observations and adjoint modeling is used to provide an explicit estimate of the variation δe in terms of the innovation vector in the observation space.

The necessity of considering higher-than-first-order approximations is discussed by Errico (2007, hereafter E07) and Gelaro et al. (2007, hereafter GZE07) who derive various-order approximation schemes and analyze the results using the fifth-generation National Aeronautics and Space Administration (NASA) Goddard Earth Observing System (GEOS-5) forecast model and DAS. The approach developed by Langland and Baker (2004, hereafter LB04) and first implemented in the Naval Research Laboratory DAS provides an observation impact estimate based on a higher-order approximation to the variation δe in the forecast error (with a third-order error, as shown in E07) by combining adjoint sensitivity gradients from two trajectories: background and analysis. The potential of the nonlinear approximations to introduce ambiguities in the impact estimates of individual observations is investigated in E07 and GZE07. In their studies it is also emphasized that further research in the design of new observation impact measures is required and that a judicious theoretical framework to high-order observation impact estimation is yet to be formulated.

In the present work a parametric approach to the adjoint estimation of the variation in a model functional output due to assimilation of data is considered as a tool to analyze and develop observation impact measures. The parametric approach is specialized to a linear analysis scheme and it is used to derive various δe approximation equations. This framework includes the Kalman filter and incremental three-and four-dimensional variational data assimilation schemes (3DVAR and 4DVAR, respectively) implementing a single outer loop iteration (Daley 1991; Courtier et al. 1994). Distinction is made between the Taylor series methods and numerical quadrature methods. The novel quadrature approximations derived in this study require a minimal additional software development and are suitable for testing and implementation at operational NWP centers where data assimilation schemes and the associated adjoint DAS are in place. Their potential use as tools for observation impact estimates needs to be further investigated.

Section 2 includes a brief review of current adjointbased observation impact measures in data assimilation. The parametric methodology to adjoint estimation of the variation in model functional output due to the assimilation of data is described in section 3; a table of approximation formulas is provided together with an order analysis and the associated error estimates. Preliminary numerical results are presented in section 4 using the NASA GEOS-5 atmospheric DAS. Summary and further research directions are presented in section 5.

2. Adjoint-based observation impact measures

Consider a data assimilation scheme that provides an optimal estimate (analysis) \mathbf{x}_a to the initial conditions of an atmospheric model (Daley 1991; Kalnay 2002)

$$\mathbf{x}_a = \mathbf{x}_b + \mathbf{K}[\mathbf{y} - \mathbf{h}(\mathbf{x}_b)], \tag{1}$$

where \mathbf{x}_b is a background estimate to the initial conditions, \mathbf{y} is the vector of observational data, \mathbf{h} is the observation operator, and

$$\mathbf{K} = \mathbf{B}\mathbf{H}^{\mathrm{T}}[\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}} + \mathbf{R}]^{-1}$$
(2)

is the optimal gain matrix expressed in terms of the background error covariance matrix **B**, the observation error covariance matrix **R**, and the linearized observation operator **H**. Denoting the analysis increment $\delta \mathbf{x}_a = \mathbf{x}_a - \mathbf{x}_b$ and the innovation vector $\delta \mathbf{y} = \mathbf{y} - \mathbf{h}(\mathbf{x}_b)$, the analysis Eq. (1) is written as

$$\delta \mathbf{x}_a = \mathbf{K} \delta \mathbf{y}. \tag{3}$$

The analysis provided by Kalman filter-based methods as well as incremental 3DVAR and 4DVAR schemes implementing a single outer loop iteration is formally expressed as (3).

The observation sensitivity and impact estimation are specific to a forecast aspect of interest. A typical scalar measure of the error in a forecast initiated from \mathbf{x}_0 is defined as (LB04; GZE07)

$$e(\mathbf{x}_0) = (\mathbf{x}_0^f - \mathbf{x}^t)^{\mathrm{T}} \mathbf{C} (\mathbf{x}_0^f - \mathbf{x}^t), \qquad (4)$$

where $\mathbf{x}_0^f = \mathcal{M}(\mathbf{x}_0)$ is the nonlinear model forecast at time *t* initiated at $t_0 < t$ from \mathbf{x}_0 , \mathbf{x}^t is the verifying analysis at time *t*, the superscript T denotes the transpose operator, and **C** is a symmetric and positive definite matrix that defines the metric on the state space (e.g., an appropriate energy norm).

For the purpose of this work we consider a general model functional output $e(\mathbf{x}_0)$, assumed to be a smooth function of the initial conditions. The change in *e* due to assimilation of data is

$$\delta e = e(\mathbf{x}_a) - e(\mathbf{x}_b). \tag{5}$$

In particular, for the forecast error measure (4)

$$\delta e = (\mathbf{x}_a^f - \mathbf{x}^t)^{\mathrm{T}} \mathbf{C} (\mathbf{x}_a^f - \mathbf{x}^t) - (\mathbf{x}_b^f - \mathbf{x}^t)^{\mathrm{T}} \mathbf{C} (\mathbf{x}_b^f - \mathbf{x}^t) \quad (6) \quad a.$$

and the gradient of *e* evaluated at $\mathbf{x}_0 = \mathbf{x}_a$ and $\mathbf{x}_0 = \mathbf{x}_b$ is expressed, respectively, as

$$\nabla_{\mathbf{x}_0} e(\mathbf{x}_a) = 2\mathbf{M}^{\mathrm{T}}(\mathbf{x}_a)\mathbf{C}(\mathbf{x}_a^f - \mathbf{x}^t)$$
(7)

$$\nabla_{\mathbf{x}_0} e(\mathbf{x}_b) = 2\mathbf{M}^{\mathrm{T}}(\mathbf{x}_b)\mathbf{C}(\mathbf{x}_b^f - \mathbf{x}^t).$$
(8)

In Eqs. (7) and (8), $\mathbf{M}^{\mathrm{T}}(\mathbf{x}_{a})$ and $\mathbf{M}^{\mathrm{T}}(\mathbf{x}_{b})$ denote the adjoint of the tangent linear model from t_{0} to t evaluated along the analysis trajectory and background trajectory, respectively. To a first-order approximation, from Eqs. (3) and (5) the variation δe due to assimilation of data \mathbf{y} may be estimated using a linearization around the background \mathbf{x}_{b} :

$$\delta e \approx (\delta \mathbf{x}_a)^{\mathrm{T}} \nabla_{\mathbf{x}_0} e(\mathbf{x}_b) = (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_0} e(\mathbf{x}_b) \stackrel{\mathrm{def}}{=} \delta e_1^b, \quad (9)$$

or, alternatively, using a linearization around the analysis \mathbf{x}_a :

$$\delta e \approx (\delta \mathbf{x}_a)^{\mathrm{T}} \nabla_{\mathbf{x}_0} e(\mathbf{x}_a) = (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_0} e(\mathbf{x}_a) \stackrel{\text{def}}{=} \delta e_1^a.$$
(10)

The measure in (10) has been initially considered for observation impact studies since it relates directly to the concept of observation sensitivity introduced in Baker and Daley (2000). From (1) the analysis sensitivity to observations is expressed as

$$\nabla_{\mathbf{y}}\mathbf{x}_a = \mathbf{K}^{\mathrm{T}}.$$
 (11)

Chain rule differentiation provides the sensitivity of the forecast initiated from \mathbf{x}_a to the observations:

$$\nabla_{\mathbf{y}} e(\mathbf{x}_a) = \nabla_{\mathbf{y}} \mathbf{x}_a \nabla_{\mathbf{x}_0} e(\mathbf{x}_a) = \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_0} e(\mathbf{x}_a)$$
(12)

and from (10) and (12) it follows that

$$\delta e_1^a = (\delta \mathbf{y})^{\mathrm{T}} \nabla_{\mathbf{y}} e(\mathbf{x}_a) \tag{13}$$

such that δe_1^{a} is the inner product in the observation space between the innovation vector and the observation sensitivity vector. The observation impact methodology first introduced in LB04 estimates the variation δe using sensitivity gradients along both background and analysis trajectories:

$$\delta e \approx (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \left[\frac{1}{2} \nabla_{\mathbf{x}_{0}} e(\mathbf{x}_{a}) + \frac{1}{2} \nabla_{\mathbf{x}_{0}} e(\mathbf{x}_{b}) \right] \stackrel{\text{def}}{=} \delta e_{2}^{a,b}, \quad (14)$$

which is a second-order accurate (third-order error) approximation to δe , as shown in E07 and in section 3b below.

a. Remark 1

In the δe -approximation measures derived throughout this work a subscript is used to specify the order of accuracy and a superscript is used to specify the trajectories involved in the computation. In LB04 $\delta e_2^{a,b}$ is denoted δe_3^e , whereas E07 and GZE07 use the notation δe_3 to specify the same expression.

b. Remark 2

From Eqs. (9), (10), and (14) one notices that $\delta e_2^{a,b}$ may be obtained by averaging the first-order approximations δe_1^a and δe_1^b . This property is also reflected in the tables of numerical data provided in GZE07.

With an appropriate definition of the response functional *e*, the measures δe_1^a and $\delta e_2^{a,b}$ have been used by Fourrié et al. (2002), Zhu and Gelaro (2008), Langland and Baker (2004), and Langland (2005) to assess the impact of individual data components in the assimilation scheme by taking the element-wise product between the innovation vector and the corresponding δy amplification factor. The validity and the appropriate use of these approximations as well as the interpretation of the observation impact are thus closely determined by the forecast model \mathcal{M} and the specification of the model functional output *e*. Various-order observation impact measures are analyzed in GZE07, including δe_1^b and $(1/2) \delta e_1^b$. A relationship between the measures $\delta e_2^{a,b}$ and $(1/2) \delta e_1^b$ is further discussed in the appendix.

The experience gained from the above-mentioned studies is that in practice first-order estimates are not accurate approximations to the variation δe in the forecast aspect induced by the assimilation of data. In the next section a parametric approach is considered to obtain high-order δe approximations and it is used to derive various adjoint-based approximation schemes, determine their order of accuracy, and provide the associated error estimates.

3. High-order adjoint-based estimation of δe

Consider a family of suboptimal analyses defined by a parameter *s*, $0 \le s \le 1$:

$$\mathbf{x}(s) \stackrel{\text{def}}{=} \mathbf{x}_b + s(\mathbf{x}_a - \mathbf{x}_b) = \mathbf{x}_b + s\mathbf{K}\delta\mathbf{y}$$
(15)

such that $\mathbf{x}(0) = \mathbf{x}_b$ and $\mathbf{x}(1) = \mathbf{x}_a$. The midpoint of the segment from \mathbf{x}_b to \mathbf{x}_a is denoted as

$$\mathbf{x}(1/2) = \frac{1}{2}(\mathbf{x}_b + \mathbf{x}_a) \stackrel{\text{def}}{=} \mathbf{x}_{(a+b)/2}.$$
 (16)

Corresponding to (15) and to the model functional output e we associate the function defined as

$$\hat{e}:[0,1] \to \mathbb{R}, \quad \hat{e}(s) \stackrel{\text{def}}{=} e[\mathbf{x}(s)].$$
 (17)

As the parameter *s* describes the segment [0, 1] on the real axis, $\mathbf{x}(s)$ describes the segment from \mathbf{x}_b to \mathbf{x}_a in the state space; accordingly, the function \hat{e} evolves from $\hat{e}(0)$ to $\hat{e}(1)$ and the model functional output evolves from $e(\mathbf{x}_b)$ to $e(\mathbf{x}_a)$ such that the variation $\delta \hat{e}$ is identical to the variation δe :

$$\delta \hat{e} = \hat{e}(1) - \hat{e}(0) = e(\mathbf{x}_a) - e(\mathbf{x}_b) = \delta e.$$
(18)

The process is illustrated in Fig. 1. Taking into account that $\mathbf{x}(s)$ depends linearly on *s* and has a constant derivative:

$$\mathbf{x}'(s) = \mathbf{K}\delta \mathbf{y}, \quad \text{for } 0 \le s \le 1, \tag{19}$$

from (17) and (19) using chain rule differentiation the first- and second-order derivatives of \hat{e} are expressed, respectively, as

$$\hat{e}'(s) = (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_0} e[\mathbf{x}(s)], \text{ for } 0 \le s \le 1, \text{ and } (20)$$

$$\hat{e}''(s) = (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_0}^2 e[\mathbf{x}(s)] \mathbf{K} \delta \mathbf{y}, \quad \text{for } 0 \le s \le 1, \quad (21)$$

where $\nabla_{\mathbf{x}_0}^2 e[\mathbf{x}(s)]$ denotes the Hessian matrix of *e* with respect to initial conditions, evaluated at $\mathbf{x}(s)$. In particular,

$$\hat{e}'(0) = (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_{0}} e(\mathbf{x}_{b}), \quad \hat{e}''(0) = (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_{0}}^{2} e(\mathbf{x}_{b}) \mathbf{K} \delta \mathbf{y},$$
(22)

and



FIG. 1. Illustration of the parametric approach for estimating the variation in the model's functional output induced by assimilation of data.

$$\hat{e}'(1) = (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_{0}} e(\mathbf{x}_{a}), \quad \hat{e}''(1) = (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_{0}}^{2} e(\mathbf{x}_{a}) \mathbf{K} \delta \mathbf{y}.$$
(23)

In general, the *m*-order derivatives of \hat{e} are expressed in terms of the gain matrix **K**, the innovation vector $\delta \mathbf{y}$, and the *m*-order derivatives of the functional *e* with respect to initial conditions, evaluated at $\mathbf{x}(s)$:

$$\hat{e}^m(s) = \nabla^m_{\mathbf{x}_0} e[\mathbf{x}(s)] (\mathbf{K} \delta \mathbf{y})^m, \quad \text{for } 0 \le s \le 1, \qquad (24)$$

where the right-hand-side term in (24) is defined recursively as

$$\nabla_{\mathbf{x}_0} e[\mathbf{x}(s)] (\mathbf{K} \delta \mathbf{y}) = (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_0} e[\mathbf{x}(s)], \text{ and}$$

$$\nabla_{\mathbf{x}_0}^m e[\mathbf{x}(s)] (\mathbf{K} \delta \mathbf{y})^m = (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_0} \{\nabla_{\mathbf{x}_0}^{m-1} e[\mathbf{x}(s)] (\mathbf{K} \delta \mathbf{y})^{m-1}\}, \text{ for } m \ge 2$$

a. Remark 3

If the forecast model is linear, $\mathcal{M} = \mathbf{M}$, and a quadratic functional output in (4) is considered then the Hessian $\nabla_{\mathbf{x}_0}^2 e$ is a state-independent matrix:

$$\nabla_{\mathbf{x}_0}^2 e = 2\mathbf{M}^{\mathrm{T}}\mathbf{C}\mathbf{M}.$$
 (25)

b. The δ*e*-*approximation equations and their error estimates*

The fundamental theorem of calculus:

$$\hat{e}(1) - \hat{e}(0) = \int_0^1 \hat{e}'(s) ds$$
 (26)

together with the relationship in (18) and Eqs. (20)–(24) are used next to derive several high-order approximations to δe and to provide the associated error estimates based on Taylor series and the theory of numerical integration (Atkinson 1988). The error in the δe approximation is expressed in terms of high-order derivatives of e with respect to the initial conditions evaluated at a certain point $x(\tau)$, $0 \le \tau \le 1$ in the state space, specific to each measure.

- 1) Approximations based on Taylor series at \mathbf{x}_{b} .
 - (i) First-order accurate: $\hat{e}(1) \hat{e}(0) = \hat{e}'(0) + 1/2\hat{e}''(\tau)$,

$$\delta e_1^b = (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_0} e(\mathbf{x}_b), \text{ and } (27)$$

$$\delta e - \delta e_1^b = \frac{1}{2} (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_0}^2 e[\mathbf{x}(\tau)] \mathbf{K} \delta \mathbf{y}.$$
 (28)

(ii) Second-order accurate: $\hat{e}(1) - \hat{e}(0) = \hat{e}'(0) + 1/2\hat{e}''(0) + 1/6\hat{e}'''(\tau),$

$$\delta e_2^b = (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_0} e(\mathbf{x}_b) + \frac{1}{2} (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_0}^2 e(\mathbf{x}_b) \mathbf{K} \delta \mathbf{y}, \text{ and } (29)$$

$$\delta e - \delta e_2^b = \frac{1}{6} \nabla_{\mathbf{x}_0}^3 e[\mathbf{x}(\tau)] (\mathbf{K} \delta \mathbf{y})^3.$$
(30)

2) Approximations based on Taylor series at \mathbf{x}_a .

(i) First-order accurate: $\hat{e}(1) - \hat{e}(0) = \hat{e}'(1) - 1/2\hat{e}''(\tau)$,

$$\delta e_1^a = (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_0} e(\mathbf{x}_a), \text{ and } (31)$$

$$\delta e - \delta e_1^a = -\frac{1}{2} (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_0}^2 e[\mathbf{x}(\tau)] \mathbf{K} \delta \mathbf{y}.$$
(32)

(ii) Second-order accurate: $\hat{e}(1) - \hat{e}(0) = \hat{e}'(1) - 1/2\hat{e}''(1) + 1/6\hat{e}'''(\tau),$

$$\delta e_2^a = (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_0} e(\mathbf{x}_a) - \frac{1}{2} (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_0}^2 e(\mathbf{x}_a) \mathbf{K} \delta \mathbf{y}, \text{ and } (33)$$

$$\delta e - \delta e_2^a = \frac{1}{6} \nabla_{\mathbf{x}_0}^3 e[\mathbf{x}(\tau)] (\mathbf{K} \delta \mathbf{y})^3.$$
(34)

3) Approximations based on numerical quadrature schemes.

Numerical quadrature schemes applied to (26) provide a δe approximation:

- (i) Second-order accurate:
- (a) Trapezoidal rule (LB04):

$$\int_{0}^{1} \hat{e}'(s) ds = \frac{1}{2} [\hat{e}'(0) + \hat{e}'(1)] - \frac{1}{12} \hat{e}'''(\tau),$$

$$\delta e_{2}^{a,b} = \frac{1}{2} [\hat{e}'(0) + \hat{e}'(1)]$$

$$= (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \frac{1}{2} [\nabla_{\mathbf{x}_{0}} e(\mathbf{x}_{b}) + \nabla_{\mathbf{x}_{0}} e(\mathbf{x}_{a})], \text{ and}$$
(35)

$$\delta e - e_2^{a,b} = -\frac{1}{12} \hat{e}'''(\tau) = -\frac{1}{12} \nabla^3_{\mathbf{x}_0} e[\mathbf{x}(\tau)] (\mathbf{K} \delta \mathbf{y})^3.$$
(36)

(b) Midpoint rule:

$$\int_{0}^{1} \hat{e}'(s) ds = \hat{e}'(1/2) + \frac{1}{24} \hat{e}'''(\tau),$$

$$\delta e_{2}^{(a+b)/2} = \hat{e}'(1/2) = (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_{0}} e[\mathbf{x}_{(a+b)/2}], \text{ and } (37)$$

$$\delta e - \delta e_2^{(a+b)/2} = \frac{1}{24} \hat{e}'''(\tau) = \frac{1}{24} \nabla_{\mathbf{x}_0}^3 e[\mathbf{x}(\tau)] (\mathbf{K} \delta \mathbf{y})^3.$$
(38)

(ii) Fourth-order accurate (Simpson's rule):

$$\int_{0}^{1} \hat{e}'(s)ds = \frac{1}{6} [\hat{e}'(0) + 4\hat{e}'(1/2) + \hat{e}'(1)] - \frac{1}{2880} \hat{e}^{5}(\tau),$$

$$\delta e_{4}^{a,b,(a+b)/2} = \frac{1}{6} [\hat{e}'(0) + 4\hat{e}'(1/2) + \hat{e}'(1)]$$

$$= (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \frac{1}{6} \{ \nabla_{\mathbf{x}_{0}} e(\mathbf{x}_{b}) + 4 \nabla_{\mathbf{x}_{0}} e[\mathbf{x}_{(a+b)/2}] + \nabla_{\mathbf{x}_{0}} e(\mathbf{x}_{a}) \}, \text{ and}$$
(39)

$$\delta e - \delta e_4^{a,b,(a+b)/2} = -\frac{1}{2880} \hat{e}^5(\tau)$$

= $-\frac{1}{2880} \nabla_{\mathbf{x}_0}^5 e[\mathbf{x}(\tau)] (\mathbf{K} \delta \mathbf{y})^5.$ (40)

A summary of the adjoint-based approximations to the variation δe in the model functional output due to assimilation of data using a linear analysis scheme is in Table 1.

c. Computational aspects and discussion

Theoretically, δe -approximation formulas of any order may be derived using both Taylor series and numerical quadrature; however, only the quadrature

TABLE 1. Adjoint-based δe approximations in a linear data assimilation scheme. A subscript is used to specify the order of accuracy of the approximation and a superscript is used to specify the trajectories involved in the computation.

| Measure | Equation | | | | | | |
|----------------------------|--|--|--|--|--|--|--|
| | Taylor series | | | | | | |
| δe_1^b | $(\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_{0}} e(\mathbf{x}_{b})$ | | | | | | |
| $\delta e_1^{\dot{a}}$ | $(\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_{0}} e(\mathbf{x}_{a})$ | | | | | | |
| $\delta e_2^{\bar{b}}$ | $(\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_{0}} e(\mathbf{x}_{b}) + (1/2) (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_{0}}^{2} e(\mathbf{x}_{b}) \mathbf{K} \delta \mathbf{y}$ | | | | | | |
| $\delta e_2^{\tilde{a}}$ | $(\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_{0}} e(\mathbf{x}_{a}) - (1/2) (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_{0}}^{2^{\circ}} e(\mathbf{x}_{a}) \mathbf{K} \delta \mathbf{y}$ | | | | | | |
| Numerical quadrature | | | | | | | |
| $\delta e_2^{a,b}$ | $(\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}}(1/2) [\nabla_{\mathbf{x}_{0}} e(\mathbf{x}_{b}) + \nabla_{\mathbf{x}_{0}} e(\mathbf{x}_{a})]$ | | | | | | |
| $\delta e_2^{(a+b)/2}$ | $(\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}_{0}} e[\mathbf{x}_{(a+b)/2}]$ | | | | | | |
| $\delta e_4^{a,b,(a+b)/2}$ | $(\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}}(1/6) \{ \nabla_{\mathbf{x}_{0}} e(\mathbf{x}_{b}) + 4 \nabla_{\mathbf{x}_{0}} e[\mathbf{x}_{(a+b)/2}] + \nabla_{\mathbf{x}_{0}} e(\mathbf{x}_{a}) \}$ | | | | | | |

approach is (currently) feasible for the practical implementation of high-order estimates. Taylor series approximations to δe are expressed explicitly in terms of the innovation vector and derivatives at one of the endpoints \mathbf{x}_b or \mathbf{x}_a . The equations of the second-order accurate approximations δe_2^b and δe_2^a clearly illustrate the presence of the innovation-component cross products $(\delta y)_i (\delta y)_i$ in the higher-than-first-order estimates. The quadrature schemes make use of information from both end nodes \mathbf{x}_b and \mathbf{x}_a such that implicitly the $\delta \mathbf{y}$ amplification factor associated to these schemes depends on all $\delta y'$ s components. Whether or not this trade-off may result in potential ambiguities when highorder δe approximations are used to assess the impact of individual observation components needs to be further investigated (GZE07).

The Hessian-vector products involved in the secondorder Taylor series may be evaluated with a secondorder adjoint model (Le Dimet et al. 2002) or approximated by gradient differences, for example, $\nabla_{\mathbf{x}_0}^2 e(\mathbf{x}) \, \delta \mathbf{x}_a \approx [\nabla_{\mathbf{x}_0} e(\mathbf{x} + \epsilon \delta \mathbf{x}_a) - \nabla_{\mathbf{x}_0} e(\mathbf{x})]/\epsilon$. Increasing the accuracy of quadrature approximations requires only additional adjoint model integrations along trajectories properly initiated on the segment from \mathbf{x}_b to \mathbf{x}_a . The midpoint in Eq. (37) provides a second-order accurate estimation to δe using a single gradient that is evaluated along the model trajectory initiated from $\mathbf{x}_{(a+b)/2}$. This point defined by (16) is obtained at virtually no additional computational cost once the analysis \mathbf{x}_a is available and, given the error estimates in (36) and (38), $\delta e_2^{(a+b)/2}$ may provide a potentially more accurate approximation to δe than the measure $\delta e_2^{a,b}$. Associated with the functional output (4), the measure $\delta e_2^{(a+b)/2}$ is

$$\delta e_2^{(a+b)/2} = 2(\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \mathbf{M}^{\mathrm{T}} [\mathbf{x}_{(a+b)/2}] \mathbf{C} [\mathbf{x}_{(a+b)/2}^f - \mathbf{x}^t], \quad (41)$$

where $\mathbf{x}_{(a+b)/2}^{f}$ is the forecast initiated from the midpoint $\mathbf{x}_{(a+b)/2}$ and $\mathbf{M}^{\mathrm{T}}[\mathbf{x}_{(a+b)/2}]$ is the adjoint model evaluated along the midpoint trajectory. In practice, when forecasts are issued for every analysis time, the state trajectories initiated from the background \mathbf{x}_b and the analysis \mathbf{x}_a can easily be made available, whereas obtaining the midpoint trajectory requires an additional run of the nonlinear forecast model. However, calculation of midpoint observation impact estimate requires only a single integration with the adjoint model \mathbf{M}^{T} , whereas the trapezoidal estimate requires two such integrations. The computational cost of implementing $\delta e_2^{(a+b)/2}$ is thus roughly equivalent to the cost of implementing $\delta e_2^{a,b}$. The midpoint calculation may become more desirable in certain situations for instance, when using the impact calculation to tune an Observation System Simulation Experiment (OSSE; R. M. Errico 2008, personal communication). In this case, forecasts are only issued with the sole purpose of calculating observation impact estimates, and therefore one might as well avoid the extra adjoint model integration required to calculate the trapezoidal expression.

The Simpson's rule in Eq. (39) gives a fourth-order accurate (fifth-order error) estimate to δe at the expense of only one additional forecast and adjoint model integration, as compared to the second-order accurate estimate $\delta e_2^{a,b}$. This measure provides a feasible tool for validating the observation sensitivity computations and for assessing the impact of the nonlinearities on the errors in the lower-order approximations.

The error estimates provided in this section show that the accuracy of the δe approximation measures depends on the innovation vector δy , the DAS **K**, the functional aspect *e*, the adjoint **M**^T, and the high-order derivatives of the nonlinear forecast model. Theoretically, for linear dynamics and quadratic functional output all second-andhigher-order accurate measures derived in this study provide the exact value of the variation δe and identical results when used for observation impact assessment.

To our knowledge, the measures in (37) and (39) have not been previously considered for estimating the observation impact and whether or not these measures may provide viable tools for practical applications to observation impact studies needs to be further investigated. Their implementation requires no additional software development as compared, for example, to the observation impact estimates based on the $\delta e_2^{a,b}$ measure and testing may be easily performed at operational NWP centers.

4. Illustrative numerical experiments

Preliminary numerical experiments are provided to illustrate the parametric approach to the analysis and design of observation impact measures using GEOS-5 (Rienecker et al. 2008). GEOS-5 assimilates observations using the incremental analysis update technique of Bloom et al. (1996). It consists of a global atmospheric model developed at Goddard and an analysis system developed jointly by the National Centers for Environmental Prediction (NCEP) and the NASA Global Modeling and Assimilation Office (GMAO). The atmospheric general circulation model (GCM) of GEOS-5 retains an updated version of the finite-volume hydrostatic dynamical core (Lin 2004) from its predecessor GEOS-4. The GEOS-5 GCM is built under the infrastructure of the Earth System Modeling Framework (Collins et al. 2005) used to couple together various physics packages including a modified version of the relaxed Arakawa-Schubert convective parameterization

scheme of Moorthi and Suarez (1992), the catchmentbased hydrological model of Koster et al. (2000), the multilayer snow model of Stieglitz et al. (2001), and the radiative transfer model of Chou and Suarez (1999). Furthermore, the GCM is accompanied by its adjoint model (ADM), which is essentially the ADM of the finite-volume dynamical core GEOS-4 (Giering et al. 2003), with added vertical diffusion and polar filter (Errico et al. 2007).

The GEOS-5 analysis component consists of the gridpoint statistical interpolation (GSI) system. The GSI implements a 3DVAR using the incremental approach of Courtier et al. (1994) for minimization with the preconditioning strategy of Derber and Rosati (1989). The background error covariance is implemented as a series of recursive filters producing nearly Gaussian and isotropic correlation functions (Wu et al. 2002). Satellite radiances are processed using the Community Radiative Transfer Model (CRTM; Kleespies et al. 2004) and bias corrected online following the algorithm of Derber and Wu (1998). Furthermore, the GSI used in the experiments here includes the adjoint capability of Trémolet (2007, 2008).

This adjoint of GSI differs from its previous incarnation in Zhu and Gelaro (2008) in that it is not a line-by-line adjoint, but rather it is derived from a swap of operations used in the forward GSI. Combining the GSI adjoint with the GCM adjoint, GEOS-5 has all the ingredients to calculate the approximations discussed earlier.

Two sets of experiments were performed and the results are discussed in what follows. In the first experimental setup, hereafter referred to as DAS-1, for compatibility with the assumptions in the theory presented in the previous sections, we replace the GEOS-5 two outer loop GSI-based 3DVAR with a single outer loop. In this way nonlinearities in the observation operator and therefore in the K operator are avoided. Accordingly, when the analysis adjoint is used, this first experiment, only executes a single outer loop of the adjoint analysis. The second experimental setup, hereafter referred to as DAS-2, leaves the default settings of the analysis minimization untouched, therefore using two outer loops to calculate analysis increments at each synoptic time. This experiment essentially ignores the fact that K is indeed nonlinear. In the DAS-1 setup firstorder Taylor series and second-order quadrature measures in Table 1 are implemented for a single forecast in early February 2007; experiments in the DAS-2 setup compare δe to the trapezoidal and midpoint approximations and the observation impact estimations provided by these measures for a full month of forecasts, valid at 0000 UTC, in August 2007. All experiments are performed at a horizontal resolution of $2.5^{\circ} \times 2^{\circ}$ with 72 hybrid levels in the vertical. The model functional aspect is specified as the 24-h forecast error in (4) with a diagonal matrix **C** taken such that e measures the 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.

Over the time periods of interest, GEOS-5 DAS assimilates observations from the conventional network: radiosondes; wind profilers, pilot balloon (PIBAL) winds, Aircraft to Satellite Data Relay (ASDAR) and Meteorological Data Collection and Reporting System (MDCARS) aircraft wind and temperature reports, Next Generation Weather Radar (NEXRAD) radar winds, dropsonde winds, paid observations (PAOB) surface pressure, Geostationary Meteorological Satellite (GMS), and Meteorological Satellite (Meteosat) cloud drift infrared (IR) and visible winds, Moderate Resolution Imaging Spectroradiometer (MODIS) clear-sky and water vapor winds, Geostationary Operational Environmental Satellite (GOES) cloud drift IR and water vapor cloud-top winds, surface land observations, Special Sensor Microwave Imager (SSM/I) rain rates and wind speeds, Tropical Rainfall Measuring Mission (TRMM) Microwave Imager (TMI) rain rates, and Quick Scatterometer (QuikSCAT) wind speeds and directions. Satellite radiances include the following: the Television and Infrared Observation Satellite (TIROS) Operational Vertical Sounder (TOVS) level 1b Advanced Microwave Sounding Unit-A (AMSU-A) from the National Oceanic and Atmospheric Administration (NOAA) satellites NOAA-15, NOAA-16, and NOAA-18; AMSU-B from NOAA-15, NOAA-16, and NOAA-17; High Resolution Infrared Radiation Sounder-2 (HIRS-2) from NOAA-14; HIRS-3 from NOAA-16 and NOAA-17; Microwave Sounding Unit (MSU) from NOAA-14; Earth Observing Satellite (EOS) Aqua level 1b radiances Atmospheric Infrared Sounder (AIRS) and AMSU-A; GOES-10 and GOES-12 sounders brightness temperatures; and Solar Backscatter Ultraviolet-2 (SBUV-2; version 6) layer and total column ozone from NOAA-16.

a. Results in the DAS-1 setup

In the DAS-1 setup the analysis state \mathbf{x}_a is obtained by assimilation of data valid at 0000 UTC 1 February 2007 and the verifying state \mathbf{x}^t is provided at 0000 UTC 2 February 2007 by performing 6-h analysis cycles.

The parametric approach may be used to identify appropriate δe -approximation measures and to quantify the approximation error introduced by the evaluation of the derivatives in the observation space. Theoretically, given the relationships (18) and (20), approximations based on derivatives estimated in the parameter space are equivalent to approximations based on derivatives estimated in the observation space. As an alternative to (20), from (17) the derivatives $\hat{e}'(s)$ may be estimated from nonlinear model forecasts and finite-difference schemes. The graphs of the function $\hat{e}(s)$ and of the derivative $\hat{e}'(s)$ as the parameter s spans the interval [01] are displayed in Fig. 2. This information was obtained using nonlinear model forecasts initiated from $\mathbf{x}(s) = \mathbf{x}_b + \mathbf{x}_b$ $s\delta \mathbf{x}_a$ to evaluate $\hat{e}(s) = e[\mathbf{x}(s)]$ at an s increment of 0.1 (a total of 11 forecasts were performed) and second-order accurate finite-difference schemes to estimate $\hat{e}'(s)$. At parameter value s = 0, $\hat{e}(0) = e(\mathbf{x}_b)$, and the average forecast error was found to be $e(\mathbf{x}_b) = 9.80 \text{ J kg}^{-1}$. At parameter value s = 1, $\hat{e}(1) = e(\mathbf{x}_a)$ and the average forecast error was found to be $e(\mathbf{x}_a) = 6.75 \text{ J kg}^{-1}$. The average forecast error reduction $\delta e = -3.05 \text{ J kg}^{-1}$ is the overall impact of the observations in the data assimilation scheme, indicative of the effectiveness of assimilating observations as measured by the (dry) total energy norm. Insight on the δe -approximation measures is provided by the graph of the derivative $\hat{e}'(s)$ in Fig. 2. The first-order measure δe_1^b approximates $\hat{e}'(s)$ in (26) by the constant value $\hat{e}'(0)$, whereas δe_1^a approximates $\hat{e}'(s)$ by the constant value $\hat{e}'(1)$. The derivative $\hat{e}'(s)$ exhibits a linear dependence on the parameter s and indicates that $\hat{e}(s)$ is close to a quadratic function. Second-order measures are thus appropriate and are expected to provide accurate δe approximations in these experiments.

It must be emphasized that the functionals $\hat{e}(s)$ and $\hat{e}'(s)$ provide only information regarding the approximation properties of the δe measures and that observation impact studies require an observation-space evaluation of the derivatives. In practice, the accuracy in the adjoint-based δe approximations is impaired by various simplifications used in the derivation and implementation of the adjoint model \mathbf{M}^{T} and/or the adjoint DAS operator \mathbf{K}^{T} . For example, the adjoint model is

often run at a coarse resolution, as compared to the nonlinear forecast model, and may not properly account for moist physics or nonlinearities in the dry dynamics (LB04). Issues in the development of an adjoint DAS that is fully consistent to the assimilation scheme are discussed in the work of Zhu and Gelaro (2008).

Table 2 provides the values of various δe approximations based on finite-difference derivative estimates in the parameter space and adjoint-based derivatives in the observation space. It is noticed that the secondorder measures based on finite-difference derivative estimation in the parameter space provided accurate approximations, whereas the observation-space computation of the derivatives introduced an approximation error of \sim 30%. Relative errors of similar magnitude were reported in LB04 and GZE07. The adjoint relationship between the operators \mathbf{K} and \mathbf{K}^{T} was checked and proved to be valid and evaluating the δe measures in the state space did not improved the estimates. Therefore, the increased uncertainty in the adjoint-based secondorder δe approximations is mainly due to inconsistencies between the nonlinear forecast model and the implementation of the adjoint model \mathbf{M}^{T} .

First- and second-order adjoint-based observation impact estimates and the corresponding estimates of the contribution of various observing system components to the average forecast error reduction are provided in Fig. 3. The observation impact is largely overestimated in the measure δe_1^b and largely underestimated in the measure δe_1^{a} . The second-order quadrature measures $\delta e_2^{a,b}$ and δe_2^{a+b} provided consistent estimates of the impact of each observing system component. Based on the second-order estimates, the largest percentage contribution to the forecast error reduction is attributed to the radiance data (45%) and wind data (37%) followed by the temperature (12%) and surface pressure data (5%).



FIG. 2. Evolution of the average forecast error function (left) $\hat{e}(s)$ and (right) its derivative $\hat{e}'(s)$ as the parameter *s* spans the interval [0 1].

TABLE 2. Approximations to the average forecast error reduction δe (J kg⁻¹) based on finite-difference derivative estimates in the parameter space and adjoint-based derivative estimates in the observation space.

| δe | Derivative estimation | δe_1^b | δe_1^a | $\delta e_2^{a,b}$ | $\delta e_2^{(a+b)/2}$ | $\delta e_4^{a,b,(a+b)/2}$ |
|-------|------------------------------------|------------------|------------------|--------------------|------------------------|----------------------------|
| -3.05 | Finite difference Adjoint based | $-4.66 \\ -5.88$ | $-1.32 \\ -2.06$ | -2.99 -3.97 | $-3.06 \\ -4.04$ | -3.04 -4.02 |

The impact of other observations in the assimilation scheme such as humidity and ozone data was estimated to be less than 0.5%. Estimates based on the fourth-order measure $\delta e_4^{a,b,(a+b)/2}$ (not shown) were in close agreement to the second-order estimates and it is noticed that $\delta e_4^{a,b,(a+b)/2} = 1/3\delta e_2^{a,b} + 2/3\delta e_2^{(a+b)/2}$. The use of the fourth-order measure may be of interest in assessing the observation impact on forecasts beyond 24 h when nonlinearities in the model forecast may result in a large deviation from quadratic of the forecast error aspect.

b. Results in the DAS-2 setup

Our second illustration involves evaluating the trapezoidal and midpoint estimates for the calculation of observation impact on the 24-h forecasts, valid at 0000 UTC, over the month of August 2007. Aside from resolution, this experiment mimics precisely the normal mode of execution of GEOS-5 DAS, where in particular, the analysis uses two outer loops for its minimization. Figure 4 shows the time series of the actual forecast error reduction δe (thin line) calculated directly from the differences between the 24-h forecasts with the corresponding verifications (analyzes), where the fore-



FIG. 3. First- and second-order adjoint-based estimations of the observation impact on the average forecast error reduction. The estimated impact of all observations (all) and of observing system components including radiances (rad), winds (uv), temperatures (temp), and surface pressures (spr). Units are J kg⁻¹.



FIG. 4. Time series of forecast error reduction in GEOS-5 due to assimilation of observations for 0000 UTC 24-h forecasts in August 2007. The thin line shows the actual error reduction, the *X*-marked line shows the estimate error reduction calculated using the trapezoidal formula, and the *O*-marked line shows the case in which the midpoint formula is used instead. Units are J kg⁻¹.

cast errors are evaluated in terms of total (dry) energy. The actual forecast error reduction shown here is similar to that shown in Fig. 1 of GZE07, but now for a different time period. The 1-day forecast error reduction due to the assimilation of observations oscillates between 1 and 3.5 J kg⁻¹, with the negative sign indicating that the assimilation of observations improved the forecasts as a whole. Estimates from the secondorder quadrature measures $\delta e_2^{a,b}$ (trapezoidal) and $\delta e_2^{(a+b)/2}$ (midpoint) are also displayed in Fig. 4, as indicated by the X- and O-marked lines, respectively. Both estimates are quite close to each other, and are reasonable approximations to the actual error reduction. At times, the trapezoidal calculation tends to get closer to the actual error reduction than the midpoint; at other times, this seems to reverse. Both estimates here are closer to the actual error reduction than what appears in GZE07. This is attributed mainly to the way the line-by-line adjoint of Zhu and Gelaro handles the analysis outer loop versus the adjoint of Trémolet (2007, 2008).

A more detailed examination is shown in Fig. 5 where the contribution of various observing systems to the forecast error reduction is displayed. The black bars are for the trapezoidal estimates; and the clear bars are for the midpoint estimates. Figure 5a shows the observation impacts in J kg⁻¹, and Figure 5b shows the fractional observational impacts (i.e., the observation impacts divided by the total estimate and multiplied by 100). Both estimates are completely consistent. For example, they both show AMSU-A being the dominant observing system when it comes to impacting the 24-h forecasts,



FIG. 5. (a) Estimate observation impact $(J \text{ kg}^{-1})$ and (b) fractional observation impact (%) for various instruments for all 0000 UTC 24-h forecasts in August 2007. The black bars are for trapezoidal estimates; the clear bars are for midpoint estimates. The abbreviations along the vertical axis indicate different types of observations: Ships, ships and buoy temperature, wind-specific humidity, and near-surface pressure; SatWind, cloud-drift winds; SSMIspd, Special Sensor Microwave Imager wind speeds; SBUV2, backscatter ultraviolet instrument total column ozone; RaobDsnd, radiosonde and dropsonde temperature, winds, specific humidity; Qscat, Scatterometer winds; MODIS, Moderate-resolution Imaging Spectroradiometer clear-sky and water vapor winds; LandSfc, land observations of temperature, winds, surface pressure, and specific humidity; HIRS, radiances from the HIRS-3 from *NOAA-16* and *-17*; GOESND, radiances from the GOES; Aircraft, aircraft temperature and winds; AMSUA, radiances from the AMSU-A on the *NOAA-15*, *-16*, and *-17*, as well as on *Aqua*; AIRS, NASA *Aqua*, AIRS radiances.

followed by the radiosonde and dropsonde observations. The trapezoidal estimate sees AMSU-A contributing slightly less than the midpoint estimate; and reversely, the midpoint estimate sees the radiosonde and dropsonde network contributing slightly more to the reduction in forecast error than the trapezoidal estimate. These small differences between the two estimates become even less noticeable when considering the fractional impact (Fig. 5b). For all practical purposes, the existing subtle differences between the two estimates are negligible, particularly when viewed in the context of approximations such as the nonlinearity of **K** and the lack of physics in the adjoint, to cite a few.

5. Conclusions and further work

This study provides insight on the adjoint-based observation impact measures implemented in NWP and contributes toward the development of a judicious theoretical framework to high-order observation impact estimates. In E07 it was first noticed that the δy -amplification factor in the LB04 observation impact measure is not per se a gradient, but a weighted combination of two gradients and that a proper interpretation of this term needs to be further investigated. The parametric approach allows an interpretation and analysis of the LB04 measure as a quadrature scheme to express the variation in the model functional output due to the assimilation of data. Approximation formulas associated with standard numerical integration schemes were provided together with their order of accuracy and error estimates. The parametric approach provides a tool to assess the approximation properties of the δe measures using nonlinear model forecasts. In practice, the accuracy of high-order adjoint-based measures is limited by the deficiencies in the current adjoint forecast models (e.g., moist physical processes are not properly incorporated in the adjoint model).

An attractive feature of the quadrature methods is that high-order δe approximations may be derived using gradients evaluated along trajectories properly initiated on the segment from \mathbf{x}_b to \mathbf{x}_a . Their potential drawback is that information from both ends of the integration interval is involved in the approximation formulas. Whether or not ambiguities are introduced when these schemes are used to estimate the impact of individual observations in the DAS needs to be further investigated and a judicious validation using OSEs needs to be performed.

The theoretical framework developed in this work is specialized to a linear analysis scheme and further research is needed in the design and implementation of high-order observation impact measures in nonlinear data assimilation. Computation of observation sensitivity and observation impact estimation in variational data assimilation (VDA) schemes with multiple outer loops is presented in the work of Trémolet (2008). The sensitivity equations of a 4DVAR DAS are discussed by Daescu (2008). An extension of the parametric approach to derive high-order δe -approximation measures for observation impact estimates in a nonlinear VDA scheme may be formulated using continuation theory for solving nonlinear equations and optimization problems (Ortega and Rheinboldt 1970; Watson 2000; Dunlavy and O'Leary 2005) and it will be provided in a subsequent study.

Acknowledgments. The numerical results in this work were obtained on the Linux Explore System through a cooperation with the NASA Center for Computational Sciences at Goddard Space Flight Center. The work of D. N. Daescu was supported by the NASA Modeling, Analysis, and Prediction Program under Award NNG06GC67G. The work of R. Todling was partially supported by the Atmospheric Data Assimilation Development component of the NASA Modeling, Analysis, and Prediction Program (MAP/04-0000-0080). We thank two anonymous reviewers whose thoughtful comments and suggestions helped to improve the manuscript.

APPENDIX

On the Observation Impact Measure (1/2) δe_1^b

In the study of GZE07 using the forecast error measure in (4) it was found that δe_1^b largely overestimated the actual variation δe , δe_1^a largely underestimated δe , and that a significantly improved approximation was obtained by taking (1/2) δe_1^b . While this estimate appears to have been first considered on an empirical basis, further insight is provided by Trémolet (2007) where it is shown that if the response functional e is quadratic as a function of the initial conditions (thus linear forecast model) and \mathbf{x}_a minimizes e (i.e., $\mathbf{x}_a^f = \mathbf{x}^t$) then $\delta e = (1/2) \delta e_1^b$.

From Eqs. (9) and (14) one notices that, including the case of nonlinear dynamics,

if
$$\nabla_{\mathbf{x}_0} e(\mathbf{x}_a) = 0$$
 then $(1/2)\delta e_1^b = \delta e_2^{a,b}$. (A1)

Thus, if the analysis \mathbf{x}_a is the initial state that (nearly) minimizes the model functional aspect, that is,

$$\mathbf{x}_a \simeq \operatorname{Arg\,min}_{\mathbf{x}_0} e(\mathbf{x}_0), \qquad (A2)$$

then $(1/2) \delta e_1^b$ is (nearly) equal to $\delta e_2^{a,b}$ and the estimate $\delta e \approx (1/2) \delta e_1^b$ is (nearly) second-order accurate. This situation may be encountered in idealized observation impact experiments when the functional aspect is defined as the variance of the error in the initial conditions and the specification of the matrices **R** and **B** is statis-

tically consistent to the observation and background errors, respectively. Most general, (A1) holds for any response functional *e* and merely requires \mathbf{x}_a to be a stationary point (initial condition) to the functional *e*; for linear dynamics and quadratic *e*, in addition $\delta e_2^{a,b} =$ $(1/2) \delta e_1^b = \delta e$. Loss of information will result when firstorder observation impact estimates are based on derivatives at (nearly) stationary points. It is also noticed that

if
$$\nabla_{\mathbf{x}_0} e(\mathbf{x}_b) = 0$$
 then $(1/2)\delta e_1^a = \delta e_2^{a,b}$, (A3)

which applies to the quadratic functional

$$e(\mathbf{x}_0) = \frac{1}{2} (\mathbf{x}_0 - \mathbf{x}_b)^{\mathrm{T}} \mathbf{C} (\mathbf{x}_0 - \mathbf{x}_b)$$
(A4)

used in the study of Zhu and Gelaro (2008) and to the functional

$$e(\mathbf{x}_0) = (\mathbf{x}_0^f - \mathbf{x}_b^f)^{\mathrm{T}} \mathbf{C} (\mathbf{x}_0^f - \mathbf{x}_b^f)$$
(A5)

used in the study of Fourrié et al. (2002).

REFERENCES

- Atkinson, K. E., 1988: An Introduction to Numerical Analysis. John Wiley & Sons, Inc., 693 pp.
- Atlas, R., 1997: Atmospheric observations and experiments to assess their usefulness in data assimilation. J. Meteor. Soc. Japan, 75 (1B), 111–130.
- Baker, N. L., and R. Daley, 2000: Observation and background adjoint sensitivity in the adaptive observation-targeting problem. *Quart. J. Roy. Meteor. Soc.*, **126**, 1431–1454.
- Bloom, S. C., L. L. Takacs, A. M. da Silva, and D. Ledvina, 1996: Data assimilation using incremental analysis updates. *Mon. Wea. Rev.*, **124**, 1256–1271.
- Chou, M.-D., and M. J. Suarez, 1999: A shortwave radiation parameterization for atmospheric studies. Vol. 15, NASA Tech. Memo. 104606, 40 pp.
- Collins, N., and Coauthors, 2005: Design and implementation of components in the earth system modeling framework. *Int. J. High Perform. Comput. Appl.*, **19**, 341–350.
- Courtier, P., J. N. Thépaut, and A. Hollingsworth, 1994: A strategy of operational implementation of 4D-Var using an incremental approach. *Quart. J. Roy. Meteor. Soc.*, 120, 1367–1388.
- Daescu, D. N., 2008: On the sensitivity equations of four-dimensional variational (4D-Var) data assimilation. *Mon. Wea. Rev.*, 136, 3050–3065.
- Daley, R., 1991: Atmospheric Data Analysis. Cambridge University Press, 457 pp.
- Derber, J. C., and A. Rosati, 1989: A global oceanic data assimilation technique. J. Phys. Oceanogr., 19, 1333–1347.
- —, and W.-S. Wu, 1998: The use of TOVS cloud-cleared radiances in the NCEP SSI analysis system. *Mon. Wea. Rev.*, **126**, 2287–2299.

- Doerenbecher, A., and T. Bergot, 2001: Sensitivity to observations applied to FASTEX cases. *Nonlinear Processes Geophys.*, **8**, 467–481.
- Dunlavy, D. M., and D. P. O'Leary, 2005: Homotopy optimization methods for global optimization. Sandia National Laboratories, Rep. SAND2005-7495, 32 pp.
- Errico, R. M., 2007: Interpretations of an adjoint-derived observational impact measure. *Tellus*, **59A**, 273–276.
- —, R. Gelaro, E. Novakovskaia, and R. Todling, 2007: General characteristics of stratospheric singular vectors. *Meteor. Z.*, 16 (6), 621–634.
- Fourrié, N., A. Doerenbecher, T. Bergot, and A. Joly, 2002: Adjoint sensitivity of the forecast to TOVS observations. *Quart. J. Roy. Meteor. Soc.*, **128**, 2759–2777.
- Gelaro, R., Y. Zhu, and R. M. Errico, 2007: Examination of various-order adjoint-based approximations of observation impact. *Meteor. Z.*, **16** (6), 685–692.
- Giering, R., T. Kaminski, R. Todling, and S.-J. Lin, 2003: Generating the tangent linear and adjoint models of the DAO finite volume GCM's dynamical core by means of TAF. *Geophysical Research Abstracts*, Vol. 5, Abstract 11680. [Available online at http://www.cosis.net/abstracts/EAE03/11680/EAE03-J-11680. pdf.]
- Kalnay, E., 2002: Atmospheric Modeling, Data Assimilation and Predictability. Cambridge University Press, 364 pp.
- Kelly, G., J. N. Thépaut, R. Buizza, and C. Cardinali, 2007: The value of observations. I: Data denial experiments for the Atlantic and the Pacific. *Quart. J. Roy. Meteor. Soc.*, 133, 1803–1815.
- Kleespies, T. J., P. van Delst, L. M. McMillin, and J. Derber, 2004: Atmospheric transmittance of an absorbing gas. 6. OPTRAN status report and introduction to the NES-DIS/NCEP Community Radiative Transfer Model. *Appl. Opt.*, 43, 3103– 3109.
- Koster, R. D., M. J. Suarez, A. Ducharne, M. Stieglitz, and P. Kumar, 2000: A catchment-based approach to modeling land surface processes in a GCM. Part I: Model structure. J. Geophys. Res., 105, 24 809–24 822.
- Langland, R. H., 2005: Observation impact during the North Atlantic TReC-2003. Mon. Wea. Rev., 133, 2297–2309.

- —, 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., I. M. Navon, and D. N. Daescu, 2002: Second order information in data assimilation. *Mon. Wea. Rev.*, 130, 629–648.
- Lin, S.-J., 2004: A vertically Lagrangian finite-volume dynamical core for global models. *Mon. Wea. Rev.*, **132**, 2293–2307.
- Liu, J., and E. Kalnay, 2008: Estimating observation impact without adjoint model in an ensemble Kalman filter. *Quart. J. Roy. Meteor. Soc.*, **134**, 1327–1335.
- Moorthi, S., and M. J. Suarez, 1992: Relaxed Arakawa–Schubert: A parameterization of moist convection for general circulation models. *Mon. Wea. Rev.*, **120**, 978–1002.
- Ortega, J. M., and W. C. Rheinboldt, 1970: Iterative Solution of Nonlinear Equations in Several Variables. Academic Press, Inc., 572 pp.
- Rienecker, M. M., and Coauthors, 2008: The GEOS-5 Data Assimilation System—Documentation of versions 5.0.1, 5.1.0, and 5.2.0. NASA/TM-2008-104606, Vol. 27, Tech. Rep. Series on Global Modeling and Data Assimilation, 118 pp.
- Stieglitz, M., A. Ducharne, R. D. Koster, and M. J. Suarez, 2001: The impact of detailed snow physics on the simulation of snow cover and subsurface thermodynamics at continental scales. J. Hydrometeor., 2, 228–242.
- Trémolet, Y., 2007: First-order and higher-order approximations of observation impact. *Meteor. Z.*, **16** (6), 693–694.
- —, 2008: Computation of observation sensitivity and observation impact in incremental variational data assimilation. *Tellus*, **60A**, 964–978, doi:10.1111/j.1600–0870.2008.00349.x.
- Watson, L. T., 2000: Theory of globally convergent probability-one homotopies for nonlinear programming. SIAM J. Optim., 11, 761–780.
- Wu, W. S., R. J. Purser, and D. F. Parrish, 2002: Three-dimensional variational analysis with spatially inhomogeneous covariances. *Mon. Wea. Rev.*, **130**, 2905–2916.
- Zhu, Y., and R. Gelaro, 2008: Observation sensitivity calculations using the adjoint of the Gridpoint Statistical Interpolation (GSI) analysis system. *Mon. Wea. Rev.*, 136, 335–351.