Tellus (2003), 55A, 371–384
Printed in UK. All rights reserved

TELLUS
ISSN 0280–6495

Second-order approximation to the 3DVAR cost function: application to analysis/forecast

By S. LAKSHMIVARAHAN[1]*, YUKI HONDA[†] and J. M. LEWIS[3‡], [1]*School of Computer Science, University of Oklahoma, 200 Felgar str., Norman, OK 73019, USA;* [2]*School of Meteorology, University of Oklahoma;* [3]*National Severe Storms Laboratory*

(Manuscript received 18 March 2002; in final form 15 April 2003)

ABSTRACT

The analysis/forecast cycling scheme used in operational weather prediction centers involves repeated application of a 3DVAR assimilation phase followed by a forecast phase. In this paper we first derive a closed-form expression for the complete Hessian of the 3DVAR objective function. This facilitates the use of Newton-like algorithms in the 3DVAR assimilation phase. It is also shown that this algorithm includes the standard first-order method as a special case. Notwithstanding the method used in this optimization phase, if the iterative optimization is terminated prematurely before convergence (generally for the sake of economy), the resulting analysis incurs an error that will corrupt the initial condition of the model and thereby affect the forecast. Using Lorenz's maximum simplification form of the barotropic vorticity equation, we examine the assimilation error and its dependency on the following factors: observational and background error covariances and the optimization strategy.

1. Introduction

Nearly 50 years ago, in the period of scientific excitement and challenge that followed the first successful numerical prediction of weather, the variational approach to meteorological analysis was introduced by Sasaki (1958). The problem was posed in the least-squares context. A cost function, defined as the sum of weighted squared departures between the optimal state and corresponding observations of the state, was minimized under the constraint of various forms of the mass/wind balance. This problem was solved by recourse to the classical theory of calculus of variations. In succeeding decades, with advances in both computing power and optimization strategies, more complicated constraints and more diverse observations have been included in the problem, yet the principle has essentially remained unchanged (see Le Dimet and Talagrand, 1986; Lewis and Derber, 1985; and Talagrand and Courtier, 1987; for example). In the nomenclature of meteorology, this methodology has become known as 3DVAR, the three-dimensional variational method (all space coordinates but excluding time), and 4DVAR when time is included. The careful and didactic development of the theory is found in Tarantola (1987) and Daley (1991).

At about the same time that Sasaki introduced the variational analysis method to meteorology, Thompson (1957) explored the limits of deterministic prediction that stem from uncertainty in the initial state. Although he used the simplest, yet operationally meaningful dynamical prediction system (the barotropic model), he clearly identified the mechanism of error growth and tabulated the rate of growth. Initial errors grew as the result of nonlinear interaction between the dynamical modes of the system. Again, in this period of the mid- to late-1950s, operational numerical weather prediction forecasts commenced (See Bergthorsson and Döös, 1955; Thiébaux and Pedder, 1987; and Wiin-Nielsen, 1991).

*Corresponding author.
e-mail: varahan@ou.edu
[†]On leave from the Japan Meteorological Agency.
[‡]On assignment to the Desert Research Institute.

One of the pressing problems of modern-day 3DVAR is handling observations of physical quantities such as radiation and radar reflectivity that are not among the basic model variables. Empirical approaches to address this problem, generally statistically based, have given way to physically based strategies that use "model counterparts." In essence, model variables are used in conjunction with a physical law, e.g. the radiative transfer equation, to determine the model's estimate of the measurement.

The general nonlinearity of the physical law (observation operator) adds complication to the geometric structure of the variational cost function in the space of the control variables. However, complication can also arise in the presence of a linear relation. As shown by Andersson and Järvinen (1999), non-Gaussian error covariances that appear in the functional lead to problems that are fundamentally the same as those encountered when the observation operator is nonlinear.

Concerns over these sources of nonlinearity in the 3DVAR problem have prompted studies that have explored advantages of using the second-order approximation to the variational cost function. The principal element of the second-order approximation is the Hessian, the matrix of second derivatives of the cost function or aspect with respect to the control variables. The recent paper by LeDimet et al. (2002) provides a comprehensive survey of issues related to the derivation and use of the Hessian information, and Wang et al. (1992; 1995; 1997) have addressed issues related to computational advantages when using the Hessian information to locate minima of the cost function.

In this paper we derive a new class of full quadratic approximation that underlies the second-order method. By way of providing an alterative derivation of this second-order method, we show that the standard first-order method used in operations is a special case of this second-order method. We compare the performance of the first-order and the second-order methods in the context of Lorenz's minimum equations (Lorenz, 1960).

2. Problem statement: conceptual view

Our aim is to assess the errors that accrue in variational analysis and subsequent forecast. Current practice at operational centers assumes that noisy observations y (with model counterparts constructed from the state vector x) are available for assimilation periodically at an interval of T units of time (the forecast horizon). Given the observations y and the background state x_b (which could be based on any combination of prior information such as forecast and/or climatology), an optimum analysis x_a^* is obtained using the 3DVAR method. Using x_a^* as the initial condition for the chosen dynamical system, a forecast to time $= T$ is generated. Based on this forecast, a new background state x_b is determined which then is combined with observations y at T to obtain a new optimum analysis x_a^*. This analysis/forecast cycle is repeated and the repetitive process is the basis for operational forecasts.

We assume that the forecast variables are not observed. Rather, the model counterparts of the observations are constructed from the basic variables. We represent the observations y as follows:

$$y = h(x) + v$$

where $h(x)$ is the model counterpart of the observation and v is the error with known mean and covariance structure.

Let us look at the analysis error. The optimum analysis refers to the state of the system that minimizes a chosen criterion function $J(x)$ which is quadratic in $(x_b - x)$ and $[y - h(x)]$ background and observation error, respectively. Thus, unless $h(x)$ is linear in x, this criterion function can be more complex than the usual quadratic in x and can exhibit multi-modes as well. In practice, to overcome the "curse of dimensionality" one may choose to cut corners. One approach [as found in Lorenc (1986), Tarantola (1987) and Daley and Barker (2001)] is to linearize $h(x)$ around the given background field. That is, $h(x)$ is replaced by a linear approximation (the first-order Taylor series expansion) at x_b in the hope that the new optimum analysis is "close" to the background, and then the resulting quadratic expression is minimized to obtain an analysis x_a. Except in those cases where $h(x)$ is strictly linear, this analysis x_a is generally quite different from the optimum analysis x_a^*. The difference $(x_a^* - x_a)$ denotes the analysis error. Reduction in this error is achieved by iterative methods, i.e. successive reductions of the norm $\|x_a^* - x_a\|$ until it is within a tolerable limit.

One strategy developed by Huang (2000) is fashioned as follows: Starting with x_b, replace $h(x)$ in $J(x)$ by the first-order Taylor expansion around x_b and solve the resulting quadratic minimization problem where the solution is denoted by x_a. Notice that this x_a optimizes only an approximation to $J(x)$, not the original $J(x)$. Now considering x_a as the new operating point, once again compute a linear approximation to $h(x)$,

substitute this into the original $J(x)$ and solve the resulting quadratic optimization problem to obtain a new value of x_a. The premise is that the new x_a is closer to x_a^* than the old x_a. This process is repeated until there is insignificant change in the successive iterates of x_a. When $h(x)$ is nonlinear, there will always be an error in the estimate of x_a^* unless a convergent iterative method is used.

From the above discussion it is clear that for a given $J(x)$, where the weight matrices for the background term and observation term are perfectly specified, the lack of statistical optimality of the analysis is largely a result of premature termination of the iterative optimization procedure where the rate of convergence of x_a to x_a^* is governed by: (a) the approximation used to represent $h(x)$ in the vicinity of the current operating point and (b) the type of optimization algorithm used. In this paper, we analyze the relative merits of using (a) the full quadratic approximation to $J(x)$ resulting from using a quadratic (second-order Taylor) approximation to $h(x)$ around the current operating point (which we call as the second-order method) and (b) the partial quadratic approximation to $J(x)$ resulting from using a linear approximation (first-order Taylor series approximation) to $h(x)$ around the current operating point (which is called the first-order method) as advocated in Lorenc (1986), Tarantola (1987) and Daley and Barker (2001).

3. Mathematical statement of the problem

Our notation follows the conventions found in Lorenc (1986) and Tarantola (1987):

$x \in \mathbf{R^n}$: state vector

$x_b \in \mathbf{R^n}$: background vector

$R \in \mathbf{R^{m \times m}}$: observation error covariance matrix, symmetric and positive definite

$B \in \mathbf{R^{n \times n}}$: background error covariance matrix, symmetric and positive definite

$h : \mathbf{R^n} \rightarrow \mathbf{R^m}$: $h(x) = (h_1(x), h_2(x), \ldots, h_m(x)^T$: model counterpart to $y \in \mathbf{R^m}$: observation vector

$v \in R^m$: the observation noise vector where $E(v) = 0$ and $E(vv^T) = R$, the observational error covariance matrix, symmetric and positive definite, and $y = h(x) + v$, where E is the expectation operator

Let $J_0 : \mathbf{R^n} \rightarrow \mathbf{R}$ denote the weighted misfit between the observation y and its model counterpart $h(x)$:

$$J_0(x) = \frac{1}{2}[y - h(x)]^T R^{-1}[y - h(x)]. \tag{3.1}$$

Similarly, let $J_b : \mathbf{R^n} \rightarrow \mathbf{R}$ denote the weighted misfit between the given background x_b and the desired optimal state x:

$$J_b(x) = \frac{1}{2}(x_b - x)^T B^{-1}(x_b - x). \tag{3.2}$$

The functional to be minimized is the sum of these two terms. Thus, our problem is mathematically stated as follows:

Given x_b, B, y, $h(x)$ and R, find x that minimizes

$$J(x) = J_0(x) + J_b(x). \tag{3.3}$$

4. The second-order method

We begin by describing the framework for developing the full quadratic approximation to $J(x)$, the second-order method, which is deeply rooted in the contemporary theory of nonlinear optimization (Nash and Sofer, 1996; Dennis and Schnabel, 1996). Let $J : R^n \rightarrow R$ be the nonlinear functional to be minimized, and let x^* be a minimizer for $J(x)$. Although x^* is unknown, we have an operating point, say x_c, which is hopefully close to x^*. Instead of minimizing $J(x)$ directly, the idea is to replace $J(x)$ by a quadratic approximation, say $Q(z)$ around x_c where $x = x_c + z$. Then, we have

$$Q(z) = J(x_c + z) = J(x_c) + [\nabla J(x_c)]^T z + \frac{1}{2} z^T \left[\nabla^2 J(x_c)\right] z \tag{4.1}$$

which is the second-order Taylor series representation for $J(x)$ around x_c (refer to FACT A5 in the Appendix). At the minimum, the gradient of $Q(z)$ vanishes. This condition takes the form:

$$\nabla Q(z) = \nabla J(x_c) + \nabla^2 J(x_c) z = 0 \tag{4.2}$$

or equivalently,

$$\nabla^2 J(x_c) z = -\nabla J(x_c). \tag{4.3}$$

The solution of eq. (4.3) produces the minimizer for $Q(z)$. Equation (4.3) is the basis for the well known Newton's method for optimization (Dennis and Schnabel, 1996; Nash and Sofer, 1996).

We now apply this framework to the $J(x)$ in eq. (3.3). It follows from eq. (3.3) that

$$\nabla J(x) = \nabla J_0(x) + \nabla J_b(x) \tag{4.4}$$

and

$$\nabla^2 J(x) = \nabla^2 J_0(x) + \nabla^2 J_b(x) \tag{4.5}$$

Now,

$$\nabla J_b(x) = B^{-1}(x - x_b), \quad \nabla^2 J_b(x) = B^{-1} \tag{4.6}$$

and

$$\nabla J_0(x) = -D_h^T(x)R^{-1}[y - h(x)] \tag{4.7}$$

where $D_h(x)$ denotes the Jacobian of $h(x)$ which is a $m \times n$ matrix (Definition A2 in the Appendix). The expressions for the gradients of $J_0(x)$ and $J_b(x)$ are found by using FACT A3 and FACT A2, respectively.

Since eq. (4.7) involves product of matrices and vectors that are functions of the state vector x, computation of $\nabla^2 J_0(x)$ requires care and deliberation. Using Definition A1, note that the k^{th} column [also the k^{th} row since $\nabla^2 J_0(x)$ is symmetric] of $\nabla^2 J_0(x)$ is the gradient of the k^{th} element of the vector $\partial \nabla J_0(x)/\partial x_k$. We first identify this element in eq. (4.7). To this end, let

$$[h(x) - y] = g(x) = [g_1(x), g_2(x), \ldots, g_m(x)]^T \tag{4.8}$$

where

$$g_j(x) = [h_j(x) - y_j]. \tag{4.9}$$

Notice that the negative sign in eq. (4.7) is absorbed in the definition of $g(x)$. Also, recall that the transpose of $h(x)$ is a $n \times m$ matrix (Definition A2)

$$D_h^T(x) = \left[\frac{\partial h_j}{\partial x_i}\right] \tag{4.10}$$

where $1 \le i \le n$ is the row index and $1 \le j \le m$ is the column index. Let

$$e(x) = [e_1(x), e_2(x), \ldots, e_m(x)]^T$$

denote the m-vector corresponding to the k^{th} row of $D_h^T(x)$. That is,

$$e(x) = \left(\frac{\partial h_1}{\partial x_k}, \quad \frac{\partial h_2}{\partial x_k}, \quad .... \quad \frac{\partial h_m}{\partial x_k}\right)^T \tag{4.11a}$$

and

$$e_i(x) = \frac{\partial h_i}{\partial x_k} \quad \text{for} \quad 1 \le i \le m. \tag{4.11b}$$

In terms of this simplified notation, the k^{th} element of $\nabla J_0(x)$ is given by

$$\frac{\partial J_0(x)}{\partial x_k} = e^T(x)R^{-1}g(x). \tag{4.12}$$

Now applying FACT A4, we obtain the k^{th} column of the Hessian, $\nabla^2 J_0(x)$, as the sum of two vectors

$$\nabla\left(\frac{\partial J_0(x)}{\partial x_k}\right) = D_e^T(x)R^{-1}g(x) + D_g^T(x)R^{-1}e(x) \tag{4.13}$$

where $D_e(x)$ and $D_g(x)$ are the Jacobians of $g(x)$ in eq. (4.8) and $e(x)$ in eq. (4.11), respectively. Further simplifying our notation, we label the first and second terms on the RHS of eq. (4.13) as vector1 and vector2, respectively. From this we see that the required Hessian of $J_0(x)$ can be computed as the sum of two matrices, call them E_2 and E_2, and the mathematical expression for this Hessian is written as:

$$\nabla^2 J_0(x) = E_1 + E_2 \tag{4.14}$$

where the k^{th} column of E_1 is given by vector1 and that of E_2 by vector2.

4.1. *Computation of E_1 from vector1*

Let

$$R^{-1}g(x) = b(x) = [\, b_1(x), \quad b_2(x), \quad .... \quad b_m(x)]^T. \tag{4.15}$$

From Definition A2, using eq. (4.11), we have

$$D_e^T(x) = \left[\frac{\partial e_j}{\partial x_i}\right] = \left[\frac{\partial^2 h_j}{\partial x_i \partial x_k}\right] \tag{4.16}$$

where $1 \le i \le n$ is the row index and $1 \le j \le m$ is the column index. Thus, the k^{th} column of E_1 is given by the matrix-vector product $D_h^T(x)b(x)$. That is,

$$k^{\text{th}} \text{ column of } E_1 = \text{Vector1} = D_e^T(x)b(x)$$

$$= \begin{bmatrix} \sum_{j=1}^{m} \left(\frac{\partial^2 h_j}{\partial x_1 \partial x_k}\right) b_j(x) \\ \sum_{j=1}^{m} \left(\frac{\partial^2 h_j}{\partial x_2 \partial x_k}\right) b_j(x) \\ \sum_{j=1}^{m} \left(\frac{\partial^2 h_j}{\partial x_n \partial x_k}\right) b_j(x) \end{bmatrix}. \tag{4.17}$$

We can now recover each of the n columns of E_1 by simply varying k from 1 through n. Now, since each element of the matrix is the sum of exactly m terms, we can express E_1 as the sum of exactly m matrices as follows:

$$E_1 = \nabla^2 h_1(x)b_1(x) + \nabla^2 h_2(x)b_2(x) + ... + \nabla^2 h_m(x)b_m(x) \tag{4.18}$$

where $\nabla^2 h_i(x)$ is the Hessian of the i^{th} component $h_i(x)$ of $h(x)$.

4.2. *Computation of E_2 from Vector2*

Recall that the k^{th} column of E_2 is given by

$$\text{vector2} = D_g^T(x) R^{-1} e(x) \tag{4.19}$$

where from eq. (4.11) we know that $e(x)$ is a column vector that is the k^{th} row of $D_h^T(x)$ [which is the same as the k^{th} column vector of $D_h(x)$]. Further, from eq. (4.9), since $g(x) = [h(x) - y]$, where y is a known constant vector, it immediately follows from the definition that

$$D_g(x) = D_h(x). \tag{4.20}$$

Combining these arguments with eq. (4.19) we have

$$k^{\text{th}} \text{ column of } E_2 = \text{vector } 2 = D_h^T(x) R^{-1} \times \{k^{\text{th}} \text{ column of } D_h(x)\}$$

and hence

$$E_2 = D_h^T(x) R^{-1} D_h(x). \tag{4.21}$$

We are now ready to assemble the Hessian $\nabla^2 J(x)$. Combining eqs. (4.5), (4.6), (4.14), (4.18) and (4.21) it follows that

$$\nabla^2 J(x) = \left[B^{-1} + D_h^T(x) R^{-1} D_h(x) + \sum_{i=1}^{m} \nabla^2 h_i(x) b_i(x) \right] \tag{4.22}$$

where $b(x) = R^{-1}[h(x) - y]$. We now return to Newton's equation (4.3) that defines the second-order method. By combining eq. (4.22) with eqs. (4.4), (4.6) and (4.7) and evaluating all the quantities at x_c (since x_c is the operating point), from eq. (4.3) we get

$$\left[B^{-1} + D_h^T(x_c) R^{-1} D_h(x_c) + \sum_{i=1}^{m} \nabla^2 h_i(x_c) b_i(x_c) \right] z = D_h^T(x_c) R^{-1} [y - h(x_c)] - B^{-1}(x_c - x_b) \tag{4.23}$$

The solution to eq. (4.23) yields $z = x - x_c$, the so-called second-order analysis increment at x_c.

5. Special case: first-order method

In deriving the first-order method as a special case, let us look at the second-order method from an alternative point of view. To this end, expand $h(x)$ around x_c using the second-order approximation as shown below.

Recall from FACT A5 that (with $x = x_c + z$)

$$h(x) = h(x_c) + D_h(x_c) z + \psi(z) \tag{5.1}$$

where for simplicity in notation we have let

$$\psi(z) = \frac{1}{2} z^T D_h^2(x_c) z, \tag{5.2}$$

a vector with $\psi(z) = [\psi_1(z), \psi_2(z) \ldots\ldots \psi_n(z)]^T$, $\psi_i(z) = z^T B_i z$ and $B_i = \nabla^2 h_i(x_c)$ (These Hessian matrices B_i are not to be confused with the background error covariance matrix B.) Thus, each component of $\psi(z)$ is a quadratic form in z. Now substituting eq. (5.1) into eq. (3.1) and using eqs. (3.2), (3.3), (4.8) and (4.9), we get

$$J(x) = \frac{1}{2}[-g(x_c) - D_h(x_c) z - \psi(z)]^T \times R^{-1}[-g(x_c) - D_h(x_c) z - \psi(z)] + \frac{1}{2}(z + x_c - x_b)^T B^{-1}(z + x_c - x_b). \tag{5.3}$$

It can be verified that the RHS of eq. (5.3) is a fourth-degree polynomial in z. To obtain a quadratic approximation, we neglect the third- and fourth-degree terms in eq. (5.3). This quadratic approximation is given by

$$Q'(z) = (1/2) g^T(x_c) R^{-1} g(x_c) + g^T(x_c) R^{-1} D_h(x_c) z + (1/2) z^T \times \left[B^{-1} + D_h^T(x_c) R^{-1} D_h(x_c) \right] z + g^T(x_c) R^{-1} \psi(z) + \frac{1}{2}(z + x_c - x_b)^T B^{-1}(z + x_c - x_b). \tag{5.4}$$

It can be verified that $Q'(z)$ as given in eq. (5.4) is indeed the same as $Q(z)$ in eq. (4.1).

As preparation for computation of the gradient of $Q'(z)$, let us first compute the gradient of the next to the last term in eq. (5.4). Using eq. (4.15) and FACT A6, we have

$$\nabla \left[g^T(x_c) R^{-1} \psi(z) \right] = \nabla \left[b^T(x_c) \psi(z) \right] = (1/2) \nabla \left[\sum_{i=1}^{n} b_i(x_c) \left(z^T B_i z \right) \right] = \sum_{i=1}^{n} b_i(x_c)(B_i z) = \sum_{i=1}^{n} b_i(x_c) \left[\nabla^2 h_i(x_c) z \right]. \tag{5.5}$$

Using eq. (5.5), it can be verified that

$$\nabla Q'(z) = D_h^T(x_c)R^{-1}g(x_c) + \left[B^{-1} + D_h^T(x_c)R^{-1}D_h(x_c)\right]z + \sum_{i=1}^{n} b_i(x_c)\left[\nabla^2 h_i(x_c)\right]z + B^{-1}(x_c - x_b). \quad (5.6)$$

Setting eq. (5.6) to zero, we find the optimum z as the solution of the following equation

$$\left[B^{-1} + D_h^T(x_c)R^{-1}D_h(x_c) + \sum_{i=1}^{n} b_i(x_c)\nabla^2 h_i(x_c)\right]z = D_h^T(x_c)R^{-1}[y - h(x_c)] - B^{-1}(x_c - x_b) \quad (5.7)$$

which is identical to eq. (4.23).

And as we might expect, by setting $D_h^2(x_c) = 0$ in eq. (5.2), eq. (5.7) reduces to

$$\left[B^{-1} + D_h^T(x_c)R^{-1}D_h(x_c)\right]z = D_h^T(x_c)R^{-1}[y - h(x_c)] - B^{-1}(x_c - x_b) \quad (5.8)$$

which is the first-order method used in Daley and Barker (2001), Lorenc (1986) and Tarontola (1987). In short, the standard first-order method achieves a quadratic form of J (second-degree polynomial in z) by assuming that h can be approximated by a Taylor expansion up to the first-degree term in z. However, if we assume h is approximated by the expansion out to the second-degree term, then J will be a fourth degree polynomial in z. When we examine this form of J up to the second degree polynomial in z ("quadratic J"), we find that there are terms involving the Hessian of $h(x)$ that are unaccounted in the first-order method. We thus say that the first-order method is a "partial" quadratic approximation, whereas the second-order method is a "full" quadratic approximation to J.

The Hessians of $Q(z)$ and $Q'(z)$ are identical and given by

$$\nabla^2 Q(z) = \nabla^2 Q'(z) = \left[B^{-1} + D_h^T(x_c)R^{-1}D_h(x_c) + \sum_{i=1}^{n} b_i(x_c)\nabla^2 h_i(x_c)\right]. \quad (5.9)$$

Recall that $[B^{-1} + D_h^T(x_c)R^{-1}D_h(x_c)]$ is positive definite by assumption. However, the positive definiteness of the matrix on the RHS of eq. (5.9) depends on the second-order properties of the nonlinear forward operator $h(x)$ and the scaled or normalized observation innovation $b(x_c) = -R^{-1}[y - h(x_c)]$.

6. Dynamical constraint: forecast equations and model counterparts to the observations

We will test our assimilation scheme by assuming that the dynamical equations governing the forecast are the maximum simplification equations or "minimum" equations of Lorenz (1960). The first sentence of the abstract to his paper reads: When the dynamic equations are to be used to further our understanding of atmospheric phenomena, it is permissible to simplify them beyond the point where they can yield acceptable weather predictions.

The equations Lorenz derives under this philosophy are fundamentally based on the spectral form of the barotropic vorticity equation. Through deft manipulation of the governing equations, Lorenz succeeds in reducing the system to a Spartan set of three nonlinear ordinary differential equations. These equations govern the interaction between the large-scale mode and the modes of two disturbances: finite disturbances on a zonal flow with exchanges of kinetic energy between the zonal flow and the disturbances. In Lorenz's notation, the large-scale (zonal flow) amplitude is denoted by A and the disturbance amplitudes by F and G. For consistency with our development, this triad of amplitudes is represented by our state vector x, i. e.

$$x = (x_1, x_2, x_3)^T = (A, F, G)^T. \quad (6.1)$$

In component form, the governing equations are:

$$\frac{dx_1}{dt} = -\left(\frac{1}{k^2} - \frac{1}{k^2 + l^2}\right) klx_2x_3$$
$$\frac{dx_2}{dt} = \left(\frac{1}{l^2} - \frac{1}{k^2 + l^2}\right) klx_1x_3$$
$$\frac{dx_3}{dt} = -\frac{1}{2}\left(\frac{1}{l^2} - \frac{1}{k^2}\right) klx_1x_2 \quad (6.2)$$

where $2\pi/l$ is the distance between successive zonal wind maxima and $2\pi/k$ is the wavelength of the disturbances. One of Lorenz's experiments with these equations is called "disturbed unstable zonal flow" where $k/l = 0.95$ and the initial state vector is $x_0 = (1.0, 0.1, 0.0)$. The dynamics associated with this regime is the growth of disturbances due to nonlinear interaction with the zonal flow. This set of equations was used by Epstein (1969, sect. 7) to study stochastic–dynamic prediction and it is an ideal platform for our study of assimilation.

For this case of unstable flow, the governing equations are given by:

$$\frac{dx_1}{dt} = -0.553 \times x_2 x_3$$
$$\frac{dx_2}{dt} = 0.451 \times x_1 x_3 \quad (6.3)$$
$$\frac{dx_3}{dt} = 0.051 \times x_1 x_2$$

which is eq. (33) of Lorenz (1960). Although Lorenz used a time-centered scheme to integrate these equations, we use the fourth-order Runge–Kutta scheme to reduce the truncation error (Press et al. 1992, pp. 704 ff.). We examine the solution at the incremental time steps used by Lorenz, i.e. $t_n = n\Delta t$ where n is an integer starting from $n = 0$ (initial time). Lorenz scaled the time by 3 h, and this implies that the time step used in the integration is $\Delta t = 2$ (non-dimensional). [See pages 248–249 of Lorenz (1960) for a more detailed discussion of the scaling.] Thus, $n = 4$ corresponds to a time 24 h after initial time.

In our idealized experiment, we assume that the model counterparts to observations are given by the RHS of these forecast equations. In essence, these observations are surrogates for the time derivatives of the amplitudes. The model counterparts take the form:

$$h(x) = [h_1(x), h_2(x), h_3(x)]^T = (-0.553 \times x_2 x_3, 0.451 \times x_1 x_3, 0.051 \times x_1 x_2)^T \quad (6.4)$$

7. Numerical experiments

7.1. Ground plan for the experiment

In operational forecast cycling, determination of the appropriate background error covariance matrix remains a challenging component of the data assimilation process in meteorology. Essentially, the true state of the atmosphere is unknown, and consequently measuring forecast error is always an approximation. Nevertheless, advances have been made that work from the premise that there exist surrogate quantities whose error statistics are similar to those of background error: forecast differences and differences between background fields from an ensemble of analyses. In our idealized experiment, we have the luxury of knowing the true state of the system and can therefore calculate the error covariance matrix B through an ensemble of forecasts that begin with initially known error. The performance of our assimilation strategies is seen in its best light under such circumstances, yet it is the relative weighting between B^{-1} and R^{-1} (rather than their exact values) that underpins the study.

The true state of the Lorenz system is the state vector that is generated by the finite-difference solution to eq. (6.3). The exact initial state is perturbed in accord with prescribed error. We have chosen to use normally distributed error with zero mean and standard deviations the order of 10% of the amplitudes—0.1 for the zonal component x_1 and 0.01 for the disturbances x_2 and x_3. Beginning with this perturbed state, a forecast is made to $n = 4$ and the difference between this forecast and the true state gives the forecast error. An ensemble of 10^5 forecasts is used to determine the error statistics: error variances and error covariances associated with the three components of the state vector. These errors determine the elements of the background error covariance matrix B^{-1}. The true state of the system is never again used in the experiment. Having found the B^{-1} matrix, we now construct a set of observation error covariance matrices R^{-1} to represent those cases where observations are given more, equal and less weight than the background field. These matrices are represented by $(R^{-1})_1$, $(R^{-1})_2$ and $(R^{-1})_3$, respectively. The observational errors will be assumed to be uncorrelated, and accordingly these matrices will be diagonal. Furthermore, we assume that the errors associated with each observation are equal and thus the diagonal elements of the matrices are identical. Table 1 displays B, B^{-1}, and the various R matrices that will be used in our experiment.

Table 1. *Background error covariance matrix associated with forecast from* n = *0 to* n = *4 using Lorenz's minimum equations (6.3)*

B		
5.39×10^{-3}	-2.16×10^{-3}	-5.50×10^{-4}
-2.16×10^{-3}	1.86×10^{-2}	5.47×10^{-3}
-5.50×10^{-4}	5.47×10^{-3}	1.64×10^{-3}
B^{-1}		
2.03×10^{2}	1.76×10^{2}	-5.19×10^{2}
1.76×10^{2}	2.82×10^{3}	-9.33×10^{3}
-5.19×10^{2}	-9.33×10^{3}	3.16×10^{4}

The values of three observation error covariance matrices for this case (where I_k is the identity matrix of order k) are: $R_1 = 3.125 \times 10^{-5}\ I_3$; $R_2 = 8.68 \times 10^{-5}\ I_3$ and $R_3 = 5.00 \times 10^{-3}\ I_3$.

From a given observation error covariance matrix R, we construct the corresponding observation vectors $y = h(x) + v$. The model counterpart, $h(x)$, is found from the forecasted model state at $n = 4$. To this we add the noise: assumed mean of zero and variance given by the diagonal element of the appropriate R matrix.

Given B, x_b, R and h, the functional J at $n = 4$ is minimized by the various algorithms: first-order, second-order and hybrid of the combination. The first-order method uses the conventional method discussed in the paper and mathematically expressed by eq. (5.8). We execute two iterations of this method. The second-order method uses eq. (5.7), again two iterations. The "hybrid" method begins with first-order but switches to second order on the second iteration. We also find an optimal assimilated state that represents the "true" minimum, the result of iteration until convergence. Standard criteria to determine termination of the iterative process (whether first-order, second-order or hybrid) are found in Dennis et al. (1981) and Nash and Sofer (1996). The optimal assimilated state is used as the benchmark to determine the goodness of the various assimilation strategies. In our difference calculations, the optimal state is subtracted from the other states.

We will test the assimilation methods in a non-cyclic mode, i.e. we will make a forecast to $n = 4$ and assimilate observations at that point in time. Although this procedure is only one step of the operational cycling process, it will demonstrate the basic performance characteristics of the various schemes.

Once we obtain the state vector at $n = 4$ (24 h) by the various assimilation strategies, we make a forecast to $n = 12$ (72 h) and verify this against the optimal state obtained by integration of the dynamical equations from the optimal state at $n = 4$. Thus, a given realization of the experiment yields errors in the assimilation methods (distance from the optimal state) and an error in the forecast that emanates from the estimated state vector. This process is executed 10^5 times for each of the three primary experiments discussed above. We average the errors to determine the ensemble error statistics.

Since the forecast horizon we have chosen is a fraction of the timescale of the energy exchange between the zonal flow and the disturbances, we have made the crucial assumption that the background error covariance matrix B and the observational covariance matrix R are fixed. When the assimilation is accomplished in a cycling mode that is commensurate with the timescale of the phenomena, this assumption of constant error covariance may not hold. This issue, although important and basic, is not considered in this contribution.

7.2. *Results*

The results are presented in tabular form. In Table 2 we exhibit the ensemble mean error vector. The errors in the amplitudes of the three components of x are tabulated (x_1, x_2, x_3, top to bottom). Table 3 shows the mean of the error norm associated with the various assimilation strategies, and Table 4 shows the error norm of the forecast from each assimilation method [a forecast from $n = 4$ to $n = 12$ (72 h)]. Table 5 displays the true and optimal states of the system between $n = 4$ and $n = 12$. Table 6 displays the errors

Table 2. *Ensemble mean of the analysis error vector*

Background/Observation error covariance combination	Time horizon $n = 4$		
	1st-order	2nd-order	Hybrid
(B, R_1)	1.2314×10^{-2}	-1.9346×10^{-2}	4.1057×10^{-2}
	-2.5430×10^{-2}	3.1713×10^{-5}	-1.3264×10^{-2}
	-7.2612×10^{-3}	6.6243×10^{-4}	-2.6524×10^{-3}
(B, R_2)	1.1111×10^{-2}	$+4.5744 \times 10^{-3}$	$+2.0941 \times 10^{-2}$
	-2.5411×10^{-2}	-1.7228×10^{-3}	-1.1910×10^{-2}
	-7.2669×10^{-3}	-3.5975×10^{-4}	-2.9452×10^{-3}
(B, R_3)	2.0561×10^{-5}	9.4510×10^{-7}	-1.0100×10^{-8}
	2.3999×10^{-4}	1.0265×10^{-5}	1.5357×10^{-5}
	7.1799×10^{-5}	3.0483×10^{-6}	4.5830×10^{-6}

Table 3. *Norm of the ensemble analysis error*

Background/observation error covariance	Time horizon $n = 4$		
	1st-order	2nd-order	Hybrid
(B, R_1)	1.0378×10^{-1}	1.1677×10^{-1}	9.314×10^{-2}
(B, R_2)	7.7288×10^{-2}	6.8161×10^{-2}	5.5606×10^{-2}
(B, R_3)	1.6990×10^{-3}	4.1980×10^{-5}	6.7900×10^{-5}

Table 4. *Ensemble forecast error at time* n = *12*

Background/observation error covariance	Starting with the analysis at time $n = 4$		
	1st-order	2nd-order	Hybrid
(B, R_1)	2.360×10^{-1}	2.144×10^{-1}	1.462×10^{-1}
(B, R_2)	2.129×10^{-1}	1.528×10^{-1}	1.083×10^{-1}
(B, R_3)	3.267×10^{-3}	0.536×10^{-4}	0.918×10^{-4}

Table 5A. *The evolution of the forecast of the true state from time* n = *4 to 12*

FORECAST HORIZON	x1	x2	x3
4	0.98564	0.18233	0.51269
5	0.97146	0.23639	0.72028
6	0.94585	0.30972	0.98574
7	0.90043	0.40535	0.13210
8	0.82224	0.52359	0.17283
9	0.69412	0.65771	0.21860
10	0.50022	0.78832	0.26295
11	0.23942	0.88248	0.29485
12	−0.06089	0.90691	0.30311

Table 5B. *The evolution of the ensemble mean of the forecast of the state variable from time* n = *4 to 12 for the optimal scheme*

FORECAST HORIZON	x1	x2	x3
4	0.96936	0.18406	0.05153
5	0.95331	0.23670	0.07178
6	0.92498	0.30715	0.09734
7	0.87611	0.39722	0.12898
8	0.79493	0.50546	0.16633
9	0.66785	0.62342	0.20664
10	0.48564	0.73288	0.24383
11	0.25301	0.80876	0.26951
12	−0.00657	0.83032	0.27671

in the forecasts as a function of time step for the case where observations and background field are given equal weight (error covariance matrices B and R_2).

Recall that the standard deviations of the amplitude errors at $n = 0$ were 10^{-1} and 10^{-2} for zonal flow and disturbances, respectively, and the mean errors were zero. Table 2 indicates that the amplitude ensemble mean errors at $n = 4$ are generally less than these standard deviations. The errors for the case of observational error covariance R_3 (observations receiving less weight than background) are significantly less than for the other two experiments.

Examination of Table 3 (mean of the error norm) yields the general result that the second-order or hybrid methods generally yield a better result than the first-order method. Again, the experiment where the observational error covariance receives less weight ($= R_3$) yields the smallest errors.

Forecast errors at $n = 12$ (Table 4), starting from the analyses at $n = 4$, indicate that better forecasts result from the hybrid analyses. Tables 5 and 6 are included to show the evolution of the ensemble statistics in the case of (B, R_2), equal weight for observations and background. Table 5 compares the true evolution with that derived from the optimal state. A comparison of the corresponding elements in Tables 5A and B indicates that the model evolution from the optimal analysis at $n = 4$ is faithful to the true model evolution of the system. In Table 6A, B, and C, we have the comparison of forecast errors (for each of the components of the state vector) as a function of time step. Results generally indicate that the errors grow with time, but

Table 6A. *The evolution of the ensemble mean and variance of the error of the first component x1 of the state variable from time* n = *4 to 12 for the first-order, second-order and hybrid schemes. The error is defined as the departure from the optimal state. The first column* n *refers to the forecast horizon*

	FIRST		SECOND		HYBRID	
n	MEAN	VARIANCE	MEAN	VARIANCE	MEAN	VARIANCE
4	$-0.58490.10^{-3}$	$0.12190.10^{-4}$	$0.42234.10^{-3}$	$0.36918.10^{-5}$	$0.60717.10^{-3}$	$0.95367.10^{-5}$
5	$-0.52627.10^{-3}$	$0.16192.10^{-4}$	$0.14717.10^{-3}$	$0.47446.10^{-5}$	$0.50319.10^{-3}$	$0.72468.10^{-5}$
6	$-0.41425.10^{-3}$	$0.25148.10^{-4}$	$-0.32532.10^{-3}$	$0.10606.10^{-4}$	$0.31918.10^{-3}$	$0.52541.10^{-5}$
7	$-0.20533.10^{-3}$	$0.45347.10^{-4}$	$-0.10922.10^{-2}$	$0.29958.10^{-4}$	$0.66237.10^{-5}$	$0.78837.10^{-5}$
8	$0.16745.10^{-3}$	$0.89092.10^{-4}$	$-0.22255.10^{-2}$	$0.78152.10^{-4}$	$-0.49026.10^{-3}$	$0.27054.10^{-4}$
9	$0.78363.10^{-3}$	$0.17474.10^{-3}$	$-0.36612.10^{-2}$	$0.16819.10^{-3}$	$-0.12029.10^{-2}$	$0.84173.10^{-4}$
10	$0.16858.10^{-2}$	$0.31757.10^{-3}$	$-0.50709.10^{-2}$	$0.28655.10^{-3}$	$-0.20821.10^{-2}$	$0.19637.10^{-3}$
11	$0.27968.10^{-2}$	$0.51238.10^{-3}$	$-0.59137.10^{-2}$	$0.38660.10^{-3}$	$-0.29632.10^{-2}$	$0.34648.10^{-3}$
12	$0.38888.10^{-2}$	$0.72883.10^{-3}$	$-0.57943.10^{-2}$	$0.43379.10^{-3}$	$-0.36222.10^{-2}$	$0.48060.10^{-3}$

Table 6B. *The evolution of the ensemble mean and variance of the error of the first component x2 of the state variable from time* n = *4 to 12 for the first-order, second-order and hybrid schemes. The error is defined as the departure from the optimal state. The first column* n *refers to the forecast horizon*

	FIRST		SECOND		HYBRID	
n	MEAN	VARIANCE	MEAN	VARIANCE	MEAN	VARIANCE
4	$-0.58351.10^{-3}$	$0.29456.10^{-4}$	$0.12033.10^{-2}$	$0.21619.10^{-4}$	$0.59288.10^{-3}$	$0.12650.10^{-4}$
5	$-0.79256.10^{-3}$	$0.46021.10^{-4}$	$0.15669.10^{-2}$	$0.34934.10^{-4}$	$0.79747.10^{-3}$	$0.22578.10^{-4}$
6	$-0.10789.10^{-2}$	$0.71899.10^{-4}$	$0.19994.10^{-2}$	$0.54815.10^{-4}$	$0.10619.10^{-2}$	$0.39500.10^{-4}$
7	$-0.14529.10^{-2}$	$0.10962.10^{-3}$	$0.24283.10^{-2}$	$0.79784.10^{-4}$	$0.13748.10^{-2}$	$0.65286.10^{-4}$
8	$-0.19047.10^{-2}$	$0.15908.10^{-3}$	$0.26878.10^{-2}$	$0.10246.10^{-3}$	$0.16910.10^{-2}$	$0.97463.10^{-4}$
9	$-0.23757.10^{-2}$	$0.21534.10^{-3}$	$0.25146.10^{-2}$	$0.11220.10^{-3}$	$0.19153.10^{-2}$	$0.12478.10^{-3}$
10	$-0.27352.10^{-2}$	$0.27120.10^{-3}$	$0.16694.10^{-2}$	$0.10999.10^{-3}$	$0.19167.10^{-2}$	$0.13166.10^{-3}$
11	$-0.28083.10^{-2}$	$0.32627.10^{-3}$	$0.18965.10^{-3}$	$0.11711.10^{-3}$	$0.15988.10^{-2}$	$0.11671.10^{-3}$
12	$-0.24855.10^{-2}$	$0.39094.10^{-3}$	$-0.14867.10^{-2}$	$0.15233.10^{-3}$	$0.98739.10^{-3}$	$0.98906.10^{-4}$

Table 6C. *The evolution of the ensemble mean and variance of the error of the first component x3 of the state variable from time* n = *4 to 12 for the first-order, second-order and hybrid schemes. The error is defined as the departure from the optimal state. The first column* n *refers to the forecast horizon*

	FIRST		SECOND		HYBRID	
n	MEAN	VARIANCE	MEAN	VARIANCE	MEAN	VARIANCE
4	$-0.17958.10^{-3}$	$0.24394.10^{-5}$	$0.35987.10^{-3}$	$0.18447.10^{-5}$	$0.18189.10^{-3}$	$0.12029.10^{-5}$
5	$-0.25526.10^{-3}$	$0.43157.10^{-5}$	$0.49326.10^{-3}$	$0.33521.10^{-5}$	$0.25548.10^{-3}$	$0.23288.10^{-5}$
6	$-0.35529.10^{-3}$	$0.72512.10^{-5}$	$0.64572.10^{-3}$	$0.56011.10^{-5}$	$0.34752.10^{-3}$	$0.42458.10^{-5}$
7	$-0.48368.10^{-3}$	$0.11537.10^{-4}$	$0.79380.10^{-3}$	$0.84286.10^{-5}$	$0.45459.10^{-3}$	$0.71646.10^{-5}$
8	$-0.63737.10^{-3}$	$0.17173.10^{-4}$	$0.88228.10^{-3}$	$0.11014.10^{-4}$	$0.56178.10^{-3}$	$0.10807.10^{-4}$
9	$-0.79698.10^{-3}$	$0.23618.10^{-4}$	$0.82286.10^{-3}$	$0.12186.10^{-4}$	$0.63725.10^{-3}$	$0.13908.10^{-4}$
10	$-0.91864.10^{-3}$	$0.30084.10^{-4}$	$0.53511.10^{-3}$	$0.12097.10^{-4}$	$0.63700.10^{-3}$	$0.14724.10^{-4}$
11	$-0.94366.10^{-3}$	$0.36546.10^{-4}$	$0.31357.10^{-4}$	$0.13182.10^{-4}$	$0.52855.10^{-3}$	$0.13119.10^{-4}$
12	$-0.83528.10^{-3}$	$0.44177.10^{-4}$	$-0.54161.10^{-3}$	$0.17544.10^{-4}$	$0.32049.10^{-3}$	$0.11250.10^{-4}$

that the hybrid method exhibits smaller variance than the other two methods.

8. Conclusions

The ever-challenging problem of producing an estimate of the atmospheric state by using the background field (forecast) and observations has been investigated in the context of a simple yet meaningful dynamical system: Lorenz's maximum simplification equations (the so-called "minimum" equations). Our aim has been two-fold. First and foremost, we have derived a method of solution to the 3DVAR analysis problem that accounts for the complete Hessian of the cost function. Essentially, the nonlinear model counterparts to observations, terms in the cost function, are expanded to second-order around the current operating point in the iterative method of solution. This differs from the present operational practice that accounts for only the first-order terms in the expansion. Secondly, we have tested the various strategies in the context of Lorenz's minimum equations.

A set of numerical experiments has been performed to elucidate the advantages/disadvantages of the second-order method, but also to indicate the penalties of premature termination of the iterative process, no matter what method is used. We have found that the second-order method converges faster when the current operating point is close to the minimum. The first-order method, on the other hand, works well and is sometimes superior to the second-order method when the operating point is far from the minimum; here the word "far" is used to indicate that the full quadratic approximation afforded by the second-order method is not representative of the curvature near the minimum in these cases. The stated performances of the first- and second-order method dictated a "hybrid" approach that commences with the first-order method and then switches to the second-order method as the minimum is approached. This appears to be the most prudent strategy for the case of the minimum equations in the unstable zonal flow situation. One suspects that this strategy would also be appropriate for dynamical systems that have model counterparts constructed from quadratic products of the model forecast variables. That is, the geometric structure of the cost functions would most likely have strong resemblances to those associated with the system we tested.

The computational burden associated with the second-order method is not excessive; the cost is basically associated with function evaluation in the pre-processing stage of the data assimilation. The additional matrix operations associated with the second-order method are multiplications, not inversions. The optimal equations used to find the increments in the first-order or second-order methods exhibit comparable difficulty [see eqs. (5.7) and 5.8)]. Although the mechanics of the analysis/forecast have been developed for a low-order spectral system of ordinary differential equations, the steps that lead to the calculation of the Hessian are readily transferable to dynamical systems that have more complicated model counterparts.

9. Acknowledgments

Basic ideas relating to the full quadratic approximation based on the second-order method described in section 4 were presented in the seminar at the National Center for Environmental Prediction (NCEP) in Washington D.C. in May 2000. We are grateful to Jim Purser for hosting the visit and to Jim Purser, John Derber and Dusanka Zupanski for their interest and encouragement. Y. Honda would like to thank Brian Fiedler, Yoshi K. Sasaki and the Japan Meteorological Agency for their support. We are grateful to three anonymous referees whose comments helped us restructure the paper and clarify the experimental plan.

10. Appendix

In this appendix we assemble a series of basic building blocks that are useful in the derivation of the gradient and Hessian of the nonlinear objective function of interest in 3DVAR data assimilation problems.

Let $x = (x_1, x_2, ..., x_n)^T$ be a column vector denoted succinctly by $\mathbf{x} \in \mathbf{R^n}$. (All the vectors are column vectors by definition and T denotes the transpose). Symbols A, B, etc. with and without subscripts denote matrices of appropriate dimensions.

Definition A1. Gradient and Hessian of a real-valued function

Let $f : \mathbf{R^n} \rightarrow \mathbf{R}$. Then the gradient of $f(x)$, denoted by $\nabla f(x)$, is a column vector given by

$$\left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, ..., \frac{\partial f}{\partial x_n}\right)^T.$$

The Hessian of $f(x)$ denoted by $\nabla^2 f(x)$ is the $n \times n$ matrix of second partial derivatives, given by

$$\nabla^2 f(x) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & .... & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_1 \partial x_2} & \frac{\partial^2 f}{\partial x_2^2} & .... & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ . & . & .... & . \\ . & . & .... & . \\ \frac{\partial^2 f}{\partial x_1 \partial x_n} & \frac{\partial^2 f}{\partial x_2 \partial x_n} & .... & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

$$= \left[\frac{\partial^2 f(x)}{\partial x_i \partial x_j} \right] \quad 1 \le i, j \le n.$$

Thus, the i^{th} column/row of $\nabla^2 f(x)$ is the gradient of $\partial f/\partial x_i$, i.e. $\nabla(\partial f/\partial x_i)$.

Definition A2. Jacobian of a vector valued function of a vector

Let $h : \mathbf{R^n} \to \mathbf{R^m}$, where $h(x) = [h_1(x), h_2(x), ..., h_m(x)]^T$. Then the Jacobian of h, denoted by $D_h(x)$, is the $m \times n$ matrix of first partial derivatives of the components of $h(x)$ and is given by

$$D_h(x) = \begin{bmatrix} \frac{\partial h_1}{\partial x_1} & \frac{\partial h_1}{\partial x_2} & .... & \frac{\partial h_1}{\partial x_n} \\ \frac{\partial h_2}{\partial x_1} & \frac{\partial h_2}{\partial x_2} & .... & \frac{\partial h_2}{\partial x_n} \\ . & . & .... & . \\ . & . & .... & . \\ \frac{\partial h_m}{\partial x_1} & \frac{\partial h_m}{\partial x_2} & .... & \frac{\partial h_m}{\partial x_n} \end{bmatrix}_{m \times n}$$

$$= \begin{bmatrix} [\nabla h_1(x)]^T \\ [\nabla h_2(x)]^T \\ . \\ . \\ [\nabla h_m(x)]^T \end{bmatrix} = \left[\frac{\partial h_i}{\partial x_j} \right],$$

$$1 \le i \le m \quad \text{and} \quad 1 \le j \le n.$$

Notice that the i^{th} row of $D_h(x)$ is $[\nabla h_i(x)]^T$, the transpose of the gradient of $h_i(x)$, $i = 1, 2, ..., m$. If $h(x)$ is linear, i.e. $h(x) = Hx$, where $H \in \mathbf{R^{m \times n}}$, then the Jacobian $D_h(x) = H$.

FACT A1. Gradient of a scalar product

Let $a \in \mathbf{R^n}$, $b \in \mathbf{R^n}$, $h(x) = [h_1(x), h_2(x), ... h_m(x)]^T$. Let

$$f(x) a^T x = x^T a \quad \text{and} \quad g(x) = h^T(x) b.$$

Then

$$\nabla f(x) = a \quad \text{and} \quad \nabla g(x) = D_h^T(x) b.$$

FACT A2. Gradient of a quadratic form

Let $\mathbf{A} \in \mathbf{R^{n \times n}}$ be a symmetric matrix and let

$$f(x) = \frac{1}{2} x^T A x.$$

Then

$$\nabla f(x) = Ax.$$

FACT A3. Quadratic form involving vector valued function

Let $h : \mathbf{R^n} \to \mathbf{R^m}$ where $h(x) = [h_1(x), h_2(x), \ldots, h_n(x)]^T$ and $A \in \mathrm{R}^{m \times m}$ be a symmetric matrix. Let

$$f(x) = \frac{1}{2} h^T(x) A h(x).$$

Then

$$\nabla f(x) = D_h^T(x) A h(x).$$

FACT A4. Gradient of another class of special functional

Let $e : \mathbf{R^n} \to \mathbf{R^n}$ with $e(x) = [e_1(x), e_2(x), ... e_n(x)]^T$ and $g : \mathbf{R^n} \to \mathbf{R^m}$ with $g(x) = [g_1(x), g_2(x), ... g_m(x)]^T$. Let $A \in \mathbf{R^{n \times m}}$, and $f(x) = e^T(x) A g(x)$. Then

$$\nabla f(x) = D_e^T(x) A g(x) + D_g^T(x) A e(x).$$

FACT A5. Second-order Taylor series

A. Scalar valued function of a scalar. Let $h : \mathbf{R} \to \mathbf{R}$. Then

$$h(x + z) \approx h(x) + \frac{\mathrm{d}h(x)}{\mathrm{d}x} z + \frac{1}{2} \frac{\mathrm{d}^2 h(x)}{\mathrm{d}x^2} z^2$$

where z denotes a small perturbation around x and $\approx$ denotes approximate equality.

B. Scalar valued function of a vector. Let $h : \mathbf{R^n} \to \mathbf{R}$. Then

$$h(x + z) \approx h(x) + [\nabla h(x)]^T z + \frac{1}{2} z^T [\nabla^2 h(x)] z.$$

C. Vector valued function of a vector. Let $h : \mathbf{R^n} \rightarrow \mathbf{R^m}$ with $h(x) = [h_1(x), h_2(x), \ldots, h_m(x)]^T$.

Then by FACT A5 (B) we have

$$h_i(x+z) = h_i(x) + [\nabla h_i(x)]^T z + \frac{1}{2} z^T \left[\nabla^2 h_i(x)\right] z.$$

By stacking in vector form, we get

$$h(x+z) = \begin{pmatrix} h_1(x+z) \\ h_2(x+z) \\ . \\ . \\ h_m(x+z) \end{pmatrix} \approx \begin{pmatrix} h_1(x) \\ h_2(x) \\ . \\ . \\ h_m(x) \end{pmatrix}$$

$$+ \begin{pmatrix} [\nabla h_1(x)]^T z \\ [\nabla h_2(x)]^T z \\ . \\ . \\ [\nabla h_m(x)]^T z \end{pmatrix} + \frac{1}{2} \begin{pmatrix} z^T \left[\nabla^2 h_1(x)\right] z \\ z^T \left[\nabla^2 h_2(x)\right] z \\ . \\ . \\ z^T \left[\nabla^2 h_m(x)\right] z \end{pmatrix}. \tag{A1}$$

The first vector on the RHS of eq. (A1) is $h(x)$. The second vector is indeed the product of the Jacobian of $h(x)$ with z, namely $D_h(x)z$. The third vector is rather special in the sense that each of its component is a quadratic form in z with the Hessian of the components of $h(x)$. We denote this vector succinctly by

$$\frac{1}{2} z^T D_h^2(x) z.$$

Combining these, we can rewrite eq. (A1) as

$$h(x+z) \approx h(x) + D_h(x)z + \frac{1}{2} z^T D_h^2(x) z. \tag{A2}$$

FACT A6. Gradient of linear combinations of quadratic forms

Let $B_i \in \mathbf{R^{n \times n}}$ for $i = 1, 2, ..., n$ be a set of symmetric matrices, $A \in \mathbf{R^{n \times n}}$ and $b \in \mathbf{R^n}$. Then, consider $f(x) : \mathbf{R^n} \rightarrow \mathbf{R}$ given by

$$f(x) = \frac{1}{2}(b_1, \quad b_2, \quad .... \quad b_n) \begin{pmatrix} x^T B_1 x \\ x^T B_2 x \\ . \\ . \\ x^T B_n x \end{pmatrix}$$

$$= \frac{1}{2} \sum_{i=1}^{n} b_i \left(x^T B_i x\right).$$

Then

$$\nabla f(x) = \sum_{i=1}^{n} b_i (B_i x).$$

REFERENCES

Andersson, E. and Järvinen, H. 1999. Variational quality control. *Q. J. R. Meteorol. Soc*. **125**, 697–722.

Bergthorsson, P. and Döös, B. 1955. Numerical weather map analysis. *Tellus* **7**, 229–240.

Daley, R. 1991. *Atmospheric data analysis*. Cambridge University Press, Cambridge, 457 pp.

Daley, R. and Barker, E. 2001. NAVDAS: Formulation and Diagnostics. *Mon. Wea. Rev.* **129**, 869–883.

Dennis, J. E., Gay, D. M. and Welsch, R.E. 1981. An adaptive nonlinear least-squares algorithm. *ACM Trans. Math. Software*, **7**, 369–383.

Dennis, J. E. Jr. and Schnabel, R. B. 1996. *Numerical methods for unconstrained optimization and nonlinear equations*. SIAM Classics in Applied Mathematics, vol. 16. 378 pp.

Epstein, E. 1969. Stochastic dynamic prediction. *Tellus* **21**, 739–759.

Huang, X.-Yu. 2000. Variational analysis using spatial filters. *Mon. Wea. Rev*. **128**, 2588–2600.

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

Le Dimet, F. X. and Talagrand, O. 1986. Variational algorithms for analysis and assimilation of meteorological observations: theoretical aspects. *Tellus* **38A**, 97–110.

Le Dimet, F. X., Navon, I. M. and Descau, D. N. 2002 Second-order information in data assimilation. *Mon. Wea. Rev*. **130**, 629–648.

Lorenc, A. C. 1986. Analysis methods for numerical weather prediction. *Quart. J. R. Meteorol. Soc*. **112**, 1177–1194.

Lorenz, E. N. 1960. Maximum simplification of the dynamic equations. *Tellus* **12**, 243–254.

Nash, G. and Sofer, A. 1996. *Linear and nonlinear programming*. McGraw Hill, New York, 692 pp.

Press, W., Teukolsky, S., Vetterling, W. and Flannery, B. 1992. *Numerical recipes in FORTRAN (art of scientific computing)*. Cambridge University Press, Cambridge, 963 pp.

Sasaki, Y. 1958. An objective analysis based on variational methods. *J. Meteorol. Soc. Jpn.* **36**, 77–88.

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

Tarantola, A. 1987. *Inverse problem theory: Methods for data fitting and model parameter estimation*. Elsevier, Amsterdam, 613 pp.

Thiébaux, H. J. and Pedder, M. A. 1987. *Spatial objective analysis*. Academic Press, New York, 299 pp.

Thompson, P. D. 1957. Uncertainty of initial state as a factor in the predictability of large scale atmosphere pattern. *Tellus* **9**, 275–295.

Wang, Z., Navon, I., Le Dimet, F. and Zhou, X. 1992. The second-order adjoint analysis: theory and application. *Meteorol. Atmos. Phys*. **50**, 3–20.

Wang, Z., Navon, I., Zhou, X. and LeDimet, F. 1995. A truncated Newton optimization algorithm in meteorological application with analytic Hessian/vector products. *Comput. Optim. Appl*. **4**, 241–262.

Wang, Z., Droegemeier, K., White, L. and Navon, I. 1997. Application of a new adjoint Newton algorithm to the 3D ARPS storm scale model using simulated data. *Mon. Wea. Rev*. **125**, 2460–2478.

Wiin-Nielsen, A. 1991. The birth of numerical weather prediction. *Tellus* **43A**, 36–52.