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Analysis error covariance *versus* posterior covariance in variational data assimilation

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The problem of variational data assimilation for a nonlinear evolution model is formulated as an optimal control problem to find the initial condition function (analysis). The data contain errors (observation and background errors); hence there is an error in the analysis. For mildly nonlinear dynamics the analysis error covariance can be approximated by the inverse Hessian of the cost functional in the auxiliary data assimilation problem, and for stronger nonlinearity by the 'effective' inverse Hessian. However, it has been noticed that the analysis error covariance is not the posterior covariance from the Bayesian perspective. While these two are equivalent in the linear case, the difference may become significant in practical terms with the nonlinearity level rising. For the proper Bayesian posterior covariance a new approximation via the Hessian is derived and its 'effective' counterpart is introduced. An approach for computing the mentioned estimates in the matrix-free environment using the Lanczos method with preconditioning is suggested. Numerical examples which validate the developed theory are presented for the model governed by Burgers equation with a nonlinear viscous term. **Copyright © 2012 Royal Meteorological Society**

Key Words: large-scale flow models; nonlinear dynamics; data assimilation; optimal control; analysis error covariance; Bayesian posterior covariance; Hessian

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1. Introduction

Over the past two decades, methods of data assimilation (DA) have become vital tools for analysis and prediction of complex physical phenomena in various fields of science and technology, but particularly in large-scale geophysical applications such as numerical weather and ocean prediction. Among the few feasible methods for solving these problems the variational data assimilation method called '4D-Var' is the preferred method implemented at some major operational centres, such as the UK Met Office, ECMWF, Meteo France and GMAO (USA). The key ideas of the method were introduced by Sasaki (1955), Penenko and Obraztsov (1976) and Le Dimet and Talagrand (1986). Assuming that an adequate dynamical model describing the evolution of the state u is given, the 4D-Var method consists in minimization of a specially designed cost functional $J(u)$ which includes two parts: the squared weighted residual between model predictions and instrumental observations taken over the finite observation period $[0, T]$; and the squared weighted difference between the solution and the prior estimate of u, known as the 'background term' u_b. Without this term one would simply get the generalized nonlinear least square problem (Hartley and Booker, 1965), whereas in the presence of the background term the cost functional is similar that considered in Tikhonov's regularization theory (Tikhonov,

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1963). The modern implementation of the method in meteorology is known as the 'incremental approach' (see Courtier *et al.*, 1994). Curiously, it took over a decade for the data assimilation community to realize that the incremental approach is nothing else but the Gauss–Newton method applied for solving the optimality system associated with $J(u)$ (see Lawless *et al.*, 2005).

The error in the optimal solution (or 'analysis error') is naturally defined as a difference between the solution u and the true state u^t; this error is quantified by the analysis error covariance matrix (see, for example, Thacker, 1989; Rabier and Courtier, 1992; Fisher and Courtier, 1995; Yang *et al.*, 1996; Gejadze *et al.*, 2008). This perception of uncertainties in the 4D-Var method is probably inherited from the nonlinear least square (or nonlinear regression) theory (Hartley and Booker, 1965). A less widespread point of view is to consider the 4D-Var method in the framework of Bayesian methods. Among the first to write on the Bayesian perspective on DA one should probably mention Lorenc (1986) and Tarantola (1987). For a comprehensive review on the recent advances in DA from this point of view see, for example, Wikle and Berliner (2007) and Stuart (2010). So far, it has been recognized that for the Gaussian data errors (which include observation and background/prior errors) the Bayesian approach leads to the same standard 4D-Var cost functional $J(u)$ to be minimized. However, it is not yet widely recognized that the conception of the estimation error in the Bayesian theory is somewhat different from the nonlinear least squares theory and, as a result, *the Bayesian posterior covariance is not exactly the analysis error covariance*. These two are conceptually different objects, which can sometimes be approximated by the same estimate. In the linear case they are quantitatively equal; in the nonlinear case the difference may become quite noticeable in practical terms. Note that the analysis error covariance computed at the optimal solution can also be named 'posterior', because it is, in some way, conditioned on the data (observations and background/prior). However, this is not the same as the Bayesian posterior covariance.

An important issue is the relationship between the analysis error covariance, the Bayesian posterior covariances and the Hessian $\mathcal{H} = J''(u)$. A well-known fact which can be found in any textbook on statistics (e.g. Draper and Smith, 1966) is that in the case of the linear dependence between the state variables (exogenous variables) and observations (endogenous variables) the analysis error covariance is equal to $\mathcal{H}^{-1}$. For the nonlinear case this is transformed into the statement that the analysis error can be *approximated* by H^{-1}, where H is a linearized approximation to $\mathcal{H}$. Since the analysis error covariance is often being confused with the Bayesian posterior covariance, the latter is also thought to be approximately equal to H^{-1}. This misconception often becomes apparent when one applies, or intends to apply, elements of the variational approach in the framework of sequential methods (filtering) (see, for example, Dobricic, 2009, p. 274; Auvinen *et al.*, 2010, p. 319; Zupanski *et al.*, 2008, p. 1043). In the 4D-Var framework, the analysis error covariance must be considered to evaluate the confidence intervals/regions of the analysis or corresponding forecast. However, it is the Bayesian posterior covariance which should be used as a basis for evaluating the background covariance for the next assimilation window if the Bayesian approach is to be consistently followed.

In this paper we carefully consider relationships between the two mentioned covariances and the Hessians $\mathcal{H}$ and H. A new estimate of the Bayesian posterior covariance via the Hessians has been suggested and its 'effective' counterpart (similar to the 'effective inverse Hessian') (see Gejadze *et al.*, 2011) has been introduced. We believe these are new results which may have both theoretical and applied value as for data assimilation, so in a more general framework of the inverse problems and parameter estimation theory (Tarantola, 2005). The issue of computational efficiency is not considered to be of major importance in this paper; however, all introduced estimates are, in principle, computable in large-scale problem set-ups.

The paper is organized as follows. In section 3 we state the variational DA problem to identify the initial conditions for a nonlinear evolution model. In section 4 the equation for analysis error is given through the errors in the input data using the Hessian of the auxiliary DA problem, and the basic relationship between analysis error covariance and the inverse of this Hessian is established. Similarly, in section 5 the expression for the Bayesian posterior covariance involving the original Hessian of $J(u)$ and the Hessian of the auxiliary DA problem is derived. In section 6 the 'effective' estimates are introduced and in section 7 the key implementation issues are considered. In section 8 the asymptotic properties of the regularized least square estimator and of the Bayesian estimator are briefly discussed. The details of numerical implementation are presented in section 9 and the numerical results which validate the presented theory in section 10. The main results of this paper are summarized in the Conclusions. The Appendix contains additional material on the asymptotic properties of the estimators.

2. Overview

Let u be the initial state of a dynamical system and y incomplete observations of the system. It is possible to write the initialization-to-data map as

$$y = G(u) + \xi_o,$$

where G represents the mapping from the initial state to the observations and ξ_o is a random variable from the Gaussian $\mathcal{N}(0, V_o)$. The objective is to find u from y.

In the Bayesian formulation u has the prior density ρ_{prior} from the Gaussian $\mathcal{N}(u_b, V_b)$. The posterior density ρ_{post} is given by Bayes' rule as

$$\rho_{\text{post}}(u) = \text{const} \cdot \exp(-\Phi(u) - \frac{1}{2}\|V_b^{-1/2}(u - u_b)\|^2),$$

where

$$\Phi(u) = \frac{1}{2}\|V_o^{-1/2}(y - G(u))\|^2$$

(for details see section 5).

The 4D-Var solution, which coincides with the maximizer of the posterior density, is found by minimizing $\Phi(u) + \frac{1}{2}\|V_b^{-1/2}(u - u_b)\|^2$ (see Eqs (2)–(3)). The minimizer $\bar{u}$ solves the optimality system

$$D\Phi(\bar{u}) + V_b^{-1}(\bar{u} - u_b) = 0$$

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(see Eqs (4)–(6)).

With this notation the paper addresses the following issues:

(i) The posterior covariance is given by

$$E^{\text{post}}((u-u^{\text{mean}})(u-u^{\text{mean}})^*),$$

where $u^{\text{mean}} = E^{\text{post}}u$ and E^{post} denotes averaging (expectation) with respect to ρ_{post} (see Eq. (32)). The posterior covariance is often approximated by trying to find the second moment of ρ_{post} centred around $\bar{u}$ instead of u^{mean} (see Eq. (33)), which is natural because $\bar{u}$ is the output of 4D-Var. In the linear Gaussian set-up u^{mean} and $\bar{u}$ coincide. This is not true in general, but can be expected to be a good approximation if the volume of data is large and/or noise is small (see section 8).

(ii) The analysis error covariance is associated with trying to find an approximation around the truth u^t, whereas the data are also assumed to come from the truth: $y = G(u^t) + \xi_o$, $u_b = u^t + \xi_b$, where $\xi_o \sim \mathcal{N}(0, V_o)$ and $\xi_b \sim N(0, V_b)$ are the observation and background error, respectively. The analysis error is defined as $\delta u = u - u^t$ and its covariance is given by

$$E^a((u-u^t)(u-u^t)^*) = E^a(\delta u \delta u^*)$$

(see Eq. (22)), where E^a denotes averaging (expectation) with respect to the analysis error density ρ_a which, taking into account the definitions of the data y and u_b, can be defined as follows:

$$\rho_a(u) = \text{const} \cdot \exp(-\Phi(u) - \frac{1}{2}\|V_b^{-1/2}(u-u^t)\|^2),$$

where

$$\Phi(u) = \frac{1}{2}\|V_o^{-1/2}(G(u^t) - G(u))\|^2.$$

The analysis error covariance can be approximated by the inverse of the Hessian H of the auxiliary cost function

$$\frac{1}{2}\|V_o^{-1/2}DG(u^t)v\|^2 + \frac{1}{2}\|V_b^{-1/2}v\|^2,$$

where v is a function belonging to the state space (see Eqs (20)–(21)). Since u^t is not known, $\bar{u}$ is used instead of u^t.

(iii) Owing to different centring of Gaussian data, the posterior covariance and the analysis error covariance are different objects and should not be confused. They are equal in the linear case.

(iv) Computing $D\Phi$ to find the 4D-Var solution requires computing $(DG)^*$ and this may be found from an adjoint computation (see Eq. (5)). Computing the approximation of the posterior covariance at $\bar{u}$ requires finding the Hessian

$$\mathcal{H}(\bar{u}) = D^2\Phi(\bar{u}) + V_b^{-1}$$

(see Eqs (45)–(47)) and inverting it. The second derivative $D^2\Phi(\bar{u})$ requires computing $D^2G(\bar{u})$. Important (and sometimes expensive to compute) terms coming from $F''(\bar{u})$ in the notation to follow cannot be neglected here.

(v) The posterior covariance can be approximated using the formula which includes both the Hessians $\mathcal{H}$ and H (see Eq. (51)). Other subsequently coarse approximations include $\mathcal{H}^{-1}$ and H^{-1}. The latter coincides with the approximation of the analysis error covariance. Actual implementation of the algorithms for computing the above estimates is detailed in the paper. Owing to the presence of linearization errors, the 'effective' values of all the covariance estimates have to be preferred (see section 6) if they are computationally affordable.

(vi) We put a distance metric (see Eq. (68)) on operators/matrices and use this to compare all of the different notions of covariance. It is important to distinguish between differences arising from conceptual shifts of perspective and those arising from approximations. For example, H^{-1} must be used for estimating the analysis error covariance, not $\mathcal{H}^{-1}$. In this case, the latter (if available by means of a different approach; see, for example, Yang *et al.*, 1996), can be used as an approximation to H^{-1}. Vice versa, it is $\mathcal{H}^{-1}$ that should be used for estimating the posterior covariance, not H^{-1}. However, the latter can be used to approximate $\mathcal{H}^{-1}$.

3. Statement of the problem

Consider the mathematical model of a physical process that is described by the evolution problem:

$$\frac{\partial \varphi}{\partial t} = F(\varphi) + f, \quad \varphi\big|_{t=0} = u, \tag{1}$$

where $\varphi = \varphi(t)$ is the unknown function belonging, for any $t \in (0, T)$, to a state space X, $u \in X$, F is a nonlinear operator mapping X into X. Let $Y = L_2(0, T; X)$ be a space of functions $\varphi(t)$ with values in X, $\|\cdot\|_Y = (\cdot,\cdot)_Y^{1/2}$, $f \in Y$. Suppose that for a given $u \in X, f \in Y$ there exists a unique solution $\varphi \in Y$ to Eq. (1).

Let u^t be the 'true' initial state and φ^t the solution to the problem (Eq. (1)) with $u = u^t$, i.e. the 'true' state evolution. We define the input data as follows: the background function $u_b \in X$, $u_b = u^t + \xi_b$ and the observations $y \in Y_o$, $y = C\varphi^t + \xi_o$, where $C : Y \to Y_o$ is a linear bounded operator (observation operator) and Y_o is an observation space. The functions $\xi_b \in X$ and $\xi_o \in Y_o$ may be regarded as the background and the observation error, respectively. We assume that these errors are normally distributed (Gaussian) with zero mean and the covariance operators $V_b \cdot = E[(\cdot, \xi_b)_X \xi_b]$ and $V_o \cdot = E[(\cdot, \xi_o)_{Y_o} \xi_o]$, i.e. $\xi_b \sim \mathcal{N}(0, V_b)$, $\xi_o \sim \mathcal{N}(0, V_o)$, where '$\sim$' is read 'is distributed as'. We also assume that ξ_o, ξ_b are mutually uncorrelated and V_b,V_o are positive definite, and hence invertible.

Let us formulate the following DA problem (optimal control problem) with the aim to identify the initial condition: for given $f \in Y$ find $u \in X$ and $\varphi \in Y$ such that they satisfy Eq. (1), and on the set of solutions to Eq. (1) a cost functional $J(u)$ takes the minimum value, i.e.

$$J(u) = \inf_{v \in X} J(v), \tag{2}$$

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where

$$J(u) = \frac{1}{2}(V_b^{-1}(u-u_b), u-u_b)_X, \\ + \frac{1}{2}(V_o^{-1}(C\varphi - y), C\varphi - y)_{Y_o}. \quad (3)$$

The necessary optimality condition reduces the problem (Eqs (2)–(3)) to the following system (Lions, 1968):

$$\frac{\partial \varphi}{\partial t} = F(\varphi) + f,\ \varphi\big|_{t=0} = u, \quad (4)$$

$$-\frac{\partial \varphi^*}{\partial t} - (F'(\varphi))^*\varphi^* = -C^*V_o^{-1}(C\varphi - y), \quad (5)$$

$$V_b^{-1}(u-u_b) - \varphi^*\big|_{t=0} = 0, \quad (6)$$

with the unknowns φ, φ^*, u, where $(F'(\varphi))^*$ is the adjoint to the Frechet derivative of F, and C^* is the adjoint to C defined by $(C\varphi, \psi)_{Y_o} = (\varphi, C^*\psi)_Y,\ \varphi \in Y, \psi \in Y_o$. All adjoint variables throughout the paper satisfy the trivial terminal condition, e.g. $\varphi^*\big|_{t=T} = 0$. Having assumed that the system (Eqs (4)–(6)) has a unique solution, we will study the impact of the errors ξ_b, ξ_o on the optimal solution u.

4. The analysis error covariance via inverse Hessian

In this section an equation for the analysis error is derived through the errors in the input data, the approximate relationship between the analysis error covariance and the Hessian of the auxiliary DA problem is established and the validity of this approximation is discussed.

Let us define the analysis (optimal solution) error $\delta u = u - u^t$ and the corresponding (related via Eq. (7)) field deviation $\delta\varphi = \varphi - \varphi^t$. Assuming F is continuously Frechet differentiable, there exists $\tilde{\varphi} = \varphi^t + \tau(\varphi - \varphi^t),\ \tau \in [0,1]$, such that the Taylor–Lagrange formula (Marchuk *et al.*, 1996) is valid: $F(\varphi) - F(\varphi^t) = F'(\tilde{\varphi})\delta\varphi$. Then from Eqs (4)–(6) we get

$$\frac{\partial \delta\varphi}{\partial t} - F'(\tilde{\varphi})\delta\varphi = 0,\ \delta\varphi|_{t=0} = \delta u, \quad (7)$$

$$-\frac{\partial \varphi^*}{\partial t} - (F'(\varphi))^*\varphi^* = -C^*V_o^{-1}(C\delta\varphi - \xi_o), \quad (8)$$

$$V_b^{-1}(\delta u - \xi_b) - \varphi^*|_{t=0} = 0. \quad (9)$$

Let us introduce the operator $R(\varphi): X \to Y$ as follows:

$$R(\varphi)\nu = \psi,\ \nu \in X, \quad (10)$$

where ψ is the solution of the tangent linear problem

$$\frac{\partial \psi}{\partial t} - F'(\varphi)\psi = 0,\ \psi|_{t=0} = \nu. \quad (11)$$

The adjoint operator $R^*(\varphi): Y \to X$ acts on the function $g \in Y$ according to the formula

$$R^*(\varphi)g = \psi^*|_{t=0}, \quad (12)$$

where ψ^* is the solution to the adjoint problem

$$-\frac{\partial \psi^*}{\partial t} - (F'(\varphi))^*\psi^* = g. \quad (13)$$

Then, the system for errors (Eqs (7)–(9)) can be represented as a single operator equation for δu:

$$H(\varphi, \tilde{\varphi})\delta u = V_b^{-1}\xi_b + R^*(\varphi)C^*V_o^{-1}\xi_o, \quad (14)$$

where

$$H(\varphi, \tilde{\varphi}) = V_b^{-1} + R^*(\varphi)C^*V_o^{-1}CR(\tilde{\varphi}). \quad (15)$$

The operator $H(\varphi, \tilde{\varphi}): X \to X$ can be defined by the successive solutions of the following problems:

$$\frac{\partial \psi}{\partial t} - F'(\tilde{\varphi})\psi = 0,\ \psi|_{t=0} = \nu, \quad (16)$$

$$-\frac{\partial \psi^*}{\partial t} - (F'(\varphi))^*\psi^* = -C^*V_o^{-1}C\psi, \quad (17)$$

$$H(\varphi, \tilde{\varphi})\nu = V_b^{-1}\nu - \psi^*|_{t=0}. \quad (18)$$

In general, the operator $H(\varphi, \tilde{\varphi})$ is neither symmetric nor positive definite. However, if both its entries are the same, i.e. $\varphi = \tilde{\varphi} = \theta$, it becomes the Hessian $H(\theta)$ of the cost function J_1 in the following optimal control problem: find δu and $\delta\varphi$ such that

$$J_1(\delta u) = \inf_{\nu} J_1(\nu), \quad (19)$$

where

$$J_1(\delta u) = \frac{1}{2}(V_b^{-1}(\delta u - \xi_b), \delta u - \xi_b)_X \\ + \frac{1}{2}(V_o^{-1}(C\delta\varphi - \xi_o), C\delta\varphi - \xi_o)_{Y_o}, \quad (20)$$

and $\delta\varphi$ satisfies the problem

$$\frac{\partial \delta\varphi}{\partial t} - F'(\theta)\delta\varphi = 0,\ \delta\varphi\big|_{t=0} = \delta u. \quad (21)$$

We shall call the problem (Eqs (19)–(20)) the 'auxiliary DA problem' and the entry θ in Eq. (21) the 'origin' of the Hessian $H(\theta)$. Let us note that any $\xi_b \in X$ and $\xi_o \in Y_o$ can be considered in Eq. (20), including $\xi_b = 0$ and $\xi_o = 0$.

Further, we assume that the optimal solution (analysis) error δu is unbiased, i.e. $E[\delta u] = 0$ (the validity of this assumption in the nonlinear case will be discussed in section 8), with the analysis error covariance operator

$$V_{\delta u}\cdot = E[(\cdot, \delta u)_X\ \delta u] = E[(\cdot, u - u^t)_X\ (u - u^t)]. \quad (22)$$

In order to evaluate $V_{\delta u}$ we express δu from Eq. (14), then apply the expectation E to $(\cdot, \delta u)_X \delta u$. Let us note, however, that the functions $\varphi, \tilde{\varphi}$ in Eqs (7)–(9) are dependent on ξ_b, ξ_o and so are the operators $R(\tilde{\varphi}), R^*(\varphi)$, and it is not possible to represent δu through ξ_b, ξ_o in an explicit form. Therefore, before applying E we need to introduce some approximations of the operators involved in Eq. (14) independent of ξ_b, ξ_o. Consider the functions $\tilde{\varphi} = \varphi^t + \tau\delta\varphi$

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and $\varphi = \varphi^t + \delta\varphi$ in Eqs (7)–(9). As far as we assume that $E[\delta u] \approx 0$, it is natural to consider $E[\delta\varphi] \approx 0$. Thus the best value of φ and $\tilde{\varphi}$ independent of ξ_o, ξ_b is apparently φ^t and we can use the following approximations:

$$R(\tilde{\varphi}) \approx R(\varphi^t),\ R^*(\varphi) \approx R^*(\varphi^t). \tag{23}$$

Then Eq. (14) reduces to

$$H(\varphi^t)\delta u = V_b^{-1}\xi_b + R^*(\varphi^t)C^*V_o^{-1}\xi_o, \tag{24}$$

where

$$H(\cdot) = V_b^{-1} + R^*(\cdot)C^*V_o^{-1}CR(\cdot). \tag{25}$$

Now we express δu from Eq. (24):

$$\delta u = H^{-1}(\varphi^t)(V_b^{-1}\xi_b + R^*(\varphi^t)C^*V_o^{-1}\xi_o)$$

and obtain the expression for the analysis error covariance as follows:

$$\begin{aligned} V_{\delta u} &= H^{-1}(\varphi^t)(V_b^{-1} + R^*(\varphi^t)C^*V_o^{-1}CR(\varphi^t))H^{-1}(\varphi^t) \\ &= H^{-1}(\varphi^t)H(\varphi^t)H^{-1}(\varphi^t) = H^{-1}(\varphi^t). \end{aligned} \tag{26}$$

In practice the 'true' field φ^t is not known (apart from the 'identical twin experiment' set-up); thus we have to use its best available approximation $\bar{\varphi}$ associated to a certain unique optimal solution $\bar{u}$ defined by the real data $(\bar{u}_b, \bar{y})$, i.e. we have to use

$$V_{\delta u} = H^{-1}(\bar{\varphi}). \tag{27}$$

This formula is equivalent to a well-established result (see Thacker, 1989; Rabier and Courtier, 1992; Courtier *et al.*, 1994), which is usually deduced (without considering the exact equation (14)) by straightforwardly simplifying the original nonlinear DA problem (Eqs (2)–(3)) under the assumption that

$$F(\varphi) - F(\varphi^t) \approx F'(\varphi)\delta\varphi,\ \ \forall\varphi, \tag{28}$$

which is called the 'tangent linear hypothesis' (TLH). In particular, in Rabier and Courtier (1992, p. 671), the error equation is actually derived in the form

$$\begin{aligned} &(V_b^{-1} + R^*(\varphi)C^*V_o^{-1}CR(\varphi))\delta u \\ &= V_b^{-1}\xi_b + R^*(\varphi)C^*V_o^{-1}\xi_o. \end{aligned} \tag{29}$$

It is obvious that the operators $R(\varphi)$, $R^*(\varphi)$ in this equation depend on the errors via φ and they cannot be treated as being constant with respect to δu when computing the expectation $E\,[(\cdot, \delta u)_X \delta u]$, as has been done by Rabier and Courtier (1992). From Eq. (29) the authors nevertheless deduce the formula (27); hence there is no difference in practical terms between the two approaches. However, it is clear from our derivation that the best estimate of $V_{\delta u}$ via the inverse Hessian can be achieved given the origin φ^t. The error in this estimate is an averaged (over all possible implementations of φ and $\tilde{\varphi}$) error due to transitions $R(\tilde{\varphi}) \to R(\varphi^t)$ and $R^*(\varphi) \to R^*(\varphi^t)$; we shall call it the 'linearization' error. The use of $\bar{\varphi}$ instead of φ^t in the Hessian computations leads to another error, which we shall call the 'origin' error. It is important to distinguish these two errors. The first one is related to the method in use and can be eliminated if the error equation (14) for each ξ_1, ξ_2 is satisfied exactly. This can be achieved by solving the perturbed original DA problem in the Monte Carlo loop with a large sample size, for example. The second one, however, cannot be eliminated by any method, given that the state estimate almost always differs from the 'truth'. It should be mentioned in advance that the origin error can be significantly larger than the linearization error. This means, for example, that the use of the computationally expensive Monte Carlo instead of the inverse Hessian may lead to only marginal quality improvement. This issue is discussed in Gejadze *et al.* (2011) and a method of accessing the possible magnitude of the origin error is a subject of a forthcoming paper.

In the context of our approach, the 'tangent linear hypothesis' should be rather considered in the form

$$F(\varphi) - F(\varphi^t) \approx F'(\varphi^t)\delta\varphi,\ \ \forall\varphi. \tag{30}$$

There is a clear difference between Eqs (30) and (28). For example, if we assume that $E[\delta\varphi] = 0$ then $E[F'(\varphi^t)\delta\varphi] = 0$; however, $E[F'(\varphi)\delta\varphi] = E[F'(\varphi^t + \delta\varphi)\delta\varphi] \neq 0$. One can easily imagine situations in which the condition (30) is far less demanding than (28). It is customarily said in the geophysical literature that $V_{\delta u}$ can be approximated by the inverse Hessian if the TLH (Eq. (28)) is valid, which should be true if the nonlinearity is mild and/or the error δu and, subsequently, $\delta\varphi$ are small. We would say more precisely that the linearization error in $V_{\delta u}$ approximated by $H^{-1}(\varphi^t)$ is small if the TLH (Eq. (30)) is valid. Moreover, we derive Eq. (26) via Eq. (14). From this derivation one can see that the validity of Eq. (26) depends on the accuracy of the approximations (23), which may still be accurate though Eq. (30) is not satisfied. This partially explains why in practice the approximation (26) is reasonably accurate if Eq. (30) is evidently not satisfied. Another reason is rooted in the stochastic properties of the nonlinear least squares estimator, as discussed in section 6. However, it is hardly possible to judge on the magnitude of the origin error in relation to the condition (30) being valid or not.

5. Posterior covariance

In this section the expression for the Bayesian posterior covariance involving the Hessians of the original functional $J(u)$ and the auxiliary functional $J_1(\delta u)$ is derived, and its possible approximations are discussed. The results of this section demonstrate that the analysis error covariance and Bayesian posterior covariance are different objects and should not be confused.

Given $u_b \sim \mathcal{N}(\bar{u}_b, V_b)$, $y \sim \mathcal{N}(\bar{y}, V_o)$, the following expression for the posterior distribution of u is derived from the Bayes theorem (for details see Stuart, 2010):

$$\begin{aligned} p(u|\bar{y}) = \text{const} \cdot \exp\,(&-\frac{1}{2}(V_b^{-1}(u - \bar{u}_b), u - \bar{u}_b)_X) \\ &\times \exp(-\frac{1}{2}(V_o^{-1}(C\varphi - \bar{y}), C\varphi - \bar{y})_{Y_o}). \end{aligned} \tag{31}$$

It follows from Eq. (31) that the solution to the variational DA problem (Eqs (2)–(3)) with the data $y = \bar{y}$ and $u_b = \bar{u}$

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is equal to the mode of $p(u,\bar{y})$ (see, for example, Lorenc, 1986; Tarantola, 1987). Accordingly, the Bayesian posterior covariance has to be defined by

$$\mathcal{V}_{\delta u}\cdot = E[(\cdot, u-E[u])_X\,(u-E[u])], \tag{32}$$

with $u\sim p(u|\bar{y})$. Clearly, in order to compute $\mathcal{V}_{\delta u}$ by the Monte Carlo method, one must generate a sample of pseudo-random realizations u_i from $p(u|\bar{y})$. In particular, in the ensemble filtering methods (see Evensen, 2003; Zupanski *et al.*, 2008) these are produced by solving the optimal control problem (i.e. inverse problem!) for independently perturbed data at the current time step by explicitly using the Kalman update formula in the EnKF of Evensen (2003) or by minimizing the nonlinear cost function in the MLEF of Zupanski *et al.* (2008). Then, the sample mean and the sample covariance (equivalent to Eq. (32)) are computed. As far as the ensemble filtering methods are considered a special case of the Bayesian sequential estimation (Wikle and Berliner, 2007, p. 10), we may call the covariance obtained by the described method the 'Bayesian posterior covariance'. Following a similar approach in variational DA, one should consider u_i to be the solutions to the DA problem (Eqs (2)–(3)) with the perturbed data $u_b=\bar{u}_b+\xi_b$, and $y=\bar{y}+\xi_o$, where $\xi_b\sim\mathcal{N}(0,V_b)$, $\xi_o\sim\mathcal{N}(0,V_o)$. Further, we assume that $E[u]=\bar{u}$, where $\bar{u}$ is the solution to the unperturbed problem (Eqs (2)–(3)), in which case $\mathcal{V}_{\delta u}$ can be approximated as follows:

$$\mathcal{V}_{\delta u}\cdot = E[(\cdot, u-\bar{u})_X\,(u-\bar{u})] = E[(\cdot,\delta u)_X\,\delta u]. \tag{33}$$

We will show that this covariance is different from the classical analysis error covariance (Rabier and Courtier, 1992) evaluated at the optimal solution $\bar{u}$.

Now, in order to build the posterior error covariance, let us consider the unperturbed optimality system (Eqs (4)–(6)) with fixed $u_b=\bar{u}_b$, $y=\bar{y}$:

$$\frac{\partial\bar{\varphi}}{\partial t}=F(\bar{\varphi})+f,\ \varphi\big|_{t=0}=\bar{u}, \tag{34}$$

$$-\frac{\partial\bar{\varphi}^*}{\partial t}-(F'(\bar{\varphi}))^*\bar{\varphi}^*=-C^*V_o^{-1}(C\bar{\varphi}-\bar{y}), \tag{35}$$

$$V_b^{-1}(\bar{u}-\bar{u}_b)-\bar{\varphi}^*\big|_{t=0}=0, \tag{36}$$

with the solution $\{\bar{u},\bar{\varphi},\bar{\varphi}^*\}$. Let us now introduce the perturbations as follows: $u_b=\bar{u}_b+\xi_b$, $y=\bar{y}+\xi_o$, where $\xi_b\in X,\xi_o\in Y_o$. The perturbed solution $\{u,\varphi,\varphi^*\}$ satisfies Eqs (4)–(6). Let us denote $\delta u=u-\bar{u}$, $\delta\varphi=\varphi-\bar{\varphi}$ and $\delta\varphi^*=\varphi^*-\bar{\varphi}^*$. Then from Eqs (4)–(6) and (34)–(36) we obtain for $\{\delta u,\delta\varphi,\delta\varphi^*\}$

$$\frac{\partial\delta\varphi}{\partial t}=F(\varphi)-F(\bar{\varphi}),\ \delta\varphi\big|_{t=0}=\delta u, \tag{37}$$

$$\begin{aligned}&-\frac{\partial\delta\varphi^*}{\partial t}-(F'(\varphi))^*\delta\varphi^*\\&=[(F'(\varphi))^*-(F'(\bar{\varphi}))^*]\bar{\varphi}^*-C^*V_o^{-1}(C\delta\varphi-\xi_o),\end{aligned} \tag{38}$$

$$V_b^{-1}(\delta u-\xi_b)-\delta\varphi^*\big|_{t=0}=0. \tag{39}$$

Using the Taylor–Lagrange formulas $F(\varphi)=F(\bar{\varphi})+F'(\tilde{\varphi}_1)\delta\varphi$, $F'(\varphi)=F'(\bar{\varphi})+F''(\tilde{\varphi}_2)\delta\varphi$, and introducing $\tilde{\varphi}_1=\bar{\varphi}+\tau_1\delta\varphi$, $\tilde{\varphi}_2=\bar{\varphi}+\tau_2\delta\varphi$, $\tau_1,\tau_2\in[0,1]$, we derive the system for errors:

$$\frac{\partial\delta\varphi}{\partial t}=F'(\tilde{\varphi}_1)\delta\varphi,\ \delta\varphi\big|_{t=0}=\delta u, \tag{40}$$

$$\begin{aligned}&-\frac{\partial\delta\varphi^*}{\partial t}-(F'(\varphi))^*\delta\varphi^*\\&=[(F'(\tilde{\varphi}_2))^*\bar{\varphi}^*]'\delta\varphi-C^*V_o^{-1}(C\delta\varphi-\xi_o),\end{aligned} \tag{41}$$

$$V_b^{-1}(\delta u-\xi_b)-\delta\varphi^*\big|_{t=0}=0, \tag{42}$$

which is equivalent to a single operator equation for δu:

$$\mathcal{H}(\varphi,\tilde{\varphi}_1,\tilde{\varphi}_2)\delta u=V_b^{-1}\xi_b+R^*(\varphi)C^*V_o^{-1}\xi_o, \tag{43}$$

where

$$\begin{aligned}&\mathcal{H}(\varphi,\tilde{\varphi}_1,\tilde{\varphi}_2)=V_b^{-1}\\&+R^*(\varphi)(C^*V_o^{-1}C-[(F'(\tilde{\varphi}_2))^*\bar{\varphi}^*]')R(\tilde{\varphi}_1).\end{aligned} \tag{44}$$

Here, the operators R and R^* are defined in section 4 and $\mathcal{H}(\varphi,\tilde{\varphi}_1,\tilde{\varphi}_2):X\to X$ can be defined by the successive solution of the following problems:

$$\frac{\partial\psi}{\partial t}=F'(\tilde{\varphi}_1)\psi,\ \psi\big|_{t=0}=\nu, \tag{45}$$

$$\begin{aligned}&-\frac{\partial\psi^*}{\partial t}-(F'(\varphi))^*\psi^*\\&=[(F'(\tilde{\varphi}_2))^*\bar{\varphi}^*]'\psi-C^*V_o^{-1}C\psi,\end{aligned} \tag{46}$$

$$\mathcal{H}(\varphi,\tilde{\varphi}_1,\tilde{\varphi}_2)\nu=V_b^{-1}\nu-\psi^*\big|_{t=0}. \tag{47}$$

Let us underline that the term involving F'' on the right-hand side of Eq. (41) is of first-order accuracy with respect to $\delta\varphi$–the same as $C^*V_0^{-1}C\delta\varphi$–and therefore it cannot be neglected in derivation of the covariance. In general, the operator $\mathcal{H}(\varphi,\tilde{\varphi}_1,\tilde{\varphi}_2)$ is neither symmetric nor positive definite. However, if all its entries are the same, i.e. $\varphi=\tilde{\varphi}_1=\tilde{\varphi}_2$, it becomes the Hessian $\mathcal{H}(\varphi)$ of the cost function in the original DA problem (Eqs (2)–(3)), which is symmetric and, also, positive definite if u is a minimum point of $J(u)$. Equation (46) is often referred to as the 'second-order' adjoint model (Le Dimet *et al.*, 2002). Technically, this is simply an adjoint model with a specially defined source term.

As before, we assume that $E(\delta u)\approx 0$. Let us accept the following approximations:

$$R(\tilde{\varphi}_1)\approx R(\bar{\varphi}),\ R^*(\varphi)\approx R^*(\bar{\varphi}),$$

$$[(F'(\tilde{\varphi}_2))^*\bar{\varphi}^*]'\approx[(F'(\bar{\varphi}))^*\bar{\varphi}^*]'. \tag{48}$$

Then the exact error equation (43) is approximated as follows:

$$\mathcal{H}(\bar{\varphi})\delta u=V_b^{-1}\xi_b+R(\bar{\varphi})^*C^*V_o^{-1}\xi_o, \tag{49}$$

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where

$$\mathcal{H}(\cdot) = V_b^{-1} + R^*(\cdot)(C^* V_o^{-1} C - [(F'(\cdot))^* \bar{\varphi}^*]')R(\cdot). \quad (50)$$

Now, we express δu from Eq. (49):

$$\delta u = \mathcal{H}^{-1}(\bar{\varphi})(V_b^{-1}\xi_b + R(\bar{\varphi})^* C^* V_o^{-1}\xi_o),$$

and obtain an approximate expression for the posterior error covariance:

$$\begin{aligned}\mathcal{V}_{\delta u} \approx \mathcal{V}_1 &= \mathcal{H}^{-1}(\bar{\varphi})(V_b^{-1} + R^*(\bar{\varphi})V_o^{-1}R(\bar{\varphi}))\mathcal{H}^{-1}(\bar{\varphi}) \\ &= \mathcal{H}^{-1}(\bar{\varphi})H(\bar{\varphi})\mathcal{H}^{-1}(\bar{\varphi}),\end{aligned} \quad (51)$$

where $H(\bar{\varphi})$ is the Hessian of the cost function J_1 in the auxiliary DA problem (Eqs (19)–(20)), computed at $\theta = \bar{\varphi}$.

Obviously, the above double-product formula could be overly sensitive to the errors due to the approximations (48). By assuming $H(\bar{\varphi})\mathcal{H}^{-1}(\bar{\varphi}) \approx I$ we obtain a more stable (but, possibly, less accurate) approximation:

$$\mathcal{V}_{\delta u} \approx \mathcal{V}_2 = \mathcal{H}^{-1}(\bar{\varphi}). \quad (52)$$

It is interesting to note that $\mathcal{H}^{-1}(\bar{\varphi})$ is known as the asymptotic Bayesian covariance in the framework of the Bayesian asymptotic theory (see Heyde and Johnstone, 1979; Kim, 1994). By assuming $\mathcal{H}^{-1}(\bar{\varphi}) \approx H^{-1}(\bar{\varphi})$ we obtain from Eq. (51) yet another (more crude than Eq. (52)) approximation:

$$\mathcal{V}_{\delta u} \approx \mathcal{V}_3 = H^{-1}(\bar{\varphi}), \quad (53)$$

i.e. the inverse Hessian of the auxiliary DA problem can be considered as an approximation to both the posterior error covariance and the analysis error covariance evaluated at $\bar{\varphi}$.

6. 'Effective' covariance estimates

At the end of section 4 the linearization and origin errors in the analysis error covariance were discussed. We say that the linearization error can be relatively small even though the TLH is violated to a certain degree. However, when the nonlinearity becomes stronger and/or the input data errors become larger, the inverse Hessian may not properly approximate the analysis error covariance (even for the known 'true' state), in which case the 'effective' inverse Hessian (see Gejadze *et al.*, 2011) should be used instead:

$$V_{\delta u} = E\left[H^{-1}(\varphi)\right]. \quad (54)$$

Apparently, the same must be true for the posterior error covariance computed by Eq. (51). By following the reasoning of Gejadze *et al.* (2011), let us consider the discretized nonlinear error equation (43) and write down the expression for δu:

$$\delta u = \mathcal{H}^{-1}(\varphi, \tilde{\varphi}_1, \tilde{\varphi}_2)(V_b^{-1}\xi_b + R^*(\varphi)C^* V_0^{-1}\xi_o).$$

For the covariance $\mathcal{V}_{\delta u}$ we have an expression as follows:

$$\begin{aligned}\mathcal{V}_{\delta u} = {} & E[\mathcal{H}^{-1}V_b^{-1}\ \xi_b\xi_b^T\ V_b^{-1}\mathcal{H}^{-1}] \\ & + E[\mathcal{H}^{-1}R^*(\varphi)C^*V_0^{-1}\ \xi_o\xi_o^T\ V_0^{-1}CR(\varphi)\mathcal{H}^{-1}] \\ & + E[\mathcal{H}^{-1}V_b^{-1}\ \xi_b\xi_o^T\ V_o^{-1}CR(\varphi)\mathcal{H}^{-1}] \\ & + E[\mathcal{H}^{-1}R^*(\varphi)C^*V_o^{-1}\ \xi_o\xi_b^T\ V_b^{-1}\mathcal{H}^{-1}],\end{aligned} \quad (55)$$

where $\mathcal{H}^{-1} = \mathcal{H}^{-1}(\varphi, \tilde{\varphi}_1, \tilde{\varphi}_2)$. As discussed in Gejadze *et al.* (2011), we approximate the products $\xi_b\xi_b^T$, $\xi_o\xi_o^T$, $\xi_b\xi_o^T$ and $\xi_o\xi_b^T$ in (55) by $E[\xi_b\xi_b^T] = V_b$, $E[\xi_o\xi_o^T] = V_o$, and $E[\xi_b\xi_o^T] = 0$, $E[\xi_o\xi_b^T] = 0$ (since ξ_b and ξ_o are mutually uncorrelated), respectively. Thus we write an approximation of $\mathcal{V}_{\delta u}$ as follows:

$$\mathcal{V}_{\delta u} = E\left[\mathcal{H}^{-1}(\varphi, \tilde{\varphi}_1, \tilde{\varphi}_2)\ H(\varphi)\ \mathcal{H}^{-1}(\varphi, \tilde{\varphi}_1, \tilde{\varphi}_2)\right].$$

First, we substitute a possibly asymmetric and indefinite operator $\mathcal{H}(\varphi, \tilde{\varphi}_1, \tilde{\varphi}_2)$ with the Hessian $\mathcal{H}(\varphi)$, in which case we obtain

$$\mathcal{V}_{\delta u} \approx \mathcal{V}_1^e = E\left[\mathcal{H}^{-1}(\varphi)\ H(\varphi)\ \mathcal{H}^{-1}(\varphi)\right]. \quad (56)$$

Here we keep in mind that $\varphi := \varphi(u) = \varphi(\bar{u} + \delta u)$, where δu is a random vector; therefore it is the variable of integration in E. Next, by assuming $H(\varphi)\mathcal{H}^{-1}(\varphi) \approx I$ we obtain a more stable (but, possibly, less accurate) approximation:

$$\mathcal{V}_{\delta u} \approx \mathcal{V}_2^e = E\left[\mathcal{H}^{-1}(\varphi)\right]. \quad (57)$$

Finally, by assuming $\mathcal{H}^{-1}(\varphi) \approx H^{-1}(\varphi)$ we obtain yet another (more crude than Eq. (57)) approximation:

$$\mathcal{V}_{\delta u} \approx \mathcal{V}_3^e = E\left[H^{-1}(\varphi)\right], \quad (58)$$

which is equivalent to Eq. (54). Therefore, the 'effective' inverse Hessian can also be considered as an approximation to the posterior error covariance.

7. Implementation remarks

In this section the key implementation issues, including preconditioning, regularization and computation of the 'effective' covariance estimates, are considered.

7.1. *Preconditioning*

Preconditioning can be used to accelerate computation of the inverse Hessian by iterative methods such as BFGS or Lanczos. The latter evaluates the eigenvalues and eigenvectors (or, more precisely, the Ritz values and Ritz vectors) of an operator using the operator–vector action result. Since $\mathcal{H}$ is self-adjoint, we must consider a projected Hessian in a symmetric form:

$$\tilde{\mathcal{H}}(\cdot) = (B^{-1})^* \mathcal{H}(\cdot)B^{-1},$$

with some operator $B : X \to X$, defined in such a way that: (a) most eigenvalues of $\tilde{\mathcal{H}}$ are clustered around 1; (b) there are only a few eigenvalues significantly different from 1 (dominant eigenvalues). A sensible approximation of $\tilde{\mathcal{H}}^{-1}$ can be obtained using these dominant eigenvalues and the corresponding eigenvectors, the number of which is expected to be much smaller than the state-vector dimension M. After that, having computed $\tilde{\mathcal{H}}^{-1}$, one can easily recover $\mathcal{H}^{-1}$ using the formula

$$\mathcal{H}^{-1}(\cdot) = B^{-1}\tilde{\mathcal{H}}^{-1}(\cdot)(B^{-1})^*.$$

By comparing Eq. (50) to (25) we notice that $\mathcal{H}(\cdot)$ is different from $H(\cdot)$ due to the presence of the second-order

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term $[(F'(\cdot))^*\bar{\varphi}^*]'$. If we assume that the difference between $\mathcal{H}(\cdot)$ and $H(\cdot)$ is not large, then $H^{-1/2}(\cdot)$ can be used for efficient preconditioning of $\mathcal{H}(\cdot)$. Thus we will look for the projected Hessian:

$$\tilde{\mathcal{H}}(\cdot) = H^{-1/2}(\cdot)\mathcal{H}(\cdot)H^{-1/2}(\cdot), \tag{59}$$

in which case the posterior error covariance $\mathcal{V}_{\delta u}$ can be approximated by the following estimates:

$$\mathcal{V}_1 = H^{-1/2}(\bar{\varphi})\tilde{\mathcal{H}}^{-2}(\bar{\varphi})H^{-1/2}(\bar{\varphi}), \tag{60}$$

$$\mathcal{V}_2 = H^{-1/2}(\bar{\varphi})\tilde{\mathcal{H}}^{-1}(\bar{\varphi})H^{-1/2}(\bar{\varphi}). \tag{61}$$

It is clear, therefore, that $H^{-1/2}(\bar{\varphi})$ has to be computed first. For computing $H^{-1}(\cdot)$ itself the preconditioning in the form $B^{-1} = V_b^{1/2}$ is used. The result can be presented in limited-memory form:

$$H^{-1}(\cdot) = V_b^{1/2}\tilde{H}^{-1}(\cdot)V_b^{1/2}, \tag{62}$$

with

$$\tilde{H}^{-1}(\cdot) = I + \sum_{i=1}^{K_1}(s_i^{-1} - 1)U_iU_i^T, \tag{63}$$

where $\{s_i, U_i\}, i = 1, \ldots, K_1 << M$ are the eigenvalues and eigenvectors of $\tilde{H}(\cdot)$ for which the values of $|s_i^{-1} - 1|$ are most significant. The matrix functions theory (see, for example, Bellman, 1960) asserts that for any symmetric matrix A (which may be presented in the form $A = BDB^T$, where D is a diagonal matrix, B is an orthogonal matrix) and for any function f the following definition holds:

$$f(A) = Bf(D)B^T.$$

In particular, if f is the power function, we obtain as follows:

$$A^\alpha = BD^\alpha B^T,\ \alpha \in \mathcal{R}. \tag{64}$$

For example, if $\tilde{H}$ is presented in the form $\tilde{H} = USU^T$ (symmetric eigenvalue decomposition), then $\tilde{H}^{-1} = US^{-1}U^T$. Assuming that only K_1 first eigenvalues are distinct from 1, i.e. $(s_i^{-1} - 1) \approx 0,\ \forall i > K_1$, we obtain Eq. (63). Let us mention that in geophysical literature the expression (63) is usually derived in a more cumbersome way by considering the Sherman–Morrison–Woodbury inversion formula (see, for example, Powell and Moore, 2009). Given the pairs $\{s_i, U_i\}$, the limited-memory square root operator $\tilde{H}^{-1/2}(\cdot)$ can be computed as follows:

$$\tilde{H}^{-1/2}(\cdot) = I + \sum_{i=1}^{K_1}(s_i^{-1/2} - 1)U_iU_i^T. \tag{65}$$

Thus we can compute $H^{-1/2}(\cdot)v = V_b^{1/2}\tilde{H}^{-1/2}(\cdot)v$, which is needed for Eq. (59). Another way to compute $\tilde{H}^{-1/2}(\cdot)v$ is the recursive procedure suggested in Tshimanga *et al.* (2008, Appendix A, Theorem 2). The operators $\tilde{\mathcal{H}}^{-1}(\cdot)$ and $\tilde{\mathcal{H}}^{-2}(\cdot)$ can also be computed by the Lanczos algorithm in the limited-memory form equivalent to (Eq. (63)):

$$\tilde{\mathcal{H}}^{-1}(\cdot) = I + \sum_{i=1}^{K_2}(\lambda_i^{-1} - 1)\mathcal{U}_i\mathcal{U}_i^T, \tag{66}$$

$$\tilde{\mathcal{H}}^{-2}(\cdot) = I + \sum_{i=1}^{K_2}(\lambda_i^{-2} - 1)\mathcal{U}_i\mathcal{U}_i^T, \tag{67}$$

where $\{\lambda_i, \mathcal{U}_i\}, i = 1, \ldots, K_2$ are the dominant eigenvalues and eigenvectors of $\tilde{\mathcal{H}}(\cdot)$, the number of which is expected to be much smaller than K_1. The advantage of computing $\mathcal{V}_1$ or $\mathcal{V}_2$ in the form (60), (61) is therefore obvious: the second-order adjoint model has to be called only K_2 times.

7.2. *Regularization*

Let us consider two symmetric positive definite $M \times M$ matrices A and B and introduce the divergence matrix $\Gamma(A, B) = B^{-1/2}AB^{-1/2}$. We define the Riemann distance between A and B as follows:

$$\mu(A, B) = \left\|\log \Gamma(A, B)\right\| = \left(\sum_{i=1}^{M} \log^2 \gamma_i\right)^{1/2}, \tag{68}$$

where γ_i are the eigenvalues of $\Gamma(A, B)$ (see, for example, Moakher, 2005).

Comparing Eqs (60) and (61) and taking into account Eqs (66) and (67), we notice that the Riemann distance between $\mathcal{V}_3 = H^{-1}$ and $\mathcal{V}_2$ is defined by $(\lambda_i^{-1} - 1)$, whereas the distance between $\mathcal{V}_3$ and $\mathcal{V}_1$ is defined by $(\lambda_i^{-2} - 1)$. Therefore, the norm of $\mathcal{V}_1$ can be significantly larger than that of $\mathcal{V}_2$, which clearly explains the increased sensitivity of $\mathcal{V}_1$ to the approximation error due to transitions (Eq. (48)) (as compared to $\mathcal{V}_2$). A simple approach to regularize $\mathcal{V}_1$ is to present it in the form

$$\mathcal{V}_1 = H^{-1/2}(\bar{\varphi})\tilde{\mathcal{H}}^{-(1+\alpha)}(\bar{\varphi})H^{-1/2}(\bar{\varphi}), \tag{69}$$

with

$$\tilde{\mathcal{H}}^{-(1+\alpha)}(\cdot) = I + \sum_{i=1}^{K_2}(\lambda_i^{-(1+\alpha)} - 1)\mathcal{U}_i\mathcal{U}_i^T, \tag{70}$$

where $\alpha = \alpha(\lambda_1, \ldots, \lambda_{K_2}) \in (0, 1)$. The idea of this approach is to bound the distance between $\mathcal{V}_1$ and $\mathcal{V}_2$ dependent on the values $(\lambda_i^{-1} - 1)$. For example, the following rule defining α is suggested and used in computations:

$$\alpha = \begin{cases} \cos(\frac{\pi}{2}x), & |x| \le 1 \\ 0, & |x| > 1 \end{cases}, \tag{71}$$

$$x = \log_\beta(\lambda_{\max}),$$

where $\lambda_{\max} < 1$ is the eigenvalue for which $1 - \lambda_i$ takes the largest positive value, and $\beta > 1$ is the regularization parameter to be chosen. Let us note that if all $\lambda_i \ge 1$, no regularization is required, i.e. $\alpha = 1$.

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7.3. *Computation of the 'effective' estimates*

Let us consider, for example, Eq. (58):

$$\mathcal{V}_{\delta u} \approx \mathcal{V}_3^e = E\left[H^{-1}(\varphi)\right].$$

The field $\varphi = \varphi(x,t)$ in this equation corresponds to the perturbed optimal solution $u = \bar{u} + \delta u$, which is the solution to the optimality system (Eqs (4)–(6)) with the perturbed data $u_b = \bar{u}_b + \xi_b$ and $y = \bar{y} + \xi_o$. Given a set of independent perturbations $\xi_b^i, \xi_o^i,\ i = 1, \ldots, L$, where L is the sample size, one can compute a set of u^i and then $\mathcal{V}_3^e$ as a sample mean:

$$\mathcal{V}_3^e = \frac{1}{L}\sum_{i=1}^{L}\left[H^{-1}(\varphi(u^i))\right]. \tag{72}$$

Clearly, this method is very expensive because it requires a set of optimal solution to be computed. A far more feasible method is suggested in Gejadze *et al.* (2011). The idea of the method is to substitute a set of optimal solutions by a set of functions which belong to and best represent the same (as the optimal solutions) probability distribution. Assuming that u has a close-to normal distribution we are looking for $\mathcal{V}_3^e$ which satisfies the system as follows:

$$\begin{cases} \mathcal{V}_3^e = E\left[H^{-1}(\varphi(u))\right], \\ u \sim \mathcal{N}\left(\bar{u}, \mathcal{V}_3^e\right). \end{cases} \tag{73}$$

A very significant reduction of computational costs can be achieved if $H^{-1/2}(\varphi(\bar{u}))$ is used for preconditioning when computing $H^{-1}(\varphi(u^i))$ (see also Gejadze *et al.*, 2011). In the same way as $\mathcal{V}_3^e$ the estimates $\mathcal{V}_2^e$ and $\mathcal{V}_1^e$ can be computed.

8. Asymptotic properties of the analysis and posterior errors

In this section the asymptotic properties of the regularized least square estimator (4D-Var) and of the Bayesian estimator are discussed. These are important properties which justify the use of the Hessian-based approximations of the covariances considered in this paper.

Let us consider the error equations (14) and (43). Both these equations can be rewritten in an equivalent form (see Appendix):

$$J''(\tilde{u})\ \delta u = -J'(\hat{u}), \tag{74}$$

where J is the cost functional (3), $\tilde{u} = \hat{u} + \tau(u - \hat{u})$, $\tau \in [0,1]$ and $\delta u = u - \hat{u}$ ($\hat{u} = u^t$ and $\hat{u} = \bar{u}$ for Eqs (14) and (43), correspondingly). This form of the error equation coincides with the equation obtained in Amemiya (1983) while considering the nonlinear least-squares estimation problem for a cost functional similar to Eq. (3), but without the penalty (background) term. In this case, the statistical properties of the nonlinear least-squares estimator have been analysed by many authors. For a univariate case, the classical result (see Jennrich, 1969) states that δu is consistent and asymptotically normal if ξ_o is an independent identically distributed (i.i.d.) random variable with $E[\xi_o] = 0$ and $E[\xi_o^2] = \sigma^2 < \infty$. In the data assimilation problem (Eqs (1)–(3)) 'asymptotically' means that, given the observation array, $T \to \infty$ given the finite observation time step dt, or d$t \to 0$ given the finite observation window $[0, T]$. Let us stress that for the asymptotic normality of δu the error ξ_o is not required to be normal. This original result has been generalized to the multivariate case and to the case of serially correlated, yet identically distributed observations, by White and Domowitz (1984), whereas an even more general case is considered in Yuan and Jennrich (1998).

In the present paper we consider the complete cost functional (Eq. (3)) and, correspondingly, both $J'' \equiv \mathcal{H}(\tilde{\varphi})$ and J' in Eq. (74) contain additional terms, i.e.

$$J''(\tilde{u}) = V_b^{-1} + R^*(\tilde{\varphi})(C^* V_o^{-1} C - [(F'(\tilde{\varphi}))^* \bar{\varphi}^*]')R(\tilde{\varphi}),$$
$$-J'(\hat{u}) = V_b^{-1}\xi_b + R^*(\hat{\varphi})C^* V_o^{-1}\xi_o.$$

To analyse a possible impact of these terms let us follow the reasoning of Amemiya (1983, pp. 337–345). It is concluded that the error δu is consistent and asymptotically normal when: (a) the right-hand side of the error equation is normal; (b) the left-hand side matrix converges in probability to a non-random value. These conditions are met under certain general regularity requirements to the function $F(\varphi)$, which are incomparably weaker than the tangent linear hypothesis and do not depend on the magnitude of the input errors. It is easy to see that the first condition holds if ξ_b is normally distributed. Since V_b^{-1} is a constant matrix, the second condition always holds, as long as it holds for $R^*(\tilde{\varphi})(C^* V_o^{-1} C - [(F'(\tilde{\varphi}))^* \bar{\varphi}^*]')R(\tilde{\varphi})$. Therefore, one may conclude that δu from Eqs (14) and (43) is bound to remain asymptotically normal. In practice, the observation window $[0, T]$ and the observation time step dt are always finite, implying the finite number of i.i.d. observations. Moreover, it is not easy to access how large the number of observations must be for the desired asymptotic properties to be reasonably approximated. Some nonlinear least-square problems in which the normality of the estimation error holds for 'practically relevant' sample sizes are said to exhibit a 'close-to-linear' statistical behaviour. The method suggested in Ratkowsky (1983) to verify this behaviour is, essentially, a normality test applied to a generated sample of optimal solutions, which is hardly feasible for large-scale applications. Nevertheless, for certain highly nonlinear evolution models it is reasonable to expect that the distribution of δu might be reasonably close to normal if the number of i.i.d. observations is significant in time (typically, in variational DA for the medium-range weather forecast one uses $T = 6$ h with the observation step d$t = 2$ min), and the observation network is sufficiently dense in space.

9. Numerical validation

In this section the details of numerical implementation are provided. These include the description of the numerical experiments and of the numerical model.

9.1. *Description of numerical experiments*

In order to validate the presented theory a series of numerical experiments has been performed. We assign a certain function u to be the 'true' initial state u^t. Given u^t, we compute a large ($L = 2500$) ensemble of optimal solutions $\{u_i(u^t)\},\ i = 1, \ldots, L$ by solving L times the data assimilation problem (Eqs (2)–(3)) with the perturbed data $u_b = u^t + \xi_b$ and $y = C\varphi^t + \xi_o$, where $\xi_b \sim \mathcal{N}(0, V_b)$ and

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$\xi_o \sim \mathcal{N}(0, V_o)$. Based on this ensemble the sample mean and sample covariance matrix are computed. The latter is further processed to filter out the sampling error (as described in Gejadze *et al.*, 2011); the result is considered to be the reference ('true') value $\hat{V}$ of the analysis error covariance matrix $V_{\delta u}$. Obviously, each ensemble member $u_i(u^t)$ may be regarded as a unique 'true' optimal solution $\bar{u}$ conditioned on a 'come true' implementation of the random processes ξ_b and ξ_o, which define the input data $\bar{u}_b$ and $\bar{y}$. Next we choose $\bar{u}$ to be a certain $u_i(u^t)$ for which the statistics $d = (u_i - u^t)^T \hat{V}^{-1}(u_i - u^t)$ are close enough to the state-vector dimension M (d has χ^2-distribution with M degrees of freedom). For any $\bar{u}$ we compute a large ($L = 2500$) ensemble of optimal solutions $\{u_i(\bar{u})\}$, $i = 1, \ldots, L$ by solving L times the data assimilation problem (Eqs (2)–(3)) with the perturbed data $u_b = \bar{u}_b + \xi_b$ and $y = \bar{y} + \xi_o$. Based on this ensemble the sample mean and sample covariance matrix are computed. The latter is further processed to filter out the sampling error; the result is considered to be the reference ('true') value $\hat{\mathcal{V}}$ of the posterior error covariance matrix $\mathcal{V}_{\delta u}$ associated with chosen $\bar{u}$. Next we compute the estimates of $\mathcal{V}_{\delta u}$: $\mathcal{V}_1$ by Eq. (51), $\mathcal{V}_2$ by Eq. (52), $\mathcal{V}_3$ by Eq. (53), $\mathcal{V}_1^e$ by Eq. (56), $\mathcal{V}_2^e$ by Eq. (57) and $\mathcal{V}_3^e$ by Eq. (58), and compare them to $\hat{\mathcal{V}}$. The accuracy of approximations of $\mathcal{V}_{\delta u}$ by different $\mathcal{V}$ can be quantified by the Riemann distance $\mu(\mathcal{V}, \mathcal{V}_{\delta u})$ defined by Eq. (68). It is also worth noting that $\tilde{H}^{-1} = \Gamma(H^{-1}, V_b)$ and $\tilde{\mathcal{H}}^{-1} = \Gamma(\mathcal{H}^{-1}, H^{-1})$. Since the computational efficiency is not the major issue in this paper, the 'effective' estimates $\mathcal{V}_1^e$, $\mathcal{V}_2^e$ and $\mathcal{V}_3^e$ are evaluated as the sample mean (see Eq. (72) for $\mathcal{V}_3^e$) using the first 100 members of the ensemble $\{u_i(\bar{u})\}$, which are available after computing the reference posterior error covariance $\hat{\mathcal{V}}$.

9.2. Numerical model

As a nonlinear evolution model for $\varphi(x,t)$ we use the 1D Burgers equation with a nonlinear viscous term:

$$\frac{\partial \varphi}{\partial t} + \frac{1}{2}\frac{\partial(\varphi^2)}{\partial x} = \frac{\partial}{\partial x}\left(\nu(\varphi)\frac{\partial \varphi}{\partial x}\right), \qquad (75)$$

$$\varphi = \varphi(x,t),\ t \in (0,T),\ x \in (0,1),$$

with the Neumann boundary conditions

$$\left.\frac{\partial \varphi}{\partial x}\right|_{x=0} = \left.\frac{\partial \varphi}{\partial x}\right|_{x=1} = 0 \qquad (76)$$

and the viscosity coefficient

$$\nu(\varphi) = \nu_0 + \nu_1\left(\frac{\partial \varphi}{\partial x}\right)^2, \quad \nu_0, \nu_1 = \text{const} > 0. \qquad (77)$$

The nonlinear diffusion term with $\nu(\varphi)$ dependent on φ'_x is introduced to mimic the eddy viscosity (turbulence), which depends on the field gradients (pressure, temperature), rather than on the field value itself. This type of $\nu(\varphi)$ also allows us to formally qualify the problem (Eqs (75)–(77)) as strongly nonlinear (see Fučik and Kufner, 1980). Let us mention that Burgers' equations are sometimes considered in DA context as a simple model of atmospheric flow motion.

We use the implicit time discretization as follows:

$$\frac{\varphi^i - \varphi^{i-1}}{h_t} + \mathrm{d}fx\left(\frac{1}{2}w(\varphi^i)\varphi^i - \nu(\varphi^i)\frac{\partial \varphi^i}{\partial x}\right) = 0, \qquad (78)$$

where $i = 1, \ldots, N$ is the time integration index and $h_t = T/N$ is a time step. The spatial operator is discretized on a uniform grid (h_x is the spatial discretization step, $j = 1, \ldots, M$ is the node number, M is the total number of grid nodes) using the 'power law' first-order scheme as described in Patankar (1980), which yields quite a stable discretization scheme (this scheme allows $\nu(\varphi)$ as small as 0.5×10^{-4} for $M = 200$ without noticeable oscillations). For each time step we perform nonlinear iterations on coefficients $w(\varphi) = \varphi$ and $\nu(\varphi)$, assuming initially that $\nu(\varphi_i) = \nu(\varphi_{i-1})$ and $w(\varphi_i) = \varphi_{i-1}$, and keep iterating until Eq. (78) is satisfied (i.e. the norm of the left-hand side in Eq. (78) becomes smaller than a threshold $\epsilon_1 = 10^{-12}M^{1/2}$). In all computations presented in this paper the following parameters are used: observation period $T = 0.32$, discretization steps $h_t = 0.004$, $h_x = 0.005$, state vector dimension $M = 200$, and parameters in Eq. (77) $\nu_0 = 10^{-4}$, $\nu_1 = 10^{-6}$.

For numerical experiments two initial conditions $u^t = \varphi^t(x,0)$ have been chosen; these will be referred to below as case A and case B. For each case, the state evolution $\varphi^t(x,t)$ is presented in Figure 1 (left) and (right), respectively. A well-known property of Burgers' solutions is that a smooth initial condition evolves into shocks. However, the diffusion term in the form Eq. (77) helps to limit the field gradients and to avoid the typical oscillations. The first initial condition is a lifted cos function. Apparently, the area to the left of the minimum points at $x = 0.5$ and $x = 1$ are the areas where the shocks form. The level of nonlinearity related to the convective term can be easily controlled in this case by adding a constant. In the second case, we combine two cos functions of different frequency and sign. Moreover, in the area $x \in (0.45, 0.55)$ one has $\varphi^t(x,0) = 0$, i.e. only the nonlinear diffusion process initially takes place in this part of the domain. Different observation schemes are used: for case A – the sensor location coordinates $\hat{x}_k = \{0.35,\ 0.4,\ 0.5,\ 0.6,\ 0.65\}$; and for case B – $\hat{x}_k = \{0.35,\ 0.45,\ 0.5,\ 0.55,\ 0.65\}$.

9.3. Additional details

The consistent tangent linear and adjoint models (operators R and R^*) have been generated by the Automatic Differentiation tool TAPENADE (Hascoët and Pascual, 2004) from the forward model code implementing Eq. (78). The consistent second-order term $[(F'(\cdot))^*\bar{\varphi}^*]'$ has been generated in the same way from the piece of the code describing the local spatial discretization stencil, then manually introduced as a source term to the adjoint model (Eq. (17)) to form the second-order adjoint model. Both adjoint models have been validated using the standard gradient tests.

Solutions to the DA problem (Eqs (2)–(3)) have been obtained using the limited-memory BFGS minimization algorithm (Liu and Nocedal, 1989). For each set of perturbations the problem is solved twice: first starting from the unperturbed state u^t (or $\bar{u}$), then starting from the background $u_b = u^t + \xi_b$ (or $u_b = \bar{u}_b + \xi_b$). If close results are obtained, the solution is accepted as an ensemble member. This is done to avoid difficulties related to a possible multi-extrema nature of the cost function (Eq. (3)). In all computations reported in this paper less than 3% of solutions have been eventually discarded for each ensemble.

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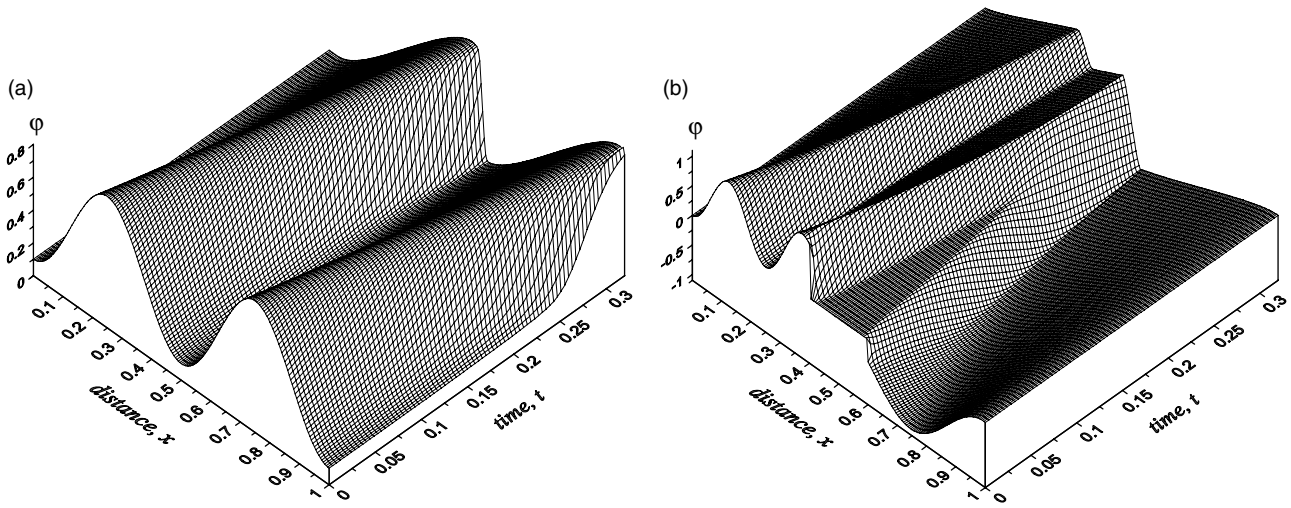

Figure 1. Field evolution. Left: case A; right: case B.

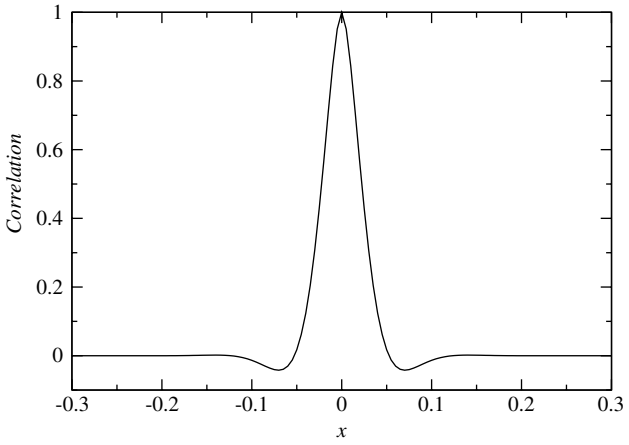

Figure 2. Correlation function.

The eigenvalue analysis of operators has been performed by the Implicitly Restarted Arnoldi Method (symmetric driver dsdrv1, ARPACK library; Lehoucq *et al.*, 1988). The operators $\tilde{H}(\varphi(\bar{u}))$ and $\tilde{\mathcal{H}}(\varphi(\bar{u}))$ needed for evaluating $\mathcal{V}_{1,2,3}$ have been computed without limiting the number of Lanczos iterations. However, when computing the effective values $\mathcal{V}^e_{1,2,3}$, the number of iterations have been limited by 20 and only the 'converged' eigenpairs (parameter tol = 0.001 in dsdrv1) has been used to form $\tilde{H}(\varphi(u^i))$ and $\tilde{\mathcal{H}}(\varphi(u^i))$.

The background error covariance V_b is computed assuming that the background error belongs to the Sobolev space $W_2^2(0,1)$ (see Gejadze *et al.*, 2010, for details). The resulting correlation function is as presented in Figure 2; the background error variance is $\sigma_b^2 = 0.02$ and the observation error variance is $\sigma_o^2 = 0.001$.

10. Numerical results

In this section we consider the numerical results which validate the presented theory.

For a given 'true' initial state (case A or case B), from the first 50 members of the corresponding ensemble $\{u_i(u^t)\}$ we choose 10 optimal solutions $\bar{u}$ such that the Riemann distance $\mu(\mathcal{H}^{-1}(\bar{u}), H^{-1}(\bar{u}))$ given by Eq. (68) is most significant. These solutions are numbered as $\bar{u}_k$, $k = 1, \ldots, 10$ and referred to below as 'case Ak' or 'case Bk'. For each $\bar{u}_k$ we compute the sample of $\{u_i(\bar{u}_k)\}$, then, consequently, the sample mean, the sample covariance and the reference posterior error covariance $\hat{\mathcal{V}}$ related to $\bar{u}_k$. Finally we compute the estimates $\mathcal{V}_{1,2,3}$ and $\mathcal{V}^e_{1,2,3}$ and the measures $\mu(\mathcal{V}_i, \hat{\mathcal{V}})$ and $\mu(\mathcal{V}^e_i, \hat{\mathcal{V}})$. The results are summarized in Table 1.

The first column of Table 1 contains $\mu^2(\mathcal{V}_3, \hat{\mathcal{V}})$, which is the squared Riemann distance between the posterior covariance $\hat{\mathcal{V}}$ and its most crude estimate $\mathcal{V}_3 = H^{-1}(\bar{\varphi})$. Thus we expect $\mu(\mathcal{V}_3, \hat{\mathcal{V}})$ to have the largest value among all measures involving other estimates of $\mathcal{V}_{\delta u}$. Let us recall that $H^{-1}(\bar{\varphi})$ is usually considered as an approximation to the analysis error covariance $V_{\delta u}$ (see Eq. (27)). The latter is sometimes regarded as the Bayesian posterior covariance, which is a conceptual mistake. Technically, the difference is clear: for computing the posterior covariance one must take into account the second-order term, whereas in computing the analysis error covariance this term simply does not appear. The second column of Table 1 contains $\mu^2(\mathcal{V}_2, \hat{\mathcal{V}})$ where $\mathcal{V}_2 = \mathcal{H}^{-1}(\bar{\varphi})$. Let us recall that $\mathcal{H}^{-1}(\bar{\varphi})$ is considered the asymptotic posterior covariance in Bayesian theory. The third column contains $\mu^2(\mathcal{V}_1, \hat{\mathcal{V}})$, where $\mathcal{V}_1 = \mathcal{H}^{-1}(\bar{\varphi})H(\bar{\varphi})\mathcal{H}^{-1}(\bar{\varphi})$ is the posterior covariance estimate suggested in this paper. According to the theory presented, for small input errors ξ_o, ξ_b one should expect

$$\mu(\mathcal{V}_1, \hat{\mathcal{V}}) < \mu(\mathcal{V}_2, \hat{\mathcal{V}}) < \mu(\mathcal{V}_3, \hat{\mathcal{V}}).$$

In practice, this relation may not stand (as can be seen from the table) due to linearization errors, as discussed in section 6. In this case one should expect this behaviour to be true at least for 'effective' estimates, i.e.

$$\mu(\mathcal{V}^e_1, \hat{\mathcal{V}}) < \mu(\mathcal{V}^e_2, \hat{\mathcal{V}}) < \mu(\mathcal{V}^e_3, \hat{\mathcal{V}}) < \mu(\mathcal{V}_3, \hat{\mathcal{V}}). \qquad (79)$$

Looking at Table 1 we note that this condition always holds, which validates the presented theory. In some cases the overall reduction of the Riemann distance (compare $\mu(\mathcal{V}^e_1, \hat{\mathcal{V}})$ to $\mu(\mathcal{V}_3, \hat{\mathcal{V}})$) is about an order of magnitude or even larger. In some cases, e.g. A5, B2, this reduction is not significant. It is difficult, therefore, to warrant a certain level of distance reduction for each particular case, and this should be accessed in an average sense. The table additionally

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Table 1. Summary of numerical experiments: squared Riemann distance $\mu^2(\cdot,\cdot)$.

Case	$\mu^2(\mathcal{V}_3,\hat{\mathcal{V}})$	$\mu^2(\mathcal{V}_2,\hat{\mathcal{V}})$	$\mu^2(\mathcal{V}_1,\hat{\mathcal{V}})$	$\mu^2(\mathcal{V}_3^e,\hat{\mathcal{V}})$	$\mu^2(\mathcal{V}_2^e,\hat{\mathcal{V}})$	$\mu^2(\mathcal{V}_1^e,\hat{\mathcal{V}})$
A1	3.817	3.058	4.738	2.250	1.418	1.151
A2	17.89	18.06	21.50	2.535	1.778	1.602
A3	10.89	9.183	8.988	4.725	3.013	2.627
A4	3.489	2.960	4.286	2.190	1.342	1.079
A5	5.832	5.070	5.778	3.710	2.886	2.564
A6	9.048	8.362	10.16	2.539	1.748	1.474
A7	20.21	19.76	22.24	4.290	3.508	3.383
A8	1.133	0.585	1.419	1.108	0.466	0.246
A9	20.18	20.65	24.52	2.191	1.986	1.976
A10	10.01	8.521	8.411	3.200	2.437	2.428
B1	7.271	6.452	6.785	2.852	1.835	1.476
B2	16.42	14.89	14.70	15.61	14.11	13.77
B3	9.937	10.70	17.70	4.125	3.636	3.385
B4	6.223	5.353	11.50	2.600	1.773	1.580
B5	10.73	9.515	9.875	4.752	3.178	2.530
B6	6.184	4.153	8.621	4.874	2.479	1.858
B7	9.551	9.818	26.51	3.912	3.195	2.971
B8	5.948	4.845	7.105	3.484	2.105	1.745
B9	17.10	15.69	16.77	5.025	4.186	3.854
B10	8.230	7.685	7.827	3.787	2.861	2.647

demonstrates the correctness and potential of the 'effective value' approach suggested in Gejadze *et al.* (2011). By comparing $\mu(\mathcal{V}_3^e,\hat{\mathcal{V}})$ and $\mu(\mathcal{V}_3,\hat{\mathcal{V}})$ in cases A2, A7, A9 and B9 one can note that the Riemann distance is drastically reduced if the 'effective' inverse Hessian is used instead of the inverse Hessian at point $\bar{u}$.

The following examples show what the Riemann distance actually means in terms of the error in covariance estimate. Let us consider the mean deviation vector σ and the correlation matrix r defined as follows:

$$\sigma(i) = \mathcal{V}^{1/2}(i,i),$$

$$r(i,j) = \mathcal{V}(i,j)/(\sigma(i)\sigma(j)), \quad i,j = 1,\dots,M,$$

and denote $\sigma_3, \sigma^e_{1,2,3}, \hat{\sigma}$ as the mean deviation vectors and r_3, $r^e_{1,2,3}, \hat{r}$ as the correlation matrices associated correspondingly with $\mathcal{V}_3$, $\mathcal{V}^e_{1,2,3}$ and $\hat{\mathcal{V}}$. Naturally, $\hat{\sigma}$ and $\hat{r}$ are used as the reference values. The mean deviation error is characterized by the vector

$$\varepsilon = \log_2(\sigma/\hat{\sigma}). \tag{80}$$

The logarithmic error (Eq. (80)) is particularly appropriate when comparing positive quantities since it shows (symmetrically!) how many times the reference value is either over- or underestimated. The error in the correlation matrix is characterized by

$$\epsilon = |r - \hat{r}|. \tag{81}$$

Let us denote by $\varepsilon_3, \varepsilon^e_{1,2,3}$ the error vectors associated with $\sigma_3, \sigma^e_{1,2,3}$, and by $\epsilon_3, \epsilon^e_{1,2,3}$ the error matrices associated with $r_3, r^e_{1,2,3}$.

For demonstration, two cases for each initial condition have been chosen: A2, A8 and B6, B9. The reference mean deviation $\hat{\sigma}$ for cases A and B is presented in Figure 3 (left) and (right), correspondingly.

In Figure 4 the logarithmic error ε (see Eq. (80)) is shown as follows: ε_3 (error associated with $\mathcal{V}_3 = H^{-1}$) as the boundary of the light-filled *area 3*; ε^e_3 (error associated with $\mathcal{V}^e_3 = E[H^{-1}]$) in *line 3e*; ε^e_2 (error associated with $\mathcal{V}^e_2 = E[\mathcal{H}^{-1}]$) in *line 2e*; and ε^e_1 (error associated with $\mathcal{V}^e_1 = E[\mathcal{H}^{-1}H\mathcal{H}^{-1}]$) as the boundary of the dark-filled *area 1e*. The presented figures confirm the main result: the mean deviation error is the largest for the posterior covariance being estimated by $\mathcal{V}_3$ (boundary of *area 3*) and the smallest - by $\mathcal{V}^e_1$. For example, see case A2 (upper/left panel), area $0.48 < x < 0.5$, or case B9 (lower/right panel), area $0.5 < x < 0.52$, where the estimated σ is about three times smaller than the actual value. If the 'effective' estimate $\mathcal{V}^3_e$ is used (*line 3e*), this error is noticeably reduced. In case B6 (upper/right panel) no benefit from using $\mathcal{V}^e_3$ instead of $\mathcal{V}_3$ can be noticed; however, the benefit of using the estimates $\mathcal{V}^e_2$ (*line 2e*) and $\mathcal{V}^e_1$ (boundary of *area 1e*) is clearly manifested. On the other hand, case B9 represents an example where no noticeable benefit is achieved when using $\mathcal{V}^e_2$ and $\mathcal{V}^e_1$ instead of $\mathcal{V}^e_3$. Nevertheless, it is obvious from the figures that $\mathcal{V}^e_1$ is, on average, the best estimate available (see also Table 1). Case B6 (upper/right panel) is also interesting in the way that σ associated with $\mathcal{V}^e_3$ and $\mathcal{V}_3$ is mainly overestimated ($\varepsilon > 0$). Relying on all 20 cases considered in numerical simulation one may conclude that $\mathcal{V}_3 = H^{-1}$ is more likely to provide underestimated values of σ.

The absolute error in the correlation matrix ϵ (see Eq. (81)) is shown in Figure 5. Here, for each case considered, sub-cases (a), (b) and (c) displaying ϵ_3, ϵ^e_3 and ϵ^e_1 correspondingly are presented. The distance between an element $\epsilon(i,j)$ and the diagonal element $\epsilon(i,i)$ is counted by $(j-i)h_x$ along the axis x'. The features to be noticed in Figure 5 are similar to those discussed previously. As before, the error associated with $\mathcal{V}_3 = H^{-1}$ (sub-case (a)) is the largest and the error associated with $\mathcal{V}^e_1$ (sub-case (c)) is the smallest. In case A2, the main error reduction is achieved by using the 'effective' estimate $\mathcal{V}^e_3$ instead of the point estimate $\mathcal{V}_3$, whereas usage of $\mathcal{V}^e_1$ instead of $\mathcal{V}^e_3$ does not make too much difference. The opposite behaviour can be observed in case B6.

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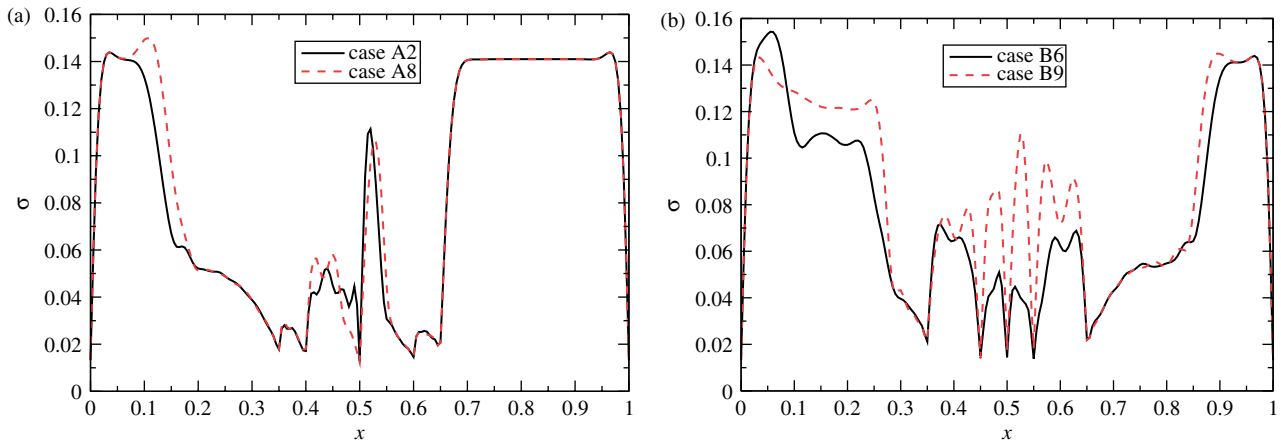

Figure 3. Reference mean deviation $\hat{\sigma}(x)$ (corresponds to $\hat{\mathcal{V}}$). Left: cases A2, A8; right: cases B6, B9. This figure is available in colour online at wileyonlinelibrary.com/journal/qj

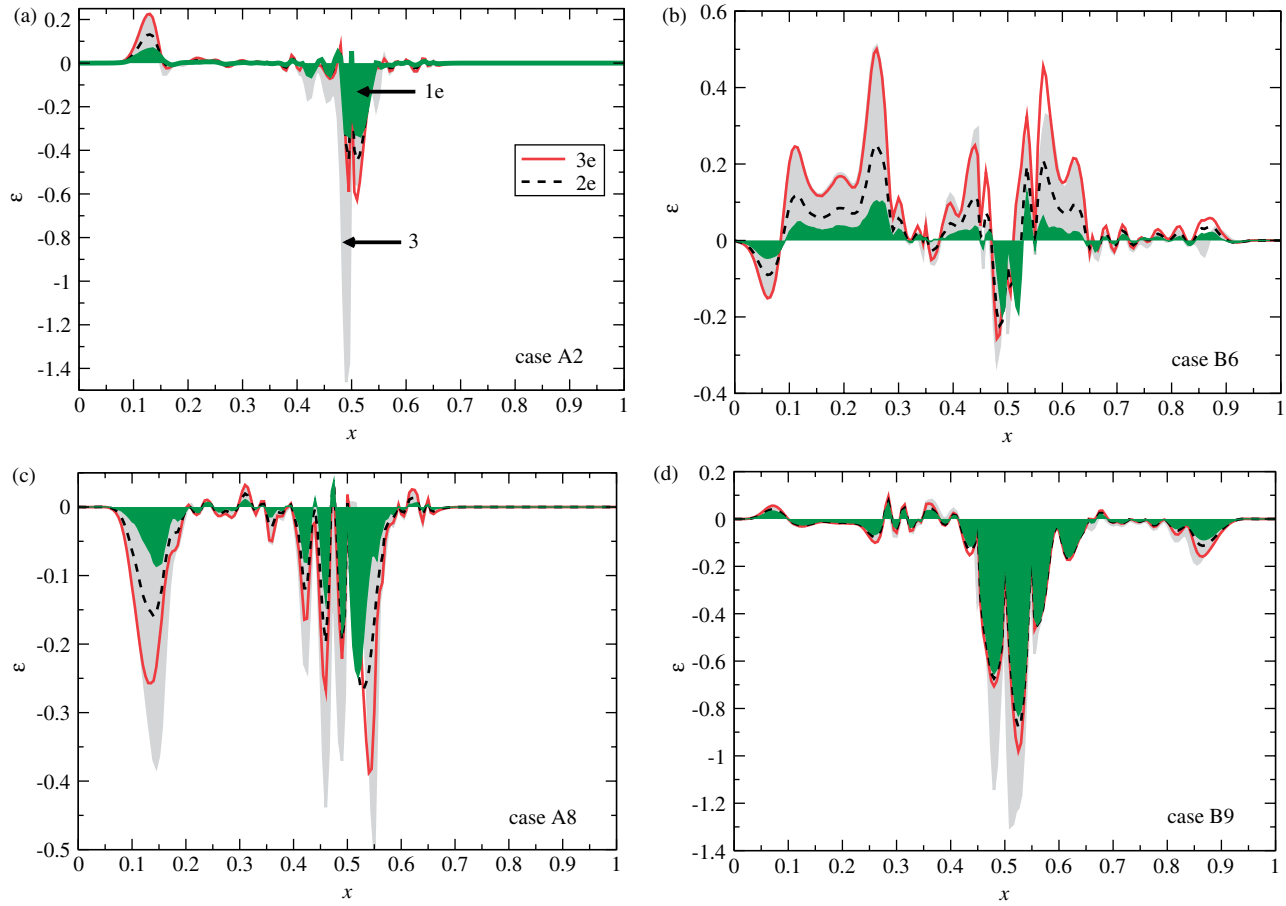

Figure 4. Logarithmic errors in the mean deviation (Eq. (80)): $\varepsilon_3(x)$, $\varepsilon_3^e(x)$, $\varepsilon_2^e(x)$ and $\varepsilon_1^e(x)$. This figure is available in colour online at wileyonlinelibrary.com/journal/qj

11. Conclusions

In this paper we consider the hind-cast (initialization) data assimilation problem, which is a typical problem in meteorology and oceanography. The problem is formulated as an initial value control problem for a nonlinear evolution model governed by partial differential equations and the solution method (called 4D-Var) consists in minimization of the cost function (Eq. (3)) under constraints (Eq. (1)). In finite dimensions this is equivalent to solving the regularized nonlinear least squares problem. The statistical properties of the optimal solution (analysis) error are usually quantified by the analysis error covariance matrix: the approach possibly inherited from the nonlinear regression theory where a similarly defined covariance matrix is used to quantify asymptotic properties of the nonlinear least-squares estimator. Less often the 4D-Var method had been considered in the Bayesian perspective, but this point of view becomes increasingly popular. In particular, it is recognized that in the case of Gaussian input errors the Bayesian approach yields the same cost functional as considered in 4D-Var. However, some authors seem to fall short in

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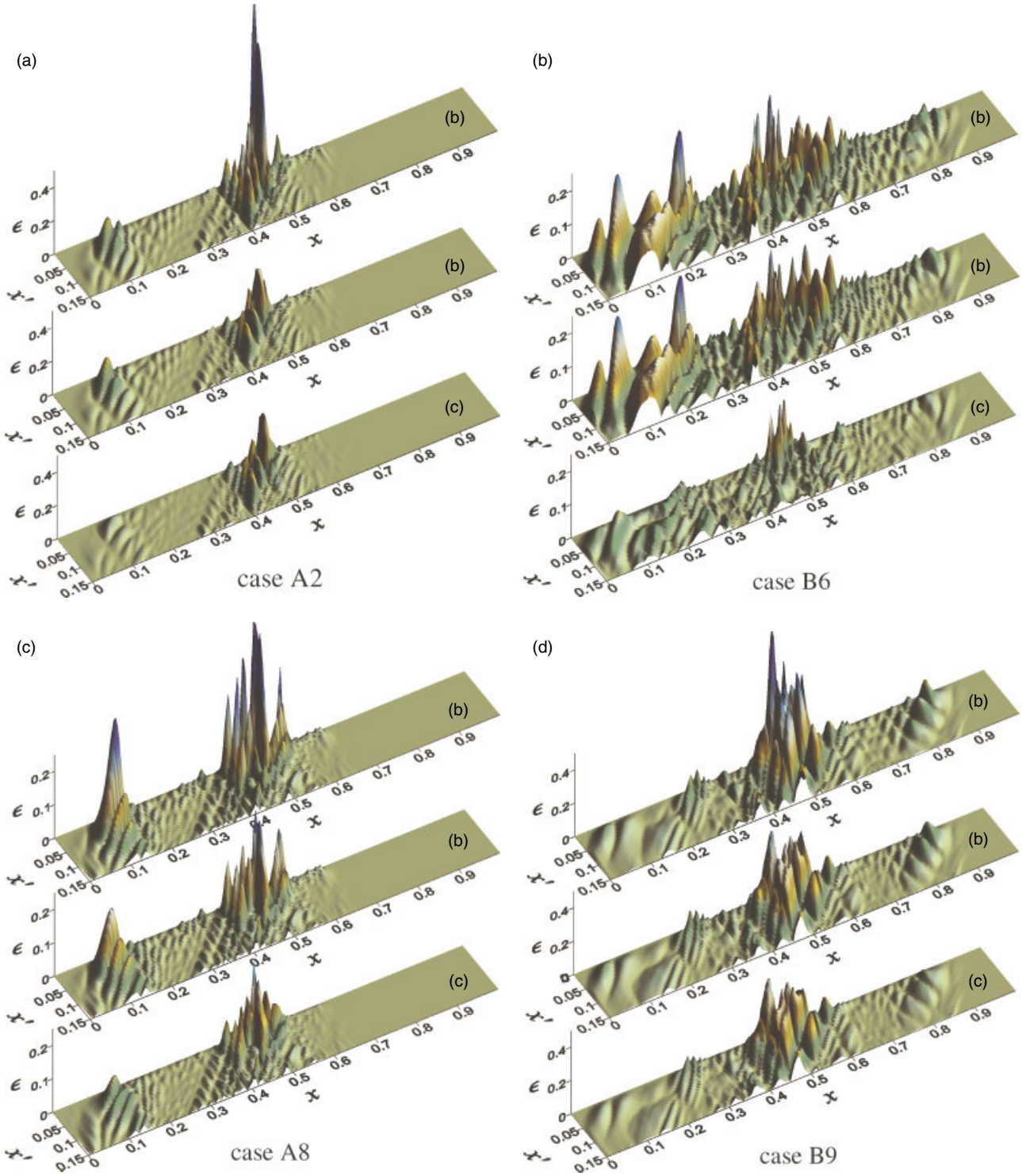

Figure 5. Absolute errors in the correlation matrix (Eq. (81)): $\epsilon_3(x,x')$, sub-case (a); $\epsilon_3^e(x,x')$, sub-case (b); $\epsilon_1^e(x,x')$, sub-case (c). This figure is available in colour online at wileyonlinelibrary.com/journal/qj

recognizing that in this case it would be consistent to utilize a somewhat different error measure, namely the proper (Bayesian) posterior covariance. Let us note that the analysis error covariance is sometimes called 'posterior' in the sense that it is conditioned on the data, i.e. it is obtained after the data have been assimilated. The main purpose of this paper has been to demonstrate that the analysis error covariance and the Bayesian posterior covariance are different objects and this difference is not merely a subtle theoretical issue.

In this paper the difference between the analysis error covariance and the Bayesian posterior covariance has been thoroughly examined. These two conceptually different objects are quantitatively equal in the linear case, but may significantly differ in the nonlinear case. The analysis error covariance can be approximated by the inverse Hessian of the auxiliary DA problem (Eqs (19)–(20)), i.e. by $\mathcal{V}_3$, or by its 'effective' value $\mathcal{V}_3^e$. The Bayesian posterior covariance has to be approximated by a double-product formula (Eq. (51)), i.e. by $\mathcal{V}_1$, or by its 'effective' value $\mathcal{V}_1^e$. The difference between $\mathcal{V}_1$ and $\mathcal{V}_3$ is due to the presence of the second-order term in Eq. (46), which vanishes in the linear case. Thus, technically, the second-order adjoint analysis is involved when dealing

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with the Bayesian posterior covariance only. As far as the authors are concerned, estimates $\mathcal{V}_1$ and $\mathcal{V}_1^e$ have never previously been suggested and studied. In Bayesian theory, the inverse Hessian of the cost function in the original DA problem (Eqs (2)–(3)), here referred to as $\mathcal{V}_2$, is considered to be the asymptotic posterior covariance and, therefore, an approximation to the posterior covariance when a finite number of observations are involved. However, no quantity similar to the 'effective' value $\mathcal{V}_2^e$ can be found. Here we demonstrate that $\mathcal{V}_2$ and $\mathcal{V}_2^e$ are just simplified versions of $\mathcal{V}_1$ and $\mathcal{V}_1^e$. A stable (regularized) method for computing $\mathcal{V}_1$ and $\mathcal{V}_1^e$ in the matrix-free environment using the Lanzcos method with preconditioning has been suggested. This method may be feasible for large-scale applications.

The results of numerical experiments fully validate the presented theory. It has been shown that the analysis error covariance and Bayesian posterior covariance can differ quite significantly. Here we do not raise a detailed discussion about which one is to be used in certain circumstances. Let us only mention that the analysis error covariance should probably be considered in relation to the confidence intervals/regions issue, and the Bayesian posterior covariance in all types of sequential estimation. An important conclusion is that due to linearization errors the point estimate $\mathcal{V}_1$, which is expected to be better than $\mathcal{V}_3$, can actually be far less accurate than $\mathcal{V}_3$. Therefore, it is likely that only the 'effective' estimate $\mathcal{V}_1^e$ may have a practical value. Surely, the computational cost of $\mathcal{V}_1^e$ is significantly higher than the cost of $\mathcal{V}_3$; however, it is still far lower than the cost of direct evaluation of the ensemble of optimal solutions, at least for a large enough observation period.

Appendix

Consider the error equation (43) in the form

$$\mathcal{H}(\varphi,\tilde{\varphi}_1,\tilde{\varphi}_2)\delta u - R^*(\varphi)C^*V_o^{-1}\xi_o - V_b^{-1}\xi_b = 0. \tag{A1}$$

We show below that the left-hand side of Eq. (A1) is related to the difference of the gradients of the cost function J at the point u, which is the solution of the optimality system (Eqs (4)–(6)), and at the point $\bar{u}$, which is the solution of the unperturbed optimality system. By definition of $\mathcal{H}(\varphi,\tilde{\varphi}_1,\tilde{\varphi}_2)$ (see Eq. (44)), we get

$$\mathcal{H}(\varphi,\tilde{\varphi}_1,\tilde{\varphi}_2)\delta u = V_b^{-1}\delta u - \psi^*|_{t=0}, \tag{A2}$$

where

$$\frac{\partial\delta\varphi}{\partial t} = F(\varphi) - F(\bar{\varphi}),\ \delta\varphi|_{t=0} = \delta u, \tag{A3}$$

$$\begin{aligned} &-\frac{\partial\psi^*}{\partial t} - (F'(\varphi))^*\psi^* \\ &= [(F'(\varphi))^* - (F'(\bar{\varphi}))^*]\bar{\varphi}^* - C^*V_o^{-1}C\delta\varphi. \end{aligned} \tag{A4}$$

From the definition of $R^*(\varphi)$ (see Eqs (12)–(13)), we have

$$R^*(\varphi)C^*V_o^{-1}\xi_o = \theta^*|_{t=0}, \tag{A5}$$

where

$$-\frac{\partial\theta^*}{\partial t} - (F'(\varphi))^*\theta^* = C^*V_o^{-1}\xi_o,\ \theta^*\big|_{t=T} = 0. \tag{A6}$$

Then

$$\mathcal{H}(\varphi,\tilde{\varphi}_1,\tilde{\varphi}_2)\delta u - R^*(\varphi)C^*V_o^{-1}\xi_o = V_b^{-1}\delta u - \delta\varphi^*|_{t=0}, \tag{A7}$$

where $\delta\varphi^* = \psi^* + \theta^*$, and $\delta\varphi^*$ is the solution of the adjoint problem (Eq. (38)). Therefore, the left-hand side of Eq. (A1) is reduced to

$$\begin{aligned} &\mathcal{H}(\varphi,\tilde{\varphi}_1,\tilde{\varphi}_2)\delta u - R^*(\varphi)C^*V_o^{-1}\xi_o - V_b^{-1}\xi_b \\ &= V_b^{-1}\delta u - \delta\varphi^*|_{t=0} - V_b^{-1}\xi_b, \end{aligned} \tag{A8}$$

and we can represent Eq. (A1) in the form

$$V_b^{-1}\delta u - \delta\varphi^*|_{t=0} - V_b^{-1}\xi_b = 0. \tag{A9}$$

The gradient $J'(u)$ is calculated by the formula

$$J'(u) = V_b^{-1}(u - u_b) - \varphi^*\big|_{t=0}, \tag{A10}$$

where φ^* is defined by Eqs (4)–(5). The gradient $J'(\bar{u})$ is given by

$$J'(\bar{u}) = V_b^{-1}(\bar{u} - u_b) - \varphi_1^*\big|_{t=0}, \tag{A11}$$

where φ_1^* satisfies the adjoint problem

$$-\frac{\partial\bar{\varphi}_1^*}{\partial t} - (F'(\bar{\varphi}))^*\bar{\varphi}_1^* = -C^*V_o^{-1}(C\bar{\varphi} - y). \tag{A12}$$

The function φ_1^* can be represented as $\varphi_1^* = \bar{\varphi}^* + \eta^*$, where $\bar{\varphi}^*$ is the solution to Eq. (35), and η^* is the solution to the problem

$$-\frac{\partial\eta^*}{\partial t} - (F'(\bar{\varphi}))^*\eta^* = C^*V_o^{-1}\xi_o,\ \ \eta^*\big|_{t=T} = 0. \tag{A13}$$

From Eqs (A10)–(A11) we get

$$J'(u) - J'(\bar{u}) = V_b^{-1}\delta u - \delta\varphi^*\big|_{t=0} + \eta^*\big|_{t=0}, \tag{A14}$$

i.e.

$$V_b^{-1}\delta u - \delta\varphi^*\big|_{t=0} = J'(u) - J'(\bar{u}) - \eta^*\big|_{t=0}.$$

Hence the left-hand side of Eq. (A9) has the form

$$\begin{aligned} &V_b^{-1}\delta u - \delta\varphi^*|_{t=0} - V_b^{-1}\xi_b \\ &= J'(u) - J'(\bar{u}) - \eta^*\big|_{t=0} - V_b^{-1}\xi_b, \end{aligned} \tag{A15}$$

and we can represent (A1) in the form

$$J'(u) - J'(\bar{u}) = V_b^{-1}\xi_b + \eta^*\big|_{t=0}, \tag{A16}$$

or, applying the Taylor–Lagrange formula,

$$J''(\tilde{u})\delta u = V_b^{-1}\xi_b + \eta^*\big|_{t=0}, \tag{A17}$$

where $J''(\tilde{u})$ is the Hessian of the original functional J at $\tilde{u} = \bar{u} + \tau(u - \bar{u})$, $\tau \in [0,1]$, i.e. it coincides with $\mathcal{H}(\tilde{\varphi})$ (see Eq. (50) for the definition of $\mathcal{H}$). It is not difficult to see that the right-hand side of Eq. (A17) is

$$V_b^{-1}\xi_b + \eta^*\big|_{t=0} = V_b^{-1}\xi_b + R^*(\bar{\varphi})C^*V_o^{-1}\xi_o = -J'(\bar{u}).$$

Hence Eq. (A1) is equivalent to the following:

$$J''(\tilde{u})\delta u = -J'(\bar{u}). \tag{A18}$$

The equation in the form Eq. (74) can be similarly derived from Eq. (14).

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