

NOTES AND CORRESPONDENCE

On the Theoretical Equivalence of Differently Proposed Ensemble–3DVAR Hybrid Analysis Schemes

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(Manuscript received 5 October 2005, in final form 7 April 2006)

ABSTRACT

Hybrid ensemble–three-dimensional variational analysis schemes incorporate flow-dependent, ensemble-estimated background-error covariances into the three-dimensional variational data assimilation (3DVAR) framework. Typically the 3DVAR background-error covariance estimate is assumed to be stationary, nearly homogeneous, and isotropic. A hybrid scheme can be achieved by 1) directly replacing the background-error covariance term in the cost function by a linear combination of the original background-error covariance with the ensemble covariance or 2) through augmenting the state vector with another set of control variables preconditioned upon the square root of the ensemble covariance. These differently proposed hybrid schemes are proven to be equivalent. The latter framework may be a simpler way to incorporate ensemble information into operational 3DVAR schemes, where the preconditioning is performed with respect to the background term.

1. Introduction

Present three-dimensional variational data assimilation schemes (3DVAR; e.g., Parrish and Derber 1992; Courtier et al. 1998; Gauthier et al. 1999) commonly assume that the background-error covariances are stationary, and nearly homogeneous and isotropic, while in fact the error covariances may vary substantially with the flow of the day (Hamill et al. 2002). Several approaches have been proposed to relax these assumptions in 3DVAR. Fisher and Courtier (1995) suggested explicitly estimating the leading eigenvectors of the background-error covariance matrix and using a simple

stationary covariance model in the orthogonal subspace. Techniques are also being developed to include some spatial inhomogeneity and anisotropy in the standard covariance models used in 3DVAR (e.g., Desroziers 1997; Riishøjgaard 1998; Purser et al. 2003; Wu et al. 2002). Another approach is to blend in flow-dependent error covariances estimated from an ensemble into the variational framework (Barker 1998; Hamill and Snyder 2000; Lorenc 2003; Buehner 2005). These latter methods are known as hybrid ensemble–variational schemes, or more simply here as hybrid schemes. In this paper we focus on discussing different proposed hybrid ensemble–variational schemes.

A hybrid scheme was proposed and tested by Hamill and Snyder (2000, hereafter HS00). In that study, the background-error covariance was explicitly replaced by a weighted sum of the 3DVAR background-error covariance and the sample ensemble covariance. Each

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member was then updated by assimilating perturbed observations with the hybrid scheme. Parallel assimilations and forecasts were cycled forward, as in a traditional ensemble Kalman filter scheme (e.g., Houtekamer and Mitchell 1998, 2001; Houtekamer et al. 2005). Later, Etherton and Bishop (2004) and Wang et al. (2007) provided an implementation of HS00, where the ensemble perturbations were updated by the ensemble transform Kalman filter (ETKF; Bishop et al. 2001; Wang and Bishop 2003; Wang et al. 2004) and the background-error covariance for updating the mean state was given by an explicit sum of the ETKF ensemble covariance and the static covariance.

Lorenc (2003, hereafter L03) proposed another form of the hybrid variational scheme for updating the state, where the control variables in the cost function were augmented by another set of control variables, preconditioned upon the square root of the ensemble covariance. He also showed how a localizing Schur product, which will reduce the effects of sampling error in the ensemble covariances, could be implemented in the variational framework with preconditioning. Buehner (2005, hereafter B05) adopted a hybrid framework similar to L03 to incorporate the ensemble covariance output from the ensemble Kalman filter into the 3DVAR system. Another implementation of the Schur product for covariance localization was proposed by B05.

Hybrid schemes present a possible alternative to more conventional ensemble data assimilation schemes (e.g., Evensen 1994; Burgers et al. 1998; Anderson 2001; Bishop et al. 2001; Whitaker and Hamill 2002, 2005; Snyder and Zhang 2003; Zhang et al. 2004; Ott et al. 2004; Szunyogh et al. 2005; Houtekamer and Mitchell 1998, 2001, 2005; Houtekamer et al. 2005). Unlike those ensemble data assimilation schemes, which adopt a framework completely different from existing variational scheme, the hybrid schemes begin with existing variational systems and thus can be implemented with minor changes to the existing variational codes. If properly preconditioned, hybrids may be less computationally expensive than other ensemble data assimilation schemes. Because many of the ensemble data assimilation schemes assimilate observations serially, their computational expense typically scales not only with the number of ensemble members and the number of state variables updated by each observation, but also with the number of observations. This may be a concern for operational applications, as the number of observations is huge and still growing with each passing year. In comparison, the computational expense of variational techniques currently used in operational centers such as the National Centers for Environmental Prediction do not scale linearly with the number of observations (Da-

ley and Barker 2000; J. Derber 2005, personal communication). Another potential advantage of hybrids is the ease of applying variational quality control (L03). Consequently, if hybrid methods can achieve much of the potential error reduction of these ensemble filters (Wang et al. 2007), then they may provide an attractive alternative for operational centers where variational data assimilation is established and ensemble forecasts are available or a suitable and efficient method can be found to form the background ensemble.

The hybrid schemes proposed by HS00, and by L03 and B05 differ in the way that they incorporate the ensemble covariance information into the cost function, though L03 and B05 state without proof that the schemes are equivalent or similar. The purpose of this note is to provide a proof that the variational state update steps for the two hybrid schemes proposed by HS00, and by L03 and B05 are mathematically equivalent. We also show that the methods that L03 and B05 proposed to implement a localizing Schur product in the variational framework with preconditioning are equivalent. Because augmenting the control variables as in L03 and B05 may be easier to implement within those variational systems in which the preconditioning is with respect to the background term, this may provide a convenient pathway for the incorporation of ensemble information into many operational analysis schemes.

Section 2 will provide a detailed proof of the equivalence of the two proposed hybrid schemes and section 3 summarizes the paper.

2. Proof of equivalence of the hybrid schemes

In HS00, the cost function associated with the hybrid ensemble-3DVAR background-error covariance is

$$J = \frac{1}{2} (\mathbf{x} - \mathbf{x}^b)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}^b) + \frac{1}{2} [H(\mathbf{x}) - \mathbf{y}]^T \mathbf{R}^{-1} [H(\mathbf{x}) - \mathbf{y}], \quad (1)$$

where \mathbf{x}^b is a column vector of the N -dimensional background forecast state, \mathbf{y} contains the observations, \mathbf{R} is the observation-error covariance matrix, and H is the operator mapping from the model space to the observation space. The hybrid background-error covariance matrix \mathbf{B} is given by a weighted sum of the 3DVAR covariance matrix \mathbf{B}_1 and the ensemble covariance \mathbf{B}_2 , that is,

$$\mathbf{B} = \alpha_1 \mathbf{B}_1 + \alpha_2 \mathbf{B}_2, \quad (2)$$

where α_1 and α_2 are scalar coefficients. In HS00, $\alpha_1 = 1 - \alpha_2$. Further defining the analysis increment as $\Delta \mathbf{x} = \mathbf{x} - \mathbf{x}^b$, then Eq. (1) becomes

$$J = \frac{1}{2} (\Delta \mathbf{x})^T \mathbf{B}^{-1} (\Delta \mathbf{x}) + \frac{1}{2} [H(\mathbf{x}^b + \Delta \mathbf{x}) - \mathbf{y}]^T \mathbf{R}^{-1} [H(\mathbf{x}^b + \Delta \mathbf{x}) - \mathbf{y}]. \quad (3)$$

After expanding $H(\mathbf{x}^b + \Delta \mathbf{x})$ in a Taylor series at \mathbf{x}^b , this is the quadratic minimization problem solved in the “inner loop” of incremental variational schemes. The goal of HS00’s hybrid scheme, is then to find $\Delta \mathbf{x}$ to minimize (3).

L03 and B05 employ a different approach to incorporate ensemble information in the cost function. They represent the analysis increment as

$$\Delta \mathbf{x} = \beta_1 \Delta \mathbf{x}_1 + \beta_2 \Delta \mathbf{x}_2, \quad (4)$$

$$\Delta \mathbf{x}_1 = (\mathbf{B}_1)^{1/2} \mathbf{v}_1, \quad \text{and} \quad (5)$$

$$\Delta \mathbf{x}_2 = (\mathbf{B}_2)^{1/2} \mathbf{v}_2, \quad (6)$$

so that the associated cost function is

$$J = \frac{1}{2} \mathbf{v}_1^T \mathbf{v}_1 + \frac{1}{2} \mathbf{v}_2^T \mathbf{v}_2 + \frac{1}{2} [H(\mathbf{x}^b + \Delta \mathbf{x}) - \mathbf{y}]^T \mathbf{R}^{-1} [H(\mathbf{x}^b + \Delta \mathbf{x}) - \mathbf{y}]. \quad (7)$$

Here, \mathbf{v}_1 is a vector of the standard 3DVAR control variables associated with the traditional 3DVAR transform $(\mathbf{B}_1)^{1/2}$, while the vector \mathbf{v}_2 is the augmented part of the control variable, which is associated with the ensemble covariance. The scalars β_1 and β_2 are the weighting coefficients to combine the two increments $\Delta \mathbf{x}_1$ and $\Delta \mathbf{x}_2$. This choice of control variables also preconditions the background term in Eq. (7), as is common in variational methods (e.g., Parrish and Derber 1992; Gauthier et al. 1999; Courtier et al. 1998).

In Eq. (6), $(\mathbf{B}_2)^{1/2}$ is the square root of the ensemble covariance. If no covariance localization is applied, $(\mathbf{B}_2)^{1/2}$ is simply the rectangular matrix whose columns are the ensemble perturbations divided by $\sqrt{K-1}$, where K is the ensemble size.

Both L03 and B05 proposed methods to implement covariance localization on the ensemble covariance in a variational system with preconditioning. As shown in the appendix of this note [and Eq. (B.3) of B05], B05 found the square root of the localized ensemble covariance. Thus, the form of the cost function by B05 with covariance localization implemented is still the same as Eqs. (4)–(7). After incorporating covariance localization, the cost function of L03 [his Eq. (17)] is somewhat different from Eq. (7). As shown in the appendix, the cost function incorporating the correlation matrix by L03 can be manipulated into the same form of B05.

Thus, in the following proof, for simplicity, we use the general formulation Eqs. (4)–(7) to represent the extended control variable method for both L03 and B05. The goal of L03 and B05’s hybrid scheme is then to find the control vectors \mathbf{v}_1 and \mathbf{v}_2 to minimize Eq. (7) and reconstruct the increment through Eqs. (4)–(6).

When $\beta_1 = \sqrt{\alpha_1}$ and $\beta_2 = \sqrt{\alpha_2}$, the hybrid variational methods proposed by HS00 and L03 are mathematically equivalent in the sense that minimizing Eqs. (3) and (7) produces the same analysis increment. This can be shown as follows.

To find $\Delta \mathbf{x}$ that minimizes Eq. (3), we set the first-order derivative of Eq. (3) with respect to $\Delta \mathbf{x}$ equal to zero, that is, $\partial J / \partial \Delta \mathbf{x} = 0$, which gives

$$\Delta \mathbf{x} + \mathbf{B} \mathbf{H}^T \mathbf{R}^{-1} [H(\mathbf{x}^b + \Delta \mathbf{x}) - \mathbf{y}] = 0, \quad (8)$$

where $\mathbf{H} \equiv \partial H / \partial \mathbf{x}$, evaluated at the \mathbf{x} that satisfies Eq. (8). Solutions for Eq. (8) can be found iteratively when the observation operator H is nonlinear. If the observation operator is linear or if it is weakly nonlinear and \mathbf{x}^b is reasonably accurate, then explicit solutions can be derived. For details, see Lorenc (1986, 1988), Daley (1991), Parrish and Derber (1992), Cohn (1997), and Daley and Barker (2001).

Next we find the analysis increment associated with minimizing Eq. (7) with respect to \mathbf{v}_1 and \mathbf{v}_2 . To minimize Eq. (7), \mathbf{v}_1 and \mathbf{v}_2 must satisfy $\partial J / \partial \mathbf{v}_1 = 0$ and $\partial J / \partial \mathbf{v}_2 = 0$, which gives

$$\mathbf{v}_1 + [\mathbf{H} \beta_1 (\mathbf{B}_1)^{1/2}]^T \mathbf{R}^{-1} [H(\mathbf{x}^b + \Delta \mathbf{x}) - \mathbf{y}] = 0, \quad (9)$$

$$\mathbf{v}_2 + [\mathbf{H} \beta_2 (\mathbf{B}_2)^{1/2}]^T \mathbf{R}^{-1} [H(\mathbf{x}^b + \Delta \mathbf{x}) - \mathbf{y}] = 0, \quad (10)$$

where $\Delta \mathbf{x}$ is given by Eqs. (4)–(6). Premultiplying Eq. (9) by $\beta_1 (\mathbf{B}_1)^{1/2}$, premultiplying Eq. (10) by $\beta_2 (\mathbf{B}_2)^{1/2}$, adding both sides of the subsequent two equations, and using Eq. (4), yields

$$\Delta \mathbf{x} + (\beta_1^2 \mathbf{B}_1 + \beta_2^2 \mathbf{B}_2) \mathbf{H}^T \mathbf{R}^{-1} [H(\mathbf{x}^b + \Delta \mathbf{x}) - \mathbf{y}] = 0. \quad (11)$$

So, if $\beta_1 = \sqrt{\alpha_1}$ and $\beta_2 = \sqrt{\alpha_2}$, we can further substitute Eq. (2), the HS00 background-error covariance, into Eq. (11) and then obtain Eq. (8). Consequently, the analysis increments from the schemes of L03 and B05 satisfy the same equation as that of HS00.

The above proof shows that the analysis increment from Eq. (3) and Eqs. (4)–(7) will converge to the same solution and thus the two hybrid schemes are equivalent.

3. Summary and discussion

In hybrid ensemble–variational data assimilation schemes, ensemble covariances that reflect flow-depen-

dent forecast-error uncertainty are incorporated into the variational framework. Methods have been proposed to achieve this. In HS00, the background-error covariance was defined explicitly as a linear combination of the standard 3DVAR covariance and the ensemble covariance. In L03 and B05, the original variational control variables were extended by another set of control variables preconditioned upon the square root of the ensemble covariance. They also suggested how to incorporate a localizing Schur product to the variational framework with preconditioning. Here we have demonstrated that the hybrid schemes proposed by HS00, L03, and B05 are mathematically equivalent. The L03 and B05 framework should be easier to apply in model-space variational schemes where preconditioning is performed with respect to the background term (e.g., Parrish and Derber 1992; Lorenc et al. 2000; Gauthier et al. 1999; L03; Barker et al. 2004). For observation-space schemes, such as the Naval Research Laboratory Atmospheric Variational Data Assimilation System (Daley and Barker 2001), the ensemble covariance can be hybridized by directly linearly combining the ensemble covariance with the standard 3DVAR covariance (C. H. Bishop 2005, personal communication). The hybrid scheme may provide an effective and feasible way to improve the analysis at the operational centers without the cost of a full implementation of an ensemble-based data assimilation approach. The improvement in hybrid analysis accuracy over a standard variational approach may depend substantially upon how accurately the short-range (e.g., 6 h) ensemble forecasts used in the hybrid estimate the flow-dependent forecast error covariance. Because operational ensembles are not optimized for this application (Hamill et al. 2000, 2003; Wang and Bishop 2003), alternative ensemble generation schemes may need to be explored.

Acknowledgments. Discussions with M. Buehner and C. H. Bishop clarified important aspects of this problem. The participation of the first author was fully funded by National Science Foundation Grant ATM-0205612. The participation of the second author was supported by National Science Foundation Grant ATM-0205665.

APPENDIX

On the Equivalence of L03 and B05 in Implementing Localized Ensemble Covariances in the Variational Framework with Preconditioning

Denote $\mathbf{X}^f = (\mathbf{x}'_1, \mathbf{x}'_2, \dots, \mathbf{x}'_K)$ as the deviation from the ensemble mean normalized by $\sqrt{K-1}$, where K is

the ensemble size. The sample ensemble covariance is $\mathbf{P} = \mathbf{X}^f(\mathbf{X}^f)^T$. Thus, if no covariance localization is applied, in Eq. (6), $(\mathbf{B}_2)^{1/2} = \mathbf{X}^f$. This is an $N \times K$ rectangular matrix, where N is the dimension of the state vector, and also note in Eq. (6), \mathbf{v}_2 is a vector of K elements.

Further denote \mathbf{S} as the prescribed correlation matrix used for covariance localization. Then the localized ensemble covariance is the Schur product of \mathbf{P} and \mathbf{S} (i.e., $\mathbf{P} \circ \mathbf{S}$). To match this localized ensemble covariance in the variational framework with preconditioning, B05 modified Eq. (6) as follows. First, $(\mathbf{B}_2)^{1/2}$ is defined as

$$(\mathbf{B}_2)^{1/2} = [\text{diag}(\mathbf{x}'_1)\mathbf{S}^{1/2}, \dots, \text{diag}(\mathbf{x}'_K)\mathbf{S}^{1/2}, \dots, \text{diag}(\mathbf{x}'_K)\mathbf{S}^{1/2}], \tag{A1}$$

where $\text{diag}(\mathbf{x}'_k)$, $k = 1, \dots, K$, represents a matrix with vector \mathbf{x}'_k along its diagonal. Denote the rank of \mathbf{S} as r . There are $K \times r$ columns in (A1). It was shown in B05 that (A1) satisfies $(\mathbf{B}_2)^{1/2}[(\mathbf{B}_2)^{1/2}]^T = \mathbf{P} \circ \mathbf{S}$. The associated extended control variables are defined as

$$\mathbf{v}_2 = \begin{pmatrix} \mathbf{v}_{21} \\ \mathbf{v}_{22} \\ \vdots \\ \mathbf{v}_{2k} \\ \vdots \\ \mathbf{v}_{2K} \end{pmatrix}, \tag{A2}$$

where \mathbf{v}_{2k} , $k = 1, \dots, K$, is a vector of r elements. With other terms in Eq. (7) unchanged, the second term of the cost function is then given by the inner product of (A2) and the $\Delta\mathbf{x}_2$ term in Eq. (6) is given by Eq. (A1) times Eq. (A2) instead. B05's cost function with covariance localization has the same form as Eqs. (4)–(7).

L03 incorporated \mathbf{S} in the cost function in a different form [see Eq. (17) of L03]. The second term of the cost function is redefined as

$$J_2 = \frac{1}{2} \mathbf{a}^T \begin{pmatrix} \mathbf{S} & 0 \\ & \ddots \\ 0 & \mathbf{S} \end{pmatrix}^{-1} \mathbf{a}, \tag{A3}$$

where the block diagonal matrix is constructed by listing K correlation matrices \mathbf{S} . In Eq. (A3) the newly defined extended control variables are

$$\mathbf{a} = \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \vdots \\ \mathbf{a}_{2k} \\ \vdots \\ \mathbf{a}_K \end{pmatrix}, \tag{A4}$$

where \mathbf{a}_k , $k = 1, \dots, K$, is a vector of N elements. The $\Delta \mathbf{x}_2$ term is modified as

$$\Delta \mathbf{x}_2 = (\mathbf{X}^f \circ \mathbf{A})\mathbf{l}, \quad (\text{A5})$$

where $\mathbf{A} = (\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_K)$, $\mathbf{X}^f \circ \mathbf{A}$ is the Schur product of \mathbf{X}^f and \mathbf{A} , and \mathbf{l} is a vector of K elements that are all equal to 1.

Next we show that by linearly transforming \mathbf{a} , L03's cost function with covariance localization incorporated, can be manipulated into the same format as that of B05. Thus, they will lead to the same solution.

We further define a new set of extended control variables \mathbf{v}_2 , which are linearly related to \mathbf{a} by

$$\mathbf{a} = \begin{pmatrix} \mathbf{S}^{1/2} & 0 \\ & \ddots \\ 0 & \mathbf{S}^{1/2} \end{pmatrix} \mathbf{v}_2, \quad (\text{A6})$$

where \mathbf{v}_2 is given by Eq. (A2). Substituting Eq. (A6) into (A3), then the second term of the cost function becomes the inner product of \mathbf{v}_2 , the same as B05.

Further substituting Eq. (A6) into \mathbf{A} , we obtain

$$\mathbf{A} = \mathbf{S}^{1/2} \mathbf{V}, \quad (\text{A7})$$

where $\mathbf{V} = (\mathbf{v}_{21}, \mathbf{v}_{22}, \dots, \mathbf{v}_{2K})$. Thus, Eq. (A5) becomes

$$\Delta \mathbf{x}_2 = [\mathbf{X}^f \circ (\mathbf{S}^{1/2} \mathbf{V})]\mathbf{l}. \quad (\text{A8})$$

Next we need to show that, $\Delta \mathbf{x}_2$, defined as Eq. (A1) times (A2) by B05 and as Eq. (A8) by L03 are the same.

Denoting $\mathbf{V} = \mathbf{v}_{ij}$, $i = 1, \dots, r$, $j = 1, \dots, K$; $\mathbf{S}^{1/2} = (s_{ij})$, $i = 1, \dots, N$, $j = 1, \dots, r$; $\mathbf{X}^f = (x_{ij})$, $i = 1, \dots, N$, $j = 1, \dots, K$; $\mathbf{A} = \mathbf{S}^{1/2} \mathbf{V} = (a_{ij})$, $i = 1, \dots, N$, $j = 1, \dots, K$, and writing Eq. (A8) in element format, we obtain the i th element of $\Delta \mathbf{x}_2$ by L03 as

$$(\Delta \mathbf{x}_2)_i = \sum_{j=1}^K x_{ij} a_{ij} = \sum_{j=1}^K x_{ij} \sum_{m=1}^r s_{im} v_{mj} = \sum_{j=1}^K \sum_{m=1}^r x_{ij} s_{im} v_{mj}. \quad (\text{A9})$$

Substituting Eqs. (A1) and (A2) into (6), we obtain $\Delta \mathbf{x}_2$ by B05 as

$$\Delta \mathbf{x}_2 = \sum_{k=1}^K [\text{diag}(\mathbf{x}_k) \mathbf{S}^{1/2}] \mathbf{v}_{2k}. \quad (\text{A10})$$

Denote $\mathbf{D}_k = \text{diag}(\mathbf{x}_k) \mathbf{S}^{1/2} = (d_{ij})_k$, $i = 1, \dots, N$, $j = 1, \dots, r$, $k = 1, \dots, K$, and note that $(d_{ij})_k = s_{ij} x_{ik}$. Substituting $(d_{ij})_k$ into Eq. (A10) and writing in element format, we obtain the i th element of $\Delta \mathbf{x}_2$ by B05 as

$$\begin{aligned} (\Delta \mathbf{x}_2)_i &= \sum_{k=1}^K \left[\sum_{j=1}^r (d_{ij})_k v_{jk} \right] = \sum_{k=1}^K \left(\sum_{j=1}^r s_{ij} x_{ik} v_{jk} \right) \\ &= \sum_{k=1}^K \sum_{j=1}^r s_{ij} x_{ik} v_{jk}. \end{aligned} \quad (\text{A11})$$

From Eqs. (A9) and (A11), the $\Delta \mathbf{x}_2$ terms in L03 and B05, with the localized ensemble covariance incorporated, are the same.

To summarize, the above shows that after linear transformation on the extended control variables, L03's cost function with covariance localization applied has the same form as B05. In other words, it can be written as Eqs. (4)–(7).

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