

Incorporating Ensemble Covariance in the Gridpoint Statistical Interpolation Variational Minimization: A Mathematical Framework

XUGUANG WANG

School of Meteorology, University of Oklahoma, and Center for Analysis and Prediction of Storms, Norman, Oklahoma

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ABSTRACT

Gridpoint statistical interpolation (GSI), a three-dimensional variational data assimilation method (3DVAR) has been widely used in operations and research in numerical weather prediction. The operational GSI uses a static background error covariance, which does not reflect the flow-dependent error statistics. Incorporating ensemble covariance in GSI provides a natural way to estimate the background error covariance in a flow-dependent manner. Different from other 3DVAR-based hybrid data assimilation systems that are preconditioned on the square root of the background error covariance, commonly used GSI minimization is preconditioned upon the full background error covariance matrix. A mathematical derivation is therefore provided to demonstrate how to incorporate the flow-dependent ensemble covariance in the GSI variational minimization.

1. Introduction

Gridpoint statistical interpolation (GSI; Wu et al. 2002; Kleist et al. 2009), a three-dimensional variational data assimilation method (3DVAR) has been widely used in operations and research in numerical weather prediction (NWP). GSI is capable of ingesting a large variety of atmospheric observations and has developed capabilities for data thinning, quality control, and satellite radiance bias correction. The operational GSI uses a static background error covariance, which does not reflect the flow-dependent error statistics. The anisotropic recursive filter (e.g., Purser et al. 2003a,b) provides the possibility to introduce anisotropic and inhomogeneous covariances. How to determine the parameters used in the anisotropic recursive filter to realistically represent varying background error covariance, however, still remains an issue.

A four-dimensional variational data assimilation system (4DVAR) implicitly includes a time-evolving covariance model through the evolution of initial errors

under tangent linear dynamics (Lorenc 2003). However, the evolved, flow-dependent covariance model may still be limited by the usage of a static covariance model at the beginning of each 4DVAR cycle (Buehner et al. 2010a,b).

On the other hand, the ensemble Kalman filter (EnKF) has been extensively explored as an alternative data assimilation method (e.g., Houtekamer et al. 2005; Whitaker et al. 2008; Szunyogh et al. 2005; Liu et al. 2008; Torn and Hakim 2008; Zhang et al. 2009; Aksoy et al. 2009; Jung et al. 2008). The main advantage of the EnKF is that it can conveniently provide, through ensemble covariance, flow-dependent estimate of the background error covariance, and therefore the background forecast and the observations are more appropriately weighted during the assimilation.

A hybrid method was proposed (e.g., Hamill and Snyder 2000; Lorenc 2003; Zupanski 2005; Wang et al. 2007a) and has been developed and implemented recently for real NWP models (e.g., Buehner 2005; Wang et al. 2008a,b; Buehner et al. 2010a,b). The hybrid method combines the advantages of both the variational method and the EnKFs and therefore demonstrates great potential for future research and operations. In the hybrid method, the variational framework is used to conduct data assimilation within which the flow-dependent ensemble covariances are effectively incorporated to

Corresponding author address: Dr. Xuguang Wang, School of Meteorology, University of Oklahoma, 120 David L. Boren Blvd., Norman, OK 73072.
E-mail: xuguang.wang@ou.edu

estimate the background error covariance. Studies using simple models and full NWP models have demonstrated the potential of the hybrid method as compared with a standalone variational method (VAR; e.g., Hamill and Snyder 2000; Wang et al. 2007b, 2008a,b, 2009; Buehner et al. 2010a,b). Recent studies also suggest potential advantages of the hybrid method in comparison with a stand-alone EnKF. For example, Wang et al. (2007b, 2009) suggested that for large-scale application the hybrid EnKF–3DVAR was more robust than the EnKF for small ensemble size and large model errors since the static covariance used in 3DVAR helped to reduce the sampling errors, which indicates smaller ensemble size may be needed by the hybrid than by the EnKFs to achieve similar performance. This is particularly attractive for operational forecasts for which the size of the ensemble may be constrained by the availability of the computational resources and the timing of the forecasts. Studies by Buehner et al. (2010a,b) suggested the 4DVAR-based hybrid is better than the stand-alone EnKF, likely because the temporal evolution of the background error covariance was in a space with much higher dimension by the 4DVAR-based hybrid method than the EnKF. Another advantage of the hybrid is that it is built based on the existing operational variational framework so that the established capability in VAR can be easily adopted. In addition, since the hybrid adopts the variational framework, the dynamic constraint can be conveniently added during the data assimilation (Kleist et al. 2009). In the current implementation of the hybrid method, the ensemble covariance is incorporated in the variational framework through the extended control variable method (Lorenc 2003; Buehner 2005; Wang et al. 2007a, 2008a), and the ensemble covariance localization is conducted in the model state variable space (i.e., model space localization); therefore, no assumption about the explicit position of the observation is required during this procedure of the covariance localization. For widely used EnKFs, explicit positions of the observations are needed to apply covariance localization (so-called observation space localization; Hamill et al. 2001). For satellite radiances, for which there is no explicit vertical position, such observation space localization is thus inappropriate. Results in Campbell et al. (2010) suggested that model space localization such as used in the hybrid framework is more sensible and effective in assimilating satellite radiances.

In an operational variational data assimilation system, the background error covariance and its inversion are never explicitly formed during the minimization because of the large dimension of the problem. Incorporating the ensemble covariance therefore cannot be conducted by a simple weighted sum of the static and ensemble

covariances. For VAR that is preconditioned upon the square root of the background error covariance, Buehner (2005) and Wang et al. (2008a,b) described a method to modify the variational minimization to incorporate the ensemble covariance. Different from Buehner (2005) and Wang et al. (2008a,b), in the widely used GSI the minimization procedure is preconditioned upon the full background error covariance (Derber and Rosati 1989). A framework to define how to incorporate the ensemble covariance in GSI is therefore needed. The goal of this paper is to provide a mathematical derivation demonstrating this framework. Such a framework can be applied in the variational system with similar preconditioning. Given the popularity of the GSI and encouraging results from previous work on hybrid data assimilation, this paper represents the first step toward developing and investigating the hybrid data assimilation method based on the GSI.

Section 2 briefly summarizes the key components in GSI minimization, and section 3 provides mathematical details on how ensemble covariance is incorporated in the GSI minimization. Section 4 suggests using the existing GSI capabilities to conduct ensemble covariance localization and discusses ways to reduce computational cost. Section 5 summarizes the paper and provides further discussion.

2. The GSI minimization algorithm

GSI adopts a 3DVAR cost function as

$$J(\mathbf{x}'_1) = 0.5(\mathbf{x}'_1)^T \mathbf{B}_1^{-1}(\mathbf{x}'_1) + 0.5(\mathbf{y}^{or} - \mathbf{H}\mathbf{x}'_1)^T \mathbf{R}^{-1}(\mathbf{y}^{or} - \mathbf{H}\mathbf{x}'_1), \quad (1)$$

where \mathbf{x}'_1 is the analysis increment, \mathbf{B}_1 is the static background error covariance, \mathbf{y}^{or} is the innovation vector, \mathbf{H} is the linearized observation operator, and \mathbf{R} is the observation error covariance. A preconditioned conjugate gradient algorithm is applied for minimizing Eq. (1) (Derber and Rosati 1989): that is, the minimization is preconditioned through defining a new variable:

$$\mathbf{z}'_1 = \mathbf{B}_1^{-1} \mathbf{x}'_1. \quad (2)$$

Then the gradients of the cost function with respect to \mathbf{x}'_1 and \mathbf{z}'_1 become

$$\nabla_{\mathbf{x}'_1} J = \mathbf{z}'_1 + \mathbf{H}^T \mathbf{R}^{-1}(\mathbf{H}\mathbf{x}'_1 - \mathbf{y}^{or}) \quad \text{and} \quad (3)$$

$$\nabla_{\mathbf{z}'_1} J = \mathbf{B}_1 \mathbf{z}'_1 + \mathbf{B}_1 \mathbf{H}^T \mathbf{R}^{-1}(\mathbf{H}\mathbf{x}'_1 - \mathbf{y}^{or}) = \mathbf{B}_1 \nabla_{\mathbf{x}'_1} J. \quad (4)$$

After establishing Eqs. (3)–(4), the iterative minimization steps are then followed (Derber and Rosati 1989; Wu et al. 2002) to find the final analysis. In other words, the GSI minimization is preconditioned on the full background error covariance, and there is no need to invert the background error covariance explicitly.

3. Incorporating ensemble covariance in GSI minimization

The goal of this section is to provide a mathematical framework to show how the GSI minimization described in section 2 will be modified to incorporate the ensemble covariance as part of the background error covariance. The idea is to follow the same preconditioning of the original GSI. We first briefly summarize the changes needed in the GSI cost function, following the method of Wang et al. 2008a. Then the derivation on how changes need to be made to fit the GSI minimization outlined in Eqs. (2)–(4) is given.

As in Wang et al. 2008a, in the hybrid system, the analysis increment, denoted as \mathbf{x}' , is a sum of two terms, defined as

$$\mathbf{x}' = \mathbf{x}'_1 + \sum_{k=1}^K (\mathbf{a}_k \circ \mathbf{x}'_k). \quad (5)$$

The first term, \mathbf{x}'_1 , in Eq. (5) is the increment associated with the GSI static background covariance. The second term is the increment associated with the flow-dependent ensemble covariance. In the second term of Eq. (5), \mathbf{x}'_k is the k th ensemble perturbation normalized by $(K - 1)^{1/2}$, where K is the ensemble size. The vectors \mathbf{a}_k , $k = 1, \dots, K$, denote the extended control variables for each ensemble member. The open-circle symbol denotes the Schur product (element by element product) of the vectors \mathbf{a}_k and \mathbf{x}'_k . In other words, the second term of Eq. (5) represents a local linear combination of ensemble perturbations.

The analysis increment \mathbf{x}' is obtained by minimizing the following hybrid cost function:

$$\begin{aligned} J(\mathbf{x}'_1, \mathbf{a}) &= \beta_1 J_1 + \beta_2 J_e + J_o = \beta_1 0.5(\mathbf{x}'_1)^T \mathbf{B}_1^{-1}(\mathbf{x}'_1) \\ &+ \beta_2 0.5(\mathbf{a})^T \mathbf{A}^{-1}(\mathbf{a}) \\ &+ 0.5(\mathbf{y}^{or} - \mathbf{H}\mathbf{x}')^T \mathbf{R}^{-1}(\mathbf{y}^{or} - \mathbf{H}\mathbf{x}'). \end{aligned} \quad (6)$$

As compared with a normal 3DVAR cost function, a weighted sum of J_1 and J_e terms in Eq. (6) replaces the usual background term. Here J_1 is the traditional GSI background term associated with the static covariance \mathbf{B}_1 . In the term J_e , \mathbf{a} is a vector formed by concatenating

K vectors \mathbf{a}_k , $k = 1, \dots, K$. The extended control variables are constrained by a block-diagonal matrix \mathbf{A} . Each of the K blocks contains the same prescribed correlation matrix, which constrains the spatial variation of \mathbf{a}_k . In other words, \mathbf{A} defines the spatial covariance, here spatial correlation (since variance is equal to 1) of \mathbf{a} . The term J_o in Eq. (6) is the observation term as in the traditional 3DVAR except that \mathbf{x}' is replaced by Eq. (5). In Eq. (6), there are two factors β_1 and β_2 that define the weights placed on the static background-error covariance and the ensemble covariance. Note that although ensemble covariance is not explicitly shown in Eq. (6), the ensemble covariance was incorporated through the second term in Eq. (5) during the minimization. To understand further how ensemble covariance is incorporated in Eqs. (5)–(6), Wang et al. (2007a) and Wang et al. (2008a) proved the equivalence of using Eqs. (5)–(6) to find the analysis to that by replacing the background error covariance in Eq. (1) with the weighted sum of the static background error covariance and the ensemble covariance modulated by the correlation matrix in \mathbf{A} . The same papers also show that \mathbf{A} determines the covariance localization on the ensemble covariance. For details please see Wang et al. (2007a) and Eqs. (6)–(8) in Wang et al. (2008a).

As described by Eqs. (2)–(4), the GSI minimization is conducted through the conjugate gradient method preconditioned on the full background error covariance. Next we derive that to minimize the new cost function in Eq. (6) we can follow the same minimization procedure used in the original GSI. The key of the new derivation is that the minimization of the new cost function can be preconditioned in the same way as shown in Eqs. (2)–(4). In other words, the same conjugate gradient minimization procedure from the original GSI will be followed, except that we will just need to extend the control variable and extend the background error covariance. Note also that the second term in Eq. (6) is preconditioned on \mathbf{A} and not on the ensemble covariance. In other words, similar to the fact that the preconditioning for the first term in Eq. (6) is with respect to the static covariance, the added second term in Eq. (6) is preconditioned with respect to \mathbf{A} , which plays a role of constraining the covariance of extended control variables that is similar to that of the static covariance to the original control variables.

Denote the new control variable as

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}'_1 \\ \mathbf{a} \end{pmatrix}. \quad (7)$$

The hybrid increment in Eq. (5) can be expressed as

$$\mathbf{x}' = \mathbf{x}'_1 + \sum_{k=1}^K \mathbf{a}_k \circ \mathbf{x}'_k = \mathbf{x}'_1 + [\text{diag}(\mathbf{x}'_1) \dots \text{diag}(\mathbf{x}'_K)]\mathbf{a}, \quad (8)$$

where diag is an operator that turns a vector into a diagonal matrix where the n th diagonal element is given by the n th element of the vector (Wang et al. 2007a). We further denote $\mathbf{D} = [\text{diag}(\mathbf{x}'_1) \dots \text{diag}(\mathbf{x}'_K)]$ and $\mathbf{C} = (\mathbf{I}, \mathbf{D})$, where \mathbf{I} is an identity matrix. Then the hybrid increment becomes

$$\mathbf{x}' = \mathbf{x}'_1 + \mathbf{D}\mathbf{a} = (\mathbf{I}, \mathbf{D}) \begin{pmatrix} \mathbf{x}'_1 \\ \mathbf{a} \end{pmatrix} = \mathbf{C}\mathbf{x}. \quad (9)$$

Denote the new background error covariance as

$$\mathbf{B} = \begin{pmatrix} \frac{1}{\beta_1} \mathbf{B}_1 & \mathbf{0} \\ \mathbf{0} & \frac{1}{\beta_2} \mathbf{A} \end{pmatrix}. \quad (10)$$

As in the original GSI, the hybrid is preconditioned by defining a new variable:

$$\mathbf{z} = \mathbf{B}^{-1}\mathbf{x} = \begin{pmatrix} \beta_1 \mathbf{B}_1^{-1} & \mathbf{0} \\ \mathbf{0} & \beta_2 \mathbf{A}^{-1} \end{pmatrix} \begin{pmatrix} \mathbf{x}'_1 \\ \mathbf{a} \end{pmatrix} = \begin{pmatrix} \beta_1 \mathbf{B}_1^{-1} \mathbf{x}'_1 \\ \beta_2 \mathbf{A}^{-1} \mathbf{a} \end{pmatrix}. \quad (11)$$

In the rest of the derivation, we will show that $\nabla_{\mathbf{z}}J = \mathbf{B}\nabla_{\mathbf{x}}J$ and therefore the minimization for the hybrid cost function can follow the same conjugate gradient method used by the original GSI described in section 2.

First, we derive the gradient of the hybrid cost function with respect to

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}'_1 \\ \mathbf{a} \end{pmatrix}.$$

The gradients of the new cost function with respect to the original control variables $\nabla_{\mathbf{x}'_1}J$ and the extended control variables $\nabla_{\mathbf{a}}J$ are given as

$$\nabla_{\mathbf{x}'_1}J = \beta_1 \mathbf{B}_1^{-1} \mathbf{x}'_1 + \mathbf{H}^T \mathbf{R}^{-1} (\mathbf{H}\mathbf{x}' - \mathbf{y}^o) \quad \text{and} \quad (12)$$

$$\nabla_{\mathbf{a}}J = \beta_2 \mathbf{A}^{-1} \mathbf{a} + \mathbf{D}^T \mathbf{H}^T \mathbf{R}^{-1} (\mathbf{H}\mathbf{x}' - \mathbf{y}^o). \quad (13)$$

Therefore, using Eqs. (9)–(13), we obtain

$$\begin{aligned} \nabla_{\mathbf{x}}J &= \begin{pmatrix} \nabla_{\mathbf{x}'_1}J \\ \nabla_{\mathbf{a}}J \end{pmatrix} = \mathbf{B}^{-1}\mathbf{x} + \mathbf{C}^T \mathbf{H}^T \mathbf{R}^{-1} (\mathbf{H}\mathbf{C}\mathbf{x} - \mathbf{y}^o) \\ &= \mathbf{z} + \mathbf{C}^T \mathbf{H}^T \mathbf{R}^{-1} (\mathbf{H}\mathbf{C}\mathbf{x} - \mathbf{y}^o). \end{aligned} \quad (14)$$

Next we derive the gradient of the hybrid cost function with respect to \mathbf{z} . The gradients of the new cost function with respect to $\beta_1 \mathbf{B}_1^{-1} \mathbf{x}'_1$ and $\beta_2 \mathbf{A}^{-1} \mathbf{a}$ are given by

$$\nabla_{\beta_1 \mathbf{B}_1^{-1} \mathbf{x}'_1} J = \mathbf{x}'_1 + \frac{1}{\beta_1} \mathbf{B}_1 \mathbf{H}^T \mathbf{R}^{-1} (\mathbf{H}\mathbf{x}' - \mathbf{y}^o) \quad \text{and} \quad (15)$$

$$\nabla_{\beta_2 \mathbf{A}^{-1} \mathbf{a}} J = \mathbf{a} + \frac{1}{\beta_2} \mathbf{A} \mathbf{D}^T \mathbf{H}^T \mathbf{R}^{-1} (\mathbf{H}\mathbf{x}' - \mathbf{y}^o). \quad (16)$$

Using Eqs. (9), (10), (11), (15), and (16), we obtain

$$\nabla_{\mathbf{z}}J = \begin{pmatrix} \nabla_{\beta_1 \mathbf{B}_1^{-1} \mathbf{x}'_1} J \\ \nabla_{\beta_2 \mathbf{A}^{-1} \mathbf{a}} J \end{pmatrix} = \mathbf{x} + \mathbf{B}\mathbf{C}^T \mathbf{H}^T \mathbf{R}^{-1} (\mathbf{H}\mathbf{C}\mathbf{x} - \mathbf{y}^o). \quad (17)$$

Comparing $\nabla_{\mathbf{x}}J$ in Eq. (14) and $\nabla_{\mathbf{z}}J$ in Eq. (17), we thus obtain

$$\nabla_{\mathbf{z}}J = \mathbf{B}\nabla_{\mathbf{x}}J. \quad (18)$$

As in the original GSI minimization described in section 2, using Eqs. (14) and (18), the same procedure of conjugate gradient minimization procedure can be followed. As discussed in section 2, there is no need to invert both \mathbf{B}_1 and \mathbf{A} explicitly. The main differences of the hybrid system relative to the original GSI system are that 1) in the calculation of $\nabla_{\mathbf{x}}J$ in Eq. (14) extra calculation of gradient with respect to the extended control variable is needed and 2) in the calculation of $\nabla_{\mathbf{z}}J$ [Eq. (18)] the extended background error covariance associated with the matrix \mathbf{A} is needed.

4. Modeling of the error covariance of the extended control variable \mathbf{A} and thoughts to reduce computational cost

In Eq. (18), the background error covariance consists of two components, the original \mathbf{B}_1 and the error covariance \mathbf{A} that constrains the extended control variable. As discussed in section 3, effectively \mathbf{A} conducts the covariance localization on the ensemble covariance. In the original GSI, \mathbf{B}_1 is approximated by the recursive filter transform (Hayden and Purser 1995; Wu et al. 2002; Purser et al. 2003a,b). The recursive filter capability in GSI can also be used to approximate \mathbf{A} , which is different from Buehner (2005) in which the correlation was modeled with a truncated spectral expansion. Note that \mathbf{A} is a block diagonal matrix with K identical submatrices. Each submatrix will be approximated by the same recursive filter transform. As discussed in Wang et al. 2008a, the parameters in the recursive filter will determine the correlation length scale in \mathbf{A} and therefore prescribe the covariance localization length scale for the ensemble covariance.

The number of extended control variables is equal to the dimension of the model space where the covariance

localization is applied times the number of ensemble members. Because with a relatively long localization scale the extended control variables \mathbf{a} are spatially smooth fields, the extended control variables and the recursive filter transform associated with \mathbf{A} can both be on a coarser grid. A large savings in computational cost is expected without loss of accuracy. A similar idea was suggested by Wang et al. (2008a) and was adopted by Buehner (2005) in which the extended control variable was in a severely truncated spectral space and by Yang et al. (2009) in the context of the local ensemble transform Kalman filter. Wang et al. (2007c) showed that the number of iterations during the minimization in the hybrid system for the Weather and Forecasting Model (WRF) in which the ensemble covariance is incorporated is less than that of the original WRF variational system in which the static background error covariance is used, suggesting a faster convergence in the minimization of the hybrid system in which ensemble covariance and static covariance were assigned zero weights than in the original VAR system with only the static covariance. They also found that the number of iterations is not sensitive to the length of the covariance localization scales. Such tests will be conducted for the GSI-based hybrid data assimilation system.

5. Summary and discussion

The popularity of GSI and the potential advantages of the hybrid ensemble–GSI relative to GSI and a pure ensemble Kalman filter suggest a need to develop the hybrid ensemble–GSI system. Different from the hybrid system in Buehner (2005) and Wang et al. (2008a,b), in the widely used GSI the minimization procedure is preconditioned upon the full background error covariance (Derber and Rosati 1989). A framework to define how to incorporate the ensemble covariance in GSI is therefore provided. Possible ways to reduce computational cost are also discussed. The method can be applied in the variational system with similar preconditioning.

The improvement in the accuracy of the analysis obtained from a hybrid method over a standard variational approach may depend on how accurately the short-range ensemble forecasts used in the hybrid estimate the flow-dependent forecast error covariance. The current operational ensemble may not optimize for this application, and alternative ensemble-generation methods such as the ensemble Kalman filter–based method may need to be explored.

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