Representations of Inverse Covariances by Differential Operators

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ABSTRACT

In the cost function of three- or four-dimensional variational data assimilation, each term is weighted by the inverse of its associated error covariance matrix and the background error covariance matrix is usually much larger than the other covariance matrices. Although the background error covariances are traditionally normalized and parameterized by simple smooth homogeneous correlation functions, the covariance matrices constructed from these correlation functions are often too large to be inverted or even manipulated. It is thus desirable to find direct representations of the inverses of background error correlations. This problem is studied in this paper. In particular, it is shown that the background term can be written into \( \int \|Dv(x)\|^2 \), that is, a squared \( L_2 \) norm of a vector differential operator \( D \), called the D-operator, applied to the field of analysis increment \( v(x) \). For autoregressive correlation functions, the D-operators are of finite orders. For Gaussian correlation functions, the D-operators are of infinite order. For practical applications, the Gaussian D-operators must be truncated to finite orders. The truncation errors are found to be small even when the Gaussian D-operators are truncated to low orders. With a truncated D-operator, the background term can be easily constructed with neither inversion nor direct calculation of the covariance matrix. D-operators are also derived for non-Gaussian correlations and transformed into non-isotropic forms.

Key words: differential operator, inverse background covariance, data assimilation

1. Introduction

Various variational formulations have been developed and used in meteorological data analyses and assimilation since the pioneering studies of Sasaki (1958, 1970). As a powerful mathematical tool, the variational framework has great flexibility to allow various types of constraints to be incorporated into the cost function and weighted differently. For practical applications, various differential operators have sometimes been used as smoothness constraints to suppress noise and improve the smoothness of the analyses. Theoretically, however, it is not obvious how different types of constraints should be selected and weighted unless the variational formulations are derived formally based on Bayesian probabilistic principles such as those in three- and four-dimensional variational data assimilation (Jazwinski, 1970; Wahba and Wendelberger, 1980, Lorenc 1986; Cohn 1997). The paper by Wahba and Wendelberger (1980) was, perhaps, the first in meteorology that not only extended Sasaki’s variational formalism rigorously in several aspects but also put it in the context of Bayesian estimation of conditional expectation. Based on Bayesian probabilistic principles, each term in the cost function should be weighted by the inverse of its associated error covariance matrix. How to estimate these error covariances and represent their inverses then becomes the central issue. This paper concerns representations of the inverse covariances, especially the inverse background error covariances in three-dimensional variational data assimilation.

Qualitatively, it has then been well recognized that the smoothing effect of the background term can be mimicked by a smoothing penalty term in which a Laplacian or a polynomial of a Laplacian is applied to the analysis increment field as a weak constraint (Wahba and Wendelberger, 1980; Purser, 1986; Xu et al., 2001a). In the seminal paper by Wahba and Wendelberger (1980), the differential operator in the spline formulation was related to an (implicit) prior background covariance, while the averaged background error variance (inversely related to the background

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weight) and the required smoothness (related to the order of the differential operator) were estimated by the Generalized Cross Validation method from the data being analyzed. Motivated by the above and other subsequent studies, it should be interesting to explore quantitatively whether and how a differential operator can be constructed concisely and precisely in consistency with a given background error correlation among all admissible forms. This problem is addressed in this paper by using a functional approach.

Due to lack of sufficient knowledge about the true covariance structures, simplifications often have to be made in order to obtain stable error statistics as well as to facilitate computations. In this respect, background error covariances are often assumed to be describable by a small number of parameters (such as the variance and the characteristic spatial scale or truncated spectral coefficients describing the gross features of the shape of the covariance function). Then, the parameters can be estimated by fitting the parameterized covariance function to observation innovations (Gandin, 1963; Hollingsworth and Lönnberg, 1986; Lönnberg and Hollingsworth, 1986; Thiebaux et al., 1986; Bartello and Mitchell, 1992; Déványi and Schlatter, 1994; Xu et al., 2001c; Xu and Wei, 2001, 2002) or to forecast differences (Parrish and Derber, 1992; Derber and Bouttier, 1999). Although the covariance functions are parameterized with relatively simple analytical forms, the covariance matrices constructed from these functions are often too large and too complex to be inverted into the weight matrix in the background term. Thus, it is necessary to find an equivalent or approximate representation of the background covariance matrix or its inverse in the variational analysis to reduce the computational demand.

Traditionally, as reviewed in the next section, the above task was accomplished by introducing an intermediate state vector through a linear transformation of the analysis increment vector so that the cost function can be reformulated and minimized with respect to the intermediate state vector without inverting the background error covariance matrix. This paper considers a direct approach in which the inverse covariance matrix is represented by the inverse of its associated correlation function (as an operator) in the limit of infinitely high resolution for continuous fields of analysis. In this case, as an example in the one-dimensional space of \( x \), the inverse relationship between a homogeneous univariate correlation function \( C(x) \) and its inverse \( Q(x) \) is defined by

\[
\int dx’ C(x - x’)Q(x’) = \delta(x), \tag{1.1}
\]

where \( \delta(\cdot) \) is the delta function (Courant and Hilbert, 1962) and the integral \( \int dx’ \) is over the entire space.

The associated background term can then be expressed by

\[
J_b = \int dx \int dx’ v(x)Q(x - x’)v(x’), \tag{1.2}
\]

where \( v(x) \) is the increment analysis field normalized by the background error standard deviation. By applying the generalized Fourier transformation (Lighthill, 1958) to Eq. (1.1), the inverse relationship is expressed concisely in the space of wavenumber \( k \) by

\[
S(k)G(k) = (2\pi)^{-1}, \tag{1.3}
\]

where \( S(k) \) and \( G(k) \) are the Fourier transformations of \( C(x) \) and \( Q(x) \), respectively. As power spectra, \( S(k) \) and \( G(k) \) are real and even functions of \( k \), so \( G(k) \) can be derived from \( S(k) \) [or directly from \( C(x) \) as shown in the appendix] as a Taylor expansion in terms of \( k^2 \), say, \( G(k) = \sum g_n k^{2n} \), where the summation \( \sum_0 \) is over \( n = 0, 1, 2, \ldots \). The inverse Fourier transformation of this expansion gives \( Q(x) = (2\pi)^{1/2} \sum g_n (d/dx)^{2n} \delta(x) \). Substituting this into Eq. (1.2) gives

\[
J_b = \int dx |Dv(x)|^2, \tag{1.4}
\]

where integration by parts is used, and \( D = (2\pi)^{1/4}[g_0^{1/2}, g_1^{1/2}d/dx, \ldots, g_n^{1/2}(d/dx)^n, \ldots]^T \) is a vector differential operator, called the D-operator.

The functional approach outlined above in Eqs. (1.1)–(1.4) indicates that the background term can be written into a squared \( L_2 \) norm of a D-operator applied to the field of analysis increment. Similar D-operator formulations can be derived for homogeneous and isotropic univariate correlation functions in two- and three-dimensional space, and the details will be presented in sections 4–5 of this paper. Depending on the form of \( S(k) \) or \( C(x) \), the D-operator can be of either finite or infinite order. For practical applications, a D-operator of infinite order must be truncated to a finite order. With a truncated D-operator, the background term can be constructed directly just like a smoothing penalty term except that the smoothing is controlled precisely by the background correlation (rather than arbitrarily or empirically). In this case, neither inversion nor direct calculation of the background error covariance matrix is required. The background term and its gradient can be directly and easily computed.

The D-operator is very different from the generalized diffusive operator of Weaver and Courtier (2001) in correlation modeling. Their approach is to model the background correlation (rather than its inverse) by