

Accurate estimation of posterior error covariance in a 4D-Var inverse analysis

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The four-dimensional variational method (4D-Var) is one prominent data assimilation/inversion method. However, it is a non-trivial task for a conventional 4D-Var to estimate a posterior error variance-covariance matrix. This study developed a method to estimate a posterior error variance-covariance matrix especially focusing on its off-diagonal elements, i.e., covariance. Off-diagonal elements are usually difficult to be estimated but provide error correlations that are beneficial for interpreting optimized parameter variations. The method was developed within a 4D-Var framework using a quasi-Newton method with the Broyden–Fletcher–Goldfarb–Shanno (BFGS) formula. This study newly introduces numerical techniques that ensure conjugacy among the set of increment vector pairs in the BFGS formula. Through application to an inverse problem of atmospheric CO₂, the developed method was evaluated with three diagnostic measures and compared against existing methods. The evaluation revealed that the developed method could provide accurate estimates of the posterior variance-covariance matrix, in terms not only of the diagonal but also of the off-diagonal elements. Although far more expensive than optimal state estimation, the computational efficiency was found reasonable for practical use, especially in conjunction with an ensemble approach.

Keywords: inversion, data assimilation, posterior error covariance