Estimation of a posterior error covariance using a linear quasi-Newton method and its application to an inversion of CO_2 sources and sinks

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Data assimilation and inversion methods are widely used in earth science problems to estimate optimal initial/boundary conditions or parameters of a numerical model from given limited observations. A four-dimensional variational method (4D-Var), one of prominent data assimilation/inversion methods, is attractive in that it estimates optimal model variables in a high-resolution without explicitly dealing with a model operator matrix whose size is too large to store in a memory or storage. However, a conventional 4D-Var does not estimate a posterior error covariance owing to its deterministic nature based on the maximum likelihood estimation. A posterior error covariance could provide valuable information not only of uncertainties of estimated variables but also of observation impacts, which is beneficial, for instance, for designing observation networks. In this study, we have developed a new method to estimate a posterior error covariance in a 4D-Var framework. The descent scheme of the 4D-Var method is based on Preconditioned Optimizing Utility for Large-dimensional analyses (POpULar: Fujii, 2005), which employs a quasi-Newton method with Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm. One prominent feature of POpULar is that it does not require difficult decomposition of a prior error covariance matrix. In iterative calculations of the BFGS formula, an inverse Hessian is approximated and then used to determine a next search direction. If accurately approximated, this inverse Hessian can be considered as the posterior error covariance. Although the developed method assumes the model linearity and the perfect forward-adjoint relationship, it successfully calculates an accurate inverse Hessian. Furthermore, the convergence speed of the estimation of the inverse Hessian can be efficiently accelerated by ensemble calculations. Applying this method to a linear problem of CO_2 sources/sinks inversion with a system named NICAM-TM 4D-Var (Niwa et al., 2016a,b), we demonstrate its validity and practical utility.

Keywords: inversion, posterior error, quasi-Newton method

