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Iterative estimation the observation error covariance matrix for ensemble-based filters and its application to a coupled atmosphere-ocean model

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In data assimilation, covariance matrices are introduced in order to prescribe the properties of the initial state, the system noise (model error, process noise), and the observation noise (observation error). Suitable specification of the covariance matrices is essential for obtaining sensible estimates, and misspecification of the matrices may lead to over- or under-fitting of the data and/or failure of the assimilation altogether. We present a technique for optimizing covariance matrices for observation noise. Methods for estimating the optimal covariance are typically based on a common statistic, specifically the so-called "innovation," which is the difference between the observation and the predicted model state. Innovations are evaluated in the methods of minimizing the squared innovations, the maximum likelihood, Bayesian estimation, and the covariance matching. The above-mentioned methods for estimating optimal covariance are, however, originally constructed based on linear-Gaussian state space models, that is, it is assumed that both the system equation and the observation equation are linear, and that both the system noise and the observation noise follows from Gaussian distributions. However, the maximum likelihood can be extended even when the system and observation equations are nonlinear (Ueno et al., 2010). Nonlinearities in the system equation are typically introduced by the advection term in the momentum equation, and can be dealt directly with by ensemble-based assimilation methods such as the ensemble Kalman filter (EnKF) and the particle filter (PF). Ueno et al. (2010) has proposed a method of ensemble-based maximum likelihood, where the likelihood is approximated with the ensemble, and demonstrated that the method can estimate the parameters that describe the covariance for system noise and observation noise. Their procedure of maximizing the likelihood, however, requires huge computational costs; it requires assimilation runs many times that amount to the total number of combinations of the parameters. It means that the method of ensemble-based maximum likelihood may not work in practice where tens or more covariance parameters need to be optimized. Here we propose an efficient algorithm for the maximum likelihood estimation of the observation noise covariance. The algorithm is based on an analytical derivation of the derivative of the ensemble-approximated likelihood with respect to the observation noise covariance, and forms an iterative updating procedure for estimating the optimal covariance parameters. The algorithm works with the ensemble-based filters in which the likelihood can be approximated with the ensemble. Since the algorithm does not require evaluating likelihood for every combination of the covariance parameters as done in Ueno et al. (2010), it can estimate many elements in the observation noise covariance matrix.