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Improved L-BFGS diagonal preconditioners for a large-scale 4D-Var inversion system: application to CO_2 flux constraints and analysis error calculation

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This work presents improved analysis error estimates for 4D-Var systems. From operational NWP models to top-down constraints on trace gas emissions, many of today's data assimilation and inversion systems in atmospheric science rely on variational approaches. This success is due to both the mathematical clarity of these formulations and the availability of computationally efficient minimization algorithms. However, unlike Kalman Filter-based algorithms, these methods do not provide an estimate of the analysis or forecast error covariance matrices, these error statistics being propagated only implicitly by the system. From both a practical (cycling assimilation) and scientific perspective, assessing uncertainties in the solution of the variational problem is critical. For large-scale linear systems, deterministic or randomization approaches can be considered based on the equivalence between the inverse Hessian of the cost function and the covariance matrix of analysis error. For perfectly quadratic systems, like incremental 4D-Var, Lanczos/Conjugate-Gradient algorithms have proven to be most efficient in generating low-rank approximations of the Hessian matrix during the minimization. For weakly non-linear systems though, the Limited-memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS), a quasi-Newton descent algorithm, is usually considered the best method for the minimization. Suitable for large-scale optimization, this method allows one to generate an approximation to the inverse Hessian using the latest m vector/gradient pairs generated during the minimization, m depending upon the available core memory. At each iteration, an initial low-rank approximation to the inverse Hessian has to be provided, which is called preconditioning. The ability of the preconditioner to retain useful information from previous iterations largely determines the efficiency of the algorithm.

Here we assess the performance of different preconditioners to estimate the inverse Hessian of a large-scale 4D-Var system. The impact of using the diagonal preconditioners proposed by Gilbert and Le Maréchal (1989) instead of the usual Oren-Spedicato scalar will be first presented. We will also introduce new hybrid methods that combine randomization estimates of the analysis error variance with L-BFGS diagonal updates to improve the inverse Hessian approximation. Results from these new algorithms will be evaluated against standard large ensemble Monte-Carlo simulations. The methods explored here are applied to the problem of inferring global atmospheric CO_2 fluxes using remote sensing observations, and are intended to be integrated with the future NASA Carbon Monitoring System.