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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Technical Note: Variance-covariance matrix and averaging kernels for the Levenberg-Marquardt solution of the retrieval of atmospheric vertical profiles" *by* S. Ceccherini and M. Ridolfi

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The authors present a new method to estimate solution covariance matrices and averaging kernels for nonlinear retrieval problems, based on Levenberg-Marquardt minimization. They devised this method since the original LM-method of estimating these matrices assume a zero damping at the final iteration, which is not necessarily true according to the authors. So at each iteration, their method updates not only the solution vector, but also the matrix T (used to calculate the covariance matrix and averaging kernel; page 25669, top of page). Then 4 methods are tested: (1) the original LM estimate with zero damping at the final iteration, (2) LM taking into account nonzero

damping at the final iteration, (3) the proposed method, and (4) a statistical method in order to estimate the 'true' covariance and averaging kernel at the final iteration. It is found that the proposed method (3) and the statistical method (4) agree well, a finding that seems to validate the proposed method (3).

However, I would not recommend publication in ACP, because I suspect strongly that something is wrong here. An iterative method that converges properly should not be dependent on the damping at the final iteration or the path taken during the minimization. A properly converged solution covariance matrix depends locally on the first derivatives of the merit function to the solution components. The Levenberg-Marquardt damping was only invented to stabilize the search path, which means to avoid the 'overshooting' that is so typical for Gauss-Newton. After convergence, the solution should be independent on the LM term. So at least method (1), (3) and (4) should give identical results.

Then why are the results from method (1) and (3) different? Most likely because the minimizations did not converge. It is mentioned that maximum 10 iterations are allowed; perhaps it is necessary to increase this number. The estimates for method (3) and (4) do agree however. The explanation is probably: both didn't convergence but started nevertheless from the same initial guess, took the same 10 iteration steps and ended at the same position (which is not the minimum).

The best argument against the validity of the proposed method: the solution, covariances and averaging kernels depend on the search path. This is why the method needs to keep track of the iterations. But then the results depend on the first guess solution. This is hardly what we want from a minimization scheme.

Interactive comment on Atmos. Chem. Phys. Discuss., 9, 25663, 2009.