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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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In their discussion paper the authors postulate that covariance matrices and averaging kernels of Levenberg-Marquardt retrievals differ from those evaluated for Gauss-Newton or optimal estimation retrievals. In this comment we provide evidence that converged Levenberg-Marquardt retrievals are characterized by the same covariance matrices and averaging kernels as Gauss-Newton or optimal estimation retrievals.

We reorganize Eq(4) of the discussion paper:

$$(\vec{K}^T\vec{S}_y^{-1}\vec{K}+\vec{R}+\lambda_i\vec{D}_i)(\vec{x}_{i+1}-\vec{x}_i)=\left[\vec{K}^T\vec{S}_y^{-1}(\vec{y}-\vec{f}(\vec{x}_i))+\vec{R}(\vec{x}_a-\vec{x}_i)\right] \quad (1)$$

Convergence means $\vec{x}_{i+1}-\vec{x}_i\rightarrow 0$, hence

$$\vec{K}^T\vec{S}_y^{-1}(\vec{y}-\vec{f}(\vec{x}_i))\rightarrow -\vec{R}(\vec{x}_a-\vec{x}_i). \quad (2)$$

We see that $\vec{x}$ of a converged retrieval depends only on the measurement $\vec{y}$, the forward model $\vec{f}$, the Jacobian $\vec{K}$, the regularization $\vec{R}$ and $\vec{x}_a$ (if any) but not on the Levenberg-Marquardt term $\lambda_i\vec{D}_i$, regardless how large this is in the final iteration. Thus, also the covariance matrix and the averaging kernels cannot depend on the Levenberg-Marquardt term.

This can also be shown algebraically: In case of convergence we can assume $\vec{T}_{i+1}$ equals $\vec{T}_i$. With this, Eq. 9 of the discussion paper reads

$$\vec{T}_{i+1}=\vec{T}_{i+1}+\vec{G}_i(\vec{I}-\vec{K}_i\vec{T}_{i+1})-\vec{M}_i\vec{R}\vec{T}_{i+1} \quad (3)$$

and gives

$$\begin{aligned}\vec{G}_i(\vec{I}-\vec{K}_i\vec{T}_{i+1}) &= \vec{M}_i\vec{R}\vec{T}_{i+1} \quad (4)\\ \vec{M}_i\vec{K}_i^T\vec{S}_y^{-1}(\vec{I}-\vec{K}_i\vec{T}_{i+1}) &= \vec{M}_i\vec{R}\vec{T}_{i+1}\\ \vec{K}_i^T\vec{S}_y^{-1}-\vec{K}_i^T\vec{S}_y^{-1}\vec{K}_i\vec{T}_{i+1} &= \vec{R}\vec{T}_{i+1}\\ \vec{K}_i^T\vec{S}_y^{-1} &= (\vec{R}+\vec{K}_i^T\vec{S}_y^{-1}\vec{K}_i)\vec{T}_{i+1}\\ \vec{T}_{i+1} &= (\vec{R}+\vec{K}_i^T\vec{S}_y^{-1}\vec{K}_i)^{-1}\vec{K}_i^T\vec{S}_y^{-1}\end{aligned}$$

which is exactly the gain function of a retrieval without Levenberg-Marquardt damping. Since $\vec{T}$ is the derivative of the retrieval with respect to the measurements, we can use it to calculate the covariance matrix

$$\vec{S}_r=(\vec{R}+\vec{K}_i^T\vec{S}_y^{-1}\vec{K}_i)^{-1}\vec{K}_i^T\vec{S}_y^{-1}\vec{K}_i(\vec{R}+\vec{K}_i^T\vec{S}_y^{-1}\vec{K}_i)^{-1} \quad (5)$$

and the averaging kernel matrix

$$\vec{A}_r = (\vec{R} + \vec{K}_i^T \vec{S}_y^{-1} \vec{K}_i)^{-1} \vec{K}_i^T \vec{S}_y^{-1} \vec{K}_i^T \quad (6)$$

as already stated in my comment (von Clarmann, Atmos. Chem. Phys. Disc. 6, S6530-S6532,2007) to Ceccherini et al. (Atmos. Chem. Phys. Disc. 6, 13307-13321, 2006), where the authors claim that the Levenberg-Marquardt term is to be considered for the calculation of covariance matrices and averaging kernels. This does not mean that Eqs. 10–11 of the discussion paper are formally incorrect, but they are obsolete because for converged retrievals they are equivalent to our much simpler non-recursive formulations inferred above.

We suspect that all problems with the standard averaging kernels and covariance matrices presented in the discussion paper arise from the fact that these are applied to non-converged Levenberg-Marquardt retrievals. The fact that the Gauss-Newton solution is far off the Levenberg-Marquardt solution of the authors' test case supports this assumption, because from our Eq. 1 we see that the Gauss-Newton and Levenberg-Marquardt solutions should be identical. With a large Levenberg-Marquardt term it is easy to obtain a small relative variation of the chi-square although the retrieval is still far from convergence, and retrievals where the iteration has been interrupted without making sure that $\vec{x}_{i+1} - \vec{x}_i \rightarrow 0$ even without a damping term should be discarded and by no means be accepted as a solution. For non-converged retrievals, Eq. 8 of the discussion paper does not hold because a term accounting for the difference of the current and the final solution is missing. If for some reason (e.g. same initial value for all test cases) all iterations are interrupted at a similar position in the state space, it is not surprising that the a posteriori estimation of the covariance matrix underestimates the true variances.

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