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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Technical Note: Propagating correlations in atmospheric inversions using different Kalman update smoothers" *by* J. Tang and Q. Zhuang

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General authors' comments: We sincerely thank the anonymous referee for the insightful comments to help us improve the technical note. Our specific responses to each comment are below.

Anonymous Referee 1 (Comments):

This technical note deals with the covariance estimation in different implementations of Bayesian parameter estimation using the Kalman filter equations. The author first derive algebraic equations to propagate the influence of covariance of fluxes outside the state vector on those inside the state vector and arrive, at least for the fixed-lag Kalman

smoother, at similar results as Bruhwiler et al., (2005). They then extend this algebraic formulation to two different ensemble based methods, and assess the effects of the implemented mechanisms in a controlled CH4 flux inversion. 1. Although the work strikes me as mathematically quite advanced, and carried out with good intentions, I feel that this paper in its current form cannot be judged well on its scientific merits. Partly, this stems from unclear or uncompleted mathematical notations (listed below), and partly also from the narrative description that goes along. This is especially true from section 2.3 and beyond. My main question in sections 2.3 and 2.4 (Equations 20 through 57) is whether this covariance correction scheme has any relevance in an ensemble based system, where the covariance is inherently represented in lower dimensional space by the ensemble members. As the members are each propagated individually, and analyzed in each cycle, they also inherently describe the covariance of the full system, i.e., from t*=0 to* t*=current. The 'missing' covariance that was separately addressed in Bruhwiler et al and in section 2.2 is thus not missing here, and does not need correction in my understanding. If I am mistaken in this matter, the authors should write a clearer justification of their proposed methods as I am sure other readers are likely to make the same mistake otherwise.*

With the doubts above in mind, I found it very hard to work through the details of the sigma-point Kalman smoother. I also fear that the purely mathematical treatment of this method in section 2.4 will not be understandable by anyone without a specialism in such methodology.

Our reply: First, we revised the text to make the intention of this Note clear and straightforward. Second, we stated that the correction for the ensemble members (in Section 2.3 and 2.4) should be carried out before the measurement is actually used in the inversion. This has not been done in Bruhwiler et al (2005). Such correction could assure that the correlation between the on-line state variables and the off-line state variables is properly accounted for. We showed that the correlation acts effectively as a balanced constraint on the online state variable. Without incorporating such correlation constraints, the variance of the ensemble becomes exactly as the $\mathbf{Q}_{uu}$ in the Note. Third, as for the sigma-point Kalman smoother, we reduced the derivation in the revised text and made it more easily to be understood.

*2. The elaborate tests of each method using the GEOS-CHEM system in sections 2.6 and beyond are again impressive in implementation and detail, but fail to answer the question whether the algebraic additions to the three methods are mathematically more accurate than the previous 'incorrect' versions with missing covariance propagation. The analysis now focuses solely on reproducing pseudo-data CH4 concentrations in which each method succeeds with different accuracies. However, the real proof of the innovations in sections 2.3, 2.4, and 2.5 should lie in a comparison of posterior mean *and* covariance estimates of fluxes to those from a 'perfect' inversion method: the linear batch inversion. Since this latter solves the full system at once, and needs no approximations or statistics, it should be the benchmark for the other methods to agree with.*

3. I feel that when the above has been addressed, this can become a quite interesting technical note; or perhaps even a full paper if the authors focus more strongly on the testing of the different approaches in a real life application like with CH_4*. I hope the authors will consider resubmitting this work after such revisions.*

Our reply: Following the reviewer's suggestion, we re-conducted the experiments to compare the posterior mean and covariance estimated by our methods and those from the linear batch inversion. Compared to the linear batch inversion, the three methods we proposed without interval constraint on the state variables performed well to reveal the true fluxes. However, the posterior uncertainty is greater than that from the linear batch inversion, similar to the findings in Bruhwiler et al., (2005) for the CO_2 study. Further, the three methods produced some unreasonable negative fluxes because of limited constraints compared to linear batch inversion. Therefore, the interval constraint technique is needed to assure the inversions are physically reasonable. We added our findings and discussion in this revision.

4. Unclear notations in mathematics: Equation 2: Can you please give the dimensions of $\vec{z}$, $\vec{s}$, and $\vec{v}$ Equation 3: Please describe or define L Equation 11: The $\mathbf{H}$ matrices in the second and third term under brackets are not the same I presume? Should one be $\mathbf{H}_v$ and the other $\mathbf{H}_u$? Equation 13: $\mathbf{Q}_a$ is not defined. Do you mean the posterior covariance $\mathbf{Q}^+$? Equation 16: What is the matrix capital $\mathbf{S}$, and which properly scaled anomalies do you refer to? Isn't $\mathbf{H}_{vu}$ the simple propagation of posterior ensemble members in time with the transport model? Equations 20-25 and beyond: What is the subscript 1 introduced here, and subscript 2 introduced further down?

Our reply: We revised the equations, explained the symbols, and corrected typos.

Interactive comment on Atmos. Chem. Phys. Discuss., 10, 19219, 2010.