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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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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.

Although the work strikes me as mathematically quite advanced, and carried out with good intentions, I feel that this paper in its current form can not 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 be 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.

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.

In summary, I found this paper quite difficult to work through because it was not clear from the start what the authors were trying to achieve: Implement three inversion methods and compare them? Solve an issue with propagating covariance in Kalman filter based estimation methods? Or perhaps select the most suitable system for the real life application in CH4 inversions with GEOS-CHEM? In a next iteration of this paper, I suggest the authors structure their work more along one clear research goal. At the same time, they could possibly reduce their mathematical descriptions to those relevant for that problem alone, and give more elaborate physical explanation of the equations.

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 CH4. I hope the authors will consider resubmitting this work after such revisions.

Unclear notations in mathematics:

Equation 2: Can you please give the dimensions of z, s, and v Equation 3: Please describe or define L Equation 11: The H matrices in the second and third term under brackets are not the same I presume? Should one be Hv and the other Hu? Equation 13: Qa is not defined. Do you mean the posterior covariance Q+? Equation 16: What is the matrix capital S, and which properly scaled anomalies do you refer to? Isn't 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?

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