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Atmospheric Chemistry and Physics Discussions

Interactive comment on “Technical note: A geostatistical fixed-lag Kalman smoother foratmospheric inversions” *by* A. M. Michalak

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The comments submitted by Referee #1 made it clear that the specific goal and innovation of the manuscript needed to be stated more clearly. This and other comments provided by the referee contributed significantly to improvements in the revised manuscript. The replies listed below are numbered consistently with the reviewer’s original numbering.

Reply to Overall Evaluation

As the reviewer correctly points out, the main goal of this technical note is to adapt the fixed-lag Kalman smoother approach presented in Bruhwiler et al. (2005) to be applicable with the geostatistical approach presented in Michalak et al. (2004). As is discussed in both the original and revised Technical Note, the Kalman smoother as

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presented in Bruhwiler et al. (2005) increases the computational efficiency of atmospheric inverse problems, while preserving the advantage of providing a full *a posteriori* covariance matrix. However, the original approach (Bruhwiler et al., 2005) was not compatible with the geostatistical approach. This is precisely the goal and contribution of this Technical Note, and this point has been clarified in the revised manuscript.

Replies to General Comments

1)

First paragraph: The reviewer is correct that the availability of an adjoint model greatly increases the efficiency with which one can calculate the sensitivity matrices required by both batch inversions and those performed using a Kalman smoother, for cases where the number of unknowns (fluxes) is greater than the number of observations. The use of the adjoint model was described in the original manuscript, and has been further clarified in the revised Technical Note in Sections 2.2 and 5.

Second paragraph: The reviewer is also correct that there “are costs associated with trying to solve the equations for large state vectors.” And because the computational cost of solving the equations for large state vectors increases for both synthesis Bayesian inversions and Geostatistical inversions, both require numerical approaches to decrease this computational cost. This is exactly the goal of the presented approach.

2)

First paragraph: The reviewer is correct that the “use of the fixed-lag Kalman smoother to limit the data ingested in the inversion does make it more computationally feasible to use large amounts data and to conduct multi-year inversions” and that this was demonstrated by Bruhwiler et al. (ACP 2005). However, as discussed above and in the original Technical Note, the Kalman smoother presented in Bruhwiler et al. (2005) was not applicable to a geostatistical setup. This is because, if a Kalman smoother is to be applied in a geostatistical setup, the lack of *a priori* flux estimates must be accounted

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for the first time each set of fluxes is estimated, whereas these preliminary estimates must be updated in the subsequent iterations of the smoother. This is different from the setup presented in Bruhwiler et al. (2005), where an estimate of fluxes is available from the very first iteration, in the form of *a priori* flux estimates. This is the reason for which the form of the equations for the geostatistical fixed-lag Kalman smoother differs from those for a synthesis Bayesian inversion. This point has been further clarified in Section 1 of the revised Technical Note.

Second paragraph: The goal of the Technical Note is to develop a fixed lag Kalman smoother that is applicable to a geostatistical inversion, and to demonstrate that this setup yields estimates consistent with those from a batch geostatistical inversion. The Technical Note thus presents a new numerical method. These points have been clarified further in Section 1 of the revised Technical Note.

Replies to Specific Comments

1) $\mathbf{X}$ is defined prior to the inversion, and the estimate of β does depend on the observations. The true (unknown) β, however, is a function of the true (unknown) fluxes, whereas the covariance matrix $\mathbf{R}$ represents only that portion of the observation signal that could not be explained by these true (unknown) fluxes (i.e. observation error, transport model error, etc.). Therefore, the deviations of the true fluxes $\mathbf{s}$ from the true β's, as parameterized by $\mathbf{Q}$, do not depend on the observations error, as parameterized by $\mathbf{R}$. Conversely, it is quite possible that the uncertainty associated with the estimated $\mathbf{s}$ is correlated to the uncertainty associated with the estimates of β, and this would appear in the *a posteriori* uncertainty matrices. Although not explicitly presented here, one could calculate not only the *a posteriori* error covariance of the estimated fluxes, but also the a posteriori error covariance of the estimated β's (see Gourdji et al., JGR 2008, in press), and even the matrices representing the cross-covariances between the $\mathbf{s}$ and β uncertainties. In short, the correlation that the reviewer refers to would appear in the *a posteriori* covariance matrices, not the *a priori* covariance matrices.

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2) The $\mathbf{\Lambda}$ are the weights that will be applied to the available observations in obtaining the best estimates of fluxes. The $\mathbf{M}$ are Lagrange multipliers that appear as a result of the unbiasedness constraint that is placed on the estimation of $\mathbf{s}$ and β (i.e. they result from the fact that the β's are also considered unknown). These variables have been defined explicitly in the revised Technical Note, and a reference to Michalak et al. (2004) has been added for further details.

3) The geostatistical estimate is actually a MAP estimator, combining *a priori* information about the autocorrelation of the state (i.e. flux distribution) with the likelihood of the data (i.e. CO_2 observations). The uncertainties obtained in this way are smaller than those that one would obtain using a maximum likelihood estimator that includes no *a priori* information.

To return to the reviewer's specific wording, the geostatistical approach is a MAP estimator, which does produce a lower uncertainty relative to an ML estimator.

Because this topic is not directly related to the main subject of this Technical Note, and in order to keep the note succinct, this discussion was not added to the manuscript.

4) Please see reply to comment P7768, L14 by Referee #2.

5) Again, the FLKS as developed in Bruhwiler et al. (2005) could not be applied in a geostatistical setup. The goal of this Technical Note is to develop and test a geostatistical version of this approach. This is described further in replies to the reviewer's other comments above, and is clarified in the revised Technical Note as is outlined in the replies to these earlier comments.

6) The scales on panels a and b, and c and d, where kept consistent in order to allow easy visual comparison of the scale of both the best estimate and uncertainty for these two regions. The average absolute uncertainty for Temperate North America is 0.90 GtC/yr for the batch inversion and 0.92 GtC/yr for the GFLKS, averaged over the 12 months presented in Figure 5. The uncertainty for the South Atlantic is 0.65 GtC/yr

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and 0.68 GtC/yr, respectively. These are expressed as +/- one standard deviation from the best estimates, and the standard deviation is therefore half these numbers. This uncertainty is 75 times larger than the difference between the uncertainties between the methods for Temperate North America, and 35 times larger for the South Atlantic. These numbers have been added to the revised version of the Technical Note. Note also that the difference between uncertainties was amplified 10-fold in panels c and d in order to make it visible (see legend in original figure). This point has now also been clarified in the figure caption.

7) The following sentence has been added: “This is also consistent with the fact that the relative *a posteriori* uncertainty is also larger for the South Atlantic.“

8) As described in the reply to the General Comments, the reliance on an adjoint model has been further emphasized in Sections 2.2 and 5 of the revised Technical Note.

9) The section referenced by the reviewer was not intended as a review of the literature on grid-scale inverse modeling, which would have included not only the papers listed by the reviewer, but several others as well, and especially those from the CO_2 literature. The sentence referred to by the reviewer specifically discussed the application of the geostatistical approach.

Given that this work is intended as a short Technical Note, most of the references were kept to examples of work in particular fields. This is also the reason for which the references to Bayesian synthesis inversions, variational methods, and ensemble methods in the introduction were all preceded by “e.g.” in order to emphasize that this Technical Note does not provide a full literature review on the subject, but instead simply provides the context for the presented work.

With regard to the specific papers recommended by the reviewer:

Petron et al. (2002) presents a time lagged inversion for CO. Because CO has a relatively short lifetime in the atmosphere, the impact of old emissions of CO on observations is negligible, and the inversion can essentially be performed as a series of batch inversions. Such an approach is not directly application to CO_2, which is a long-lived gas.

Stavrakou et al. (2006) compare grid-scale and big regions inversions of CO, which is of course an important topic, but not directly related to the subject of this technical note.

Elbern et al. (2007) present a variational approach for estimating sources of air pollutant precursors. 4d variational methods are an important class of numerical tools increasingly being applied in atmospheric inverse modeling. Because this Technical Note described the proposed approach in the context of CO_2 flux estimation, the sample paper on variational methods that was referenced in the Introduction is from the CO_2 literature (Baker et al., 2006). Again, this paper was referenced preceded by an "e.g." to make it clear that this is only one example of work in this area. In the revised Technical Note, the Introduction now specified that the work by Baker et al. (2006) presents a variational approach, whereas the work by Peters et al. (2005) presents an ensemble approach.

Meirink et al. (2008) present a variational approach for estimating methane emissions. This is another excellent example of the application of 4D Var to atmospheric inversions, but was simply not the example that is listed as a sample of work in this area in the introduction.

In order to respond to the reviewer's implicit concern about the number of papers referenced in this Technical Note, a second reference was added for both variational (Chevallier et al., JGR 2005) and ensemble (Zupanski et al., JGR 2007) approaches to CO_2 inverse modeling, and a reference to Law (ACP, 2004) was added as a predecessor to the method presented in Bruhwiler et al. (2005).

Chevallier, F., M. Fisher, P. Peylin, et al. Inferring CO_2 sources and sinks from satellite observations: Method and application to TOVS data, J. Geophys. Res., 110 (D24),

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D24309, 10.1029/2005JD006390.

Law, R. M.: Technical note: an interannual inversion method for continuous CO_2 data, Atmos. Chem. Phys., 4, 477–484, 2004.

Zupanski, D., A.S. Denning, M. Uliasz, et al. Carbon flux bias estimation employing maximum likelihood ensemble filter (MLEF), J. Geophys.Res., 112(D17), D17107, 10.1029/2006JD008371.

Interactive comment on Atmos. Chem. Phys. Discuss., 8, 7755, 2008.

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