

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

Anonymous Referee #1

Received and published: 30 June 2008

The manuscript presents a new method for inverse modeling of atmospheric tracers, in which a geostatistical approach is combined with a fixed-lag Kalman smoother. The author argues that this new approach improves the computational efficiency of conducting multi-year inversions at high spatial resolution and without the use of a priori estimates of the fluxes. There is a clear need for new computational methods to improve the efficiency and reliability of atmospheric inversions. However, as I discuss below, I do not believe that the work presented here represents a new technical advance beyond what is already described in Michalak et al. (J. Geophys. Res., 2004) and Bruhwiler et al. (ACP, 2005). Therefore, I cannot recommend it for publication in ACP.

General Comments

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The major conclusion of the manuscript is that "this method makes it feasible to perform multi-year inversions, at fine resolutions, and with large amounts of data." However, I have the following concerns about this:

1) As described in Kitanidis (Adv. Water. Resour., 1996) and Michalak et al. (J. Geophys. Res., 2004), the main difference between the geostatistical approach and more traditional applications of the maximum a posteriori (MAP) technique is that the geostatistical approach incorporates a "structural analysis" to better capture the correlation structure of the fluxes given the information content of the data, rather than relying on a priori information. However, it does not make high-resolution inversions more feasible, as the author claims. In the work presented here, it is feasible to conduct the inversion at a resolution of $5.0^\circ \times 3.75^\circ$ because of the availability of the adjoint of the TM3 model. Without this adjoint model it would be computationally expensive to generate the high-resolution sensitivity matrix.

There are also costs associated with trying to solve the equations for large state vectors, but as noted by Michalak et al. (2004), "as the number of observations used in inversions increases and the spatial and temporal scale at which we want to estimate the fluxes continues to decrease, the numerical costs of the direct geostatistical approach will grow in the same way as those of classical Bayesian inverse modeling." It is not clear in what context the author is describing the approach in this manuscript as making these high-resolution inversions more "feasible."

2) 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. However, this approach was previously demonstrated by Bruhwiler et al (ACP, 2005).

Overall, the description of the methods and experiments presented in this manuscript do not provide any more insight into the utility of the geostatistical and fixed-lag Kalman smoother techniques beyond that shown in Michalak et al. (2004) and Bruhwiler

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et al (ACP, 2005), respectively. Bruhwiler et al. showed that the fixed-lag Kalman smoother provides estimates similar to those obtained from the traditional batch approach, whereas this study shows that the geostatistical fixed-lag Kalman smoother also provides estimates similar to the batch approach. It is not clear what new is being offered in this manuscript that warrants a technical note.

Specific Comments

1) Page 7758, equation (2): Based on this equation, it seems that the pdf in equation (1) is assumed to be Gaussian and that the errors ($z - Hs$) and ($s - X\beta$) are independent? However, I would expect that these errors would be correlated since $X\beta$ depends on the observations.

2) Page 7758, line 23: What are Λ and M ?

3) Page 7764, equation (17): It would be helpful to discuss how the a posteriori covariances compare with those obtained from a MAP estimator? As shown in equation (9), the use of an a priori (with covariance Q) in the MAP estimator produces an estimate with smaller uncertainty than one would obtain using just the information in the data - a Maximum Likelihood (ML) estimator. Since the Geostatistical approach is a ML estimator, are the a posteriori covariances generally larger than those from the MAP method?

4) Page 7768, lines 13-15: Why does a smaller error magnify the differences? The smaller error should imply more information in the data.

5) Page 7769, line 4: Since the covariances are prescribed in this experiment, the comparison between the batch and GFLKS approaches is really a comparison between batch and the FLKS, but at a high spatial resolution. The experiment shows good agreement between batch and the GFLKS, which is consistent with Bruhwiler et al. (2005), who showed good agreement between batch and the FLKS. Therefore, as I stated in my general comments, I don't see what new is being offered here, beyond

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Bruhwyler et al. (2005).

6) Figure 5: Why not change the scale on panel (b)? Since the data are only in the range of ± 1 GtC/yr, plotting them on a scale of ± 5 , GtC/yr is not helpful. Also, in panels (c) and (d), how large is the absolute uncertainty for the estimates? It would be helpful to have that information to compare with the differences between the estimates and the truth ("inventory").

7) Page 7770, lines 25-28: The relative difference between the estimates is larger, but the relative uncertainty in the estimates is also larger. An improved Figure 5, as described above, would be helpful here. From what I can see in Figure 5, the two estimates are all within the range of uncertainty, which is expected.

8) Page 7771, lines 26-27: "Overall, this method makes the solution of large-scale geostatistical inverse problems feasible, paving the way for additional studies on gridscale flux estimation." As I mentioned on the general comments, it is the availability of the adjoint that makes "gridscale flux estimation" feasible.

9) Page 7772, lines 1-4: There is a lack of citation of other studies which have explored similar issues on inverse modeling of atmospheric trace gases. For example, a lagged Kalman filter was used by Pétron et al. (2002) for their inverse modeling of CO for monthly mean emission estimates. More recently, Stavrakou and Müller (2006), Elbern et al. (2007), and Meirink et al (2008) have examined issues associated with grid-scale inverse modeling. These should be mentioned.

Pétron, G., C. Granier, B. Khattatov, J.-F. Lamarque, V. Yudin, J.-F. Müller, and J. Gille, Inverse modeling of carbon monoxide surface emissions using Climate Monitoring and Diagnostics Laboratory network observations, *J. Geophys. Res.*, 107(D24), 4761, doi:10.1029/2001JD001305, 2002.

Stavrakou, T., and J.-F. Müller, Grid-based versus big region approach for inverting CO emissions using Measurement of Pollution in the Troposphere (MOPITT) data, *J.*

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Geophys. Res., 111, D15304, doi:10.1029/2005JD006896, 2006.

H. Elbern, A. Strunk, H. Schmidt, and O. Talagrand, Emission rate and chemical state estimation by 4-dimensional variational inversion, Atmos. Chem. Phys., 7, 3749-3769, 2007.

Meirink, J. F., et al., Four-dimensional Variational Data Assimilation for Inverse Modeling of Atmospheric Methane Emissions: Analysis of SCIAMACHY Observations, J. Geophys. Res., doi:10.1029/2007JD009740, in press, 2008. (<http://www.agu.org/contents/journals/ViewPapersInPress.do?journalCode=JD>).

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

ACPD

8, S4279–S4283, 2008

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