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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Technical Note: Methods for interval constrained atmospheric inversion of methane" *by* J. Tang and Q. Zhuang

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General comments

This technical note deals with sequential schemes for atmospheric inversion. Atmospheric inversion seeks a vector sources and sinks s (in the following, for convenience, I write just "sources" or "fluxes") that are consistent with a vector of concentrations (in the present case of methane) given an atmospheric chemical transport model H:

$$z = H(s) \tag{1}$$

The authors present an algorithm (including its implementation) that restricts the components of the source vector to intervals specified by the user. The presentation of the study is very weak. A few examples are highlighted in the specific comments. It appears that the study and the manuscript were produced in a hurry. As a consequence

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Interactive Discussion

Discussion Paper

of the weak presentation, much of what follows below had to be guessed as good as possible from the presented material and the references.

In their approach the authors make several simplifications. First, they treat H as a linear function (their Eq. 1). This is a simplification, because the strength of the sink processes is proportional to the concentration. Second, they aggregate the sources to a only a few components ("big regions"), for which they compute basis functions. This is a simplification, because the space-time structure within the "region" is prescribed although it is uncertain. Third, they divide the inverse problem into a sequence of sub problems, which they solve one after another. Each sub problem uses one month of data to constrain six months of sources. The sequential scheme is set up such that the final estimate for each month of sources is influenced by six months of concentrations (from the same month plus the following five months). This is a simplification because a source affects all future concentrations. Bruhwiler et al. (2005) (Fig. 7) demonstrate that the error of this simplification can be as large as 1GtC/yr even for a linear problem and when using a "big region" non sequential setup as reference. I wonder how large the error gets in the case of a non-linear model (as here), and when benchmarked against a reference inversion that solves for the sources on the model grid. In the linear case of Bruhwiler et al. (2005) one knows (see, e.g., Enting, 2002) at least that, without imposing any error, one can set up of a sequential inversion scheme, in which each inversion step uses a sub set of the concentrations, provided that each step estimates all sources and that each step uses as prior the posterior estimate of the previous step. This does not hold in the non-linear case treated here. The authors choose a particularly favorable reference setup, namely a big region setup that is linearized in the same way as in their experiments and produce their pseudo concentrations with this setup. Hence, we don't know how the suggested method deals with concentrations that are affected by the non-linear sink processes or with source components that are unresolved by the big region setup.

Another weak point are the diagnostics. The authors don't show a single posterior

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error. Hence, we don't know, how much adding the interval constraint reduces the posterior error.

The references to Tang and Zhang (2010) are often not very helpful, because parts of the text are relatively similar, sometimes even identical. For example, understanding the details of the experimental setup is difficult if not impossible. Inspecting the corresponding subsection in Tang and Zhang (2010), one learns that “seasonal fluxes” denotes monthly resolution of the fluxes. But one has no idea how the grid cells are grouped to form the “11 seasonal fluxes” and “7 yearly constant fluxes”, and how the sink processes are treated. Except that some lines above “stratospheric fluxes” are mentioned. For the general setup of the inversion scheme, one can just guess that it is based on the scheme of Bruhwiler et al. (2005). The results section (3) then mentions a “lag length of 6” without any unit. For the calculation of the matrix dimensions in the experimental setup section of Tang and Zhang (2010) one can just guess that the lag might be 6 months.

The manuscript certainly contains some innovative material, but, as it stands, it has only a limited scientific significance.

Specific comments

Intro, p19982: The way the Kalman smoother refs are contrasted with the previous refs to Enting and Gurney et al. suggests that only the Kalman refs are based on Bayes' theorem/the theory described by Tarantola. This is not true.

Intro, p19983: The authors stress that the variable transform complicates the use of their Kalman smoother approach, because it increases the non-linearity of H. The authors claim that the variable transform method poses problems regarding the interpretation of the posterior uncertainties. In fact, at least for monotonic transformations, this interpretation is straight forward: For example, the +/- 1 σ range in the ξ space is transformed into an interval in the s-space which corresponds to the same probability.

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Methods (2.1, l 11): “Combine the term ... into the measurement”. Which mathematical operation does “combine” denote? Addition? Multiplication?

Methods (2.2, Eq 4): What are Q and R?

Methods (2.2: The presentation of the iterative procedure is seriously confusing. What is the “active set method”, “Zigzag”, “anti cycling”?

Methods (2.3): Why is the variable transform introduced? It appears that it is not used: “we find it useful to solved the problem in terms of s”.

Methods (2.3, text after Eq 20): What is the effect of the truncation in the eigenvalue spectrum on the posterior sources and posterior error. The truncation removes the leading eigenvectors of the inverse of Q, which enters Eq 18. It is that part of the source space which is only weakly constrained and large adjustments can occur. The procedure appears to suppress these adjustments.

Methods (2.3, top paragraph of p 19988): ICMLES has not be introduced. What is a “truncated multi-dimensional Gaussian distribution”?

Methods (2.5): This section is particularly difficult to follow. Why is the shape of $Q^{-1/2}$ rectangular, with dimensions m x n? What is the instrumental distribution? Use capital letters for “QR” in “QR factorization”.

Results (Second paragraph): I presume the authors want to say that the problem is “ill-posed”. The regularization through the prior should actually render the problem “well-posed”. Without the regularization the ill-posedness might also be a consequence of the sequential treatment, because 1 month of concentrations (at 211 locations) is used to estimate six months of fluxes over 18 big regions, i.e. 6 x 18 flux components. By contrast, in a non-sequential inversion the ratio of concentrations to unknowns would be 211/18, which looks less “ill-posed”.

The authors are using the term “correlation of fluxes”, when they actually mean “correlation of the error (or uncertainty) in fluxes”, e.g. in “unrealistic negative values of fluxes

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are inferred due to some spurious correlations among the different fluxes". They also switch between the use of "posterior fluxes" and "inverted fluxes". I would recommend to use the former term throughout.

Technical corrections

p 19982 l 2: replace "including" by "i.e.", since here you are listing all methods that you are testing.

p 19987 l 6: "in terms" instead of "in term"

p 19988 l 4: "for the next update" instead of "for next update"

p 19988 l 9: "after initialized" instead of "after being initialized"

p 19991 l 19: "show" instead of "showed"

Interactive comment on Atmos. Chem. Phys. Discuss., 10, 19981, 2010.

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Interactive Comment