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Interactive Comment

Interactive comment on "Atmospheric inverse modeling with known physical bounds: an example from trace gas emissions" *by* S. M. Miller et al.

Anonymous Referee #2

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Overall comments:

Inverse modeling with known physical bounds is a common problem in the atmospheric sciences. This manuscript reviews several existing statistical methods for addressing this type of problem and tests the performance of each in a case study that uses simulated observations. The advantages and disadvantages of each method are explored, with respect to aspects such as biases in the central estimate and uncertainty bounds, computational cost and flexibility in prescribing the shape of the conditional distributions at the bounds.

The manuscript is well-written and represents a valuable contribution to the literature on

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methods for the inversion of atmospheric transport. My main comment is that the application of uncertainty bounds might be better considered a modification of the priors rather than of the conditional PDFs, as I explain in more detail below. In addition, this is not the first application of MCMC methods in the context of estimating atmospheric fluxes, and the authors should clarify this statement.

I highly recommend this manuscript for publication in Atmospheric Chemistry and Physics after minor revisions addressing the detailed comments below.

Detailed comments:

p. 4550, l. 13: The authors write that one of the advantages of the Gibbs sampler over the Metropolis Hastings algorithm is that it offers "greater flexibility in determining the shape of the marginal distributions at the bounds". Isn't the same flexibility in determining the shape of the distributions also available using a Metropolis Hastings algorithm, by simply modifying the prior and conditional PDFs appropriately? I think the distinction here should be made between the methods used to enforce non-negativity (Lagrange multipliers vs. the shape of prescribed conditional and/or prior PDFS), rather than between the Metropolis-Hastings algorithm and the Gibbs Sampler.

In particular, an alternative approach for implementing a non-negative constraint in an MCMC algorithm is to apply the constraint as a prior pdf, i.e., use a step function rather than a fully uninformative prior (e.g., Burrows, et al., 2013). Since the posterior PDF is proportional to the product of the prior PDF and the conditional PDF (Tarantola, 2005), this is also mathematically equivalent to specifying the conditional PDF as a truncated Gaussian, or to repeating each random draw until it falls within uncertainty bounds as was done in Michalak (2008).

This raises the philosophical question of whether the bounds should be considered a component of the prior information or of the conditional PDF. This is perhaps a matter of taste and won't affect the calculations. But, since the bounds constitute information about the fluxes that is known prior to the inversion, and is unrelated to the observed

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concentrations, wouldn't it make more sense to consider the bounds to be a part of the prior? Stated another way, introducing bounds reduces the uncertainty of the inversion because it adds information to the problem – but this information comes in the form of (prior) physical knowledge about the system, rather than in the form of additional observations or reduced uncertainty in the observations.

p. 4545, l. 13 – 18: It is interesting to see that the unconstrained inversion sometimes violates the known bounds. Violations of known bounds in atmospheric transport inversions that use real observations could indicate a problem with the modeled transport or loss processes, which is sometimes raised as an objection to the use of bounded inversions. In this case, though, violations of the known bounds occur with synthetic observations where the sources and winds are exactly known, arising simply as a result of the uncertainty in the inversion. This is not surprising, but maybe it is worth re-emphasizing this point, since it is a good argument in favor of enforcing bounds in this type of inversion.

p. 4549, l. 26: As noted by other reviewers, this is not the first application of MCMC to the estimation of atmospheric trace gas fluxes. Further examples of similar/related applications of Monte Carlo techniques to the estimation of trace gas fluxes (and/or their uncertainties) can be found in a number of recently published papers – e.g., Berchet et al., 2013; Broquet et al., 2013; Hirst et al., 2013 – and presumably there are others. Please remove this statement and/or clarify the distinctions and relationships between this application and previously published studies.

Minor and technical comments:

p. 4543, l. 18-19: Are the synthetic concentration measurements generated using WRF as the forward model? Please clarify.

p. 4535, l. 17: "X is a m x 1 vector" – change "a" to "an"

p. 4542, l. 12: "in context" – missing "the"

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p. 4546, l. 25: the budget is cited here as “2.1 +- 0.2 TgC per month” – but in Table 2, the budget for the “Transform” inversion is “1.59 +- 0.20 TgC per month”. Possibly a typo?

References: Berchet, A., Pison, I., Chevallier, F., Bousquet, P., Conil, S., Geever, M., Laurila, T., Lavrič, J., Lopez, M., Moncrieff, J., Necki, J., Ramonet, M., Schmidt, M., Steinbacher, M., and Tarniewicz, J.: Towards better error statistics for atmospheric inversions of methane surface fluxes, Atmos. Chem. Phys., 13, 7115-7132, doi:10.5194/acp-13-7115-2013, 2013.

Broquet, G., Chevallier, F., Bréon, F.-M., Kadygrov, N., Alemanno, M., Apadula, F., Hammer, S., Haszpra, L., Meinhardt, F., Morguí, J. A., Necki, J., Piacentino, S., Ramonet, M., Schmidt, M., Thompson, R. L., Vermeulen, A. T., Yver, C., and Ciais, P.: Regional inversion of CO2 ecosystem fluxes from atmospheric measurements: reliability of the uncertainty estimates, Atmos. Chem. Phys., 13, 9039-9056, doi:10.5194/acp-13-9039-2013, 2013.

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Tarantola, A.: Inverse Problem Theory and Methods for Model Parameter Estimation, Society for Industrial and Applied Mathematics, Philadelphia, PA, 2005.

Interactive comment on Geosci. Model Dev. Discuss., 6, 4531, 2013.