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

S. M. Miller et al.

scot.m.miller@gmail.com

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We would like to thank the reviewer for feedback and suggestions on the manuscript. These comments provide an important independent perspective that have helped us improve the quality and readability of the manuscript.

Overall 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).

We agree with this comment. As the reviewer points out, one could use a different prior probability density function (pdf) in the inversion setup and sample the posterior distribution using Metropolis Hastings. In theory, a modeler is not restricted to a multivariate normal prior pdf but instead could use any number of choices (e.g., Rigby et al. 2011, Burrows et al. 2013). In this sense, Metropolis Hastings allows for a range of flexible implementations. However, it can be difficult to efficiently sample the posterior pdf using Metropolis Hastings. This consideration becomes particularly important when the number of unknown emissions ($\vec{s}$) is large. Efficient sampling often places practical limitations on the complexity of the prior pdf. We have added a new section 1 to the supplement that discusses this challenge in detail. Furthermore, we have reworded sections 3.3.1 and 5.4 in the main manuscript to account for this discussion.

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 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.*

The wording in section 3.3.2 may have unintentionally muddled the discussion on this topic. In this section, the phrase "conditional pdf" refers to the univariate probability of element s_i conditional on the probability of all other elements in $\vec{s}$. This pdf is different from the conditional pdf in Bayes theorum. For the application here, that pdf refers to the multivariate probability of the atmospheric observations conditional on the unknown emissions.

The Gibbs sampler implementation in the manuscript incorporates the bounds as a component of the prior distribution. The Gibbs sampler in Michalak et al. (2008) formulates the prior pdf as a multivariate truncated Gaussian distribution. As a result, the posterior pdf is also a multivariate truncated Gaussian distribution. In our study, we further modify the prior pdf to increase the probability of estimating zero emissions. We have reworded sections 2 and 3.3.2 in the revised manuscript to clarify this discussion.

.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.

This is a very good point. If the observations and transport operator are both positive,

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then a negative emissions might seem implausible:

$$\vec{z} = \mathbf{H}\vec{\hat{s}} + \vec{\epsilon} \tag{1}$$

In this equation, $\vec{z}$ are the observations, $\mathbf{H}$ the sensitivity or transport matrix, $\vec{\hat{s}}$ the posterior emissions estimate, and $\vec{\epsilon}$ the model data mismatch (e.g., transport, measurement, boundary condition errors, etc.). If $\vec{z}$ and $\mathbf{H}$ contain only positive elements, then it may seem illogical that $\vec{\hat{s}}$ could have negative components. In reality, $\vec{\hat{s}}$ may contain negative elements due to the effect of model-data mismatch errors ($\vec{\epsilon}$). When these errors are present, the gradients in the observations may be consistent with adjacent positive and negative sources. Furthermore, these negative emissions are not necessarily caused by any violation of the statistical assumptions in the inversion. In the methane case study, we synthetically generate model-data mismatch errors, so these errors are guaranteed to obey all assumptions of the statistical model. Positive observations and positive transport can nonetheless lead to a negative emissions estimate in some locations. We have added several sentences to section 5.1 that highlight this point.

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.

This is a useful suggestion, and we thank the reviewer for the list of references. Rigby et al. (2011) and Burrows et al. (2013) use MCMC implementations to enforce inequality constraints in the inversion. A number of other studies, including several of those referenced by the reviewer, use MCMC methods to sample the posterior uncertainties in problems without inequality constraints. We now reference the two studies above in the revised manuscript. Furthermore, we have added section 1 to the supplement; this section compares the Metropolis-Hastings implementations in Rigby et al. (2011) and Burrows et al. (2013) to an approach used in several hydrology studies.

Detailed comments

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

This is correct. The synthetic concentration measurements are generated using WRF-STILT as the forward model. Note that WRF is used here for its modeled wind fields. STILT, in contrast, is a particle-following model that transports atmospheric tracers along these modeled wind fields. We have clarified this in section 4.1.

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

Thank you for pointing this out. We have changed the manuscript as suggested.

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

We have changed the manuscript accordingly.

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

This difference is intended, and we have edited line 25 on this page to clarify the difference. The budget listed in the table is the maximum a posteriori (MAP) best estimate calculated using the transform inversion. The higher budget listed in the text (2.1 $\pm$ 0.2 TgC per month) is the mean of the conditional realizations. In the unconstrained inversion setup, these realizations sample the posterior probability space, and the mean of the realization is identical to the MAP estimate. In the data transformation case, however, this relationship no longer holds true. The difference in budgets above highlights a key point: the posterior uncertainties and conditional realizations can be difficult to interpret in the data transformation inversion.

References

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