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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.

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We would like to thank the reviewer for suggestions and comments. This feedback has helped us improve and clarify the manuscript.

Specific comments and corresponding manuscript changes

P4532 L11-12, P4549 L26-27 I don't think this is the first application of MCMC to estimate atmospheric trace gases. Please remove this comment.

We have removed this comment from the manuscript. We have further cited two atmospheric studies that use MCMC implementations to enforce inequality constraints.

P4532 L17-19 I don't agree that Lagrange multipliers offer a real alternative to MCMC methods. As far as I understand Lagrange multipliers are only able to provide a best estimate but not an estimate for the uncertainties. Therefore they are not an alternative. Please reformulate this sentence.

We agree with this suggestion. We have removed the word "alternative" in the revised manuscript.

P4537 L18-19 Why can you only enforce a single upper or lower bound that is the same for all elements in s? Surely it must be possible to use different transformation methods for different parameters.

If an optimization problem has only a few parameters, it might be reasonable to transform each parameter differently, thereby enforcing different, individual bounds on each parameter. In spatially-resolved inversions, however, the parameter vector (e.g., emissions) can have thousand to millions of elements to estimate. In this case, it would not be computationally tractable to apply individual transformations to individual parameters. Furthermore, this approach to transformations would complicate spatial and/or temporal correlations in the unknown emissions field. If one applied different transformations to different parameters, the assumption of spatiotemporal correlation in the transformed state would likely not be valid.

A transformation on the upper and lower bounds could, in principle, exist. This transformation would need to convert from a variable defined over a finite interval to one defined over all real numbers. And the inversion residuals in this transformed space would need to be approximately normally distributed. We have changed the manuscript to the following: "Furthermore, most common transformations can only enforce a single upper or lower bound that is the same for all elements of $\vec{s}$."

Could you please provide a better overview in terms of the computational requirements (i.e. number of iterations) for each method?

Both the power transform and Lagrange multipliers implementations require iterations. In other words, both require iterative calculation until the algorithm converges on the final best estimate. MCMC algorithms, in contrast, compute a large number of realizations that collectively sample the posterior probability space.

For medium to large inverse problems like the methane case study, the calculation of many realizations can be computationally demanding. We have added a paragraph to section 5.4 that discusses the computational requirements and number of realizations required by MCMC methods. In the revised manuscript, we also refer the reader to a book by Andrew Gelman, which includes an entire chapter on this topic.

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