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Geoscientific Model Development Discussions

Interactive comment on "A tuning-free method for the linear inverse problem and its application to source term determination" *by* O. Tichý et al.

Anonymous Referee #1

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This paper provides an interesting description of a Variational Bayesian approach to source term estimation that allows for the tuning of the hyper-parameters to be performed, based on the information content of the measurements. The paper is a valuable contribution, in that the optimization of the uncertainty hyper-parameters does not require pre-specified or pre-optimized uncertainties, as is often the case in Bayesian inversions. However, there are a number of issues that should be addressed before the paper is ready for publication. The authors have omitted to mention a range of studies in the literature that have previously addressed the problem of objectively defining these hyper-parameters, and how this work compares to those that have gone before. In addition, the paper is hindered by a lack of explanation in places, making it occasionally difficult to follow. A more thorough description of how this work compares to other hyper-parameter estimation approaches is required, along with the remedying of

other issues outlined below, in order for a more polished manuscript to be produced.

Specific Comments:

1. Page 1, Line 24: "...this two-pronged approach..." What exactly is meant by this? Top-down inversion studies are normally performed independently of the compilation of bottom-up inventory studies.

2. Page 2, Line 4: Could the authors be more specific as to what "other bottom-up information" entails?

3. Page 2, Lines 20-23: The authors have neglected to mention that many studies do not select these tuning parameters subjectively, and there have been a number of studies that have defined objective criteria for this purpose. For known location source-term estimation, examples include Davoine and Bocquet (2007) or Winiarek et al. (2012). In trace gas inversions Michalak et al. (2005) optimized covariance parameters using maximum likelihood estimation, and a similar approach was used in Berchet et al. (2013). In a perhaps more closely related approach to variational Bayes, Ganesan et al. (2014) used an MCMC method to estimate the hyper-parameters using the data. A discussion of these other approaches is needed, in order to contextualise this work.

4. Page 3, Line 7 & 10: The use of the term "State of the art methodology" is a bit of a push. The work of Eckhardt et al. (2008) may provide a useful reference to compare to, but there have been many examples of advances beyond the use of subjectively prescribed uncertainties since then (if not before, see above).

5. Page 4, Algorithm 1: The term "stopcond" needs explaining, or some reference made to it in the text.

6. Page 4, Line 4: What is meant by the "potential prior mean" and why is this subtracted from both sides of the equation?

7. Page 4, Line 11: "The method of Eckhardt et al. (2008) has Bayesian interpretation

as a maximum a posteriori probability estimate of the following model:" This sentence did not make sense to me, please clarify or rephrase.

8. Page 5, Line 8: Could the Variational Bayes approach also be extended to deal with this second problem?

9. Page 5, Line 10: "Approximate inference of these values does not yield acceptable results". This statement is too vague, please expand. Are the authors referring to MCMC approximations, and if so why would these be unacceptable? As I understand, the advantage of Variational Bayes over MCMC is mostly a matter of speed, but Variational Bayes may be more susceptible to bias. Perhaps this could be commented on.

10. Page 5. Line 22: "The selection of these constants will be discussed later in this paper." It would be helpful to point the reader to the exact section. As it stands, I am not certain that any discussion on the selection of these constants actually appears in the text.

11. Page 6, Lines 15-16: Given that the authors state that the expected values of l_j are either 0 or -1, is there a need for such an uninformative range on l_j (-1 +/- 100)? What would be the effect of a smaller range on l_j? Similarly what would the effect of further relaxation be, and why is this not recommended?

12. Page 7, Algorithm 2, 2 (c) and (d): It is unclear which equations in Appendix B define the covariance structure. I assume it is Eq. (B1), but this could be made more obvious.

13. Page 8, Lines 6-7: How much higher is the computational cost expected to be?

14. Page 9, Lines 29-32: In A) what is the Lagrangian timescale? It would be helpful to explain why different results are expected for different time steps, and what uncertainty running two different time steps might account for. It was a little surprising to find no subsequent discussion of the differences between configurations A and B. Why, for

instance, is the artefact in ERA-Interim A not seen in ERA-interim B?

15. Page 10, Lines 13-14: For the avoidance of doubt please make clear which of 230 kg and 340 kg is the posterior and which is the true source term. Furthermore, there surely must be some uncertainty on the posterior source term? "Quite similar" is a vague description, and may not be entirely accurate given one term is 50% larger than the other. Could the authors comment on whether the results are statistically similar?

16. Page 11, Lines 3-4: What do the top rows in Figures 5 & 6 show? It is not immediately obvious what the graphs are displaying, and it would help to explain this in the text. These graphs need more explaining both in the text and the figure caption.

17. Page 11, Lines 18-20: I assume the range of possible solutions is shown by the blue fill, but this should be made explicit in the text and the figure captions.

18. Page 11, Lines 21-23: How long does it take to run, and how much more expensive is it than the simpler techniques? How would the computational cost scale with the dimension of both the parameters and data vectors?

19. Figure 5 & 6: Which tuning parameter does the x-axis refer to and does it have a unit? Shouldn't the y-axis in the top panel also have units?

Technical Corrections:

20. Throughout the manuscript I believe equations should be referenced as "Eq. (1)". Similarly figures should appear as "Fig. 1". Details of GMD guidelines can be found here: http://www.geoscientific-model-development.net/for_authors/manuscript_preparation.html

21. Page 9, Line 13: Figure 4 is referenced before figure 3

22. Figure 2: The x-axes appear to be missing a label. The dotted lines also appear very faint and hard to see.

23. Figure 3: No x-axis label

References

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