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Discussions

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Interactive comment on "Estimation of trace gas fluxes with objectively determined basis functions using reversible jump Markov chain Monte Carlo" *by* Mark F. Lunt et al.

Anonymous Referee #2

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1 Main comments

This paper represents a very interesting description and application on synthetic and real data of tracer, of the most recent techniques in transdimensional inverse modelling. In that respect, this paper is very valuable and I believe that it should ultimately be published. However, the manuscript is not without flaws that should be corrected before the paper becomes acceptable for publication. The most important flaws to be corrected are

1. From time to time, a crucial lack of details.

2. The bibliographical account on hyperparameter estimation is very misleading. As opposed to what is implied in the manuscript, this subject has been addressed in tracer inversion and greenhouse gas inversion for more than 10 years now. I have some knowledge on all the techniques that are addressed by the authors, and I can tell that this poor bibliographical account clashes with the rather good account on the other mathematical aspects.

3. Several passages of the manuscript are odd and difficult to understand. This tells me that the manuscript has not been polished enough yet, although it is already quite enjoyable.

2 Minor points or comments related to the main points

1. Page 1, line 9, "it allows the uncertainty in our choice of aggregation to be carried through to the solution" is too vague for the abstract. Please clarify or postpone this statement.

2. Page 1, Eq.(1): It is common practice to insert equations within the flow of the article and use punctuation marks at the end of equations (or not if embedded within a sentence).

3. Page 2, line 16: "...or the solution being overly influenced by an incorrect prior, giving the so-called smoothing error": This statement is partially misleading to me. The fact that there are more degrees of freedom is not an issue *per se*. This has been shown in Bocquet et al. (2011): in theory the more resolved the grid, the better the inversion. It is in addition the fact that the prior could be incorrect that may lead to the smoothing error. If the incorrectness in the prior is low, then such a balance might be pointless. In that case, dimensional reduction is essentially

only important for computation issues (which is critical) as pointed out by Bocquet et al. (2011) and ultimately confirmed in Turner and Jacob (2015).

4. Page 2, line 28: "Various studies..." Obviously there has been only a few studies so far. Please mitigate your statement.

5. Pages 2, line 33-35: "Although a parameter dimension was successfully identified which minimised the total error, ultimately the choice of model to use was as much influenced by computational efficiency, as it was by this combination of aggregation and smoothing error": Yes, just as predicted in Bocquet et al. (2011). This could be mentioned.

6. Page 3, line 2-3: "Therefore, the uncertainties in step one do not necessarily propagate through to step two." All of he objective criteria in Bocquet et al. (2011) depend on the observation network. One of the criterion in Bocquet et al. (2011) actually depend on the data itself (section 4.1.3 and illustrated on Fig. 5 of the same paper).

7. Page 4, lines 20-30: This paragraph gives a wrong and totally biased picture of the literature on the hyperparameter estimation as used in tracer/greenhouse gas inversions, not to mention geophysical data assimilation and in particular meteorology. There are dozens of papers on the subject before the contributions of Ganesan et al. Only focusing on tracer inversions, one of the very first use for the inversion of the Chernobyl source term is in Davoine and Bocquet (2007) which has been extended to non-Gaussian inversion problems in the Fukushima case (Winiarek et al., 2012). But there really are dozens of papers on the subject. Two reviews on the matter are Michalak et al. (2005) and Wu et al. (2013). It would be fair to mention those papers before mentioning Ganesan et al.

8. Page 5, whole section 2.1: this subsection 2.1 is totally off in the flow of the paper, especially starting from line 10. I do not understand why the past tense is used.

I do not understand which numerical experiment you are referring to? This must be re-written or postponed in the manuscript.

9. Page 5, section 2.1: The use of a Lagrangian model such as NAME adds further interesting issues that were discussed in Koohkan et al. (2012). There is an additional uncertainty due the number of particles, especially when just a few of them fall into grid-cells. This issue could conflict with the transdimensional approach.

10. Page 5, line 25: "Furthermore, each grid cell within each aggregated region has an enforced correlation to it's neighbours": Why?

11. Page 5, line 25: "it's" $\longrightarrow$ "its".

12. Page 6, lines 19-24: "In this work, we approximate the form of the Voronoi cells, by restricting them to those points on the underlying finite grid which are closest to their respective nuclei. As such, the region edges are not exactly equidistant between nuclei, but this approach was taken since the exact form of the Voronoi cells is unimportant, and each underlying grid cell belongs to only one nuclei, making computation very simple." This passage is very unclear to me. Please give more details.

13. Page 6, line 7: "as shown by Ganesan et al. (2014)." You are pushing the envelope too far here. This was well known and shown a long time before Ganesan et al. (2014). Please remove this statement which is biased.

14. Page 6, line 10: "Where the assumption has been made that θ is independent of k": This is a question that has puzzled me for a long time. It may very well be that this independence is plain wrong and that it has a strong impact on the resulting inversions. At the very least, you should discuss that assumption.

15. Page 6, lines 10-20: "Whereas the hierarchical framework alone can be solved through conventional Markov Chain - Monte Carlo (MCMC) methods (Ganesan et al., 2014), since the dimension of m is variable in the transdimensional case, it must be solved by a different, though strongly related, approach." The sentence is unclear. Please rephrase.

16. Page 8, line 15, Eq.(11): $n \longrightarrow \mathbf{n}$.

17. Page 9, line 2: hyperparameter $\longrightarrow$ hyperparameter.

18. Page 9, line 3: "The other three proposals" $\longrightarrow$ "The other three proposal ratios".

19. Page 9, lines 4-5: "In effect, this means a change in the sensitivity matrix, $\mathbf{H}$, that maps the relationship between emissions and observations.": Please be more much precise as to what it implies for $\mathbf{H}$.

20. Page 9, line 9, "there are an unknown number of unknowns" $\longrightarrow$ "there is an unknown number of unknowns"?

21. Page 9, line 10, "be decomposed to two separate terms" $\longrightarrow$ "be decomposed into two separate terms".

22. Page 9, lines 10-11: "since the prior location and emissions variables are independent of each other" is not obvious to me. Can you please elaborate?

23. Page 9, lines 19: "so they may be located anywhere" $\longrightarrow$ "so they may be located a priori anywhere".

24. Page 9, line 20: "can be located on the finite underlying grid": that is an imprecise statement. Could you please be more specific?

25. Page 9, Eq.(16): Even using an – as much as possible – uninformative prior may slightly influence the number of nuclei. Can you elaborate on that?

26. Page 10, Eq.(18): Shouldn't x be bold?

27. Page 11, line 17: "and the other a correlation length between measurements, τ.": That is why I have reservation on the fact that all of the hyperparameters are independent from k.

28. Page 11, line 18: "it's" $\longrightarrow$ "its".

29. Page 11, line 18-21: Please elaborate. The statements are too concise.

30. Page 12, line 19: "it's" $\longrightarrow$ "its".

31. Page 12, line 24-27: What is $|\mathbf{J}|$ here?

32. Page 12, line 25: "In practice, this means that one does not have to define the nuclei locations as being restricted to the locations of the 25 underlying grid, and they can in fact take any position within the inversion domain." Okay, but what did you do in this study?

33. Page 13, line 9: "in order for convergence to occur" $\longrightarrow$ "in order for the convergence to occur".

34. Page 14, line 1: Can you describe the temporal dimension of the emissions. For instance, are they modulated in time?

35. Page 14, line 10: How many observations do you use? How long is the time frame?

36. Page 14, line 16: Which first guess (mean prior) did you choose? In general the reader is missing quite a few details to fully understand the experiment. Please give more information.

37. Page 16, line 30-32: What would happen without this filter?

38. Page 17, line 1-4: Please provide a figure.

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