Geoscientific Model Development Discussions

Geosci. Model Dev. Discuss., referee comment RC2
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Comment on gmd-2022-89

Anonymous Referee #2

Referee comment on "Metrics for evaluating the quality in linear atmospheric inverse problems: a case study of a trace gas inversion" by Vineet Yadav et al., Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2022-89-RC2, 2022

This paper presents methods for sensitivity analysis of the solution of the inverse problem to various input parameters, keeping in mind the cost associated with the sensitivity computations. This is important because it provides the user with some understanding of the sensitivities and may lead to better prior models or measurement strategies. The methodology is illustrated in the case of an atmospheric inverse problem. The computational costs are significant for such problems, even for computing the MAP estimate, so it is important to derive efficient methods for sensitivity analysis.

Major concerns:

- **Contributions**: I couldn't fully understand the contributions of this paper. Is it claiming to be developing new methods for inverse problems, or applying existing techniques to the case study? The methods for local sensitivity analysis involving derivatives appear to be a special case of the Hyperdifferential sensitivity analysis for linear inverse problems and the GSA method is essentially DGSM (see end of review).
- **Mathematical exposition**: I understand that this is not an applied math journal, but the standard for exposition was well below this journal. The notation is not setup properly and inconsistently used. There were a lot of vague statements (I did not fully tabulate this list).

Specific comments:

- Title: I think working in the word sensitivity is better here than “assessing”.
- The abstract does not clarify, of what quantity (i.e. MAP estimate) the sensitivity is being computed. GHG is not expanded and Jacobian should be capitalized throughout. The word Jacobian (to me) is misleading because this is a linear problem – there are other Jacobians used in the paper.
- The introduction does not clearly list the contributions (as mentioned earlier) and is missing some references.
- Section 3:
  - The inversion is not setup properly before 3.1.1-3.1.3 are explained. I essentially did not understand anything in these subsections. I am not sure what sets are being considered, how this relates to the inversion, etc. There is a small discussion at the end of 3.1.3 but it is referring to things that haven’t yet been defined.
  - Section 3.2: Someone not familiar with this material will struggle since it has not been discussed properly. I suggest reorganizing this section bringing some of this material earlier.
  - Notation/Writing: This is not consistent throughout the paper. Sometimes subscripts refer to sizes, other times they mean elements. Sometimes boldfaced, sometimes not. Sometimes lower/upper case. Sentences should not start with variables. When units are being described, the entries of vectors have units, not the vectors themselves.
  - Line 157: it’s -> its. This occurred in other places also.
  - Line 169: it can be simplified using the notation below in 172.
  - Line 173: One differentiates a function rather than an equation.
  - When referring to equations, one typically puts a parenthesis, e.g. (10).
  - Line 178: The inputs to the inverse problems are data and hyperparameters. The transport model is typically fixed, as is the drift matrix X. What does it mean to differentiate wrt them? Why is that useful in applications? Are these matrices functions of some hyperparameters?
  - Line 185: The equation is not referred to as Lambda but one of the terms there is Lambda.
  - Line 203: When differentiating a vector wrt a matrix, one should get a tensor. I think what is happening is that you are vectorizing X and then differentiating. But the notation is not clear. Same with line 227.
  - Section 3.3: I agree that full GSA is very complicated. It’s not clear how this is GSA. Is this essentially derivative based global sensitivity? Once again I did not really understand what was being discussed.
  - Section 3.4: The authors raise a good point here cautioning against sensitivity metrics since they are of different units but little has been done to address them. There are techniques in sensitivity analysis that the authors should consult (DGSMs and activity scores are some techniques, see Constantine and Diaz)
- Section 4: I didn’t understand the figures since sometimes the sizes of the quantities are not clear. Are entrywise sensitivities being plotted?
- Appendix: The notation was especially problematic here.

Returning to the major concerns: I don’t think the paper is novel in the methodology, but as an application to atmospheric inverse problems I think it has potential. In its current version, I don’t think it is worthy of publishing. In addition to the comments I raised, I would encourage the authors to think of the following questions to improve the utility. What is the computational cost of these approaches? Can they be computed when the forward model is not available entrywise? What are the challenges involved and how can they be efficiently implemented? What are the strengths and weaknesses of each approach? How does one compare sensitivities of different quantities (with different units) and rank the sources of sensitivity?

References:

- Sunseri, Isaac, et al. "Hyper-differential sensitivity analysis for inverse problems constrained by partial differential equations." *Inverse Problems* 36.12 (2020): 125001.
- Sunseri, Isaac, et al. "Hyper-differential sensitivity analysis for nonlinear Bayesian inverse problems." *arXiv preprint arXiv:2202.02219* (2022).
- Sobol, I. M., and S. Kucherenko. "Derivative based global sensitivity measures." *Procedia-Social and Behavioral Sciences* 2.6 (2010): 7745-7746.
- Constantine, Paul G., and Paul Diaz. "Global sensitivity metrics from active subspaces." *Reliability Engineering & System Safety* 162 (2017): 1-13.