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Interactive comment on "Atmospheric Inverse Modeling via Sparse Reconstruction" *by* Nils Hase et al.

Anonymous Referee #2

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General comments

The paper describes a shrinkage method to estimate methane emissions. It is clearly written and has an exposition of shrinkage, as applied to atmospheric inverse problems, that is far easier to understand than others I have encountered (mostly in image processing, under the guise of compressive sensing). I am pretty sure that the paper is the first one, in atmospheric inverse problems, that uses a dictionary of basis functions and not an orthogonal basis set. It is, I believe, one of less than half-a-dozen recent papers in atmospheric inversions that uses shrinkage, which is a key advance demonstrated by this paper.

The main contributions of this paper are as follows. Anthropogenic emission fields tend not to be smoothly distributed in space; they are rough, have hotspots and are

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Discussion paper

correlated with some aspect of human economic or social activity. Estimating these fields require bases that can accommodate roughness e.g., wavelets, as was done by Ray et al, GMD, 2016 (cited in Hase's paper). Using a non-orthogonal dictionary, as Hase et al have done, injects a much higher degree of flexibility (and efficiency) of spatial representation than is possible solely with wavelets. This is because now any shape function (basis) can be used; further, the choice of shape functions can be optimized using some covariate / prior belief of methane emissions. This is the first contribution of this paper. Of course, the dictionary no longer contains orthogonal functions, and in the presence of sparse observations, using shrinkage is a must.

Shrinkage has been known in statistical literature for some time (the famous paper on LASSO appeared in JRSS-B, 1996), but imposing non-negativity on the solutions has not been a priority. That is not the case when estimating emission fields where non-negativity is a must, and Hase et al have had to invent an updating scheme that preserves non-negativity. This is a new algorithmic development in shrinkage regression as used to infer fields and is the second contribution of this paper. Note that while Ray et al, GMD, 2016 also had to impose non-negativity, Hase et al have a rather different way of doing so.

Thus the paper is quite novel and has some significant methodological contributions.

The authors have a style of writing that is direct, and at times, the paper reads a little like a text book. Though somewhat unusual, it is welcome. It makes the exposition of their ideas very clear, which should be the prime objective of the authors.

Specific comments

The paper introduces L1 regularization in Sec 3.3 but never provides a physical motivation for it. It is offered as a contrast and an alternative to L2 regularization, which is quite correct mathematically. However, methane emissions are expected to be "spotty" (or distributed in space in a rough manner) and a sparse representation is necessary. L1 regularization can enable such a representation by picking out appropriate atoms from the dictionary. This is an intuition that is driven by physics and could be mentioned in the paper. Perhaps a paragraph in Sec. 3.3 somewhere or in the Conclusions would suffice. Further, in the same paragraph they could describe, in words, how L1 regularization enforce sparsity (by forcing as many elements of **x** to zero as possible [in Eq. (6)]). In contrast, L2 regularization exaggerates the large elements of **x** and concentrates on reducing them, producing smooth solutions.

In Sec. 4.6 the authors mention smoothing errors, but provide sensitivity analysis instead. Their argument is that a sensitivity analysis is the best one can do in real-life situations where the true emission field is not known. That is true. However, since this paper is a synthetic data study, these smoothing errors could be calculated. This would be akin to the errors computed in Table 2 (Barnett shale study), but without introducing noise into the synthetic observations (i.e., all the errors are due to smoothing and none due to measurement noise).

In Fig. 5, the authors plot fluxes (**x**) and show how a Laplacian distribution is a better prior than a Gaussian. However, they do not plot the top 5% of the fluxes, presumably because, being outliers, they do not fit either of the priors. Not plotting the super-emitters could detract from their contention that a Laplacian prior is a better choice. Perhaps the authors could plot a Fig. 5(b) with the outliers and use that to illustrate the following facts:

- Using fluxes in each grid cell is not a good idea. They don't honor the prior, due to the existence of super-emitters.
- A different representation of the fluxes, which honors the prior, is a better idea (i.e., the fluxes are sparse in the representation used)
- Capturing the outliers could be done by augmenting the representation using the atoms (like the ones in Fig. 6). This could be a good illustration of why a dictionary of non-orthogonal functions is needed.

Corrections, typos etc.

1. Abstract, Pg 1, line 6: "applied math" should be "applied mathematics". Also, "developped" has 1 'p'.
2. Pg 1, line 24: ". . . small noise on the measurements can be "largely" amplified by the inversion . . ." - largely can be omitted.
3. Pg 2, line 20: "carbondioxid" emissions . . .. - carbon dioxide
4. Pg 5, line 6: ". . .it prevents "oszillations" . . .. - oscillations. . .
5. Pg 5, line 22: ". . .. Which are called sparse "solutions". - "solutions" is missing
6. Pg 8, line 20: The projection step for the dictionary is "so" difficult because . . .. - Omit so
7. Pg 10, line 2: . . ..access to the noise characteristics, which is "a" common case - 'a' is missing.
8. Pg 10, line 22: "Realistic" synthetic methane emissions . . .. - Remove realistic? Synthetic data is never quite realistic
9. Pg 14, line 13: . . . industrial facilities and mining "all" do not extend more . . .. - remove all?
10. Pg 15, line 25: The numerical computation requires to solve one reconstruction . . ..- Change to "The numerical computation requires *one* to solve *a* reconstruction ....."
11. Pg 19, line 7: The interpretation is "a" slightly different for . . .- Remove 'a'
12. Pg 19, line 18: . . .the method is not sensitive to data "at all" - Second use of 'at all' in the same sentence. Please omit.

13. Pg 22, line 10: “adequatly “ : wrong spelling.

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