Atmospheric
Chemistry
and Physics
Discussions

Interactive comment on "Atmospheric CO$_2$ inversions at the mesoscale using data driven prior uncertainties. Part 1: Methodology and system evaluation" *by* Panagiotis Kountouris et al.

Anonymous Referee #3

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This paper presents a method for estimating a priori flux uncertainties in carbon dioxide inversion systems. The system is then evaluated using synthetic atmospheric data. Whilst the paper is generally well written, I was left wondering what we've really learnt from a study such as this. At present, the abstract and conclusions largely focus on the outcome of the synthetic data inversion, which I don't believe represent a major innovation, or provide a framework that could readily be used in other work (see below). Perhaps the paper can be re-focused on elements that the authors feel represent a true advance, that could be applied beyond the inversion system described. Alternatively, it appears that the authors have attempted to split this work into two publications: whilst I haven't read the companion paper, I wonder whether the work in this paper is

too incremental to stand on its own, and could instead be folded into the other work (provided the below comments can also be addressed)?

General comments:

1. I'm not convinced that, with a synthetic data experiment such as this, it is possible to show whether a particular prior flux uncertainty covariance is closer to the "truth" than another (aside from demonstrating that one or another was obviously very under- or over-constraining), or, put another way, that one inversion set up would perform better using real world data. The paper describes various metrics of the posterior solution. However, most of these (e.g. RMSE and correlation compared to the known fluxes), simply show that the gradient descent is probably working (i.e. these factors must improve unless there is something obviously wrong with the algorithm). The only metric that might have some ability to demonstrate that the prior uncertainty covariance is appropriate to the real world are the chi-squared tests. However, as the authors note, since this is a synthetic data study, the model is "perfect", so the model-data mismatch will be much smaller than would be achieved in the real world, making this test uninformative for real-world applications.

2. Several relevant papers have not been referenced here. Ganesan et al. (2014) tackle essentially the same problem in a hierarchical Bayesian framework. They show that inclusion of a set of hyper-parameters describing the prior uncertainty covariance necessarily moves the posterior uncertainty closer to the "truth", compared to an inversion without these factors. They were also able to include transport model-data mismatch uncertainties in the inversion. Whilst I don't believe they included a spatial or temporal component in the prior uncertainty covariance, they did explore this in the model-data mismatch, and I don't see why the framework couldn't be extended to do so with the prior (similarly the inclusion of a "bias" hyper-prior would also be possible). In a related approach, Lunt et al. (2016) included the spatial disaggregation of the flux field (and hence, presumably, the level of spatial correlation in the posterior solution) as an unknown in the inversion. Finally, Zammit-Mangion et al. (2015; 2016) present

a solution to the flux inverse problem in which only the spatial correlation lengths are used a priori, and the inversion is not constrained to a mean flux field. In summary, I think that these papers demonstrate some significant advances in this area in recent years. Ideally, this article would build on these developments, or demonstrate why the advocated approach is preferable. At the very least, these papers should be cited.

3. In Figure 7, it appears that, for several months, the derived fluxes are not between the prior and the "truth". I'm not sure how this could be the case, since the pseudo-data should always pull the solution towards the truth, and the prior should pull towards itself. Therefore, shouldn't our expectation value of the posterior fluxes be somewhere in between? Has some random error been added to the pseudo-data (this should be clarified in Section 2.2.3)? If so, is this feature a product of this particular random realisation of the pseudo-dataset? Therefore, do you need to run an ensemble of inversions to "average out" sampling errors?

Specific comments:

P4, L31: I don't see why model errors will be more easy to define that prior uncertainties? I don't think we have a very good handle on transport model error. Furthermore, this term does not need to be diagonal, as this sentence implies (see references above).

P6, L30: See references above.

P9, L9: Why limit this matrix to being diagonal? As noted on Line 13, the transport model will certainly exhibit temporal and spatial uncertainty correlations.

P11, L5: This equation is not referenced explicitly in the text. What does it show?

P11, L6 – L12: These terms are discussed before being introduced (they refer to an equation in the following subsection). I think the order needs to be changed here.

P11, L19: If I understand this correctly, synthetic eddy covariance (EC) data were extracted at several locations in both models, and these pseudo-fluxes were used to

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calculate the spatial and temporal correlation lengths for use in the inversion (please clarify that this is synthetic EC). So essentially, we are using the difference between two models as a proxy for the uncertainty correlation in the real world? I think this is fine. However, two things come to mind: 1) if we were to use "real" eddy covariance data, we would sample very much smaller length scales than the model (i.e. typically <1km, rather than 50km), so I would not expect that the derived correlations would be comparable to the same experiment using real data (as the text seems to indicate on P6); 2) since we're in model world, and in light of point (1), why not use every grid cell to calibrate the correlations? Would this come out as being very different?

P12, L12: The two experiments that are carried out focus on "tuning" the covariance matrix in two ways, so as to match the overall difference between the two models: B1, scale the covariance matrix uniformly; S1 add a bias. What is the reasoning for choosing only these two methods? Couldn't this mismatch be closed in several other ways, e.g. by increasing the correlation lengths or adding a "nugget" term to the diagonal elements, etc.?

P14, L4-L8: Please provide a reference for these choices of data filtering.

P15, L13: I don't think Thompson et al., 2011 is the most appropriate reference here.

P16, L17 – L22: The improved correlation and "variance" is simply a product of the cost function descent. This should be clarified.

P16, L23: Does "chi-squared" show us anything here that we can extend to the real world, given that the model is perfect (see general point 1 above)?

P17, L7: Again, isn't this a trivial result showing that the gradient descent is working?

P18, L11: Probably should be noted that this will largely be determined by the model-measurement mismatch uncertainty covariance, rather than the prior uncertainty.

P19, L15: I think this is a very strong conclusion to draw here. I'd contend that the suitability of EC data for "validation" of inverse model fluxes is dominated by scaling

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issues. In this paper, it is assumed that the EC data is representative of 50km^2. In reality, EC data will sample scales that are orders of magnitude smaller.

P20, L1: I think this shows that your inversion algorithm is working, not that you would get any closer to the truth in the real world.

P21, L13: See general point 1.

P22, L11: I don't think we can comment on the reliability of the results of a real world inversion here. A real world inversion will likely be dominated by chemical transport model errors, which are not quantified here.

References:

Ganesan, A. L., Rigby, M., Zammit-Mangion, A., Manning, a. J., Prinn, R. G., Fraser, P. J., Harth, C. M., Kim, K.-R., Krummel, P. B., Li, S., Mühle, J., O'Doherty, S. J., Park, S., Salameh, P. K., Steele, L. P. and Weiss, R. F.: Characterization of uncertainties in atmospheric trace gas inversions using hierarchical Bayesian methods, Atmospheric Chemistry and Physics, 14(8), 3855–3864, doi:10.5194/acp-14-3855-2014, 2014.

Lunt, M. F., Rigby, M., Ganesan, A. L. and Manning, A. J.: Estimation of trace gas fluxes with objectively determined basis functions using reversible-jump Markov chain Monte Carlo, Geoscientific Model Development, 9(9), 3213–3229, doi:10.5194/gmd-9-3213-2016, 2016.

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