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Atmospheric Measurement Techniques Discussions
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Interactive comment on "Tomographic airborne limb sounder retrievals on irregular grid with second order regularisation" *by* Lukas Krasauskas et al.

Anonymous Referee #2

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The manuscript deals with 3D tomographic inversions of limb sounding data. This is a highly challenging task. Standard approaches must be adopted or replaced in order to handle the extensive calculations required. The manuscript deals mainly with the following important issues

- How to construct the regularisation matrix (denoted as the precision matrix by the authors).
- Usage of irregular grids is explored.
- Monte Carlo estimation of the retrieval precision.

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Discussion paper

The manuscripts clearly fulfills the basic requirements. The measurements of concern are inside the scope of AMT. The issues considered are relevant and the manuscript includes a significant amount of novel material. However, the presentation and some details should be improved.

General comments

- It is not clear in all parts if the material presented is new or not. It seems that references are lacking. For example, my interpretation of Sec 2.3 is that Delaunay triangulation is claimed to be introduced for this type of measurements. If correct, this should be stated clearly, and also be mentioned in the abstract. On the other hand, in the abstract it seems that this approach is quite standard (which is clearly not the case). Further, Delaunay triangulation has at least been used in other types of radiative transfer simulations, e.g. astronomy. Some references clarifying all this should be included. Further examples are given below.
- It should be clarified to what extent the new approaches are relevant for the more standard 1D and 2D inversions. Most importantly, can 1D and 2D regularisation matrices be constructed in the same manner?
- The new way to construct the regularisation matrix is presented as an extension of Tikhonov regularisation, but I rather see it as a way to approximate the precision matrix of Equation 1? In any case, the approach bridges the gap between Bayesian and Tikhonov regularisation. This is important and should be stressed (depending a bit on if your approach works for 1D and 2D). To be clear, you argue that the simplest way to set the Tikhonov regularisation matrix is to consider statistics of the atmosphere. You use correlation structures, but that approach is essentially identical to the Bayesian approach. That is, you basically argue that the Bayesian approach is to prefer. I am trying to provoke here, on purpose,

to encourage you to extend the discussion and clarify the nice link you provide between Bayesian and Tikhonov regularisation.

- The nomenclature should be revised. Some examples are given below.

General comments on some manuscript parts

Title: Should be changed. The present title is too generic, especially considering that the manuscript doesn't involve any real observations. The manuscript deals only with technical improvements of the retrieval step. On the other hand, I don't see any reason to make a restriction to "limb sounding" and"airborne", the new methods are relevant for any 3D observations (also 1D and 2D?).

Abstract: I find the abstract vague. See comment about Delaunay triangulation above. Some hard facts would be nice. For example, what reduction in the number of grid points was achieved?

Section 2: This section is hard to digest. First of all, it contains relatively advanced mathematics. I must confess that the mathematics in some parts is above my knowledge level, and I must leave it to others to check the details. Further, the presentation is relatively lengthy and is in large parts of textbook character. This makes it hard to distinguish the purely novel contributions and core points, from background information. My suggestion is to make Section 2 more condensed and move the details to an appendix.

As a concrete example, despite Section 2.2 is detailed it is not yet clear to me, after several readings, how the result of Equation 11 shall be used to actually construct the regularisation matrix. Maybe I miss something obvious but I don't see how the result of Eq 11 shall be used to generate S_a^{-1}.

The nomenclature should also be revised. For example, the symbol used on the left-hand side of Equation 11 is not defined. Or rather, I assume it's should the same as in Equation 9. Further, it's unlucky to use y in Equation 14, as y represents the observation in Equation 1.

With respect to Eq.2 and related text: I don't know how Tikhonov formulated the approach (and it was introduced independently by others), and your reference may be correct. On the other hand, I don't think it is fair to say that Tikhonov regularisation is today restricted to consider the first derivative. For example, the description of Tikhonov regularisation in "Numerical recipes" says "... measures of smoothness that derive from first or higher derivatives." An example from the atmospheric field where the second derivative was considered:

Steck, Tilman. "Methods for determining regularization for atmospheric retrieval problems." Applied Optics 41.9 (2002): 1788-1797.

The text can be interpreted as that considering the second derivative is novel, which is not true.

Section 3: This section has similar problems as Sec 2. At least the first part dealing Cholesky decomposition contains mainly rather well-known facts (but no reference is given). Do the authors present something new in the part based on graph theory? Anyhow, most of the details can be removed as the final conclusion is that Cholesky decomposition cannot be used. Focus on the final conclusion, found on page 11, lines 7-10.

Also, the next part (page 11, lines 11-30) can be made shorter. First of all, the comments around $Mx = b$ just confused me. As I understand it, all the equations are taken from Allen et al (2000). Then no need to repeat the details, just explain that the solution of Eq 22 has the desired properties. On the other hand, it must be explained how Eq 22 shall be used practically. My understanding is that A shall be set to S_a. But we just have its inverse! Can this be clarified by just changing the notation (i.e. replace A with the symbol used elsewhere for what the matrix actually represents).

Section 4.1: Title and content do not agree. The section deals also with the forward model.

Section 4.3: The vertical correlation length is estimated from horizontal correlation. This seems backward as there should exist much better estimates of the vertical correlation. The later can simply be derived from e.g. sonde data. Take this is a comment, I don't demand a change here.

Section 4.4: A demonstration of the new features is, of course, nice to see, and maybe even a demand. However, showing results for a single retrieval case does not prove much. Statistics of an ensemble of retrievals are required to judge if one retrieval is better than another one. For a single case, specifics of the case can make the poorer method to look better. Further, it is also very unclear how "optimal" the regularisation weights used in A actually are? Anyhow, can really optimal weights be found by manually tuning? There are in fact objective methods for setting the weights.

Some of the new features can be tested in a more direct manner, compared to doing full retrievals. For example, a basic demand when selecting a grid is that discretization errors are kept at a sufficiently small level. That is, for me, the first test when introducing a new grid scheme (here Delaunay) is to simply compare forward model simulations and check that results only change in a tolerable way. This test is most critical for D.

By the way, is the same simulated measurement inverted in A to D (presumably based on A)? If a new simulated measurement is done for each case, then a possible discretization errors are swept under the carpet.

In my mind, the most interesting question in the manuscript is how well the calculations actually manage to estimate the exponential covariance assumed (Equation 7)? Is it possible to derive/estimate the S_a implied by the derived S_a^{-1}, and check how well the obtained S_a follows the start assumptions? Either for a sub-volume or a smaller test case. My interpretation of Section 2.4 is that you ensure S_a^{-1} to be positive definite and it should then be invertible (for a reasonable large case).

Conclusions: Should be extended a bit. Are all problems solved? Or something lacking to attack real observations? Are the new methods applicable in other cases (such as 1D and 2D)?

Details

Page 1, line 8, and elsewhere: It should be considered how the word "accuracy" is used. Accuracy equals systematic error or at least includes this term. See https://en.wikipedia.org/wiki/Accuracy_and_precision. There is no discussion of systematic errors in the text and I think that the word "precision" in general is more proper.

Page 1, line 20: Seems reasonable to reference some 2D retrievals.

Page 1, lines 22-23: This is not a specific 3D issue.

Page 2, line 3: The choice of regularisation constraint does affect the output of the retrieval, but I don't agree that it changes the quality. The regularisation methods are mathematical tools, and, assuming that there is no numerical issues or similar problems, they simply optimize what you have told them to do. That is, if you change regularisation constraint, you select to optimize another metrics, and the result will differ. But can it be claimed generally that one metrics is better than another one? I would say that it depends on the application.

Sec 2.3: I assume you are using some kind of external library to derive the Delaunay triangulation. Which one should be specified? Any other libraries that should be mentioned?

Page 8, line 3: A atmospheric state has been defined as x (y represents the measurement).

Page 9, line 26 and page 11, line 14: "rather difficult" is used in both places. A very vague formulation, be more specific.

Page 9, line 26: I don't agree that this is in general a difficult problem. As you point out, Rodgers (2000) explains how it should be done. Basically, all retrievals come with an error estimation, so it is, in general, a feasible task.

Page 10, line 1: Estimating the retrieval accuracy is not only "valuable", I would say that retrievals without an error estimation should not be used at all. That is, the error estimation is mandatory.

Page 10, line 10: Don't use y to denote a state vector. y denotes the measurement (Eq 1).

Page 11, line 18: "s.p.d." is not defined (I can guess what it means, but that is not good enough).

Page 13, line 15: The figures shall be introduced in order. You start with Figure 3.

Page 16, lines 3 and 13: Join these two comments about weights, to more clearly describe what has been done.

Page 17, line 14: Significant can either be interpreted as "by a large amount" or in a statistical sense. Neither seems to fit in how "significantly" is used here. It suffices to say that there is a 6% increase.

Page 18, lines 30-33: I don't follow the explanation. Why can't you compare apples with apples? If this is not possible, there is little value in the exercise.

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