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Interactive comment on “Remote sensing of atmospheric trace gas columns: an efficient approach for regularization and calculation of total column averaging kernels” by T. Borsdorff et al.

Anonymous Referee #3

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The paper by Borsdorff et al. presents a method to retrieve vertical column densities and to provide column averaging kernels for these retrievals. Unfortunately, I have major reservations with respect to the categories ‘scientific significance’ and ‘presentation’, thus I cannot recommend publication of this manuscript.

1. Scientific significance: The method claims to combine the numerical simplicity of a profile scaling retrieval with the numerical robustness of more sophisticated schemes. The Jacobian used in a profile scaling retrieval is only a vector, containing the sensitivities of the measured values with respect to the scaling factor. The method of the paper under review however, assumes availability of the full Jacobian matrix (i.e. altitude-

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resolved partial derivatives). It remains unclear, why, with the full Jacobian available, it should be disadvantageous to calculate the averaging kernel in the traditional way, e.g. either for a strongly regularized retrieval which leaves only one degree of freedom, or for an altitude-resolved profile retrieval from which finally the column is calculated. The ‘simplicity of a profile scaling retrieval’ involves that this Jacobian is NOT available. To make a strong case that this method is actually useful and advantageous is crucial for this paper. Frankly speaking, I do not quite see what the problem is with the conventional approaches.

2. Presentation (here I list also technical/scientific errors as far as they do not affect the main conclusion): At many instances the language is sloppy, misleading, or even erroneous (semantically, not syntactically). Further, the paper is organized in a way that it is virtually ununderstandable until one arrives at Eq. (30). After having seen the concept introduced by Eq. (30), I had to start again to read the paper from the beginning of Section 2. Statements made earlier in the paper are simply incorrect without the specification given by Eq. (30) and mislead the reader.

Abstract and throughout the paper: The paper tries to maintain some kind of general applicability, but without specifying e.g. the measurement geometries under consideration, it is hard to judge if the statements are true or not. More specific and thus verifiable statements are needed instead of overgeneralized commonplaces for which almost always a counterexample can be found..

General: The term ‘column averaging kernel’ is something different than the averaging kernel in the Rodgers book. The term is often used in the paper before it is defined on page 5007.

p 5001 I.22-24: This is grossly oversimplifying: The truth of this statement depends on the spectral resolution of the instrument, the measurement geometry, and the vertical grid chosen. This is a typical example where the desire to generalize leads to incorrect statements.

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p5002 I13: not quite clear what ‘normalized’ means in this context.

p5003 9-12: 1st order Tikhonov is not equivalent with profile scaling. Scaling implies a multiplicative modification of the a priori profile while 1st order Tikhonov implies an additive modification (c.f. second term in Eq.(3)). For profiles with a large dynamic range, this difference can be dramatic. This difference and its implications are not at all mentioned in the paper until Eq. (30). On the contrary, the equivalence of profile scaling and Tikhonov 1st order with large lambda is explicitly stated on page 5010 I19/20. The only thing both these methods have in common is that there is only one degree of freedom left but this common feature means by no means that this is the same! This conflict is only remedied in Eq. (30) for a particular choice of representation of the state space, but (a) here a kind of prior profile gotten rid of in Eq. (9) comes in through the back door again (via rho_ref), and (b) the whole discussion from p5004 to p5010 remains understandable with respect to the equivalence of Tikhonov 1st order and scaling until Eq. (30) is presented. The reader is misled over pages! Also, I6/7 in the abstract are very misleading because the restriction is not mentioned.

p5004-5007: This is quite a broad description of the Tikhonov smoothing approach which does not add much to the existing (often not referenced) literature of the method and its application in remote sensing.

p5004 I5 and Eq (1): e_y are not ‘error bounds’, but as used in Eq (1) these are the actual errors.

p5004 I15: Here the use of ‘error bounds’ is not consistent with Eq. (1).

p5004 Eq 3: The Se-1 and the Ln-p matrices must not appear inside the norm signs.

p5005 I3: I have not found the term ‘regularization matrix’ in the Rodgers book.

p5006 I6: "contributions of the null space": I quote the Rodgers book, p 49 second paragraph: "This component of the error budget was described incorrectly as ‘null space error’ in Rodgers (1990). The term null space error should properly be used to

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describe the contribution to the error budget from those components of the state which lie on the null space of K , and are consequently not seen by the retrieval...". Since it is, in the general case, not even clear that K has a null space, and since $(I-A)x_a$ contributes depending on how large λ is chosen, usually also to quantities not affected by the null space, I consider this terminology (here and later in the manuscript) as inappropriate.

p5006 I9 and Eq. (10): When regularization is chosen so strong that the Tikhonov retrieval actually mimics a column retrieval (i.e. a retrieval with only one degree of freedom), then the result according to Eq. (10) will be an altitude-constant profile (because the regularization forces differences between x_n and x_{n-1} towards zero. I found it bold to stretch linear theory so far that it is assumed that the Jacobians are the same for a straight line and a realistic profile, before I learned in Eq 30 how the x -vector is re-interpreted. In other words: Without having seen Eq. (30), it is not possible to see anything useful w.r.t. column retrievals in Eq. (9).

p5009: Here the meaning of the different terms are discussed but it would be helpful to finish this section with explicitly writing out the transformed retrieval equation and the transformed equation used to calculate the averaging kernel. Otherwise the reader is left with backsubstitution of all these terms. Further, it is not quite clear what is gained in comparison to the traditional method (except better insight into the anatomy of the Tikhonov method).

p5006 'integration': is the state space represented by continuous functions, or should it read 'summation'?

p5009: The term 'degrees of freedom for signal' is inferred on p29-31 of the Rodgers book explicitly for maximum a posteriori retrievals. Particularly, his Eqs 2.51-2.53 make use of the fact that x_a is actually the mean of the true state. For general regularized retrievals this is not true, so the term 'degrees of freedom for signal' should not be used. The commonly used more generic term for the latter case is to my knowledge

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'degrees of freedom of the retrieval' or 'degrees of freedom of the retrieved profile'.

p5010 I1-10: This is neither new nor relevant to this paper; it is not used in the following.

p5010 Eq. (27): This equation is involves an undefined sum because of non-matching matrix dimensions (the sum is defined only for the squares of these matrices).

p5012 I17: While the paper by von Clarmann and Grabowski might be relevant to the paper under review in a more general sense, because these authors use excessive (in their case: blockwise) Tikhonov smoothing to emulate (in their case: partial) column retrievals, as in the paper under review, this paper is quoted somehow out of context: The Tikhonov retrievals in their paper are used in the first place to find out how a reasonable altitude grid for an unregularized retrieval might look like, and everything else is linear transformation. Availability of intra-layer averaging kernels is only a side-product of their approach.

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