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Atmospheric Measurement Techniques Discussions

Interactive comment on "Harmonization and comparison of vertically resolved atmospheric state observations: Methods, effects, and uncertainty budget" *by* Arno Keppens et al.

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The response to the Referees is structured in a clear and easy-to-follow sequence: (1) comments from Referees; (2) author's response; (3) author's changes in manuscript.

The manuscript "Harmonization and comparison of vertically resolved atmospheric state observations: methods, effects, and uncertainty budget" by A. Keppens et al. presents a summary of different methods for harmonization and comparison of atmospheric profile retrievals. This paper summarizes different approaches to harmonize data using a consistent mathematical terminology, which makes it easy to contrast different methods and estimate a contribution of each manipulation to the final result.

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Discussion paper

This study fits well to the scope of the problems discussed in the AMT. This manuscript would be a good addition to the special TUNER (Towards Unified Error Reporting) issue laying a theoretical base for the atmospheric profile comparisons and error analysis. The results are presented in a consistent manner. The manuscript is very technical, but overall it is well written. I would recommend this paper for the publication in AMT after some technical corrections. My general and technical comments are listed below.

General comments: (1) Page 4, line 5: Do you mean cross-covariances here – the covariances between different error terms? Please, re-phrase this statement. (2) The current statement – "This expression assumes that the covariances of the difference error terms are not considered in the ex-ante covariance matrices" – could indeed be misleadingly interpreted. The error terms however are expected to be independent, as now stated explicitly. What is meant here is that some of the difference error estimates are sometimes provided within the ex ante uncertainty covariance matrix. If this is the case, the corresponding term should obviously be removed from Eq. (7). The authors have rephrased the first sentence below Eq. (7) to make this more clear. (3) The first sentences below Eq. (7) has been rephrased as follows: "This expression assumes that the covariance matrices of the difference error terms are independent and are not already included in the ex-ante covariance matrices. Eq. (7) should be corrected for those which are."

(1) Page 6, lines 16-19: I am not sure if I understand this part of the manuscript. To interpolate a vertical profile from a coarser vertical scale to a finer scale, one needs to assume an underlying function (linear, quadratic etc.). This interpolation might introduce an additional source of error into the comparison results that authors did not mentioned and considered here. If one degrades vertical resolution of the profile reported on a finer vertical scale, then no additional information is required. Typically, it is recommended to make comparisons on a vertical scale of the measurement with a coarser resolution. There is a discussion of effect of interpolation in section 5, but it would be good if you can mention that here as well. (2) The authors agree that "If

one degrades vertical resolution of the profile reported on a finer vertical scale, then no additional information is required." This however only generally holds when the target grid is a subset of the input grid of the regridding operation. If the target grid is not a subset of the input grid, then an underlying function is required nevertheless, just as for the coarse to fine scale regridding. The fine to coarse scale regridding however always loses information as intermediate points are removed. This is hardly the case for coarse to fine regridding. E.g., linear interpolation only inserts information-neutral grid points. The recommendation "to make comparisons on a vertical scale of the measurement with a coarser resolution" is agreed with and has therefore been included. (3) The first sentence "Straightforward regridding by (linear or other) interpolation only appropriately works when going from a coarser-resolution input grid to a finer-resolution target grid." has been extended as follows: "Straightforward regridding by (linear or other) interpolation only appropriately works, i.e. with minimum information loss, when going from a coarser-resolution input grid to a finer-resolution target grid." And at the end of the paragraph, the following sentence has been added: "The elements of W are determined by the interpolation function one applies, which introduces an additional term in the uncertainty budget (see Section 6)." Additionally, the next bullet now starts with the following sentence: "In order not to suggest a vertical resolution that is misleadingly much higher than the effective vertical resolution of (one of) the observations, atmospheric state profile comparisons are often made on the vertical grid of the product with the coarsest sampling."

(1) Page 7, equation 13: Why do you apply two operators (max/min) simultaneously? How would these two operators work? In the original paper referenced here [Langerock et al., 2015], authors use min or max, but not a combination of the two. (2) It is agreed that equation 13 is not fully clear in its present form. In fact, the nested max and min in the two terms indicated the layers' upper and lower bounds respectively, and not the mathematical max or min (as for the first occurrences). This has now been made clear in the equation and the text. (3) The second max and min in each term have been replaced by an upper height index U and L, respectively, and the first sentence

following the equation has been extended with the following: “and the indices U and L indicating the layers’ upper and lower height bounds, respectively”

(1) Page 19, Conclusions. Conclusions are not well written, and I would suggest you make some revision. I listed some suggestions below in the technical section. (2) The authors acknowledge the reviewer’s account of the conclusions and have rewritten most of the middle part, largely in agreement with the reviewer’s specific technical comments. (3) The middle part of the conclusions section has been rewritten as follows: “The harmonization of two profiles’ representations is mandatory for data comparisons and for proper quantitative $\chiˆ2$ testing of the resulting total difference covariance. Other data manipulations are needed to reduce the uncertainty budget of the comparison by minimizing the contributions due to differences in retrieval characteristics and spatiotemporal co-location. Ten matching operations have been identified and expressed in a consistent way using common matrix algebra. These operations include procedures for converting the ex-ante covariance matrix and the averaging kernel matrix (for retrieved products) associated to each atmospheric profile. It has therefore also been discussed how the information content of a retrieved product, as calculated from its AKM, is modified by each harmonization operation. Finally, it has been examined which terms of the error covariance are removed from the full comparison uncertainty budget by each harmonization operation”

Technical comments: (1) Page 1, line 11: the reference is missing. (2) A reference was not intended here. Rather, some measurements that are used in comparisons are called “reference measurements”. The adjective was put between brackets to indicate both ‘regular’ measurements and ‘reference’ measurements. The authors believe that this is clear from the current text. (3) No action has been taken.

(1) Page 2, lines1-2: there are many abbreviations here that have not been introduced earlier in the text. (2) The authors agree that the abbreviations used might not be clear to all readers. The phrasing of this sentence has been changed, with all abbreviations expanded or removed, and a reference added. (3) The phrasing has been changed

into the following: “Carried out in the context of several satellite validation studies (for Sentinel-5p, the European Space Agency’s Climate Change Initiative, the Satellite Application Facility on Atmospheric Composition Monitoring) and of the exploration of advanced data fusion methods (Cortesi et al., 2018). . .” The reference to Cortesi et al. (2018) has been added.

(1) Page 3, lines 1-10: Typically, Xa and Sa are used to define a priori profile and corresponding matrix. It might be easier for readers to follow your paper if you use the established terms. (2) Xp and Sp resulted from an in-house notation, but using Xa and Sa is equally valid, does not conflict with other notations, and might indeed better match general practice. Subscripts of prior-related vectors and matrices have therefore been changed. (3) Xp, Sp, and Rp (and variations thereof) have been replaced by Xa, Sa, and Ra.

(1) Page 4, line 18: It might be better to re-phrase: “a full assessment and quantification of all contributions to the difference error Sdelta are necessary” (2) The authors are grateful for this nice suggestion. The text has been adapted accordingly. (3) “a full assessment and quantification of all difference error contributions to S_delta is necessary” has been replaced by “a full assessment and quantification of all contributions to the difference error S_delta are necessary”

(1) Page 5, lines 6-7: I suggest to replace this phrase with “the latter may introduce a bias and increase the spread due to uncertainties in the ancillary data” (2) The original phrasing “the latter may introduce both manipulation (difference) and ancillary data uncertainties” could indeed be improved. The suggestion by the reviewer however neglects uncertainties due to data manipulations. The reviewer’s suggestion has therefore been extended in order to be in agreement with the full initial meaning of the statement. (3) The initial phrasing has been replaced by the following, more general statement: “A representation conversion may introduce a bias and reduce the precision due to uncertainties in the ancillary data and data manipulations. . .”

(1) Page 5, eq. 8 (also eq. 12): there are three equations written in one line. I suggest to have one equation in each line and have (a, b, c) labels for each equation. (2) The authors agree. (3) Eqs. (8) and (12) have been subdivided into Eqs. (8a) to (8c) and (12a) to (12c), respectively.

(1) Page 7, lines 29-30: the sentence needs some re-wording, because the meaning is not clear. (2) The substance "As any inversion approach of a retrieval outcome's vertical smoothing results in an ill-posed deconvolution. . ." might indeed be unclear to the non-expert reader. The authors have simplified this statement. (3) The original wording has been replaced by the following: "As the algebraic inversion of a retrieved profile's vertical smoothing is typically an ill-posed problem. . ."

(1) Page 19, line 1: I suggest to re-phrase with "The harmonization of a pair of atmospheric profile retrievals and their representations is required" (2) In the initial phrasing the harmonization of the profiles' representations was specifically intended. As this is different from the suggestion by the reviewer, the authors prefer keeping the text as is. (3) No changes have been made based on this comment.

(1) Page 19, lines 3-4: This sentence needs some re-wording. Maybe something like "Other data manipulations are needed to reduce the error budget of the comparison by minimizing contributions due to differences in retrieval characteristics and spatiotemporal sampling." (2) This suggestion has been included, with "sampling" replaced by the more general "co-location" in order to also include smoothing. (3) See text update at the end of the general comments section.

(1) Page 19, lines 4-5: replace with "have been identified and expressed in a consistent way using common matrix algebra." (2) This suggestion has been included. (3) See text update at the end of the general comments section. Additionally "from the literature" has been added after "identified".

(1) Page 19, lines 5-6: Suggest to replace with "These operations include procedures for converting the ex-ante covariance and averaging kernels matrices associated to

each atmospheric profile retrieval." (2) This suggestion has been included. (3) See text update at the end of the general comments section.

(1) Page 19, lines 7-10. It would be easy to read and understand if you simply say "In this study we discussed" or "Finally, we examined" (2) The authors agree with the reviewer that sometimes the active voice simplifies an expression of accomplished work. Only the passive voice however has been used throughout this manuscript, and the authors therefore prefer to stick to this voice also in the conclusions. The original phrasing however has been simplified to increase readability. (3) The initial phrasing of the first sentence has been replaced as follows: "Therefore the effect of each harmonization operation on the information content of a retrieved product, as calculated from its AKM, has also been discussed."

(1) Page 19, lines 8-10. I would rather say "what terms of the error covariance are removed" (2) This suggestion has been included (with "what" replaced by "which"). (3) See text update at the end of the general comments section.

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