Response to Report 1 (reviewer 2):

The authors have significantly modified their paper, and have taken my comments and suggestions into account. They have generalized their 'triangular' approach to estimation in the form of an interesting 'polynomial' approach (none of my suggestions). I think the paper is now acceptable for publication. I nevertheless suggest a number of modifications of mostly editing character which should not require substantial work.

General Reply: We are grateful for the thoughtful re-evaluation and valuable remarks.

1. **From a purely scientific point of view, I have only one request for correction which, without being critical for the paper, must be made.**

   The authors write, concerning positive definiteness (ll. 406-407) ... ***the generalization to covariances matrices is expected to increase the occurrence of negative values in off-diagonal elements.*** **Positive definiteness is not a question of the sign of off-diagonal elements. It is that a covariance matrix, in addition to being symmetric (and to have as such real eigenvalues) must have only positive eigenvalues (or nonnegative ones, depending on the precise definition one takes). For instance, the 2-2 matrix**

1	a
a	1

   is definite positive if $a^2 < 1$, and is not if $a^2 > 1$, independent of the sign of a.

   Reply: Thank you for pointing this out. The paragraph was actually meant to be related to the occurrence of negative elements in the covariance matrices which we incidentally mixed up with positive definiteness. We removed the mentioning of positive definiteness in the first sentence of this paragraph (underlined below) and deleted the sentence where it was mentioned again. The rest of the paragraph was left unchanged (ll. 401-407, compare also corrections to comment 5 below):
   " Estimated error covariances might even contain negative values if error dependencies are large compared to the true error covariance of a dataset. If the true error covariances differ significantly among highly correlated datasets, the neglected error dependency between two datasets might become much larger than the smaller error covariance, e.g. $\mathbf{\Delta D}_{\tilde{k};\tilde{i}} - \mathbf{\Delta D}_{\tilde{j};\tilde{k}} \approx 0$, $\frac{1}{2}\mathbf{\Delta D}_{\tilde{i};\tilde{j}} > \mathbf{C}_{\tilde{i}}\Big|_{true}$. *This phenomena was also described and demonstrated by Sjoberg et al. (2021) for scalar problems. However, the generalization to covariances matrices is expected to increase the occurrence of negative values in off-diagonal elements. Because spatial correlations and thus true covariances may become small compared to uncertainties in the assumptions or sampling noise, estimated error covariances at these locations might become negative. "*

Along with the same line of ideas, I make the following remarks

1a. **L. 727, I think the need for positive definiteness will always we there, independently of the purpose or use (using a 'covariance matrix' that is not positive definite can lead to absurd results, for instance in data assimilation)**

   Reply: Agreed. We removed the item, the sentence now reads (ll. 738-739):
   " The optimal selection is specific for each application and may depend on several requirements related to the actual purpose or use (e.g. available knowledge, accuracy of each estimate). "

1b. **And I suggest to change the words *positive definiteness might not be fulfilled* (ll. 785-786) to *there remains the risk that positive definiteness might not be fulfilled***

Reply: In alignment with the main reply to comment 1 above, we replaced the use of "positive definiteness" by "negative values". The sentence reads now (ll. 796-797):
" ... there remains a risk that negative values might occur for real applications due to inaccurate assumptions or sampling uncertainties. "

2. **L. 685,** ... ***not every possible combination of error statistics to be estimated provides a solution.* This statement, which is fundamental for the paper, is mentioned explicitly only in the conclusions. It should be mentioned in the introduction (for instance between ll. 47 and 48 or the present version, or after l. 67), with appropriate references (possibly Vogelsang and Stoffelen, 2001, or Gruber et al., 2016).**

In addition, from I understand, a better formulation would be ... ***not every possible a priori choice of error statistics to be estimated provides a solution.***

Reply: We agree that this fundamental aspect needs to be stressed clearly in the manuscript. Concerning the introduction, there is already a sentence mentioning that this point was observed by Vogelsang and Stoffelen,2021, however formulated slightly differently (ll. 58-59): *" They observed that the problem can not be solved for all possible combinations of cross-variances to be estimated. "*

We also modified the formulation based on the reviewers suggestion and added the reference to Vogelzang and Stoffelen,2021 also here (ll. 696-698):
" However not every possible choice of error statistics to be estimated provides a solution, which was also observed by Vogelzang and Stoffelen (2021) in the scalar case. "

On the number of occasions, the wording is improper, imprecise or awkward

3. **Ll. 71-72,** ... ***the exact formulations of error statistics in Sect. 3.3 remain underdetermined*** ... **to be changes to** ... ***the complete estimation of error statistics in Sect. 3.3 remains underdetermined*** ... **(it is the estimation as a whole that is underdetermined in a real situation, not the exact estimation)**

Reply: We agree, but we decided to keep the expression "exact formulation" here because it is the title of the section that is referred to. We reformulated the expression based on the reviewers remark to make clear that it refers to the complete estimation (ll. 71):
" While the exact formulation for estimating error statistics in Sect.3.3 ... "

4. **Ll. 323-324, sentence starting *It includes* ... seems awkward to me. From what I understand, I suggest *In order to achieve a complete estimation of error statistics, the Section includes the estimation, either direct or sequential, of additional error covariances, as well as of some error cross-statistics* (although it seems to me that the words *additional* and *some* are not here necessary, since it as the whole of error statistics that are in the end to be estimated. But I may be mistaken)**

Reply: The sentence was modified based on the reviewers suggestion, but skip the first part of the suggested sentence because we think that is is not essential. It reads now (ll. 323-324):
" It includes the estimation, either direct or sequential, of additional error covariances, as well as of some error cross-statistics. "

We use the words "additional" for error statistics of all datasets which are not part of the basic polygon thought the manuscript, and so also here. The word "some" refers to the fact that only a

part of the error cross-covariances can be estimated, in contrast to the ones that have to be assumed a priori.

5. **L. 326,** ***the analysis of differences from residual covariance- and cross-covariance estimates,*** ... **The formulation might be confusing. I think it would be preferable to restrict the word** ***estimate*** **to estimates of the error statistics, not to the residual statistics, which are directly computed form the data and which (contrary to the estimation of the error statistics) do not require** ***a priori*** **hypotheses. I suggest to write simply** ***the analysis of differences from residual covariances and cross-covariances.***

   A similar change may have to be made elsewhere. Please check.

   Reply: It refers to the differences of error estimates which are achieved either from residual covariances or residual cross-covariances, which was wrongly formulated. We corrected the sentence accordingly (ll. 326-327):
   " (i) the analysis of differences between error estimates from residual covariances and cross-covariances (Sect. 4.1.2) ... "

   Additionally, we checked the rest of the document and added the word "error" for estimated error statistics at some locations for clarification: l. 407, 475, 489

6. **L. 337,** ... ***the assumption of zero error cross-covariance*** ...

   Reply: Corrected.

7. **Ll. 384-385,** ... ***none of the estimates ensures positive definiteness of the estimated error covariances.***

   Reply: Corrected.

8. **Ll. 415-416, I suggest** ***As described in Sect. 2, for*** $I > 3$ ***datasets,*** $A_I > 0$ ***gives the number of error cross-statistics which can potentially be a priori assumed in addition to all error coviariances***

   Reply: As described in the replay to comment 5 above (and in accordance to the reviewers suggestion in comment 5), the word "estimated" is used for error statistics which are estimated with the proposed method, in contrast to error statistics which are need to be assumed a priori and a priori computed residual statistics. We therefore keep the current words "estimated" instead of "a priori assumed" (reviewers suggestion). Except that, we reformulated the sentence as suggested (ll. 414-415):
   " As described in Sect. 2, for $I > 3$ *datasets,* $A_I > 0$ *gives the number of error cross-statistics which can potentially be estimated in addition to all error covariances. "*

9. **L. 437,** ... ***pairwise-independent datasets*** ..., **do you mean two successive datasets in the series are independent, or more than that ?**

   Reply: Yes, but additionally the last and first elements have to be independent to "close" the series, we added the description in the sentence (ll. 435-437):
   " Similarly, a "basic polygon" can be defined from a closed series of F pairwise-independent datasets, where each two successive datasets in the series as well as the last and first element are independent from each other (compare Sect. 4.2.1). "

10. **L. 437 again,** ... ***where the referring error covariances*** ... **What to you mean here by *referring* ?**

    Reply: We reformulated consistent with the prior comment for clarification (ll. 437-438):
    " Then, the error covariance of each dataset in the series can be directly estimated from Eq. (48). "

11. **L. 464,** ... ***polygonal error covariance*** ...

    Reply: Corrected (l. 464). We also checked the rest of the document for the incidental use of the word "polynom*" and corrected it accordingly (l. 758).

12. **L. 523-524, sentence starting *The sequential estimation* ... makes no real sense to me. In any case, there is a useless repetition of the words *error covariance*, and the proper wording is *similar* ... *to* (not *similar* ... *as*)**

    Reply: We removed the incidental repetition of the words "error covariance" and reformulated for clarification (ll. 523-524):
    " The sequential estimation of an error covariance becomes favourable if the error covariance estimate of its reference dataset is as least as accurate as the assumed dependency between these two datasets $\left(\Delta\mathbf{C}_{\tilde{j}} \rightarrow \Delta\mathbf{D}_{\tilde{i};\tilde{j}}\right)$. *"*

13. **L. 546,** ... ***the true error statistics*** ... **Ambiguous. The *a priori* assumed error statistics, or the empirical statistics obtained from the 20,000-sample ? The difference may be small in the present case, but I presume you mean the latter, which would be the only ones available in a real simulation. And they would not be *error statistics* but *residual statistics.***

    Reply: We understand the reviewers concern regarding the "truth" of error statistics. This sentence indeed refers to the fact that the presented experiments are based on artificial data with predefined error statistics. In contrast to real applications where only residual error statistics can be calculated from the available data, the residual covariances were here calculated by these predefined error statistics. We understand that this was not formulated clear enough in the manuscript and added the following sentences in the introduction of the experiments for clarification (ll. 537-542):
    " The experiments use predefined error statistics which are artificially generated to fulfill certain properties concerning error covariances and dependencies. Although also being generated by a finite sample of 20,000 realizations, these predefined error statistics are used to calculate residual statistics and thus represent the true error statistics that would be unknown in real applications. Here, the artificial generation of sampled true error statistics – denoted as "true error statistics" hereafter – allows for an evaluation of uncertainties of the "estimated error statistics" that are estimated with the proposed method. "

14. **Ll. 565-566,** ... ***the independent assumption in the basic triangle(1;2;3) is an accurate approximation of the true error dependencies.* Well, have not the true error dependencies assumed to be zero by construction ?**

    Reply: Indeed, the true error dependencies are zero by construction. We reformulated the sentence to state this more clearly (ll. 568-570):
    " In the first experiment in Sect. 5.1, the true error dependencies are constructed to fulfill the independent assumption in the basic triangle$(1;2;3)$. *"*

    Please note that the true error statistics are constructed in these experiments and don't include any assumption in contrast to the "assumed" estimations of those statistics.

15. **L. 579,** ... ***true error dependencies are occurring*** ... → ... ***true error dependencies are used*** ...

    Reply: Replaced with "are generated" to stress the fact that the true statistics are artificially generated in these experiments (l. 583).

16. **L. 591,** ... ***This neglected positive error dependency*** ... **In what is that neglected error dependency positive ?**

    Reply: We removed the word "positive" to avoid confusion (l. 595).

17. **L. 594-595,** ... ***these three matrices are underestimated w.r.t. the true statistics by the half of the neglected error dependency matrix*** ... **The these matrices are underestimated by half of the neglected error dependency matrix is not visible from the figure. Say it clearly, and say how you know it. Is it consistent with error estimates that have been given in Section 4 ? If yes, say it clearly and make reference to the relevant equations. If not, explain.**
    A similar comment applies to the text ll. 615-617.

    Reply: We see that this point is not sufficiently described in the manuscript. The fact the matrices are underestimated by half the neglected error dependency can actually be seen from the equations as well as in the figure – as good as different values can be specified by the colortable. However we agree that this is not obvious for the reader and some more description is needed to guide the reader to see that conclusion. We reformulated the two paragraphs to provide more visual guidance and state more explicitly the relation to the equations in Sect.4. (ll. 596-600):
    " This agrees with the experimental results shown in Fig. 2b where the neglected error dependency$(2;4)$ *with diagonal values around 1.2 (orange colors in upper-left part of 1st row, column 5) induces an absolute uncertainty of the estimated error covariance* 4 *with diagonal values around 0.6 (purple colors in 3rd row, column 4). The sign of the uncertainty which corresponds to the underestimation can be seen from comparing the true and estimated error covariances matrices of dataset* 4 *(2nd row, column 4). "*

    And similarly (ll.624-629):
    " For the two datasets involved 2 *and* 3*, the neglected positive dependency*$(2;3)$ *is transferred with the same sign, leading to an underestimation of their error covariances (row 2, column 2-3). In contrast, the impact on the error covariance of the remaining dataset in the triangle* 1 *is reversed, leading to an overestimation of the true error covariance (2nd row, column 1). As expected from Eq. (45), the magnitude of uncertainty of the three estimated error covariances with diagonal elements around 0.4 (light purple colors in 3rd row, colomn 1-3) is half the neglected error dependency with diagonal elements around 0.2 (dark purple colors in upper-left part of 1st row, column 3). "*

18. **L. 597-598, Sentence starting** ***This experiment demonstrates*** ... **Move the word** ***accurately*** **to** ... ***to estimate accurately.***

    Reply: Corrected.

19. **L. 598,** ... ***accurate reproduction → accurate estimation***

    Reply: Corrected.

20. **L. 606** ... ***a true dependency*** ... → ... ***a non-zero dependency*** ...

    Reply: Corrected.

21. **Similarly, l. 607,** ... ***three true error dependencies*** ... → ... ***three non-zero error dependencies***

    Reply: Corrected, also in a similar case in l.630.

22. **L. 830,** ... ***the need for estimating possible asymmetric error cross-covariances*** ... **(cross-covariance matrices, if they are square in the first place, will in general be asymmetric, but there is no need for them to be so)**

    Reply: Yes. Here, we just wnated to point out that cross-covariances are (or may be) asymmetric statistics, and these asymmetric components cannot be estimated from residual covariances (as described in Sec.3.3.1). We added this information for clarification (l. 841):
    " ... the need for estimating asymmetric components of error cross-covariances ... "

The English, although perfectly understandable in most places, is occasionally incorrect

23. **In may places (starting on l. 272) the word *uneven* is used to quantify an integer that is not even. The proper word is *odd***

    Reply: Yes, thank you! We replaced it everywhere in the manuscript.

24. **L. 30,** ***This method has been widely used*** ...

    Reply: Corrected.

25. **L. 48,** ... ***the estimation [...] has been well-established for decades,*** ...

    Reply: Corrected.

26. **L. 54,** ... ***were the first to propose the additional estimation*** ...

    Reply: Corrected.

27. **L. 338,** ***thereafter → hereafter***

    Reply: Corrected.

28. **L. 498,** ***partly → partially***

    Reply: Corrected.

29. **L. 534,** ... ***the capabilities for estimating*** ...

    Reply: Corrected.

30. **L. 651,** ***If the other two error covariances 1 and 2 had also been estimated***

    Reply: Corrected.

Additional corrections to be made

31. **L. 2,** ... ***is an underdetermined problem*** ...
Reply: Corrected.

32. **L. 70, word *respectively* seems here useless**
Reply: Yes, removed.

33. **L. 96, l. 189,** ... ***as functionS of*** ...
Reply: Corrected at both locations.

34. **L. 461,** ... ***each subsequent datasetS*** $j > i$ ... **(singular)**
Reply: Corrected.

35. **L. 477,** ... ***and ~~the~~*** m_{G-1} ***the reference of*** ...
Reply: Corrected.

36. **L. 546, suppress the word *be***
Reply: Done.

37. **L. 556,** ... ***to estimated the error covariance*** ...
Reply: Corrected.

38. **L. 626,** ... ***the uncertainty in the two estimated error dependencies*** ...
Reply: Corrected.

39. **L. 526,** ... ***of the other two error dependencies*** ...
Reply: Corrected.

40. **L. 724, *datasets***
Reply: Corrected.

41. **Ll. 767-768,** ... ***a flexible setup*** ...
Reply: Corrected.

42. **L. 807, Title of Appendix *Algorithms* (plural)**
Reply: Corrected.

43. **L. 201,** ... ***or unbiased datasets*** ... **It has already been said (l. 148) that unbiasedness would be assumed in the paper. Unless the authors want to stress particularly that point (and, if so, they must do it explicitly), this kind of repetition is useless, and may even be confusing.**
Reply: Agreed. We removed the part on unibased datsets; it reads now (l. 201):
" ... without any further assumption like independent errors. "

In addition to the reviewers suggestions above, we corrected the abbreviation "Sec." by "Sect." which occurred in Sect.5-6.