## Reply to referee 1 – Report #2

Comments of referee 1 from the online report mask are in black.

Comments of referee 1 annotated in the pdf of the referee report are in brown.

The comments from the two sources were not in all cases identical. In case

- (1) they were identical, we noted that and omitted the duplicate,
- (2) only one or two sentences, or introductory words were differing, we omitted the duplicate and stated the differences,
- (3) there were more differences than in (2), we listed the complete comments from both sources.

Our explanatory notes for the first two cases are in italic.

Replies of the authors (AR) are in blue.

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## **Comments of referee 1**

Review of Technical Note: An illustrative introduction to the domain dependence of spatial Principal Component patterns by Lehr and Hohenbrink.

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The manuscript is much improved. The previous sections (prior to those added in the latest revision) are acceptable. The main revision is now to the part of the paper added in the latest revision, the application of the Varimax rotation to assess DD. Additionally, some of the comments in the new material ought to be addressed in the conclusions.

To begin, the paper is important. I suspect it will be read by those in the hydrologic sciences and beyond. My take on this is as a general issue for EOF/PC analyses is that the analyst can go one of two ways: (1) apply EOF/PCA as a data reduction technique and then stop without any physical interpretation. This seems to be the minority of applications. However, in those cases, DD is of no interest as the patterns are never examined; they serve only as a set of basis vectors. If DD patterns are the most efficient basis set, so be it. (2) However, the majority of analyses set out to interpret individual EOFs, and then DD becomes critical. In those cases, how can the analyst know the EOFs reflect patterns embedded in the covariance matrix rather than DD? You provide a set of patterns and an algorithm in this paper. Are you suggesting that algorithm be applied for everyone using EOFs for interpretation? Given all the results herein, you are in a position to make such a statement or suggest a concrete plan for those using EOF/PCA. I urge you issue a statement. More specifics follow.

AR: Thank you very much for the overall positive assessment and acknowledging the importance of our paper. Yes, our understanding is the same and we generally agree with the two ways you are pointing out. Regarding case (1) we like to add the restriction that if the subsequent use of the PC patterns requires an adequate description of multiplet subspaces, care should be taken that no multiplet is split by the selection of retained PCs (see Section 4.4). We

added corresponding statements in the conclusions at the end of the 2<sup>nd</sup> paragraph in Lines 806–809:

"If PCA is used purely for data reduction, DD is of no interest as the patterns are never examined; they serve only as an efficient set of basis vectors. If, however, the subsequent use of the PCs requires an adequate description of multiplet subspaces, for example if PCA is used as preprocessing step for other analyses, care should be taken that no multiplet is split by the selection of retained PCs."

## and in Lines 816-818:

"If the spatial PC patterns do not differ significantly from DD reference patterns, we recommend to report that and stop any interpretation of individual spatial PC patterns as distinct hydrological features."

See also our reply to points 5a and 2 of your comments to the conclusion section.

What we are suggesting is that if spatial PC patterns are used for interpretation, the patterns should be checked for DD before. We state this in Lines 803–806 of the conclusions. We recommend "visual comparison of the spatial PC patterns from subdomains with markedly different shapes and/or sizes … as quick qualitative check" (end of 3<sup>rd</sup> paragraph of the conclusion). And we recommend DD reference patterns as null hypothesis to "test whether spatial PC patterns differ significantly from DD patterns" (beginning of the 4<sup>th</sup> paragraph of the conclusion).

On the discussion of rotation and Varimax, there are some important issues that need to be addressed, mostly in Section 5.2.2. Here the level of detail should be commensurate with the rest of the manuscript. Further, the details for Varimax that match the details in the rest of the paper are partly or fully missing (see comments that follow). For example, where is there a Table equivalent to that of Table 4 for Varimax? The r and aCC are needed to evaluate the results.

AR: We highly appreciate the sincereness and precision of your comments and the amount of work you spent. It considerably helped to improve our manuscript, in particular with respect to completeness, precision and explicit statements. However, some of your suggestions point conceptually to a different direction than it is our intention for our study. As we understand it, some of the details you are missing is because of that. To be clear, our goal is not (i) to perform and include a full-scale rotation study here, and we do not want (ii) to go for physical interpretation of individual spatial PC patterns, or to analyse their validity in this regard. In our opinion, your suggestions regarding these two aspects provide material for at least one standalone paper. For us here, it is beyond our scope. And we think it would overload our manuscript. We want to emphasize that we consider these suggestions interesting, substantial and worth implementing in independent studies. We included some of your ideas in our suggestion for future work (Lines 774–780 and at the end of the conclusions).

Here, our goal is to introduce DD and its functioning to the PCA users in the hydrological community. All experiments and presented results focus on that. For this purpose, we decided to use mainly unrotated spatial PC patterns. In our paper, varimax rotation is briefly discussed as one aspect among several in the section 5 on "approaches to consider DD". Therefore, its sub-section should be commensurate to the other sub-sections of section 5. We have deliberately weighted the sub-topics in this way.

Table 4 provides the comparison of the spatial PC patterns from the precipitation data (Figure 16) and the corresponding DD reference patterns (Figure S7). The reasoning is to show how well the patterns of the precipitation data match with those of the DD reference. The DD reference patterns here and throughout the paper are calculated for unrotated correlation matrix based PCs. An equivalent comparison with varimax rotated PCs would require to calculate DD reference patterns for varimax rotated PCs, depending on the k number of PCs selected for rotation. To our knowledge, calculating DD reference patterns for varimax rotated PCs has not been done before. It could be an interesting objective in a future study focussing on rotated PCA (and physical interpretation of PC patterns). However, it is clearly beyond the scope of our study here. We think, it would overload the paper, distract from our intended focus and therefore impair the readability and practical value for PCA users in hydrology.

Here are the specifics (also annotated in the reviewed manuscript)

Line 346: added "as much as the data permit"

AR: We included this specification.

Line 349: So, in this case, the unit length eigenvectors are being rotated, I presume? Please verify/clarify.

AR: Yes, you are right. We stated this explicitly in Line 366 at the end of this section, after introducing varimax and pointing to the importance of the eigenvector scaling for the results in Lines 361–363. See also our reply to your comment to Line 743.

Line 664: A legend is needed to evaluate the magnitudes of the EOFs.

AR: Figures 16 and 17 are overview plots just as Figures 8, 9, 10, 11 and Figures S7 and S9 in the supplement. The focus is on the spatial patterns only - not their magnitudes. We discussed this already in the first review round with referee 2, see our comment there.

The magnitudes of the unrotated and the rotated spatial PC patterns from the precipitation PCAs are provided in form of the contrasts, that is the differences between the minimum and maximum of the scaled eigenvectors (correlation loadings), in Table S3 and S2 (see Lines 742–743). This is in line with the rest of the paper where we showed the contrasts in Figure 14 and Figures S4 and S5 in the supplement.

Line 682: "while" replaced with "although"

AR: We changed that.

Line 738: This new section really needs attention to bring it to the quality level of the rest of the paper. Where is the Table 4 equivalent for the Varimax PCs? The r and aCC is needed to evaluate the results.

AR: Please see our second reply to your introductory comment.

Line 743: "while" replaced with "whereas"

AR: We changed that.

Line 743: Are those patterns unit length eigenvectors or eigenvectors scaled by the square root of the corresponding eigenvalue?

Line 743: "patterns" Are the patterns unit length eigenvectors are scaled eigenvectors? It matters as Varimax was built for the latter. It might work for the former though that has not been tested widely. In either case, if one is to compare the Varimax patterns to the unrotated patterns, the vector scaling (or lack thereof) should be the same. If it is unit length eigenvectors, that might require a sentence stating that the vast majority of applications of Varimax (in all research domains of study) use scaled eigenvectors.

AR: The patterns are eigenvectors scaled by the square root of the corresponding eigenvalue (what we term "correlation loadings" here). We stated that this is the most popular scaling variant for varimax rotation in Lines 361–363. We agree that for comparison of rotated and unrotated patterns, the vector scaling should be the same. Therefore, we use the same scaling (correlation loadings) throughout the manuscript (see Lines 232–233 and 366).

Line 745: Were the unit length eigenvectors or the eigenvectors postmultiplied by the corresponding (square root of the) eigenvalue used here?

If the former (unit length eigenvectors or EOFs), are these comparable to the patterns in the earlier Figures?

If the latter (scaled eigenvectors), they won't be comparable to the EOF patterns but perhaps more amenable to the rotation algorithm by virtue of being scaled.

Some comments on the comparability are in order.

AR: We used the same scaling (eigenvectors scaled by the square root of the corresponding eigenvalue, "correlation loadings) throughout the manuscript to ensure comparability. See also our reply to your comment to Line 743.

Line 746: Was there any testing (e.g., matching the patterns to those of your covariance functions) to optimize the selection of the k=2, 3 or 4 PCs? Selecting 2 - 4 seems arbitrary. Similarly, do we know if perhaps 5, 6, ..., 10 PCs are a better choice? As you state in the paper, the eigenfunctions change as a function of k PCs retained and rotated. Further, Figures 8, 9, 10, 11 and 16 all show up to 10 patterns. Why were 2, 3 and 4 selected here? Doesn't that smaller number bias the results? I suggest rotating sets of 2, 3, ..., 10 PCs and then comparing each to the corresponding covariance matrix vector that is indexed to the largest magnitude PC loading for each PC. Then calculate the congruence coefficient for each vector for each set. By doing so, you can select the one set of k PCs that is best supported by the matrix that is diagonalized.

*The identical comment was given in the online form to* Line 746: "2 rPCs..." *and* Lines 746-747: "The first four precipitation PCs..."

AR: There was no testing to optimize the selection of the k number of PCs for rotation performed. The purpose of the varimax rotation experiment and section in our manuscript is not to identify the one set of k PCs that is best suited for physical interpretation of the rotated precipitation PC patterns or alike. It seems your suggestion is pointing in this direction. We also do not want to perform or include a full-scale rotation study here.

Within the introductory scope of our manuscript, varimax rotation is briefly discussed as one aspect among several in the section 5 on "approaches to consider DD". In this setting the results of three varimax variants are exemplarily shown. To our knowledge, in most hydrological PCA studies only the first few leading PCs are used. Therefore, we selected for our simple experiment the first 2, 3 and 4 PCs for rotation and compared the results. The exemplarily character of our selection is explicitly stated at the beginning of the 2<sup>nd</sup> paragraph of section 5.2.2 in Line 736.

The spatial patterns of the three varimax rotation variants clearly depend on the shape of the domain. We stated this and did not expand the varimax analysis any further. To clarify that we performed only a simple experiment here, and not an extensive rotation study, we (i) changed the wording in Lines 748–749 to:

"Thus, in our simple experiment here, varimax rotation was not successful in resolving DD."

and (ii) added a few sentences on the limitations of our simple experiment, including some of your ideas, at the end of the 3<sup>rd</sup> paragraph of section 5.2.2 (Lines 755–759):

"Note however, that for the introductory scope here, the experiment with the three varimax rotation variants was kept deliberately simple. Therefore, the results and their significance are limited. It is not a full-scale rotation study that would involve finding the best suitable set of rotated PCs for physical interpretation or alike. Also, we did not investigate which number of rotated PCs resulted in more or less DD, nor did we aim to find an optimum number of rotated PCs with respect to DD.".

See also our reply to your second comment to Lines 746–747 and our second reply to your introductory comment.

We like to add that we think that the proceeding you are suggesting and the concept behind is rather unknown in hydrology. We assume it is more common in atmospheric sciences for atmospheric mode detection. Thus, for us here, it would require another introduction to a rather unknown concept in our already introduction rich manuscript. It would also add another level of complexity that distracts from the focus and intention of our study. We think that experiments like those we suggest for future work at the end of the conclusions and in the last paragraph of section 5.2.2 (Lines 774–780) with synthetic data from hydrological simulation models "to test which hydrological features of the model can be uncovered by the patterns of the PCs" would be easier accessible for most hydrological readers.

Lines 746-747: This justification is unnecessary and problematic. Once a rotation is applied, it is for physical interpretation of the EOFs in terms of the matrix from which they were derived (e.g., covariance, correlation). This is a **validity issue** whereas eigenvalue degeneracy is a reliability issue. If there is little or no validity to the individual patterns, the reliability makes no difference. The set of EOFs, be they from well-separated eigenvalues, a mixture of well-separated and degenerate eigenvalues or from a full set of degenerate eigenvalues is immaterial because in all those situations, the k EOFs retained is the set that maximizes the total variance retained. It variance maximization is all that is needed from an EOF/PCA, then DD is never an issue. End of story.

However, here, and more generally for those applying EOF/PCA, they are invoking Varimax that is meant to, "*To support the interpretability of the results*" (*line 350 herein*). By invoking interpretability, the concept of what EOF/PCA is used for changes dramatically. No longer is

the data compression the sole goal. Now, the goal is to find physical signals in the individual EOFs. **Finding interpretable signal requires extra work.** The two pieces of that extra work are: (1) finding the best k PCs (something mentioned in this paper) and (2) ensuring that there are valid patterns within those k PCs (something not done yet in this work). Valid patterns arise from what the EOF/PCA does: it diagonalizes a covariance (or correlation) matrix either explicitly or implicitly into a set of k eigenpatterns and each of those k eigenpatterns are examined for physical relevance. Unless those patterns reflect the variation in the matrix that is being diagonalized, they are not valid. What the analysis does is collect a rectangular data sample, relate it via the covariance matrix and then find the most important vectors that summarize that covariance matrix. So step (2) is ensuring each of those patterns relates sufficiently well to the covariance pattern (or correlation pattern) with a congruence exceeding some threshold. In this paper you seem to adopt an aCC magnitude of 0.85 as a minimum for acceptable match. Therefore, you should rotate your various sets of k PCs over a range, such as k=2, 3, ...,10, and calculate the aCC match to the covariance vector indexed to the largest maximum magnitude loading. If there is a set where each EOF matches at that aCC level are larger (I recommend 0.9, but 0,85, 0.9 or 0.95 might be workable), it is an acceptably **valid set.** At that juncture the k PCs in the set can be examined for DD. However, if there are one or more PCs in some sets that fail to meet the aCC match threshold, that whole set is invalid. It is also possible that no set has all EOFs, in all the various k sets tested, exceeding the aCC threshold and then the Varimax solution fails for all sets of k=2, 3, ..., 10 PCs retained. In that case, another rotation might be applied to diagnose if the orthogonality constraint was the problem. If the situation persists, another analysis technique may be needed for physical interpretation. It is also possible there is a large degree of noise in the data, the covariance matrix fails to capture and physical signals that exceed the noise and the EOF/PC approach will not work for such a noisy data set. It is possible no other technique will be able to extract signal from a data set comprised mostly or noise. One need to test (1) and (2) quantitatively to know when to proceed and when to quit.

AR: We agree that, usually, rotation of PCs is applied for physical interpretation of the PCs and their patterns. However, in our study, this is not the case. We did not perform any physical interpretation of the PCA results in the paper and we never meant to. The focus is to introduce DD to the PCA users in the hydrological community. All experiments and presented results focus on that. In this setting, we performed here the comparison of the spatial patterns from unrotated and rotated PCA only, and not their interpretation (see also our replies to your first comment to Lines 746-747 and the second part of your introductory comment). To ensure that the results of the rotation were not affected by multiplet effects, we took care that no multiplets were split by the rotations. To clarify this, we changed the addressed sentence (Lines 737–738 in the revised manuscript) to:

"No multiplets were split by the rotations (Figure S7) to ensure that the results of the rotation were not affected by multiplet effects (Section 4.4)."

The extra work you are suggesting goes clearly beyond the scope of our study. We think, executing the work plan you are suggesting would be sufficient for a standalone paper, focussing on the physical interpretability of (rotated) PCA results. It could be applied for example very well in the performance assessment of our suggestion for future work in Lines 774–780 and at the end of the conclusions.

To clarify that DD is not an issue if the PCA is purely used for data reduction, we added a sentence at the end of the  $2^{nd}$  paragraph of the conclusions. Please see also our replies to the first part of your introductory comment and point 5a of your comments to the conclusion.

Line 753: The sign of the loadings in any loading vector (or EOF) is arbitrary. You can multiply any vector by -1 to make them all (or virtually all) positive with zero loss of meaning or variance explained.

*The identical comment was given in the online form to* Line 753: "only positive or..."

AR: We agree. Our sentence simply states that the loadings of most PCs were of one sign only.

Line 753: added "in"

AR: We added that.

Line 755: See comments below why the analysis of Varimax is problematic as shown. This can be fixed.

AR: We did not aim to identify the best set of k PCs for physical interpretation or alike or to perform a full-scale rotation study. Please see our replies to your two comments to Lines 746–747.

Line 755" "In all three rotation variant...". First, there is no rotation variance, only a change on the number of patterns for a single rotation, Varimax. If you had compared Varimax or several other rotation Variants (e.g., Promax, Oblimin) then the statement would have been correct. Please fix the terminology and the comments left about testing for the optimum k PCs hold.

AR: To be more precise, we changed the phrase into "In all three varimax rotation variants ...".

Lines 757-758: Two comments:

- 1. I don't think you can say this because you have not testing if 2 PCs retained is most appropriate. That testing is essential with rotated PCs.
- 2. Please square your statement with the one highlighted on line 765. Is there more, the same or less DD with rotation in your experiment?

*The identical comment was given in the online form to* Lines 757-758: "Thus, in our case here, varimax rotation was not..."

AR: 1. We changed the wording to

"Thus, in our simple experiment here, varimax rotation was not successful in resolving DD."

2. We added a few sentences at the end of the section to clarify the limitations of our study.

Please see also our reply to your first comment to Lines 746–747.

Line 758: This is vague, at best. What does this mean? Do the Varimax rotated PC loadings resemble the correlations more of less than the unrotated PC loadings? If not, state so. If so, then this suggests it is the underlying correlation patterns that are affected by the DD. If that is the case, the whole idea of explicitly or implicitly using correlations (or covariances) and a matrix to relate the data comes into question. Further, because PCA diagonalizes the correlation (or covariance) matrix, what advice can you offer the readers.

The identical comment was given in the online form to Line 758: "Instead, the patterns..."

AR: We did not investigate the underlying correlation patterns of the precipitation data in the way you are suggesting in your first comment to Lines 746–747, nor did we aim to identify the set of PCs (rotated or unrotated) that resemble best these patterns. Please see our replies to your two comments to Lines 746–747 for our reasoning, and the text we added in the revised manuscript to clarify the scope and limitations of our study (Lines 755–759).

Lines 759-760: See previous comment. The potential problem is not clear. Either this gradient reflects the correlation patterns or it does not. If it is the former, then the problem is not with Varimax but how the domain shape captures the underlying correlation pattern. If it is the latter, then it is a failure of the Varimax rotation. This needs to be addressed.

Lines 759-760: "...the new dominant patterns are..." See previous comment. The potential problem is not clear. Either this gradient reflects the correlation patterns or it does not. If it is the former, then the problem is not with Varimax but how the domain shape captures the underlying correlation pattern. If it is the latter, then it is a failure of the Varimax rotation. The relationship between the covariance/correlation patterns and selecting a domain shape should be addressed.

AR: See previous reply. We did not perform any identification of underlying correlation patterns here. Please see also our replies to your two comments to Lines 746–747 for our reasoning, and the text we added in the revised manuscript to clarify the scope and limitations of our study (Lines 755–759).

Line 760: Again, the analyst is not going to select multiple sets of Varimax PCs to move forward. They should keep a range of solutions and test those to find the optimum set for the single best set of k PCs that captures the patterns embedded in the covariance matrix. Here you show k=2, 3 and 4 with no such tests and for all we know the optimum number for k should be some other number (e.g., 5, 6, ..., 10). If that is the case, perhaps what you term DD is the distortion caused by under-retention (or over-retention) of PCs.

*The identical comment was given in the online form to* Line 760: "...4rPC variant..."

AR: We simply stated that in our simple experiment the spatial patterns of the varimax rotated PCs were clearly dependent on the domain geometries. We did not test this for other numbers k or speculate whether this would be different for other numbers k. We included a statement on the limitations of our simple varimax experiment at the end of the 3<sup>rd</sup> paragraph of section 5.2.2. Please see also our reply to your first comment to Lines 746–747.

Line 763: "while" replaced with "whereas"

AR: We changed that.

Line 764: Two comments:

1. This general web page is not a peer-reviewed publication. It is more of an opinion piece because, other than a single citation on sampling errors, there are no citations to any of the statements.

2. The statement about the possible shortcoming of Varimax EOFs from that web page is: "Still, REOF methods have issues. The patterns are may still be domain dependent and the initial number of EOFs retained is arbitrary"

Note there are no citations in this web page that support this quoted claim.

The identical comment was given in the online form to Line 764: "NCAR 2013". In bullet point one of the comment, there was in addition the following sentence at the end: ... Such flimsy non-peer reviewed web pages are best omitted.

AR: Thanks for pointing out this weakness. We removed the citation of the web page.

Line 765: Is this the finding in this paper or from the two studies cited, or both?

Line 765: "Except for being less prone to DD,..." Is this the finding in this paper or from the two studies cited, or both? Please clarify.

AR: The statement refers to the last sentence of the previous paragraph and the citation there. In the revised manuscript, we included the citation here again to clarify.

"Except from being less prone to DD (Richman, 1986; Wilks, 2006), rotated PCA results ..."

Lines 788-790: A legend is needed to evaluate the magnitudes of the EOFs.

Lines 788-790: Figure 17. A legend is needed to evaluate the magnitudes of the EOFs. Further, see other comments on adding and testing for validity 5rPCs, ..., 10rPCs.

AR: Regarding the magnitudes, see our reply to your comment to Line 664. Regarding your comments on adding and testing for validity of further PCs please see our reply to your second comment to Lines 746–747.

Line 794: Although this Table shows the changes in the variance of the Varimax PCs, we have no idea if 2, 3 or 4 is the optimal numbers. See above comments for the suggested remedy.

*The identical comment was given in the online form to* Line 794: Table 5.

AR: Please see our reply to your first comment to Lines 746–747.

## Line 795 onward:

The identical comment was given in the online form to Line 795 onward: Conclusions. ... For better readability we replied directly after each bullet point.

Somewhere in the conclusions there should be advice given to those who apply EOF/PCA for hydrological applications. Specifically:

1. How to select a domain shape? Some of the domains used herein, such as the triangle are less likely to be used compared to a rectangle, for example. However, the bigger take away is that examining the covariance functions for their shapes and then selecting a domain shape is important and a logical extension of your work. Foe pattern that is zonally oriented might be best captured by either a hemispheric domain or a large rectangular patch.

- AR: 1. We assume that in practice, the analysed domain will be mainly determined by the research task. Our take away for the practice is that for a given domain, we recommend to perform a visual comparison of the spatial PC patterns from subdomains with clearly different shapes as quick qualitative check for DD (see the end of the 3<sup>rd</sup> paragraph of the conclusions).
- 2. If their EOFs look essentially the same as your DD patterns, what do you recommend. Do they forge ahead with physical interpretation despite the similarity or terminate the analysis?
- AR: 2. We added the following statement to the conclusions in Lines 816–818: "If the spatial PC patterns do not differ significantly from DD reference patterns, we recommend to report that and stop any interpretation of individual spatial PC patterns as distinct hydrological features." Please see also our reply to the first part of your introductory comment.

However, we like to point out, that it is not sufficient to visually compare the spatial PC patterns with the patterns shown in our paper here. DD patterns are original for every combination of domain and spatial correlation properties. We stated this explicitly in the introduction Lines 112–113 and the conclusions Lines 812–813 of the manuscript.

- 3. If their EOFs look somewhat like the same as your DD patterns, but also have substantial deviations, what do you recommend. Do they forge ahead with physical interpretation despite the similarity or terminate the analysis? How can they separate the covariance part of the pattern from the DD part?
- AR: 3. We think this depends on the purpose of the analysis. For example, Dommenget (2007) "suggested using the spatial PC patterns from an analytic covariance matrix as null hypothesis to find spatial PC patterns "that are most distinguished from those of the null hypothesis". These so called Distinct Empirical Orthogonal Functions (DEOFs) are derived by rotating the eigenvectors of the observed data to maximum difference in explained variance between the EOFs of observed data and those of the analytic covariance matrix." (see the 3<sup>rd</sup> paragraph in Appendix A, Lines 849–852). However, we don't want to get more specific or explicit in our conclusions regarding this aspect, because we did not show this in our manuscript. It would require a thorough analysis focussing on signal identification and interpretation of the results, which is not our focus here (see our second reply to your introductory comment and our replies to your comments to Lines 746–747).
- 4. If their EOFs look different from your DD patterns, is it fair to say there is no DD effect?
- AR: 4. No. DD reference patterns are original for every combination of spatial domain and spatial correlation properties (see Lines 112–113 in the introduction and Lines 812–813 in the conclusions). Visual similarity or dissimilarity with patterns from different domains is not sufficient (see the 3<sup>rd</sup> paragraph of the conclusions.)
- 5. Despite the DD patterns you show throughout the paper:
- a. If the EOFs are used purely for data reduction, with no interpretation of the individual patterns, such as a preprocessing step for other analyses to lower dimensionality (e.g., to make the computing more efficient), should they care about DD at all? My thought is, no, DD makes zero difference it the EOF is used solely for data reduction with no physical interpretation of the individual patterns. However, that is not the way the majority of EOF/PC studies are analyzed.

AR: 5a. We agree, with the restriction that if the subsequent use of the PC patterns requires an adequate description of multiplet subspaces, care should be taken that no multiplet is split by the selection of retained PCs (see Section 4.4). To clarify this, we added a statement at the end of the 2<sup>nd</sup> paragraph of the conclusions in Lines 806–809:

"If PCA is used purely for data reduction, DD is of no interest as the patterns are never examined; they serve only as an efficient set of basis vectors. If, however, the subsequent use of the PCs requires an adequate description of multiplet subspaces, for example if PCA is used as preprocessing step for other analyses, care should be taken that no multiplet is split by the selection of retained PCs."

Please see also our reply to the first part of your introductory comment.

b. If the individual EOFs are to be used for physical interpretation, only then does DD become critical. In those cases, **how** can the analyst know the EOFs reflect patterns embedded in the covariance matrix rather than DD? You provide a set of patterns and an algorithm in this paper. Are you suggesting that algorithm be applied for everyone using EOFs for interpretation? Given all the results herein, you are in a position to make such a statement. I urge you to do so.

AR: 5b. Prior physical interpretation, we suggest (i) visual comparison of the spatial PC patterns from domains with clearly different shapes as quick qualitative check (see the end of the 3<sup>rd</sup> paragraph of the conclusions) and (ii) the comparison with DD reference patterns to check for significant differences (see the beginning of the 4<sup>th</sup> paragraph of the conclusions).

Line 882: "while" replaced with "yet"

AR: We changed that.

A couple of additional issues:

1. Please add color legends to Figures, where possible.

AR: For the overview figures we deliberately did not include legends. See also our reply to your comment to Line 664.

2. A few minor wording issues (e.g., use of "while" that should be reserved for time comparisons). I attempted to locate and replace those.

AR: Thank you. We changed that.