Reply to referee 2

Comments of referee 2 are in black.

Replies of the authors (AR) are in blue.

Comments of referee 2

https://hess.copernicus.org/preprints/hess-2024-172#RC2

This paper highlights a largely overlooked issue called domain dependence (DD), where the PCA results are influenced more by the size and shape of the spatial domain being analyzed than by the actual hydrological processes. This effect, caused by spatial autocorrelation in hydrological data, can lead to misleading patterns, accumulation of variance in leading PCs, and closely related (degenerate) PCs that are difficult to distinguish. The paper emphasizes the need to account for DD when interpreting PCA results and introduces two methods—stochastic and analytic—for generating DD reference patterns. These methods are demonstrated using synthetic examples, and R-scripts are provided to help users explore and address DD in their analyses. The results presented are solid. The paper covers all the aspects that are important for a user. However, there are redundancy and a lack of clarity in some of the sections. I suggest a major revision that's focused on organizing and presenting the materials. Please see my detailed comments below.

AR: Thank you for the clear and comprehensive summary of our work. Thank you furthermore for your helpful and motivating comments. We appreciate the work you have spent on the review.

Major comments:

It is good to have all the relevant terms explained in Section 2. However, as a hydrologist, I personally found the section 2 quite challenging to follow. Since the objective of this technical note is to raise attention to the DD effects among PCA users in the hydrology community, it is better to use terminologies and displayable items accessible/understandable to hydrologists especially in the method section.

I suggest adding 1) equations when necessary and 2) conceptual diagrams like hypothetical spatial and temporal PC graphs to explain PCA and S-mode PCA (they can be put in the appendix). The authors can also add workflow diagrams in both the method and discussion sections when they illustrate to practitioners how to consider DD, how to diminish DD, etc. Also, consider adding a real hydrological case at the end of the paper to illustrate the DD effects and how to deal with DD. That way, the value of the paper to hydrologists and other PCA users can be greatly improved.

AR: Thank you for your suggestions. In the revised manuscript, we will provide more equations in the main text, e.g. the equation for the calculation of the correlation loadings in section 2.1.2,

$$c_j = a_j * \sqrt{\lambda_j} \quad (1)$$

and in additional schemes. We will add the following schemes:

- a conceptual diagram for S-mode PCA (first draft in Figure 1) and
- workflow diagrams in the method section for (a) the stochastic method and (b) for the analytic method (first drafts in Figure 2 and Figure 3).

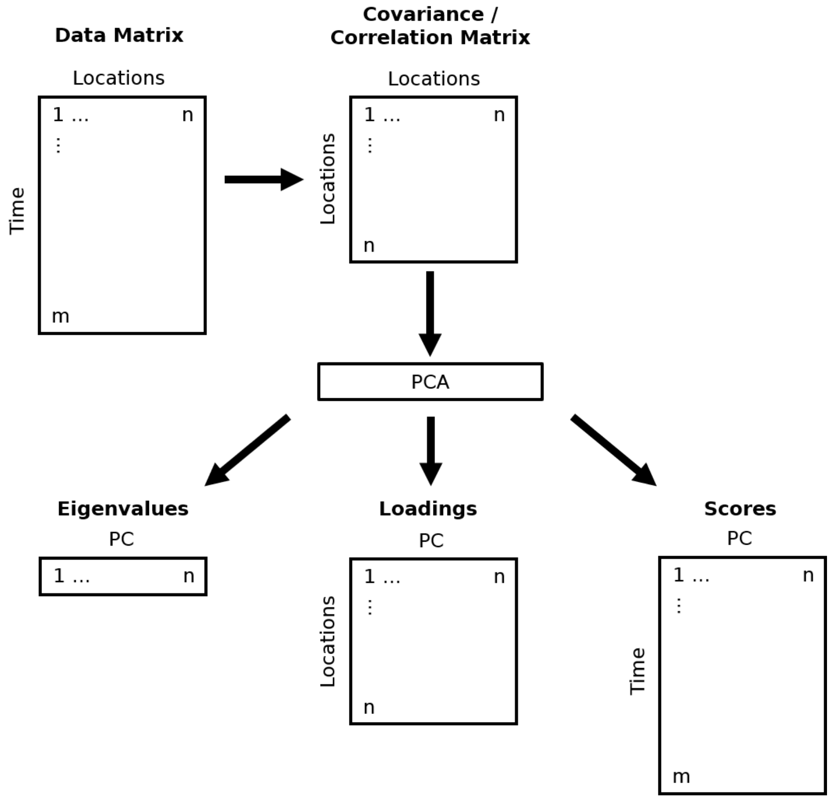

Figure 1: S-mode PCA, adapted after Fig. 9 in Richman (1986). n: number of locations, m: number of time steps. The eigenvalues define the explained variance, the loadings the unscaled spatial PC patterns and the scores the temporal PC patterns.

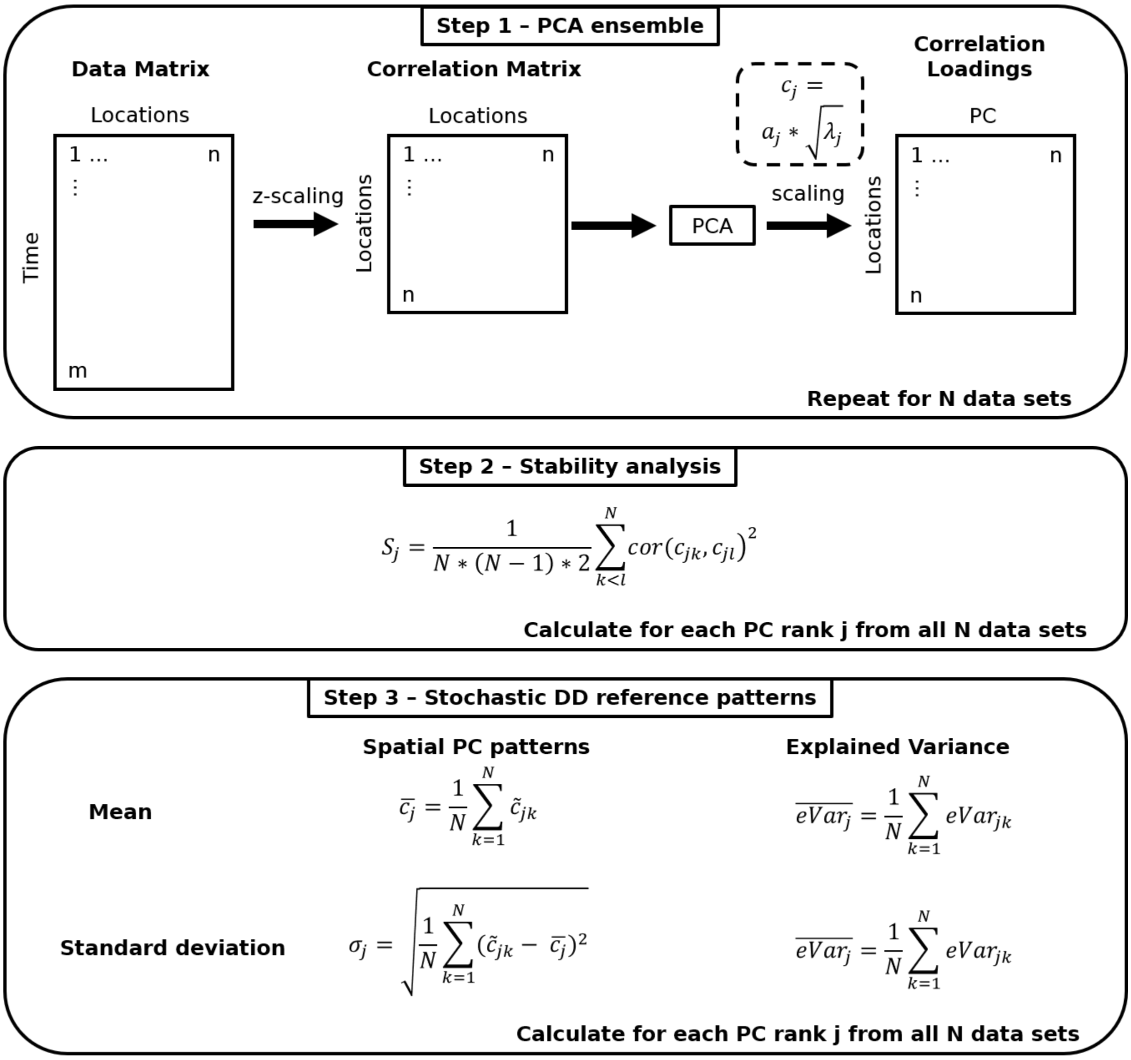

Figure 2: Stochastic DD reference method. n: number of locations, m: number of time steps, N: number of data sets, respectively PCAs, index j: PC rank, c: correlation loadings, a: loadings, λ: eigenvalue, S: stability, indices k, l: running indices for PCAs from the ensemble, $\tilde{c}$: harmonized correlation loadings, eVar: explained variance.

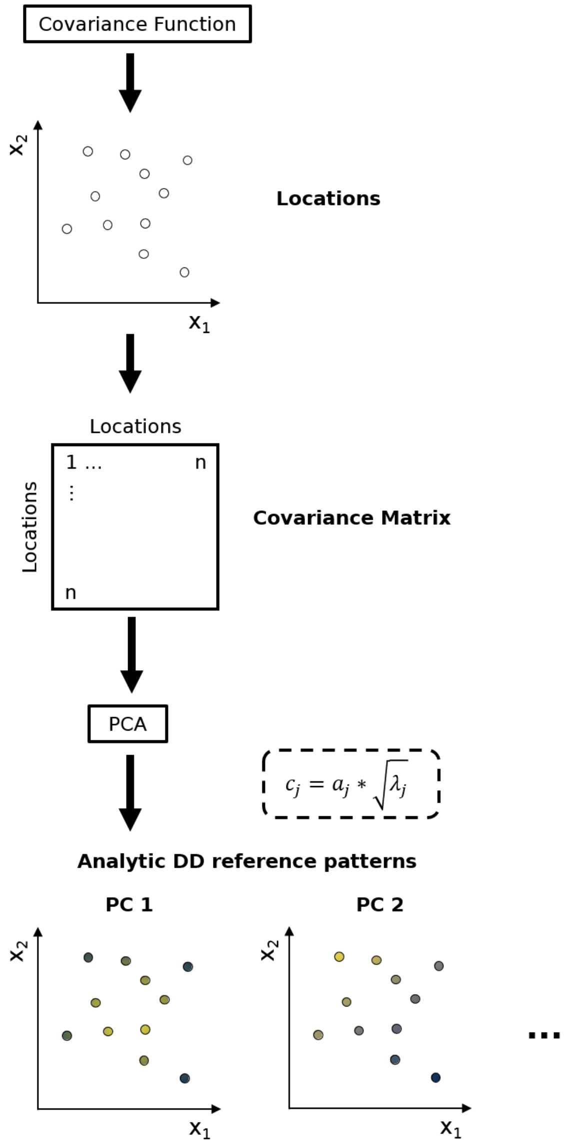

Figure 3: Analytic DD reference method.

We see your point with adding a real hydrological case at the end of the paper. However, for a number of reasons we like to refrain from it. The focus of our work is to illustrate the functioning of DD and its side effects. For this, we believe that it is best to use synthetic examples only. It (1) ensures clearly defined statistical properties, (2) clarifies that "all observed effects are solely caused by the specified statistical properties" and (3) enables "to study the effects of specific properties, e.g. spatial correlation length or spatial extent, on the PCA results." These points are already mentioned in the second last paragraph of the introduction (lines 106–110). For further clarification, we want to add a short phrase in line 106:

"To focus on the functioning of DD and its side effects, we illustrate our introduction with synthetic examples only. This ensures ..."

Furthermore, the manuscript is already quite extensive and we prefer not to extend it further. An analysis of a real hydrological data case would be material for another manuscript. As a matter of fact, the current manuscript evolved out of the work on a manuscript with spatially distributed groundwater level and precipitation series. In that manuscript handling DD is just one aspect. Given the lack of knowledge about DD in the hydrological literature, we tried first to include an introduction to DD on top of the other analysis. We realized very quickly that both together is too much and that we have material for two standalone manuscripts. We decided to provide first an introduction to DD for the hydrological community - including all the different aspects that we consider important and that we discussed in the presented manuscript here - before presenting the application to real hydrological data cases.

Minor comments:

Combine data set to be one word "dataset".

AR: We will do so.

Avoid using the word "system" which is too broad a term and could mean different things to different people. Be more specific. If you are talking about a catchment, use catchment. If you are talking about a soil column, use soil column.

AR: Here we are using the broad term "system" on purpose because we are presenting the functioning of DD irrespective of the analysed system, be it a catchment or a soil column. We will clarify what we mean by "hydrological system" by adding the following sentence to line 37 in the very beginning of the introduction:

"The approach can be applied to data from very different hydrological systems such as catchments or soil columns."

Abstract: The abstract needs reworking. Currently, the authors spend three quarters of the abstract on describing what DD is and why it's important to consider DD. Only 3-4 sentences are focused on what the paper does. The abstract needs to be re-organized such that the first quarter gives the introduction and background information about DD. The middle two quarters focus on the methodology and results. The last few sentences focus on the implications of the findings.

AR: We will re-organize the abstract trying to follow your suggestions. However, we must consider that the manuscript is not a classic research paper. A central aim of this work is to provide HESS readers an introduction to DD and effectively degenerate multiplets. We will therefore need more space than a quarter of the abstract to introduce these concepts and warn of the resulting pitfalls for hydrological interpretations.

Line 45-50: Could expand the list by adding references of PCA/EOF to hydro-climate research like:

Li et al. (2023): https://link.springer.com/article/10.1007/s00382-021-06017-y

Bieri et al. (2021): https://journals.ametsoc.org/view/journals/hydr/22/3/JHM-D-20-0116.1.xml

AR: Thank you. We will do so.

Line 105: You've defined domain dependence to be DD. Use DD here.

AR: We will do so.

Line 118: ”Considering DD is discussed”. I don’t quite understand. Do the authors mean “in practical, when and how to consider DD is discussed”? Be a bit more specific here.

AR: In this section we want to provide the reader with options how to check for DD and how to deal with it. For clarification, we like to change the quoted sentence in L118 to:

"Finally, different options to consider DD are discussed with respect to detecting DD and diminishing DD."

Move section 3 to data and code availability statement.

AR: We will do so.

Figures 5-6: Show the colorbars for the color shadings.

Figure 7 is just a repeat of the square experiments in Figures 5 and 6. I suggest showing one figure of square experiments, one figure of rectangle experiments, and one figure of triangle experiments. On all the PCs, show the colorbar, the information you showed in the title of Figure 7a.

AR: The overview plots in figures 5, 6, 8, 9 and Figure S5 in the supplement are meant for direct visual comparison (1) with the "classical Buell patterns" shown in Figure 1, and (2) among each other. Therefore, we always provide the same structure, with PC 1–10 as columns and the domain boundaries (a) square, (b) rectangular, (c) triangular in the rows. The focus is here on the spatial patterns only - not their magnitudes. Like in Buell´s original work, we therefore don´t show the scales. This way the overview character of the figure is ensured and the plots can be conveniently compared. In contrast to Buell, we use colour gradients - instead of +/- schemes - to picture the spatial patterns (see caption of Figure 5). We think that this further improves the readability of the figures, especially for the more fine structured patterns of the PCs with small eigenvalues (lower ranked PCs).

The detail plots of Figures 7, 13 and Figure S7 in the supplement are meant as examples to demonstrate what magnitudes of (1) contrasts in the spatial PC patterns and (2) explained variance associated with the PCs can result from DD alone. We think that it is important and informative to show this level of detail once in the presentation of the stochastic DD patterns (Figure 7) and in the discussion of the effective multiplets (Fig 13). In case of the overview plots we think this level of detail would be distracting for the readers. In this logic, Figure S7 in the Supplement is merely the anisotropic counterpart for Figure 7 in the main text, meant to complete the anisotropic set of figures S5–7.

To clarify the different purposes of overview and detail plots, we like to separate their introduction in section 4.1. into separate paragraphs with paragraph breaks in lines 260 and 264.

The section titles can be more informative. Like “4.1 First examples, 4.2 Domain shape, 5 Considering DD”… The authors should use short phrases instead of words for the subheaders. This is a good opportunity to provide more information to summarize the subsections.

AR: Thanks for your suggestion. We will change the section titles of section 4 and 5 to:

4. Exploring the DD effect
4.1. Exploring Buell patterns and their stability

4.2. Effects of the domain shape
4.3. Effects of the domain size and spatial correlation length
4.4. Effectively degenerate multiplets

5 Approaches to consider DD
5.1. Detecting DD
5.1.1. Comparing spatial PC patterns from markedly different subdomains
5.1.2. Comparison with DD reference patterns

5.2 Approaches to diminish DD
5.2.1. Subsampling of domains
5.2.2. Rotation of PCs

Table 1: When the PC of the subsampled variant does not correlate the best with the all-cell PC of the same rank, i.e., the values with “\”, the correlation is significantly lower. For example, 0.52 for PC4 in Square patter, 0.45 for PC5 in Square, 0.52 for PC6 in Rectangle. They are significantly lower than other values in the table. Is there an explanation for that?

AR: Best correlating PCs with different ranks do not always exhibit rather low correlation. What we can see in Table 1 are different levels of variation of the patterns from the homogeneous subsampling variant when compared with the patterns from the all cells variant (the classical Buell patterns). The patterns of the subsampling variant can be:

1) simply noisy variants of the all cells patterns (e.g. PC 1 and 2 from all domains),
2) simply noisy variants of the all cells patterns but with different ranking (e.g. PC 3 and 4 from the rectangular domains),
3) a mix of all cells patterns (e.g. PC 4 and 5 from the square domains[1]), or
4) very different from the all cells patterns (e.g. PC 10 from all domains[2]).

In this sequence of increasing differences between the patterns from both variants, the last example you were addressing (PC 6 from the rectangular pattern) would be placed somewhere in between 3) and 4). Generally, the differences increase towards the low ranked PCs with the more detailed patterns. But, there are also substantial differences between the patterns from relatively high ranked PCs possible (e.g. PC 4 and 5 from the square domains). Thus, even for rather homogeneous subsampling, the DD patterns are not necessarily simply noisy variants of the classical Buell patterns.

This underlines the main message of section 4.2: " For data sets with identical spatial correlation properties and similar domain size, the DD patterns are original for every domain shape." (L316).

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[1] In the all cells variant, PC 4 exhibits two maxima in the upper left and lower right corner and two minima in the lower left and upper right corner, PC 5 exhibits the maximum in the center and four minima in the four corners. In the subsampling variant, PC 4 exhibits two maxima in the upper left and lower right corner and the minimum in the center, PC 5 exhibits basically the same structure but rotated by 90°.

[2] For PC 10, the patterns of the all cells variant are for all domains already so fine structured that the subsampling results in quite different patterns.

We suggest to integrate the above details, including the footnotes, and extend the paragraph in line 340-347 to:

"For the spatial patterns of the homogeneous subsampling variant and the all cells variant, the correlation analysis confirmed the visual impression of overall similarity (Table 1). But it also showed that there are differences. The patterns of the subsampling variant can be:

1) simply noisy variants of the all cells patterns (e.g. PC 1 and 2 from all domains),
2) simply noisy variants of the all cells patterns but with different ranking (e.g. PC 3 and 4 from the rectangular domains),
3) a mix of all cells patterns (e.g. PC 4 and 5 from the square domains[1]), or
4) very different from the all cells patterns (e.g. PC 10 from all domains[2]).

Transitions between 3) and 4) are possible (e.g. PC 6 and 7 of the rectangular domain). Generally, the differences increase towards the low ranked PCs with the more detailed patterns. But, there are also substantial differences between the patterns from relatively high ranked PCs possible (e.g. PC 4 and 5 from the square domains). Thus, even for rather homogeneous subsampling, the DD patterns are not necessarily simply noisy variants of the classical Buell patterns. The comparison with the heterogeneous variant yielded substantially stronger deviations (Table 2). Thus, generally, visual recognition of Buell like patterns in S-mode PCA results is a concrete indication for DD. However, it is so in particular for the leading PC patterns from domains with rather homogeneous spatial arrangement of locations within boundaries similar to Buell´s archetypes. Even for domains of similar size and identical spatial correlation properties, deviations from strictly regular distribution of locations alone can result in DD patterns substantially deviating from what one might expect with the classical Buell patterns in mind."

It is unclear to me how exactly did you calculate stability. Suggest showing equation when it is first mentioned to illustrate.

AR: The stability S_j of the spatial patterns of PC rank j is calculated as the mean R^2 of the pairwise correlations of all spatial patterns with PC rank j from the PCA ensemble:

$$S_j = \frac{1}{N * (N-1) * 2} \sum_{k<l}^{N} cor(c_{jk}, c_{jl})^2$$

N is the number of PCAs which equals the number of analysed data sets, from the ensemble; k and l are the running indices of the PCAs that are compared.

We will add the above equation and a scheme to the description of step 2 (lines 195–197). A first draft of the scheme is given in Figure 2. The abbreviations from the scheme will be introduced in the main text as well.