EGUsphere, author comment AC3
https://doi.org/10.5194/egusphere-2022-434-AC3, 2022

Reply on EC1

Tobias Necker et al.

Author comment on "Guidance on how to improve vertical covariance localization based on a 1000-member ensemble" by Tobias Necker et al., EGUsphere, https://doi.org/10.5194/egusphere-2022-434-AC3, 2022

We would like to thank the editor for taking the time to review our manuscript and for providing additional comments. Below we respond to the editor's comments and explain how we plan to address them in the revised manuscript. The original queries are bold, and our responses are normal text. Planned changes in the manuscript are italic.

EC1: 'Comment on egusphere-2022-434', Olivier Talagrand, 17 Aug 2022

Following the comments of the two referees, I would like as Editor to raise a point that I think is important, and possibly critical for acceptance of the paper. It is the symmetric positive semi-definite character of the matrices that are defined in the paper for representing localized covariances and correlations.

As reminded by the authors, a covariance matrix (and in particular a correlation matrix) must be symmetric positive semi-definite (SPSD, meaning without negative eigenvalues). If that condition is not verified in an EnKF, the minimization of the variance of the estimation error that is implicit in the analysis step of the EnKF (as also in variational assimilation) may lead to negative 'minima' (actually saddle-points) and to absurd results.

I understand that all localized correlations determined in the paper are obtained through formulas of the type of Eq. (3), i. e., through Schur-multiplication of an original covariance matrix P by a localization matrix C. For a given localization matrix C, the localized matrix Ploc defined by the Schur-product will be SPSD for any covariance matrix P, if, and only if, the localization matrix is itself SPSD.

Is the condition that the obtained matrices are SPSD verified in the paper? As a precise example, do the quantities obtained through the EOL minimization Eq. (5-7) define (as it seems to be the authors' purpose) a correlation matrix, i.e. an SPSD matrix with 1's on its diagonal (the remark ((ll. 374-375) … the EOL exhibited values larger than one when estimated after applying the SEC suggests that all 'correlations' defined in the paper are not proper correlations)?

These questions are not discussed, nor even mentioned, in the paper. I think they should be. It is possible that they have been discussed in previous papers (either by the authors of the present paper or by other authors), where responses that are relevant for the present paper can be found. If so,

appropriate references and explanations must be given.

If not, I think it is necessary to check the SPSD character of either the localization matrix C or the localized matrix Ploc (or both). That can be done on the basis of theoretical considerations (it is not clear to me if the correlation matrices defined by the EOL minimization Eq. (5-7) are even symmetric). Or it can be done alternatively through numerical computations. There are in the present case 4 physical variables and 20 vertical levels, so that the relevant matrices have dimension 80 x 80, of which it must be possible to determine explicitly their full spectrum of eigenvalues. And if that is too costly, it is possible to consider submatrices, for instance by reducing the number of vertical levels.

If matrices that are meant to be SPSD, while being symmetric, turn out not to be SPSD, but with only a small number of small negative eigenvalues, one solution may be to set those eigenvalues to 0 (or to small positive values). If the negative character of the matrices is significant, there will be a real problem, which will have to be solved or at least discussed in depth. It may be that the conclusion of the paper will be that difficulties remain, to be solved in future works.

In any case, I consider as Editor that a proper discussion of those SPSD aspects is critical for acceptance of the paper.

Reply: Thank you for raising this important point. Overall, one central aim of our study was to analyse how an optimal vertical localization should look without given algorithmic constraints. The SPSD requirement is one of those constraints. We agree that it would be helpful to discuss this aspect to make the reader and future studies aware of this constraint. Following your comment, we performed some additional analysis in this regard, which we discuss below. Furthermore, we will discuss the SPSD aspect in the revised manuscript, given its importance for EnKF and variational systems.

The localization matrix C based on the SINGLE EOL is symmetric by definition given Eq. 7. The diagonal contains all 1's. As suggested, we analysed the C matrix with dimensions 80x80 (see the Appendix/Supplement, Figure 1). In this example, the resulting localization matrix was symmetric but not PSD. The eigenvalues of this C matrix range from -0.5 to 50, while more than half of the eigenvalues are positive. Setting all negative eigenvalues to zero and constructing a C' matrix that is SPSD (see Figure 2) changes the localization values by up to 15% (see Figure 3).

We will add discussion in Sec. 2.5: *"Applying the EOL by construction yields a symmetric but not necessarily a positive semi-definite localization matrix. In our case, the computed localization matrices are not symmetric positive semi-definite (SPSD), which can result in non-SPSD localized covariance matrices. As some DA algorithms require an SPSD covariance matrix (Gaspari and Cohn 1999, Bannister 2008), additional steps would be required to apply the EOL results to such algorithms."*

We will add the following discussion in the conclusion section: *"For a serial filter (e.g., the Ensemble Adjustment Kalman Filter (EAKF) by Anderson2001), an EOL-based localization can be applied directly and easily tested in future studies. Yet, each filter can exhibit algorithm-specific requirements for localization. For example, covariances or localization matrices often need to be symmetric positive semi-definite, which the EOL methodology might not fulfil. However, in all cases, EOL results can serve as guidance for finding better localization functions or methods that resemble the results of the EOL but also fulfil the criteria of a symmetric positive semi-definite matrix."*

"(the remark ((ll. 374-375) … the EOL exhibited values larger than one when estimated after applying the SEC suggests that all 'correlations' defined in the

paper are not proper correlations)?"

Reply: In our study, correlations are proper correlations. EOL values larger than one occur when the SEC was previously applied to statistically correct sampling error in correlations. Yet, correlations sometimes are damped too much due to the suboptimal behaviour of the SEC. In this case, the EOL allows the diagnosis of deficiencies in the applied localization approach. EOL values larger than one indicate that the SEC damps correlations too much, while EOL values smaller than one reveal that the SEC did not successfully correct sampling errors.

I add one remark. The authors mention on several occasions (e.g. ll. 44-45) distancedependent tapering functions with a cut-off at finite distance. A distance-dependent SPSD function that is continuous at the origin (i.e. at distance 0) cannot have a discontinuity elsewhere (that would be inconsistent with the requirement that the correlation between two close points must tend to 1 when the distance between those points tends to 0). It may be that people who have used such 'cut-off' functions have not run into difficulties because of the 'small' negativity of the corresponding covariances-correlations, but those functions cannot mathematically be SPSD.

Reply: Thanks for this interesting remark. Indeed, a cut-off could lead to discontinuities. However, our paper only applies and refers to the Gaspari-Cohn (GC) function when discussing cut-offs. The GC function is a piecewise rational function which is continuous (Gaspari and Cohn, 1999). This property explains why people do not run into difficulties caused by negativity when using the GC function that exhibits a cut-off (damps correlations to zero after a defined distance).

We changed the following sentences to be more precise and to make people aware of the importance of continuity:

"Distance-dependent localization always requires tuning of localization scales ***and cut-off distances*** *(deleted)."*

"This behaviour motivates most distance-based localization approaches with a predefined tapering function that damp ***or cut-off (deleted)*** *distant correlations."*

"However, other considerations, e.g., ***continuity****, computational efficiency or matrix rank, also may need to be considered when deciding on a cut-off."*

Please also note the supplement to this comment:
https://egusphere.copernicus.org/preprints/2022/egusphere-2022-434/egusphere-2022-434-AC3-supplement.pdf