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Atmospheric Measurement Techniques Discussions

Interactive comment on "Methods for estimating uncertainty in factor analytic solutions" *by* P. Paatero et al.

Anonymous Referee #3

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Methods for estimating uncertainty in factor analytic solutions

This article describes three different methods, i.e. bootstrap analysis (BS), displacement analysis (DISP) and a combination of the two (BS-DISP), for estimating the confidence interval for PMF solutions. In the manuscript the confidence interval is well-described as the combination of the random errors and the rotational uncertainty occurring in bilinear multivariate factor analytic models. The article is very nicely written, clearly structured and totally within the scope of the AMT journal.

An important point that is overlooked is that normally PMF users would estimate the amount of rotational uncertainty using the global fpeak tool. It would have been more complete to have discussed this approach as a fourth case in order to show the

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strengths/limitations of the fpeak tool.

Below are listed some suggestions/questions to the manuscript:

p. 7597, l.17-20

The idea that the rotational ambiguity scales with the amount of zero entries in G and F is, to my understanding, only valid within the discussion of rotations understood as linear combinations of the entire factor time series or factor profile in G and/or F. What about rotations that involve only a change in one or few entries in G and/or F? For these rotations, whether the neighboring variable in G and/or F shows a zero or not should be irrelevant.

p. 7598, l.28

Why have you chosen dQ 20? Is there a specific reason for this value? If not, then "for example" before dQ 20 could be inserted. I can't really follow why this limit should be independent. Shouldn't dQ be always scaled by Qexp to account for the size and the number of factors? Since the PMF users are more used to the discussion based on Q/Qexp, a comparison with this entity could be of interest.

p. 7599, l.22-27

This paragraph describes the uncertainty estimation based on the perturbed original data. On page 7600 line 13 this approach is repeated. I suggest merging this to one paragraph.

p. 7601, l.7

I was asking myself why only the entries of the matrix F have been displaced. Why haven't the entries of the matrix G also been displaced?

p. 7601, l.11 and l.17

It is somehow contradictory, since in line 11 DISP is supposed to capture first the data

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error (random errors) and afterwards the rotational ambiguity in line 17. I would agree with the statement in line 17.

p. 7603, l.1

Since the Frobenius norm is explicitly mentioned I would quickly define it. Not all PMF users are aware of this norm.

p. 7603, l.9-1

I can't really follow this sentence. Does the word "problem" at the end refer to the G-T approach?

p. 7606, l.14

The fact that only a subset of variables in F and or G is displaced is the biggest limitation for the full estimation of the rotational uncertainty. This is most probably due to the high computational effort involved with such immense model runs. For the reader, it would be interesting to know what is feasible using the aforementioned approaches with the actual technology. In other words, how many tests are necessary or how much time is required for a series of test runs that you carried out? Could one make some suggestions on the number of tests in relation to the size of the data matrix and/or the number of factors? This is especially important, since the data acquisition techniques are generating more and more input data for e.g. the PMF algorithm. Could such an approach still make sense for data set with e.g. 50'000 to 100'000 points in time? It would also be interesting to address this question to the approach dealing with the perturbed original data for the estimation of the random errors for the model solution that was briefly mentioned in the introduction.

p. 7609, l.20

Could a valid alternative be the internal definition, i.e. within the script file of a slightly higher dQmax, such as 5 or 10%. This could allow finding the maximal increase of e.g. fkj for the given dQmax and as such would avoid the assumptions of interpolation and

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linearization.

p. 7610, l.7

Does DISP alone really comprise both the rotational uncertainty and the random errors? I understood that this would be only in combination with BS, i.e. BS-DISP.

p. 7610, l.18

What does “well” describe? The full rotational ambiguity is not captured here, right? If this is the case, then I would state this.

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