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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 #2

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General comments

The manuscript deals with the challenging issue of the rotational uncertainty in multivariate receptor models introducing a new method that may represent a major breakthrough in the estimation of model output uncertainty.

The manuscript is quite exhaustive and the explanation of methodological aspects and results is appropirate. Nevertheless, restructuring the text and removing redundancy would result in a more synthetic and fluent document.

As the authors recognize, this study is only a starting point and more experience with synthetic and real-world datasets is necessary to understand the strengths and the limitations of the method. For instance, more replicates would be required to assess the

repeatability of the method including also replicates with the same number of zeroes. In addition, comparison with other techniques for overall output uncertainty estimation such as intercomparison exercises or benchmarking tools could be beneficial to validate the method.

The uncertainty estimation with DISP seems to be sensitive to the user's defined maximum allowed change in Q (dQmax) which is in turn linked to the modeling errors and the size of the dataset. In addition, it is unclear what portion of the total uncertainty is represented by the estimated intervals.

Moreover, the selection of active and passive species may impact the evaluation of the uncertainty. For example, the combined effect of many species each of which with small individual mass but high uncertainty could significantly contribute to the overall output uncertainty.

More effort is needed to provide reference values for the Q drop in DISP aiming at defining standardized thresholds (e.g. based on the dataset size) for rejecting solutions. For users concerned by the resource-intensity of the method, a reasonable choice would be to run only BS-DISP. It combines re-arrangement of samples and factor profiles perturbation to obtain an estimation that represents the rotational and the random components of uncertainty. In addition, it is less impacted by data uncertainties inaccuracies than DISP and provides more satisfactory intervals for downweighted variables.

Specific comments

Page 5 line 11. "Classical type of error" is a rather vague expression. Also systematic bias is part of the classical interpretation of error.

Page 6 line 7. Also wrong decisions about outliers introduce errors that may lead to loss of true environmental information (e.g. temporary sources, advection episodes).

Page 7 line 22. Please, specify that you are referring to model output uncertainty estimation.

Page 7 line 23. Also intercomparison exercises and benchmarking tools provide information about models repeatability and bias.

Page 8 line 7. According to the guide for the expression of uncertainty in measurements, also Monte Carlo Methods are suitable for propagation of distributions in uncertainty estimation (Joint Committee for Guides in Metrology 101:2008).

Page 8 line 8 and 19. The concept of noise insertion is not clear. Resampling is associated with observation rearrangement but no modification of observations is made. Perturbation/noise insertion seems a different kind of technique. Please, put some words here.

Page 15 lines 1-2. Please, explain better what is Qopt. Is it the Q of the base case PMF solution? What do you mean by “varying all factor elements”? Explaining this variable to the reader is fundamental for understanding dQ in DISP analysis.

Page 15 lines 16 and following. It seems that the length of the intervals is quite dependent on dQmax and that little is known about the portion of total uncertainty represented by the intervals. Are intervals obtained with different dQmax comparable?

Page 17 line 21. Why do you consider F (factor profile identity) rather than G (factor time trend) in DISP? Is it a way to complement BS that deals only with samples?

Page 20 line 6: Pearson is widely used in chemistry and engineering as well. It is also used in EPA-PMF 3.

Page 20 lines 9-10. This is true but cosine similarity is sensitive to scale and location changes.

Page22 lines 11-15. In the three cases the relative uncertainties for values close to zero may be too small.

Page 23 line 11. Why did you set the correlation threshold to 0.8? In EPA PMF 3 the

default value for comparing bootstrap results is 0.6.

Page 23 line 25. Is there any relationship between the choice of dQmax and the drop of Q?

Page 26 line 26. I suggest to mention “Table 3” here to help the reader following your explanation.

Page 27 line 5. Two replicates seems not enough and in any case an odd number is recommended.

Page 28 line 3. I suggest testing synthetic replicates with the same number of zeroes.

Page 29 line 21. It is also recommended to report the variations of Q as absolute and relative values (percentage) for a better interpretation and comparison between different cases.

Page 31 lines 9 -14. You should also consider the uncertainty of the source profile.

Page 31 lines 15-18. I don’t think factor uncertainty should be used for estimating source uncertainty. In addition, how can be defined what is “small enough”.

Technical corrections

Page 8 lines 1-5. there is a repetition of two sentences.

Page10 line 20. Use only first name initials.

Interactive comment on Atmos. Meas. Tech. Discuss., 6, 7593, 2013.