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Atmospheric Measurement Techniques Discussions

Interactive comment on "A method for random uncertainties validation and probing the natural variability with application to TROPOMI/Sentinel5P total ozone measurements" *by* Viktoria F. Sofieva et al.

Anonymous Referee #1

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The manuscript presents a method based on estimation of the nugget of the structure function (or variogram) for validation of "random" uncertainty estimates in remote sensing retrievals. The method is illustrated on TROPOMI total column ozone measurements and is used to show that the reported random uncertainty estimates are typically reasonable in regions with low-moderate variability but can underestimate the uncertainty in regions of high ozone variability. The methods proposed are a potentially very valuable tool for validating random uncertainty estimates but I have the following comments. After addressing these, I think the manuscript is worthy of acceptance.

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Discussion paper

Major Comments:

1. I would like to see further explanation of the methodology and its necessary assumptions, most explicitly the importance of stationarity. The paper appears to be focused on presenting a new methodology to the community that is applicable to many other areas beyond the TROPOMI analysis (which I certainly agree with), but the authors do not give a reader who is not already familiar with variogram analysis the tools to know how to apply it to another application. Overall, there is very little explanation (or references) of the structure function/variogram method, how it's estimated or it's assumptions, beyond a couple of lines in Section 2. As an example, in Section 4, the TROPOMI variogram analysis is separated into latitude bins, by month, and across orbits presumably in an attempt to satisfy stationarity assumptions, but there is no explanation to the reader of why this needs to be done in order for the variogram estimates to be meaningful.

2. Related to 1., the literature review is sparse and inclusion of additional references in spatial statistics would be extremely useful for any reader who intends to use the methodology. Examples of such references include, for general variogram analysis:

Matheron, G. (1963). "Principles of geostatistics". Economic Geology. 58 (8): 1246–1266.

Cressie, N., 1993, Statistics for spatial data, Wiley Interscience

And for methods involving estimation of the nugget effect see for example:

Kang, E. L., Cressie, N., and Shi, T. (2010), "Using temporal variability to improve spatial mapping with application to satellite data,"Canadian Journal of Statistics, 38, 271–289.

3. The TROPOMI analysis focuses only on clear-sky conditions due to the fact that "some pseudo-random errors (i.e. systematic errors varying rapidly at short spatio-temporal scales) may be present in the data due to imperfect corrections for the pres-

ence of clouds in the probed scene." For validation of the propagation of only measurement error uncertainty I can see why this is necessary, but wouldn't it also be a powerful use of the method to show/find if the presence of other errors (e.g. from non-clear sky conditions) result in an underestimate of uncertainty? I.e. if the nugget estimate is substantially higher than that reported by the algorithm?

Minor Comments:

1. Define all acronyms the first time they are used, e.g. TROPOMI, rms, etc.

2. Pg2. Line 32: It would be helpful to define explicitly what is meant by random vs systematic error here.

3. Pg. 3, line 61: "The application of this method requires many measurement points with different spatial and temporal separations, including very small separations." – the methodology as presented ignores temporal correlation, so only small spatial separations are needed.

4. Section 4: How did you decide upon these spatial and temporal bins, is stationarity reasonable here?

5. Pg. 5, line 124: Replace "horizontal and vertical directions" with longitude and latitude

6. Section 4: By computing structure function estimates from each orbit separately, you have an ensemble from which you compute a final mean estimate. Why not also look at the variability information from the ensemble when assessing if the nugget is consistent with that reported by the TROPOMI algorithm? Standard deviations or quantiles of the structure function estimated from the ensemble would provide further information about how consistent the nugget estimate is with that reported from the algorithm.

7. Figure 3, center: shrink the color scale to the value range (1.4-1.6ish)

8. Figure 3, right: I am not sure exactly what is being computed here or what informa-

tion this plot provides. Is the mean being taken over all of the points that are included in the differences taken in each bin? In that case, almost all of the data should be included in each lat/long bin except at very large lags. This would mean that the averages in each bin are taken over mostly the same data and should be consistent?

9. Figure 5: Does the TROPOMI inversion algorithm provide a footprint level uncertainty estimate? If so, is the single value used in figures an average of these estimates within lat bin/month? Please provide further explanation.

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