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Response to *On the significance of Bragg reflections* by Jørgensen *et al.*

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A response to the article *On the significance of Bragg reflections* by Jørgensen *et al.* [*Acta Cryst.* (2012). A**68**, 301–303] is given.

The work of Jørgensen *et al.* (2012) identifies and remedies an important inadvertence in our work (Henn & Meindl, 2010; hereafter denoted HM). We appreciate and support their efforts and conclusions.

We would like to add the following comments:

(1) Even when the population variance is calculated from redundant data taken from area detectors, owing to correlations in the data this variance will still be underestimated, as has been pointed out, for example, in §5.2 of Blessing (1997). Blessing also recommends the use of the population variance rather than the variances of the sample means for the standard uncertainties in order to not bias model parameters obtained by a least-squares procedure towards a few highly redundant measured reflections.

(2) From today's point of view we would prefer the use of W_2 over W, because the Poisson-limit value of W_2 is strictly defined, whereas the Poisson limit for W actually might depend on the distribution of intensities in the data set, in particular when many very weak observations are included. Of course, W_2 also has to be corrected for rescaling of the data with a correction factor $1/k$ if the data and the standard uncertainties were both scaled with k.

(3) Jørgensen *et al.* (2012) also state that the redistribution of standard uncertainty values as done by *SADABS* (Bruker, 2008) does not greatly affect the model parameters for standard structure determination. It remains unclear, however, how it will affect the topology of the density and the topology of the Laplacian, *i.e.* its impact on charge-density studies.

(4) The increase in significance of individual reflections when processing data with *SADABS* was not further discussed in our paper, because it was stated before that the significance of individual reflections can only decrease during data processing and that the data-processing procedure should be carried out in such a way as to lose as little significance as possible. The use of an error model as used in *SADABS*, however, intrinsically allows for an increase in significance. This will happen when the first term in equation (4) in Jørgensen *et al.* (2012) dominates over the second one, $\sigma^2(I_{\rm Bragg}) \gg (g\langle I_{\rm Bragg}\rangle)^2$, which is to be expected *e.g.* for single or for very weak observations, AND additionally the parameter c in equation (4) in Jørgensen *et al.* (2012) is determined to be smaller than 1. The other limit, $\sigma^2(I_{\rm Bragg}) \ll (g\langle I_{\rm Bragg}\rangle)^2$, leads to the maximum significance possible, which is $1/[(c)^{1/2}g]$. As c is typically close to one, it is possible to estimate the maximum significance as a rule of thumb to be of the order of magnitude $1/g$.

(5) We clearly made a mistake by not considering the pure effect of scaling on W and W_2. The main conclusions of our paper are, however, luckily not touched, because it was argued largely that the redistribution of standard uncertainties by *SADABS* is at least questionable. This redistribution was demonstrated by means of histograms and by a graphic similar to Fig. 1 in Jørgensen *et al.* (2012). The loss of significance was demonstrated by explicitly comparing the average significance for the data sets (Table 1, column 6 in HM) as obtained from *SADABS* and from *SORTAV* (Blessing, 1997). Jørgensen *et al.* (2012) explain the seemingly contradicting findings of increasing W values and decreasing average significance for *SADABS* data correctly with the missing scale factor in W. They also find a questionable redistribution of standard uncertainties leading to a lowered mean significance compared to values obtained from *SORTAV*.

We hope that the data-quality indicator W_2 is more frequently used in the future. Extensions to include redundancy of observations in W or W_2 are straightforward. This might turn W_2 into a valuable tool for daily use.

We thank Jørgensen *et al.* once again for their important contribution.

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