Addendum to


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In Eq. (33) of the original paper, of which the terminology is used here and to which all following equation and section numbers refer, a $\chi^2$ test is suggested to test the significance of a bias $\hat{b}$, i.e. the mean difference of $K$ co-incident profiles. This approach assumes a perfectly known covariance matrix $\hat{S}_{\text{bias}}$, i.e. a large size of the sample this covariance matrix is estimated from. However, it turns out that in real applications the sample size $K$ often is too small to justify this approach. In such cases the $T^2$ statistics (Hotelling, 1951) is the method of choice for profile validation. The quantity to be tested is

$$T^2 = \frac{b_{\text{diff}}^T \hat{S}_{\text{bias}}^{-1} b_{\text{diff}}}{\chi^2_{\text{bias}}}$$

but the probability function applicable to this test is the Hotelling’s $T^2$ distribution instead of the $\chi^2$ distribution. For univariate applications as discussed in Sect. 7, the Student’s $t$-test (Gosset, 1908) is the natural choice for assessment of the significance of a scalar bias in the case of small sample sizes.

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References
