Identification and Handling of Discrepant Measurements in Key Comparisons

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In an earlier report [1] the author showed that the method of least squares can be used to evaluate virtually any measurement comparison and even groups of linked comparisons under the following conditions:

1. A model for the reference values with one or more unknown parameters can be specified.
2. The measurement results of the participants and the associated covariance matrix are available.

Estimates of the unknown parameters in the model for the reference values and the associated covariance matrix can be found by the method of least squares. These estimates are valid only if the measurement results provided by the participants are consistent with the model of the reference values taking into account the covariance matrix of these measurements. A robust procedure for identifying and handling of discrepant measurement results is therefore necessary.

In this talk it will be demonstrated how *normalized deviations* [1][2] can be used to identify discrepant measurements. The normalized deviation d_i of a measurement result x_i, i=1,…, n, is defined by:

$$d_i = \frac{x_i - x_{ref,i}}{u(x_i - x_{ref,i})}, \qquad (1)$$

where $x_{ref,i}$ is the reference value corresponding to x_i calculated from the parameters estimated by the method of least squares. Due to the inherent covariance between x_i and $x_{ref,i}$, the expression (1) can be written as:

$$d_i = \frac{x_i - x_{ref,i}}{\sqrt{u^2(x_i) - u^2(x_{ref,i})}}. \qquad (2)$$

If $|d_i|>2$, the measurement result x_i is a potential discrepant result. If the chi-square value χ^2 of the fit indicates that the measurement results are not consistent with the model[1], it is suggested that the measurement result x_k with the largest value $|d_k|$ is removed as input to the least squares adjustment. New estimates of the model parameters and a new full set of reference values $x_{ref,i}$ (including $x_{ref,k}$) are then calculated. Modified normalised deviations d_i, $i \neq k$ are calculated from (2), whereas the normalized deviation d_k of the measurement x_k excluded from the least squares adjustment is calculated from the expression:

$$d_k = \frac{x_k - x_{ref,k}}{\sqrt{u^2(x_k) + u^2(x_{ref,k}) - 2u(x_k, x_{ref,k})}} \,. \tag{3}$$

Note that if the result x_k is independent of the results x_i, $i \neq k$, then x_k is independent of the reference value $x_{ref,k}$ and as a result, the covariance $u(x_k, x_{ref,k})$ is equal to zero. It can be shown that if a single result x_k is excluded from the least squares adjustment, the new value of the corresponding normalized deviation d_k calculated from (3) is identical to the old value d_k calculated from (2). In other words, the normalized deviation of a result is independent of whether the result is included in the least squares adjustment or not! This is the key to the robustness of the presented procedure for identifying discrepant measurement results.

If the reduced set of measurement results is still inconsistent with the model, the next discrepant measurement result is identified and excluded from the least squares adjustment as well. This procedure is repeated until a consistent set of measurement results is achieved.

In the key comparison report, the results of all participants and the associated normal deviations should be reported but the measurements excluded from the least squares adjustment should be identified. Since the purpose of a key comparison is to provide evidence for the uncertainties claimed by NMI's in the Calibration and Measurement Capabilities (CMC) tables, the consequence of providing discrepant measurements in a key comparison have to be defined. A logical consequence would be to increase the uncertainty claimed by the NMI in the CMC table, but by how much? Since we are dealing with mutual recognition of measurements, this is actually a political rather than a scientific question. A simple solution that might be acceptable to all parties involved is the following:

Increase the standard uncertainty $u(x_k)$ of an discrepant measurement result x_k until equation (3) gives a normalised deviation d_k satisfying the criteria

$$d_k^2 = 1 \tag{4}$$

This criteria reflects the fact the normalised deviation d has expectation 0 and variance 1 which implies that $E(d^2)$=1. The standard uncertainty $u(x_k)$ satisfying (4) is given by:

$$u^2(x_k) = (x_k - x_{ref,k})^2 - u^2(x_{ref,k}) + 2u(x_k, x_{ref,k}) \,. \tag{5}$$

The expanded uncertainty U to be inserted in the CMC table is then calculated as U=$k_p u(x_k)$ were k_p is the coverage factor providing the specified coverage probability p.

The described procedure of identifying and handling discrepant measurements is quite different from an procedure for removing model and data non-conformity presented elsewhere [3]. Whereas the first procedure identifies the discrepant measurement results and increases the uncertainty of these results, the latter procedure not only increases the uncertainties of all measurement results, but also changes the results themselves. Although the latter procedure is well founded theoretically, it may be difficult to accept a procedure that corrects the measurement result submitted by an NMI to a key comparison, since the NMI would need a procedure to correct all measurements performed subsequently in a similar way.

[1] Lars Nielsen, Evaluation of measurement intercomparisons by the method of least squares, *DFM report* DFM-99-R39 (2000)

[2] Lars Nielsen, Evaluation of measurements by the method of least squares, presented at *Algorithms for Approximation IV*, Huddersfield, 16-20 June 2001

[3] K. Weise and W. Wöger, Removing model and data non-conformity in measurement evaluation, *Meas. Sci. Technol.* **11** (2000) 1649-1658