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ON THE ANALYSIS OF MULTIDIMENSIONAL QUANTITIES IN MEASUREMENT COMPARISONS

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Abstract

A method of analysis is discussed to determine the comparison reference value and the degrees of equivalence in a measurement comparison with multidimensional measurands.

Introduction

Guidelines are available for the evaluation of comparison data with univariate measurands [1] but so far nothing similar exists for multivariate quantities. Similarly does the ISO guide on the evaluation of measurement uncertainty [2] primarily deal with scalar measurement quantities. A prominent example for multivariate measurands are scattering parameters (S-parameters) which describe reflection and transmission in radio frequency and microwave measurements. This work is an attempt to provide a method of analysis for multivariate comparison data in the spirit of procedure A in [1].

In the following we use a matrix formalism. Vectors are indicated by lower case bold type, e.g. $\mathbf{x}$, and matrices by upper case bold type, e.g. $\mathbf{X}$, respectively. $\mathbf{I}$ denotes the identity matrix and a prime, $'$, the transpose.

The comparison produces the following data set: The multidimensional quantity is represented by a m-dimensional column vector $\mathbf{x} = (x_1, ..., x_m)'$. The quantity $\mathbf{x}$ is measured by n laboratories: $\mathbf{x_i}$, $i = 1, ..., n$. The laboratories also provide a $(m \times m)$ covariance matrix $\mathbf{V_i}$, which contains squared standard uncertainties as diagonal elements and covariances with the correlation information as off-diagonal elements. It is assumed that there is no correlation between the participating laboratories. Outlier identification is not considered here and for this study we assume that we have a “clean” data set with n data points.

Comparison Reference Value

A natural choice for the CRV is a weighted average $\overline{\mathbf{x}} = \sum_{i=1}^{n} \mathbf{W_i x_i}$ with $\sum_{i=1}^{n} \mathbf{W_i} = \mathbf{I}$. Procedure A in [1] promotes the usage of the inverse squared standard uncertainties as weights in the univariate case. The formal extension of this principle to the multivariate case leads to

$$\overline{\mathbf{x}}_\mathbf{W} = \mathbf{V_T^{-1}} \sum_{i=1}^{n} \mathbf{V_i^{-1} x_i} \qquad \mathbf{V_T} = \sum_{i=1}^{n} \mathbf{V_i^{-1}} \tag{1}$$

with the inverse covariance matrices as weights. If the weights are assumed to be equal then equation (1) simplifies to an arithmetic multivariate mean:

$$\overline{\mathbf{x}}_\mathbf{A} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x_i} \tag{2}$$

Equation (1) should be used if the differences in covariance matrices $\mathbf{V_i}$ (most notably the diagonal elements) seem reasonable and indeed represent the different measurement capabilities of the participating laboratories. If this is not the case the uncertainties should be disregarded for the calculation of the CRV and equation (2) should be used.

Uncertainty of the Comparison Reference Value Using linear uncertainty propagation it is possible to derive a covariance matrix of the CRV. This results for general weights in

$$\mathbf{V}_{\overline{\mathbf{x}}} = \sum_{i=1}^{n} \mathbf{W_i V_i W_i'} \tag{3}$$

From the general expression (3)we derive

$$\mathbf{V}_{\overline{\mathbf{x}}_\mathbf{W}} = \mathbf{V_T^{-1}} \tag{4}$$

for the weighted mean according to equation (1) and

$$\mathbf{V}_{\overline{\mathbf{x}}_\mathbf{A}} = \frac{1}{n^2} \sum_{i=1}^{n} \mathbf{V_i} \tag{5}$$

for the arithmetic mean according to equation (2), respectively.

It should be noted that expressions (4) and (5) only depend on the uncertainties (i.e. the covariance matrices), which assumes that the dispersion of data points is purely statistical. A more realistic approach should also take systematic bias into account. This has been recently discussed by Kacker et al [3] for the univariate case. The “systematic laboratory effects model” presented in there could be applied to the multivariate case too but is not further discussed here.

As an alternative to expression (3) it might sometimes be more appropriate to use the sample covariance matrix of the mean,

$$\mathbf{V}_{\overline{\mathbf{x}}} = \frac{1}{n\,(n-1)} \sum_{i=1}^{n} (\mathbf{x_i} - \overline{\mathbf{x}})\,(\mathbf{x_i} - \overline{\mathbf{x}})' \tag{6}$$

as a measure of uncertainty of the CRV. Expression (6) has been used for the uncertainty of the CRV in a recent analysis of S-parameter comparison data [4].

Degrees of Equivalence

The degree of equivalence (DoE) is a measure of agreement between measurements and the CRV. Discrepant data points, which are excluded for the calculation of the CRV, must be included again for the calculation of DoEs. For simplicity, it is however assumed that our data set still consists of n data points.

Two types of DoEs are calculated in the univariate case, the deviation of a laboratory from the CRV and the deviation between laboratories. A straightforward extensions of this concept for the multivariate case results in vector quantities for the DoE with respect to the CRV $\mathbf{d_i} = \mathbf{x_i} - \overline{\mathbf{x}}\,;\; i = 1, ..., n$ and for the bilateral DoE $\mathbf{d_{ij}} = \mathbf{x_i} - \mathbf{x_j}\,;\; i, j = 1, ..., n,\; i \neq j$.

Uncertainty of the Degrees of Equivalence Uncertainties for $\mathbf{d_i}$ and $\mathbf{d_{ij}}$ must again be quoted as covariance matrices. For the bilateral DoE the covariance matrix is simply $\mathbf{V_{d_{ij}}} = \mathbf{V_i} + \mathbf{V_j}$.

For $\mathbf{d_i}$ one needs to distinguish different cases. If data point i contributes to the calculation of the CRV and the uncertainty of the CRV is calculated according to equation (3) one has to take the correlation between the data point and the CRV into account and the resulting covariance matrix for general weights becomes

$$\mathbf{V_{d_i}} = (\mathbf{I} - 2\mathbf{W_i})\,\mathbf{V_i} + \mathbf{V_{\overline{x}}}$$

For the special cases we obtain

$$\mathbf{V_{d_i}} = \mathbf{V_i} - \mathbf{V_{\overline{x}_W}}$$

for the weighted mean according to equations (1) and (4) and

$$\mathbf{V_{d_i}} = \left(1 - \frac{2}{n}\right)\mathbf{V_i} + \mathbf{V_{\overline{x}_A}}$$

for the arithmetic mean according to equations (2) and (5).

If data point i does not contribute to the calculation of the CRV (e.g. if the data point was flagged as a discrepant measurement) or if $\mathbf{V_{\overline{x}}}$ is calculated according to equation (6) then no correlation between the data point and the CRV exists and the covariance matrix for $\mathbf{d_i}$ simplifies to

$$\mathbf{V_{d_i}} = \mathbf{V_i} + \mathbf{V_{\overline{x}}}$$

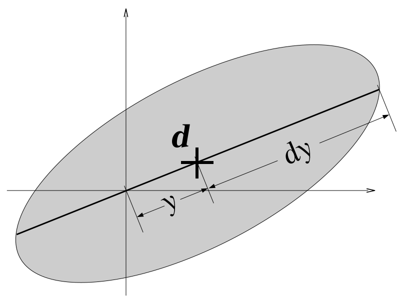
where $\mathbf{V_{\overline{x}}}$ is calculated according to equation (3).

In the univariate case, the DoE is a scalar quantity with a standard uncertainty interval centered around the DoE. It is common to expand this standard uncertainty by a factor of 2 thus creating an interval with approximately 95% confidence level under the assumption that the underlying distribution is close to normal. In the multivariate case the degree of equivalence $\mathbf{d_i}$ is a vector with dimension m and the uncertainty is described by a $m \times m$ covariance matrix. Assuming an underlying m-variate normal distribution a confidence region is described by an m-dimensional elliptical contour centered around $\mathbf{d_i}$ [5]

$$(\mathbf{x} - \mathbf{d_i})'\,\mathbf{V_{d_i}}^{-1}\,(\mathbf{x} - \mathbf{d_i}) = \chi^2_{m,\alpha}$$

where the expansion factor $\chi^2_{m,\alpha}$ is the upper $100\,(1-\alpha)$ percentage point of the χ^2-distribution with m degrees of freedom.

Graphical representation of the degrees of equivalence In the univariate case it is common to represent the DoEs graphically in an x-y graph. The DoE with expanded uncertainty interval (y) is displayed for each participating laboratory (x) and if the expanded uncertainty interval includes $y = 0$ the measurement is considered in agreement with the CRV with a confidence better than 95%. Such a graphical representation is convenient and allows a better judgement about the quality of measurements than tabulated values only. It might be possible, albeit tedious, to extend such principles to the two-dimensional case. For higher dimension, however, one needs to find a suitable reduction in dimension in order to graphically represent the results. We propose to produce a x-y graph with laboratories as the abscissa and $y \pm dy$ as the ordinate. y and dy are the absolute magnitude of $\mathbf{d_i}$ and the distance from $\mathbf{d_i}$ to the confidence boundary through the origin of the coordinate system, respectively, as shown for the 2-dimensional case in the figure below.



The general analytical expressions are $y_i = \|\mathbf{d_i}\|$ and $dy_i = \sqrt{\left(\mathbf{d_i'}\mathbf{V_{d_i}^{-1}}\mathbf{d_i}\right)^{-1}\chi^2_{m,0.05}}\;\|\mathbf{d_i}\|\,,\;\|\mathbf{d_i}\| \neq 0$

References

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