Calculation of the measurement uncertainty for the substitution measurement method

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The substitution measurement method is especially suited to correcting for a possibly present but unknown systematic measurement deviation of a measurement system. The goal of this article is to provide the formulae to calculate the systematic measurement deviation, the corrected measurement result of the quantity under consideration, as well as the measurement uncertainties associated with the measurement results from the data obtained by repeated measurements.

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1. Introduction

The substitution measurement method is quite common in metrology and industrial measurement. This method is especially suited to correcting for a possibly present but unknown systematic measurement deviation of a measurement system. This can be achieved by measuring the measurand of a measurement standard, e.g. a material measure, and subsequently the measurand of the object under consideration. The first measurement can be understood as a calibration step in order to get the necessary information about the unknown systematic measurement deviation which is possibly present, while the second measurement step is the actual measurement of the unknown quantity value. Usually each of the two measurement steps is repeated several times under well-defined repeatability conditions as defined in the VIM [1].

After the measurement results have been obtained, the estimates of the corrected measurement result of the quantity under consideration and the systematic measurement deviation, respectively, as well as their associated measurement uncertainties have to be calculated. The goal of this paper is to provide the necessary formulae, which have been derived by using the principles of probability theory and Bayesian statistics.

2. The model equations

According to the GUM [2], a measurement model must be given, in order to calculate the estimated values of the considered quantities as well as their associated measurement uncertainties. Since the substitution measurement method is a two step process, we describe the measurement model by the two model equations

$$Y_S = X_S - X_{syst} \quad \text{and} \quad Y = X - X_{syst}\,, \tag{1}$$

where X_S denotes the uncorrected value of the measurand of the measurement standard, Y_S its corresponding corrected value, X_{syst} the possibly present systematic measurement deviation, X the uncorrected value of the measurand under consideration, and Y its corresponding corrected value. The model equations are the mathematical description of the relations of the involved physical quantities [3].

3. Outline of the calculation

In Bayesian probability theory the state of knowledge concerning the physical quantities involved in the measurement is represented by a joint posterior probability density function (pdf). This pdf comprises all quantities used in the model equations, as well as the measurement data. All other interesting quantities, such as expectations or uncertainties, can subsequently be calculated from the respective marginal pdfs. Consequently, we start our calculation by assigning pdfs to the quantities under consideration.

The prior pdf comprises our state of knowledge concerning the quantities under consideration before any measurement results are available. Since Y_S denotes the measurand of the material standard, we know its value y_S and the standard uncertainty $u(y_S)$ associated with this value from the calibration certificate of the material standard. This enables us to assign a pdf to Y_S by the principle of maximum entropy [4, 5]. Since we are totally ignorant concerning Y and X_{syst}, we use Jeffreys' suggestion [6] to assign a prior pdf to these quantities.

The likelihood function describes how likely it is to obtain the measured data, if the values of the interesting quantities are all known. We assume in our calculation that the measurement values are stochastically independent and that each data set comes separately from an identical normal distribution. This assumption is implicitly made in the GUM as well.

The posterior pdf of the interesting quantities can be obtained from the prior pdf and the likelihood function by the application of Bayes' theorem. After a marginalization, we finally obtain the marginal posterior pdfs of Y and X_{syst}, respectively. From these pdfs expectations of the interesting quantities, Y and X_{syst} are subsequently calculated.

4. Results

If we denote the expectations by small letters corresponding to the respective capital letters denoting the quantities, we obtain from the marginal posterior pdfs

$$y = \bar{x} - x_{syst} \quad \text{and} \quad x_{syst} = \bar{x}_S - y_S \, , \tag{2}$$

where the bar denotes the respective mean value of the measured data. These formulae were, of course, to be expected according to the model equations (1). They enable us to calculate the value of the quantity under consideration, as well as the value of the systematic measurement deviation from the measured values, and the value of the measurement standard stated in its calibration certificate.

Using the posterior pdf, the well-known variance formula and the formula for the standard uncertainty according to the Type A evaluation method of the GUM [6], we obtain

$$u(y) = \sqrt{\frac{n-1}{n-3} s_x^2 + u^2(x_{syst})} \quad \text{and} \quad u(x_{syst}) = \sqrt{\frac{m-1}{m-3} s_{xs}^2 + u^2(y_S)} \, , \tag{3}$$

where m and n denote the respective number of measurements when measuring the material standard and the object under consideration and s_x and s_{xs} the standard deviations of the respective mean values. These formulae enable us to calculate the measurement from the measured values and the standard measurement uncertainty of the material standard stated in its calibration certificate.

The uncertainty formulae show that we need at least four measurements, in order to calculate the measurement uncertainties. Note the factors $(m-1)/(m-3)$ and $(n-1)/(n-3)$, respectively, in these formulae, which are not present, if the methods according to the GUM are used instead of the Bayesian probability theory. In comparison with the measurement uncertainties obtained by applying the methods of the GUM, these factors considerably increase the measurement uncertainties, if the number of measurements is only small. Since in metrology usually only a few measurements are taken, it is strongly recommended not to use the Type A evaluation method of the GUM in such cases but rather the formulae given here, in order to assure a more realistic estimation of the measurement uncertainty.

The reason for the discrepancy between the uncertainty evaluation given here and the one obtained according to the GUM is due to the fact, that the GUM Type A evaluation uses formulae from orthodox statistics, which are known to be valid only for large samples. For an infinite (or approximately for a very large) number of measurements, however, our uncertainty formulae agree well with those obtained according to the GUM. Since it is known that the recommendations given in the GUM lack a firm theoretical basis and can only be regarded as approximations to certain solutions obtained by a rigorous application of the probability theory [7], our results constitute no peculiarity for professional statisticians. Unfortunately, non-specialist users of the GUM are not aware of its approximative character. Thus, more research is needed in order to reveal the limitations of the GUM and to provide improvements which are easy for practitioners to use.

5. Conclusions

Formulae for the substitution measurement method have been derived by using the principles of Bayesian probability theory, which allow the calculation of the estimates of the corrected measurement result of the quantity under consideration, and the systematic measurement deviation, respectively, as well as the associated measurement uncertainties. It turns out that the formulae for the calculation of the measurement uncertainties differ from those which are obtained if the methods of the GUM are applied. The measurement uncertainties are increased considerably, if the number of measurements is only small.

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