Reduction of the bias of measurement uncertainty estimates with significant non-linearity of a model equation

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Abstract. The analysis of the non-linear model equation is carried out. The non-linear model equation in a Taylor series is expanded. It is shown that the bias in the estimation of the combined standard uncertainty by using the Law of Propagation of Uncertainty is due to the terms of the expansion of the second degree. To eliminate this bias, it is necessary to take into account the kurtosis of the input quantities distributions. A finite increments method for obtaining reliable estimates of the uncertainties contributions for non-linear model equations is proposed. A practical example of calculation of comparison loss in microwave power meter calibration by various methods was considered. Estimate of the measurement uncertainty obtained with Law of Propagation of Uncertainty in this case has a bias. The result obtained with the finite increments method coincides with the results obtained using the Monte Carlo method.

1. Introduction
In general, the model of the measurand $Y$ as a function of several input quantities $X_1, X_2, \ldots, X_N$, can be represented in the following form [1]:

$$Y = f(X_1, X_2, \ldots, X_N).$$

(1)

In the GUM [1] the value of the measurand $y$ and its standard uncertainty $u(y)$ are calculated by the formulas:

$$y_{GUM} = f(x_1, x_2, \ldots, x_N),$$

(2)

$$u(y) = \sqrt{\sum_{j=1}^{N} c_j^2 u_j^2 + 2 \sum_{j \neq i}^{N} c_i c_j \text{cov}(x_i, x_j)},$$

(3)

where $x_1, x_2, \ldots, x_N$ are estimates of the input quantities $X_1, X_2, \ldots, X_N$; $u_j$ is standard uncertainty of the $j$-th input quantity; $\text{cov}(x_i, x_j) = r(x_i, x_j) u_i u_j$ is covariance of the $i$-th and $j$-th input quantities; $r(x_i, x_j)$ is correlation coefficient; $c_j = \partial y / \partial x_j$ – sensitivity coefficient for the $j$-th input quantity.

In the nonlinear equation (1), the estimates (2) and (3) of $y$ and $u(y)$ have a bias, the value of which depends on the type of the model equation and the values of the relative uncertainties of the input quantities.
quantities [2]. The bias compensation of $y$ in [1] is not carried out, and the bias compensation of $u(y)$ is realized in [1] by taking into account the terms of the second order of the expansion (1) in the Taylor series. In this case, it is necessary to have the values of the partial second-order derivatives function (1) with respect to the input quantities $X_1, X_2, ..., X_N$. It should be noted that the expression for an unbiased estimate of the standard uncertainty of the measurand is given in [1] only for the Gaussian probability density functions (PDF) of input quantities.

The purpose of this report is to obtain expressions that provide unbiased estimate of the standard uncertainty of the measurand for nonlinear model equations and for specified PDF of input quantities.

2. Expansion in a Taylor series of the model equation

Expression (1) can be represented as a Taylor series expansion:

$$ Y = f(x_1, x_2, ..., x_N) + \sum_{j=1}^{N} c_j (X_j - x_j) + \frac{1}{2} \sum_{j=1}^{N} c_{jj} (X_j - x_j)(X_i - x_i) + R_0, $$

in which $c_j = \partial^2 f/\partial x_j \partial x_i$ – the mixed partial derivative (1) with respect to $X_j$ and $X_i$; $R_0$ – the remainder term of the series.

The mathematical expectation of the expression (4) for $R_0 = 0$ will have the following form:

$$ E(Y) = E[f(x_1, x_2, ..., x_N)] + \sum_{j=1}^{N} c_j E(X_j - x_j) + \frac{1}{2} \sum_{j=1}^{N} c_{jj} E[(X_j - x_j)(X_i - x_i)]. $$

(5)

Taking into account that $E(X_j - x_j) = 0$, and for uncorrelated input values

$$ E[(X_j - x_j)(X_i - x_i)] = \begin{cases} u_j^2, & \text{when } j = i; \\ 0, & \text{when } j \neq i, \end{cases} $$

we get the following expression:

$$ E(Y) = Y = f(x_1, x_2, ..., x_N) + \frac{1}{2} \sum_{j=1}^{N} c_{jj} u_j^2, $$

(6)

where $c_{jj} = \partial^2 f/\partial x_j^2$ – is the partial derivative of the second order of the measurand with respect to the $j$-th input quantity.

Thus, to reduce the bias of measurand estimate when the nonlinear model equation is used, it is necessary to take into account the standard uncertainties of input quantities.

Let’s write down the expression for the difference between the measurand and its mathematical expectation (6):

$$ Y - E(Y) = Y - f(x_1, x_2, ..., x_N) - \frac{1}{2} \sum_{j=1}^{N} c_{jj} u_j^2 = $$

$$ = \sum_{j=1}^{N} c_j (X_j - x_j) + \frac{1}{2} \sum_{j=1}^{N} c_{jj} [(X_j - x_j)^2 - u_j^2] + \sum_{j=1}^{N} \sum_{i=j+1}^{N} c_{ij} (X_j - x_j)(X_i - x_i). $$

(7)

The mathematical expectation of the square of the resulting expression will be an unbiased estimate of its variance $u_{ub}^2(y)$:

$$ E[Y - E(Y)]^2 = u_{ub}^2(y) = \sum_{j=1}^{N} c_j^2 u_j^2 + \frac{1}{4} \sum_{j=4}^{N} c_j^2 (\mu_j - 1) u_j^2 + \sum_{j=2}^{N} \sum_{i=1}^{j-1} c_{ij}^2 u_j^2 u_i^2, $$

(8)
where \( \mu_j = E[(X_j - x_j)\hat{u}_j^4] \) – is the normalized fourth-order central moment of the \( j \)-th input quantity.

The values of \( \mu \) for different probability density function (PDF) are given in Table 1.

**Table 1.** The values of \( \mu \) for different PDF of the input quantities.

| PDF                        | \( \mu \) |
|----------------------------|----------|
| Arcsine                    | 1.5      |
| Uniform                    | 1.8      |
| Triangular                 | 2.4      |
| Gaussian                   | 3        |
| Student’s with number of degrees of freedom \( \nu \) | \( 6/(\nu - 4) + 3 \) |

Thus, the value of the variance of the measurand will depend on the PDF of the input quantities. So, for example, for Gaussian PDF of all input quantities \( \mu = 3 \), therefore expression (8) takes the form known from the literature [3]:

\[
u^2(u) = \sum_{j=1}^{N} c_j^2 u_j^2 + \frac{1}{2} \sum_{j=1}^{N} c_{jj} u_j^4 + \frac{1}{6} \sum_{j=1}^{N} \sum_{i=1}^{N} c_{jj} u_j^4 u_i^2 . \]

(9)

For a function of single variable, the value of the standard uncertainty of the measurand takes the following form:

\[
u_{st}(y) = \sqrt{c_1^2 u_1^2 + c_2^2 u_2^2 (\mu_1 - 1)/4} . \]

(10)

For a function of two variables, the value of the standard uncertainty of the measurand takes the following form:

\[
u_{st}(y) = \sqrt{c_1^2 u_1^2 + c_2^2 u_2^2 + \frac{1}{4} c_{11} (\mu_1 - 1)u_1^4 + \frac{1}{4} c_{22} (\mu_2 - 1)u_2^4 + c_{12} u_1^2 u_2^2} . \]

(11)

It is seen from expressions (8) to (11) that in order to obtain an unbiased estimate of the standard uncertainty of the measurand, it is necessary to know the second partial derivatives of the measurand with respect to the corresponding input quantities, i.e. the model of the measurand should not only be fully known, but also twice differentiable.

**3. The finite increments method**

To calculate the unbiased estimate of the numerical value and the uncertainty of the measured quantity, the finite increment method [4] can be applied.

The difference partial derivative of the first order of the measurand with respect to the \( j \)-th input will be equal:

\[
\hat{c}_j = \frac{\hat{f}[x_1, ..., (x_j + u_j, x_j), ..., x_N] - \hat{f}[x_1, ..., (x_j - u_j, x_j), ..., x_N]}{2u_j} .
\]

(12)

The difference partial derivative of the second order of the measurand with respect to the \( j \)-th input quantity will be equal:

\[
\hat{c}_{jj} = \frac{1}{u_j^2} \{ f[x_1, ..., (x_j + u_j, x_j), ..., x_N] - 2f(x_1, x_j, ..., x_N) + f[x_1, ..., (x_j - u_j, x_j), ..., x_N] \} .
\]

(13)

The difference partial derivative of the second order of the measurand with respect to the \( j \)-th and \( i \)-th input quantities will be equal:
\[ c_i^* = \frac{1}{4u_iu_j} \left[ f(x_i\ldots(x_j+u_j),\ldots,x_j\ldots,x_j) - f(x_i\ldots(x_j+u_j),\ldots,x_j\ldots,x_j) - f(x_i\ldots(x_j-u_j),\ldots,x_j\ldots,x_j) + f(x_i\ldots(x_j-u_j),\ldots,x_j\ldots,x_j) \right] \]

\[ -f(x_i\ldots(x_j-u_j),\ldots,x_j\ldots,x_j) \]

(14)

For the function of \( N \) variables, the calculation of the partial difference derivatives (13) to (15) is easily realized by using a simple program executed in the MS Excel.

4. An example of calculation of comparison loss in the calibration of a microwave power meter

In subsection 9.4 of Appendix 1 to GUM [5], in the example of “Comparison loss in the calibration of a microwave power meter”, the function \( Y = X_1^2 + X_2^2 \) for \( x_1 = 0 \), \( x_2 = 0 \) and standard uncertainties \( u_1 = 0.005 \), \( u_2 = 0.005 \) is considered. In this case, using GUM [1], we have:

\[ u_{GUM}(y) = \sqrt{(2x_1u_1)^2 + (2x_2u_2)^2} = 0. \]

For the model equation under consideration, we get:

\[ c_1 = 2x_1 = 0; \quad c_2 = 2x_2 = 0; \quad c_{11} = 2; \quad c_{22} = 2; \quad c_{12} = c_{21} = 0. \]

Similar results can be obtained using the formulas (12) to (14):

\[ c_1^* = \frac{1}{2u_1} \left[ (x_1+u_1)^2 + x_1^2 - (x_1-u_1)^2 - x_1^2 \right] = 0; \quad c_2^* = \frac{1}{2u_2} \left[ (x_2+u_2)^2 + x_2^2 - (x_2-u_2)^2 - x_2^2 \right] = 0; \]

\[ c_{11}^* = \frac{1}{u_1^2} \left[ (x_1+u_1)^2 + x_1^2 - 2(x_1^2 + x_1^2) + (x_1-u_1)^2 + x_1^2 \right] = 2; \quad c_{22}^* = \frac{1}{u_2^2} \left[ (x_2+u_2)^2 + x_2^2 - 2(x_2^2 + x_2^2) + (x_2-u_2)^2 + x_2^2 \right] = 2; \]

\[ c_{12}^* = \frac{1}{4u_1u_2} \left[ ([x_1+u_1]^2 + x_1^2) - ([x_1-u_1]^2 + x_1^2) - ([x_1+u_1]^2 + x_1^2) + ([x_1-u_1]^2 + x_1^2) \right] = 0. \]

Therefore, for uniform distributed input quantities, from equation (11), we have:

\[ u_{m}(y) = \sqrt{c_1^2u_1^2 + c_2^2u_2^2 + 0.8 \frac{c_{11}^2u_1^4 + c_{22}^2u_2^4}{4} + c_{12}^2u_1^2u_2^2} = \sqrt{0.2(4u_1^4 + 4u_2^4)} = \sqrt{1.6 \cdot 0.005^4} = 0.005 \cdot \sqrt{1.6} = 3.162 \cdot 10^{-5}. \]

A value of \( u_{MCM}(y) = 3.159 \cdot 10^{-5} \) was obtained by Monte Carlo method (MCM) with the NIST Uncertainty Machine [6], which coincides with the value \( u_{m}(y) \).

5. Conclusions

To reduce the bias of measurand estimate when the nonlinear model equation is used, it is necessary to take into account the standard uncertainties of input quantities. This approach, in contrast to GUM, is suitable in the presence of uncertainties in the input quantities, estimated by both statistical and nonstatistical methods.

It is shown that the unbiased estimate of standard uncertainty of the measurand is depending from normalized fourth-order central moments of the input quantities.

To simplify the calculation of the unbiased estimate of the numerical value and the uncertainty of the measurand, the finite increment method can be applied.

References

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