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XXXII МЕЖДУНАРОДНЫЙ НАУЧНЫЙ СИМПОЗИУМ

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Advanced methods for measurement uncertainty evaluation

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***Abstract*—Disadvantages of the law of propagation of uncertainty underlying the implementation of the model approach in the GUM are analyzed. Advanced methods for implementing a model approach to measurement uncertainty evaluation are described, which allow eliminating the shortcomings of the GUM uncertainty framework: the law of propagation of distributions, the kurtosis method, the law of propagation of expanded uncertainty, the law of propagation of observational results for reliable evaluation of type A uncertainty for correlated and uncorrelated measurement results of input quantities.**

***Keywords*—model approach to measurement uncertainty evaluation, Monte Carlo method, kurtosis method, the law of propagation of expanded uncertainty, reduction method, transposition method**

I. Introduction

The measurement uncertainty evaluation described in the Guide to the Expression of Uncertainty in Measurement (GUM) [1] is based on the so-called model approach, which consists in the fact that any measurand *Y* is associated with a mathematical model:

$$Y = f(X_1, X_2, ..., X_N)\,, \qquad (1)$$

linking it with the input quantities $X_1, X_2, ..., X_N$. The implementation of the model approach in the GUM uncertainty framework was carried out on the basis of the law of propagation of uncertainty: having estimates of the input quantities $x_1, x_2, ..., x_N$ through the measurement model (1), an estimate of the measurand *y* is calculated, and having standard uncertainties of the input quantities $u_1, u_2, ..., u_N$, the standard uncertainty of the measurand *u*(*y*) is calculated through the law of propagation of uncertainty.

The expanded uncertainty *U*(*y*) is evaluated using the formula:

$$U(y) = k \cdot u(y)\,, \qquad (2)$$

where *k* is the coverage factor, defined as the Student's coefficient for the confidence level *p*=0.9545 and the effective degrees of freedom ν_{eff} obtained from the Welch-Satterthwaite formula [1].

This approach led to a shift in the estimates of the numerical values of the measurand and its standard uncertainty at nonlinear model equations and to the unreliability of the estimates of the expanded uncertainty due to ignoring the influence of the laws of distribution of input quantities on the law of distribution of the measurand.

The shortcomings of the GUM uncertainty framework have led to the emergence of alternative methods for measurement uncertainty evaluating [3,5-8], which are the subject of this report.

II. Law of Propagation of Distributions

The listed shortcomings of the law of propagation of uncertainty underlying the GUM are eliminated when implementing the law of propagation of distributions.

The idea of the law of propagation of distributions is that the input quantities of the model (1) are represented by the corresponding probability distribution density functions (PDF) $g_1, g_2, ..., g_N$, for which $E(X_j) = x_j$ and $V(X_j) = u_j^2$ are taken. This is followed by propagation of these PDFs through the measurement model (1) to obtain a PDF of the measurand *g*(*Y*) with subsequent determination of its parameters: mathematical expectation, standard deviation and confidence interval for a given confidence level *p*.

An effective implementation of the law of propagation of distributions was the Monte Carlo method (MCM) [2,3], which is based on the generation of input quantities values in the form of random numbers $x_{1q}, x_{2q}, ..., x_{Nq}$ (*q*=1, 2, ..., *M*) with a given PDF $g_1, g_2, ..., g_N$ and their transformation through the measurement model (1) into a set of random numbers y_q with a distribution law corresponding to the PDF of the measurand *g*(*Y*). The use of the MCM was a real breakthrough in the measurement uncertainty evaluation, since it made it possible to get rid of the shortcomings of the GUM uncertainty framework listed above.

The implementation of the Monte Carlo method consists in performing the following operations:

1) generating *N* arrays of random numbers x_{jq}, $j = 1, 2, ..., N$, $q = 1, 2, ..., M$, of large size $M=10^6$-10^7, obeying the given distribution laws;

2) obtaining an array of random numbers y_q of size M corresponding to the measured value, taking into account the correlation between the input quantities

3) calculation of estimates of the parameters of the obtained joint distribution through the ranked values of the array of estimates of the output value according to the formulas:

$$\bar{y} = \frac{1}{M}\sum_{q=1}^{M} y_q\,, \qquad (3)$$

$$u(y) = \sqrt{\frac{1}{M-1}\sum_{q=1}^{M}(y_q - \bar{y})^2}\,, \qquad (4)$$

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$$U(y)=\frac{1}{2}\left\{y_{[M(1+p)/2]}-y_{[M(1-p)/2]}\right\}. \quad (5)$$

It should be noted that despite all the advantages of MCM, its direct use for measurement uncertainty evaluating in testing and calibration laboratories accredited for compliance with the requirements of ISO/IEC 17025:2017 is hindered by the following factors:

• lack of certified software tools for measurement uncertainty evaluating based on MCM;

• the impossibility of obtaining the budget of measurement uncertainty by the existing software tools that implement the MCM;

• the impossibility of documenting a step-by-step procedure for measurement uncertainty evaluating based on MCM.

In addition, a comparison of the estimates of the combined standard uncertainty obtained using the approaches described in [1] and [3] shows their numerical difference, primarily due to the difference in finding the standard uncertainties of input quantities by type A. This posed the task of revising the GUM [4].

The first draft NewGUM was distributed by the end of 2014 to JCGM Member Organizations, National Metrology Institutes and other recipients [5]. The revised Guide retained the law of propagation of uncertainty, with Type A and Type B uncertainty estimates to be calculated based on a Bayesian approach.

However, the developers of NewGUM failed to offer methods for reliable estimation of the expanded uncertainty. This shortcoming of NewGUM was eliminated by the authors in [6-7].

III. KURTOSIS METOD

The expanded measurement uncertainty is calculated in the kurtosis method by the formula:

$$U=k_p\cdot u(y), \quad (6)$$

where k_p is the coverage factor, which for a confidence level of p is calculated using the formulas [6]:

$$k_p=\begin{cases}0{,}1085\eta^3+0{,}1\eta+1{,}96, \text{for } p=0.95;\\ 0{,}12\eta^3+0{,}1\eta+2, \text{ for } p=0.9545,\end{cases} \quad (7)$$

at $\eta<0$ and

$$k_p=t_{p;(6/\eta+4)}\sqrt{\frac{3+\eta}{3+2\eta}} \quad (8)$$

at $\eta\geq 0$.

It should be noted that at $\eta\geq 0$ with an error of no more than 2%, one can take $k_{0,95}=1{,}96$ and $k_{0,9545}=2$.

In expressions (7-8) η is the kurtosis of the distribution of the measurand, determined in the absence of correlation between the results of measurements of the input quantities as:

$$\eta=\frac{\sum_{j=1}^{N}\eta_j c_j^4 u_j^4}{u^4(y)}, \quad (9)$$

where η_j are the kurtosis of the input quantities, c_j are the sensitivity coefficients; $u(y)$ is the standard uncertainty of the measurand, determined by the formula:

$$u(y)=\sqrt{\sum_{j=1}^{N}c_j^2u_j^2}. \quad (10).$$

If there is an observed correlation between the measurement results of the k-th and l-th input quantities with the correlation coefficient r_{kl}, the kurtosis of the distribution of the measurand should be calculated by the formula:

$$\eta=\frac{\sum_{j=1;i\neq k;i\neq l}^{N}\eta_j c_j^4u_j^4+\eta_{kl}[c_k^2u_k^2+2r_{kl}c_kc_lu_ku_l+c_l^2u_l^2]^2}{u^4(y)}, \quad (11)$$

where $u(y)$ is the standard uncertainty of the measurand, determined by the formula:

$$u(y)=\sqrt{\sum_{j=1}^{N}c_j^2u_j^2+2r_{kl}c_kc_lu_ku_l}; \quad (12)$$

$\eta_{kl}=\eta_k=\eta_l=6/(n-5)$ is the kurtosis of the k-th (l-th) input quantity.

It is shown [6] that the deviation of the expanded uncertainty estimates obtained by the kurtosis method from the estimates obtained using the MCM does not exceed ±2.5%.

Because the kurtosis of Student's distributions $\eta_t=6/(\nu_t-4)$, attributed to type A standard uncertainties, exists when the number of degrees of freedom $\nu_t=n-1$ is greater than 4, then the kurtosis method is applicable for the number of repeated measurements of input quantities n greater than 5.

With a smaller number of repeated measurements, the law of propagation of expanded uncertainty should be applied to calculate the expanded uncertainty [7].

IV. LAW OF PROPAGATION OF EXPANDED UNCERTAINTY

The law of propagation of expanded uncertainty is applied to the expanded uncertainty evaluation given the number of repeated observations of input quantities $n\geq 2$.

The expression for calculating the expanded uncertainty for a probability of 0.95 in this case has the form [7]:

$$U=\sqrt{U_A^2+U_B^2}, \quad (13)$$

where $U_A(y)$, $U_B(y)$ are estimates of expanded uncertainties of type A and B of the measurand, respectively.

Type A expanded uncertainty estimate is calculated by the formula:

$$U_A=\sqrt{\sum_{j=1}^{N}t^2_{(0,95;\nu_i)}c_j^2s^2(\bar{x}_j)}. \quad (14)$$

Here

$$s(\overline{x}_j) = \sqrt{\frac{1}{n_j(n_j-1)}\sum_{i=1}^{n_j}(x_{ji}-\overline{x}_j)^2} \quad - \qquad (15)$$

standard deviation of the arithmetic mean of the results of repeated measurements of the *j*-th input quantity; $t_{(0,95;\nu_i)}$ is Student's coefficient for the probability of 0.95 and the number of degrees of freedom $\nu_i = n_i - 1$.

Type B expanded uncertainty estimate is calculated by the formula:

$$U_B = k_B \cdot u_B(y), \qquad (16)$$

where is the (combined) Type B standard uncertainty of the quantity being measured

$$u_B(y) = \sqrt{\sum_{j=1}^{N} c_j^2 u_B^2(x_j)}; \qquad (17)$$

k_B – type B coverage factor calculated by the kurtosis method according to formula (7).

It was shown [7] that the deviation of the expanded uncertainty estimates obtained by this method from the estimates obtained using the MCM does not exceed ± 4.5%.

When implementing the law of propagation of expanded uncertainty, it is necessary to draw up two uncertainty budgets: separately for components estimated according to type B and separately for components estimated according to type A [7].

V. Law of Propagation of Results of Observations

A significant drawback of all implementations of the model approach is that PDFs of input quantities are assigned based on not always reliable a priori information about their variability.

For example, the PDF parameters assigned to type *A* standard uncertainties are estimates of the mean, standard deviation, and correlation coefficients obtained from a limited number of observations assuming their normal distribution, which may not be correct, since it is not possible to test the hypothesis of normal distribution for a limited number of observations.

This shortcoming can be avoided by using the so-called the law of propagation of the results of observations. In this case, the artificially generated random numbers used in the Monte Carlo method are replaced by the results of real observations.

The implementation of the law of propagation of the results of observations is carried out depending on the presence or absence of a correlation between the results of observations of the input quantities.

If there is a correlation between the results of observations of the input quantities, the processing of the results is carried out by the ***reduction method*** [8].

The essence of the reduction method is as follows.

Let the model equation (1) contain two input quantities (for example, X_k, X_l), the results of *n*-fold measurements of which are performed simultaneously and correlate with each other with a significant correlation coefficient .

These results are recorded in the first two columns of Table. 1.

TABLE I. Scheme of Implementation of the Reduction Method

X_k	X_l	$Y=f(X_1, X_2, \dots, X_N)$
x_{k1}	x_{l1}	$y_1 = f(x_1, x_2, \dots, x_{k1}, x_{l1}, \dots, x_N)$
x_{k2}	x_{l2}	$y_2 = f(x_1, x_2, \dots, x_{k2}, x_{l2}, \dots, x_N)$
…	…	…
x_{kn}	x_{ln}	$y_n = f(x_1, x_2, \dots, x_{kn}, x_{ln}, \dots, x_N)$

For all other input quantities X_j ($j = 1,2,\dots,N$; $j \neq k,l$), evaluated from the results of single or multiple measurements, determine their numerical values , which are substituted into expression (1). From the beginning, the first pair of sample values of the *k*-th and *l*-th input quantities (x_{k1}, x_{l1}), is substituted into the same expression, obtaining the first sample value of the measurand $y_1 = f(x_1, x_2, \dots, x_{k1}, x_{l1}, \dots, x_m)$ (Table 1). Other sample values $y_2, \dots y_n$ are obtained similarly.

Based on the obtained sample values, the numerical value of the measurand is calculated:

$$y = \overline{y} = \frac{1}{n}\sum_{i=1}^{n} y_i, \qquad (18)$$

and its standard uncertainty

$$u(y) = \sqrt{\sum_{\substack{j=1 \\ j\neq k,1}}^{N} u_j^2(y) + u_{Akl}^2(y)}, \qquad (19)$$

where $u_{Akl}(y)$ is the total contribution to the uncertainty of the measurand of the standard measurement uncertainty of the correlated pair of *k* and *l* input quantities:

$$u_{Akl}(y) = \sqrt{\frac{1}{n(n-1)}\sum_{i=1}^{n}(y_i - \overline{y})^2}. \qquad (20)$$

The resulting value $u(y)$ will be evaluated taking into account the correlation between the results of observations *k* and *l* of the input quantities without calculating the estimate of this coefficient.

If there is no correlation between the results of observations of the input quantities, the processing of the results is carried out by the method of transpositions.

The essence of the transposition method is to obtain all possible values of the measured quantity obtained by transposition of all values y_i of the input quantities substituted into the measurement equation:

$$y_i = f(x_{1i}, x_{2i}, \dots, x_{Ni}). \qquad (21)$$

For two input quantities with the number of observations n_1 and n_2 the process of obtaining an array can be represented in the form of Table 2.

TABLE II. THE TRANSPOSITION METHOD FOR TWO INPUT QUANTITIES

	x_{21}	x_{22}	…	x_{2n_2}
x_{11}	$f(x_{11}, x_{21})$	$f(x_{11}, x_{22})$	…	$f(x_{11}, x_{2n_2})$
x_{12}	$f(x_{12}, x_{21})$	$f(x_{12}, x_{22})$	…	$f(x_{12}, x_{2n_2})$
…	…	…	…	…
x_{1n_1}	$f(x_{1n_1}, x_{21})$	$f(x_{1n_1}, x_{22})$	…	$f(x_{1n_1}, x_{2n_2})$

The number of values y_i obtained in this way are defined as the product $n_1 n_2$.

Obviously, with N input quantities, the process of obtaining an array of possible values y_i of the measurand will look like a N-dimensional table with a total number of cells

$$M = \prod_{j=1}^{N} n_j \; . \qquad (22)$$

Based on the resulting array of the measured value, you can get an unbiased estimate of the measurand:

$$\bar{y} = \frac{1}{M} \sum_{i=1}^{M} y_i \qquad (23)$$

and the variance of estimates of the possible values:

$$s^2(y_i) = \frac{1}{(M-1)} \sum_{i=1}^{M} (y_i - \bar{y})^2 \; . \qquad (24)$$

Since the estimate of the measurand (23) and the variance estimate (24) were obtained from M estimates of the measurand y_i, they are significantly more reliable than the estimates obtained using the traditional method.

The total standard uncertainty of type A is calculated by the formula:

$$u_A(y) = \frac{s(y_i)}{\sqrt{n_{eq}}} = \sqrt{\frac{1}{n_{eq} \cdot (M-1)} \sum_{i=1}^{M} (y_i - \bar{y})^2} \; , \qquad (25)$$

where n_{eq} is the equivalent number of degrees of freedom when using the transposition method:

$$n_{eq} = \frac{\sum_{j=1}^{N} n_j c_j^2 u_{jA}^2}{\sum_{j=1}^{N} c_j^2 u_{jA}^2} \; . \qquad (26)$$

For an equal number of observations of all input quantities $n_j = n$, we get $n_{eq} = n$.

CONCLUSIONS

1. The implementation of the model approach in the GUM framework leads to a shift in the estimates of the numerical values of the measured quantity and its standard uncertainty with nonlinear model equations and to the unreliability of the extended uncertainty estimates due to ignoring the influence of the laws of distribution of input quantities on the law of distribution of the measured quantity.

2. The listed shortcomings of the law of propagation of uncertainty underlying the GUM are eliminated when implementing the law of propagation of distributions based on MCM.

3. Despite all the advantages of MMC, its direct use for estimating measurement uncertainty in testing and calibration laboratories accredited for compliance with the requirements of ISO/IEC 17025:2017 is hindered by a number of factors.

4. The use of the kurtosis method and the law of propagation of the expanded uncertainty makes it possible to obtain estimates of the expanded uncertainty, taking into account the laws of distribution of input quantities.

5. To estimate type A uncertainties, it is advisable to apply the law of propagation of observational results. In this case, the artificially generated random numbers used in the Monte Carlo method are replaced by the results of real observations.

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