Revision of GUM: the suggested alhorythm for processing measurment results

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***Abstract* – The main requirements for the revised GUM are considered. The proposed algorithm for processing measurement results is given. Criteria for compliance with the listed requirements are described. Methods for processing the measurement results with a nonlinear model are proposed.**

Keywords – GUM revision; estimates and standard uncertainties of input quantities; estimate and standard uncertainty of the measurand; correlation; expanded uncertainty

I. INTRODUCTION

The improving of the processing results methods and measurement uncertainty evaluation has led to the need to revise the current Guide to the expression of uncertainty in measurement (GUM-93) [1]. The reason for this was its inconsistency with the supplements GUM-S1 and GUM-S2 developed on the basis of the Monte-Carlo method (MCM) [2, 3]. The main source of this inconsistency is different approach to the type A uncertainty evaluation in GUM-93 and its supplements (frequentist and Bayesian, respectively). In addition, in [1] the question of obtaining estimates of expanded uncertainty, taking into account the laws of the distribution of input quantities, was not solved. The first Committee Draft (CD) of the revised GUM [4], proposed by the Working Group 1 of JCGM, also did not resolve this issue.

The main steps of the proposed algorithm for the measurement results processing, which allow to eliminate this drawback are discussed.

II. THEORETICAL RELATIONSHIPS

The basic algorithm for evaluating and reporting uncertainty in CD contains 5 steps:

1. Modelling the measurement;
2. Evaluating input quantities, standard uncertainties and covariances;
3. Evaluating the measurand and standard uncertainty;
4. Determining a coverage interval for the measurand;
5. Reporting and recording measurement result.

The implementation of the above steps in the proposed GUM is to be considered.

<u>1. Modelling the measurement</u>

The general issues of measurement modeling will be discussed in detail in JCGM-103 [5], which is currently being developed.

The proposed GUM focuses on measurands, which can be described using a linearized univariate explicit model, in which a single output quantity (measurand) Y is determined through other (input) quantities $X_1, X_2, ..., X_N$ by the formula:

$$Y = f(X_1, X_2, ..., X_N) \,. \tag{1}$$

The uncertainty estimate for nonlinear models that cannot be linearized is covered in GUM-S1 [2]. Multivariate and implicit models are considered in GUM-S2 [3].

<u>2. Evaluating input quantities, standard uncertainties and covariances</u>

Input quantities can be classified as:

- quantities, whose values and uncertainties are directly determined in the current measurement and can be obtained from a single indication of measuring instruments (MI) or repeated indications;

- corrections for MI indications and corrections for influencing quantities, such as ambient temperature, barometric pressure and humidity;

- quantities whose values and uncertainties of which are entered into measurements from external sources, such as calibrated standards, certified reference materials and reference data are given in handbook.

If a single indication x_i of the MI quantity X_i is obtained directly in this measurement, then this indication is the value of this quantity.

The standard uncertainty of this quantity (instrumental standard uncertainty) is calculated from information taken from the calibration certificate of MI: expanded instrumental uncertainty and coverage factor k_p:

$$u_t(x_i) = \frac{U_{pi}}{k_{pi}} \,, \tag{2}$$

where p – the confidence level, which is usually "approximately 0.95", that is, exactly 0.9545. For this probability, information about probability density function (pdf) that is attributed to this input value can be obtained from Table. 1.

TABLE I. COVARAGE FACTORS AND RELEVANT PDF

k_p	1.41	1.65	1.65-1.93	1.93	2	>2
pdf	U-shaped	Uniform	Trapezoidal	Triangular	Gauss	t-distribution

The parameter $\alpha = u_2/u_1$ of the trapezoidal pdf with standard uncertainty u_{trap} is found in Fig. 1, where

$u_1 = u_{trap} \big/ \sqrt{1+\alpha^2}$, $u_2 = \alpha u_1$ – the standard uncertainties of two uniform laws of distribution, the composition of which gives the trapezoid-visible law of distribution.

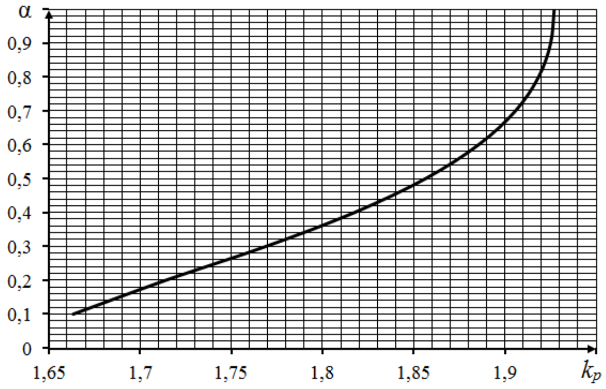

Fig.1. A nomogram for finding the parameter $\alpha = u_2/u_1$ of the trapezoidal pdf by value

The effective number of degrees of freedom ν_{eff} for the t-distribution for the probability of 0.9545 is found in Fig. 2.

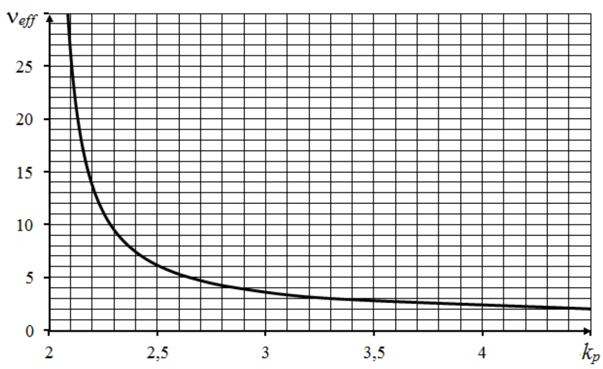

Fig.2. A nomogram for finding an effective number of degrees of freedom ν_{eff} of the t-distribution

If repeated indications of MI $x_{i1}, x_{i2}, ..., x_n$ are obtained directly in this measurement, then the value x_i of this quantity X_i is their arithmetic mean:

$$x_i = \bar{x}_i = \frac{1}{n}\sum_{r=1}^{n} x_{ir} . \quad (3)$$

In this case, the correction ε_i to X_i on the random effect is added to the measurement model, the value of which $\hat{\varepsilon}_i = 0$ and the standard uncertainty are determined by the formula:

$$u(\hat{\varepsilon}_i) = \sqrt{\frac{n-1}{n-3}}\sqrt{\frac{1}{n(n-1)}\sum_{r=1}^{n}(x_{i,r} - \bar{x}_i)^2} = \sqrt{\frac{1}{n(n-3)}\sum_{r=1}^{n}(x_{i,r} - \bar{x}_i)^2} . \quad (4)$$

This correction is attributed to the unbiased scalable t-distribution pdf with the number of degrees of freedom $\nu_i = n-1$. These statistical estimates of the standard uncertainties of the input values make sense for $n_j \geq 4$ and are valid only for normally distributed results of multiple measurements [6].

If a correlation is observed between repeated readings of two input quantities X_i and X_j measured simultaneously, then the covariance value between the corrections ε_i and ε_j is found by the formula [4]:

$$\mathrm{cov}(\hat{\varepsilon}_i, \hat{\varepsilon}_j) = \frac{1}{n(n-4)}\sum_{r=1}^{n}(x_{i,r} - \bar{x}_i)(x_{j,r} - \bar{x}_j) . \quad (5)$$

3a. Calculation of the numerical value of the measurand

The estimate y of the measurand Y in [1] is calculated by substituting into the model (1) the estimates $x_1, x_2, ..., x_N$ of the input quantities:

$$y = f(x_1, x_2, ..., x_N) . \quad (6)$$

With a non-linear model, this method of evaluation gives an accurate result only in the absence of uncertainty in these estimates. In the presence of significant uncertainties in the input quantities $u_1, u_2, ..., u_N$, this method leads to a bias in the estimate of the measurand [1].

In [8], the authors found an expression for the shift in the estimate of the measurand:

$$\Delta_y = -\left[\frac{1}{2}\sum_{i=1}^{N} c_{ii}u_i^2 + \sum_{i=2}^{N}\sum_{j=1}^{i} c_{ij}\,\mathrm{cov}(x_i, x_j)\right], \quad (7)$$

where $c_{ii} = \frac{\partial^2 y}{\partial x_i^2}$, $c_{ij} = \frac{\partial^2 y}{\partial x_i \partial x_j}$ и $\mathrm{cov}(x_i, x_j)$ — the second partial derivative of Y with respect to X_i , mixed second partial derivative of Y with respect to X_i , X_j and covariance X_i , X_j , respectively, evaluated at $X_1 = x_1, ..., X_N = x_N$.

The resulting shift Δ_y is compared with the value $u_0(y)$ that is obtained in the section 3b. If the inequality:

$$\left|\Delta_y\right| \geq \frac{1}{3}u_0(y) , \quad (8)$$

holds it is necessary to take into account the shift (6) as an correction to (5), to obtain an unbiased estimate of the measurand using the formula:

$$y_0 = y - \Delta_y . \quad (9)$$

3b. Calculation of the standard uncertainty of the measurand

If the model equation is expressed by the formula (1), then the standard uncertainty estimate of the measurand in the first approximation is performed from the expression:

$$u^2(y) = \sum_{i=1}^{N} c_i^2 u_i^2 + 2\sum_{i=2}^{N}\sum_{j=1}^{i} c_j c_i\,\mathrm{cov}(x_i, x_j) , \quad (10)$$

where $c_i = \frac{\partial y}{\partial x_i}$, $c_j = \frac{\partial y}{\partial x_j}$ — sensitivity coefficients, which are the corresponding partial derivatives Y, which are estimated at $X_1 = x_1, ..., X_N = x_N$.

To determine the shift of this estimate, the value is calculated [9]:

$$\Delta_{u^2} = -\left[\frac{1}{4}\sum_{i=1}^{N} c_{ii}^2(\eta_i + 2)u_i^4 + \sum_{i=2}^{N}\sum_{j=1}^{i} c_{ij}^2 u_i^2 u_j^2\right], \quad (11)$$

where η_i — the kurtosis of the i-th input value pdf, which is taken from the table. 2

TABLE II. THE VALUES OF KURTOSIS FOR DIFFERENT PDF OF THE INPUT QUANTITIES

pdf	η
U-shaped	-1,5
Uniform	-1,2
Trapezoidal with parameter α	$-1,2\,(1+\alpha^4)/(1+\alpha^2)^2$
Triangular	-0,6
Gaussian	0
t-distribution with number degrees of freedom ν	$6/(\nu-4)$

The resulting value of shift is compared with the value (9). If the inequality

$$\left|\Delta_{u^2}\right| \geq \frac{1}{9}u^2(y), \quad (12)$$

holds it is necessary to take into account the shift (11) as an amendment to (10), to obtain an unbiased estimate of the measurand variance using the formula:

$$u_0^2(y) = u^2(y) - \Delta_{u^2}. \quad (13)$$

4. Determining a coverage interval for the measurand;

To eliminate the above disadvantages of the GUM and JCGM-100CD approaches to evaluation of the expanded uncertainty, the authors propose to apply the kurtosis method [8].

The kurtosis of the measurand is found by the formula:

$$\eta = \frac{\sum_{j=1}^{m} \eta_j c_j^4 u_j^4}{u^4(y)}. \quad (14)$$

After finding the η, coverage factor for $p = 0,95$ is calculated by the formula [9]:

$$k_{0.95} = \begin{cases} 0,1085\eta^3 + 0,1\eta + 1,96, \text{ при } \eta < 0; \\ 1,96, \text{ при } \eta \geq 0. \end{cases} \quad (15)$$

It is shown that the deviation of the estimates of the expanded uncertainty, obtained by the kurtosis method from the estimates obtained using the MCM, does not exceed ± 2.5% for the number of repeated measurements of input values more than 5.

It should be noted that the fulfillment of the inequality about the presence of a shift of the measurand indicates the asymmetry of its distribution law. In this case, the MCM [2] must be used to find the expanded uncertainty.

III. Example. Calibration of a Ring Gauge [10]

When calibrating the ring gauge using a length comparator of the Abbe type, a specific error δ arises due to the non-coaxiality of the ring gauge and the measuring axis of the comparator (Fig. 3).

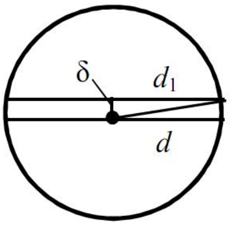

Fig.3. Non-coaxiality of the ring gauge and the measuring axis of the comparator

From fig. 3 we have:

$$d = 2\sqrt{\left(\frac{d_1}{2}\right)^2 + \delta^2} = \sqrt{d_1^2 + 4\delta^2}. \quad (16)$$

Using expression (7), we can write the expression for shift in the estimate of the measurand:

$$\Delta_d = -\left[\frac{1}{2}\frac{\partial^2 d}{\partial d_1^2}u^2(d_1) + \frac{\partial^2 d}{\partial \delta^2}u^2(\delta)\right], \quad (17)$$

where $u(d_1)$ и $u(\delta)$ – standard deviations of d_1 and δ, accordingly.

In view of (16), and also that the small distance δ has zero expectation, we get:

$$\Delta_d = -\frac{2}{d_1}u^2(\delta) \quad (18)$$

and unbiased estimate of the measurand will be equal:

$$d_0 = d_1 + \frac{2}{d_1}u^2(\delta). \quad (19)$$

Using expression (11), we can write the expression for shift in the estimate of the measurand variance:

$$\Delta_{u^2} = -\frac{1}{4}\left(\frac{\partial^2 d}{\partial \delta^2}\right)^2[\eta(\delta) + 2]u^4(\delta), \quad (20)$$

and unbiased estimate of the measurand variance will be equal:

$$u_0^2(d) = u^2(d_1) + \frac{4u^4(\delta)}{d_1^2}[\eta(\delta) + 2]. \quad (21)$$

For the given in [10] values d = 90 mm, $\delta = (0 \pm 20)\,\mu m$, and the uniform pdf of δ, we obtain $\Delta_d = -0.003\,\mu m$ and $\Delta_{u^2} = -0.007\,\mu m$.

CONCLUSIONS

1. The main approaches to the implementation of the algorithm for processing the results and measurements uncertainty evaluation based on the Bayesian method, taking into account the presence of non-Gaussian distribution of input quantities and non-linearity of model equations with significant uncertainties of the input quantities, are presented.

2. To obtain an unbiased estimate of a measurand, it is necessary to use the proposed expression suitable in the presence of uncertainties in the input quantities estimated by both statistical and non-statistical methods.

3. Obtaining an unbiased estimate of the standard uncertainty of the measurand for nonlinear model equations based on the law of propagation of uncertainty, built on expanding the measurement equation into a second-order Taylor series, for any distribution of input values can be implemented based on an expression that takes into account the kurtosis of input quantities.

4. The use of the kurtosis method allows to obtain estimates of the expanded uncertainty taking into account the laws of distribution of input quantities for symmetric distributions. It is shown that the deviation of the estimates of the expanded uncertainty obtained by the kurtosis method from the estimates obtained using the MCM does not exceed ± 2.5% for the number of repeated measurements of input quantities more than 5.

5. An example of evaluation of an unbiased estimate of a measured quantity and its variance when measuring the diameter of a ring gauge using a length comparator of the Abbe type is given.

6. The approaches proposed by the authors allow the creation of a Guide to the expression of uncertainty in measurement based on the Bayesian approach, which permits obtaining an unbiased estimate of the measurand, as well as its standard and expanded uncertainties.

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