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ESTIMATION OF EXPANDED UNCERTAINTY IN MEASUREMENT WHEN IMPLEMENTING A BAYESIAN APPROACH

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Issues with the estimation of expanded uncertainty in the first draft of the revised Guide to the Expression of Uncertainty in Measurement (GUM) based on the Bayesian approach are considered. Comparative analysis is done of the methodologies that are known and those that are proposed by the authors for estimating expanded uncertainty, based on the current version of the GUM, the GOST R 8.736–2011 standard, and the distribution law of expanded uncertainty. It is shown that the authors' technique makes it possible to achieve good correspondence of the estimates of expanded uncertainty with estimates obtained by the Monte Carlo method.
Keywords: *uncertainty in measurement, coverage factor, Bayesian approach, distribution law of expanded uncertainty.*

At the present time, Working Group 1 of the Joint Committee on Guides to Metrology (JCGM) is conducting a revision of the Guide to the Expression of Uncertainty in Measurement (GUM) [1]. The reason for the revision is the discrepancy in uncertainty estimates that are obtained in compliance with the GUM methodology [2] and the Monte Carlo method (MCM) according to Addition 1 [3] to the GUM. Since the Bayesian approach is placed at the foundation of [3] for estimating uncertainty in measurement, this approach [4] must be also used in the updated version [1] (NewGUM). By the end of 2014, the first NewGUM project was widespread among the organizations that are JCGM members, national metrological institutes, and other recipients, from whom more than 1000 generally-negative comments and responses arrived [4]. One of the main complaints against this document was that the proposed method of calculating expanded uncertainty does not depend on the distribution laws of the input values, and results in extremely overestimated estimates of this value. In this regard, it is necessary to develop a methodology of estimating expanded uncertainty in measurement, within which the estimation of expanded uncertainty will be coordinated with the estimates received by the MCM.

We will analyze various methodologies of estimating expanded uncertainty. For this purpose, we will compare the values of expanded uncertainty obtained by means of the MCM, U_{MCM}, and by the studied methodologies (SM), U_{SM}, under identical initial conditions. We define the relative deviation of values of the required value when using SM by the formula

$$\delta_{\mathrm{SM}} = (U_{\mathrm{SM}} / U_{\mathrm{MCM}} - 1)\cdot 100. \tag{1}$$

In order to simplify the analysis (reduce the number of specified variables), we divide U_{SM} and U_{MCM} by the total standard uncertainty u_{MCM} that is found using the MCM. In this case, expression (1) is recast as

$$\delta_{\mathrm{SM}} = (k^*_{\mathrm{SM}} / k_{\mathrm{MCM}} - 1)\cdot 100, \tag{2}$$

where $k_{\mathrm{MCM}} = U_{\mathrm{MCM}}/u_{\mathrm{MCM}}$ is the coverage factor for MCM, and $k^*_{\mathrm{SM}} = U_{\mathrm{SM}}/u_{\mathrm{MCM}}$ is the "Bayesian" coverage factor which in some cases differs from the coverage factor $k_{\mathrm{SM}} = U_{\mathrm{SM}}/u_{\mathrm{SM}}$ for the SM.

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Hence, in order to estimate δ_{SM}, it is necessary to derive the values of k^*_{SM} and k_{MCM} under identical initial conditions. In the course of calculating δ_{SM}, we will analyze the situation when there are two sources of uncertainty: the first one is defined by the measuring instrument (MI) being used, where information on the instrument's uncertainty is contained in the calibration certificate, and the second one is defined by the dispersion of readings of the MI during measurements [5]. In this case, the total standard uncertainty in measurement when using the MI is expressed as

$$u_{SM} = \sqrt{s^2 / n + u_B^2},$$

where s is the standard deviation (SD) of the readings of the MI; n is the number of measurements; and u_B is the standard type B uncertainty according to the certificate of calibration of the MI.

The total standard uncertainty estimated by the NewGUM methodology [4] is

$$u_{NewGUM} = \sqrt{\alpha^2 s^2 / n + u_B^2},$$

where $\alpha = \sqrt{(n-1)/(n-3)}$.

For the situation examined in [5] where $u_{NewGUM} = u_{MCM}$, then

$$k^*_{SM} = \frac{U_{SM}}{\sqrt{\alpha^2 s^2 / n + u_B^2}} = \frac{U_{SM}\sqrt{n}}{s\sqrt{\alpha^2 + \gamma^2}},$$

where $\gamma = u_B \sqrt{n} / s$.

Current version of the GUM. In accordance with [2], the expanded uncertainty taking into account type A uncertainty is calculated by the formula

$$U_{GUM} = k_{GUM} u_{GUM} = t_{0.95;\nu_{eff}} \sqrt{s^2 / n + u_B^2} = t_{0.95;\nu_{eff}} s\sqrt{1+\gamma^2} / \sqrt{n},$$

where $t_{0.95,\nu_{eff}}$ is the Student coefficient for probability 0.95 and effective number of degrees of freedom ν_{eff}, calculated from the Welch–Satterthwaite formula.

For the situation being studied [5], the effective number of degrees of freedom [6] and the Bayesian coverage factor are defined respectively by the expressions

$$\nu_{eff} = (n-1)[1 + u_B^2 n / s^2]^2 = (n-1)[1+\gamma^2]^2;$$

$$k^*_{GUM} = \frac{U_{GUM}\sqrt{n}}{s\sqrt{\alpha^2+\gamma^2}} = t_{0.95;\nu_{eff}} \sqrt{\frac{1+\gamma^2}{\alpha^2+\gamma^2}}. \quad (3)$$

First NewGUM project. It is recommended to calculate the coverage factor k_{NewGUM} when calculating the expanded uncertainty for arbitrary asymmetrical and symmetrical laws of distribution, by using the formulas [4]

$$k_{NewGUM} = 1/\sqrt{1-P};$$

$$k_{NewGUM} = 2/(3\sqrt{1-P}). \quad (4)$$

For the situation examined in [5], it is necessary to use (4), and then the coverage factor is $k_{NewGUM} = 2.98$ for $P =$ $= 0.95$, independent of the number of repeated measurements and the distribution law of type B uncertainty. Further, it will be shown that this value differs from k_{MCM} by 49–65% for normal distribution, and 49–81% for uniform distribution.

GOST R 8.736–2011. In accordance with [7], the expression for the confidence limits of the error of direct repeated measurements, calculated using the SD s of random error and the limit θ of the uniformly distributed residual systematic error (RSE), has the form

$$\Delta_{0.95} = \frac{t_{0.95;(n-1)} s/\sqrt{n} + \theta}{s/\sqrt{n} + \theta/\sqrt{3}} \sqrt{s^2/n + \theta^2/3},$$

where $t_{0.95;(n-1)}$ is the Student coefficient for probability 0.95 and number of degrees of freedom n–1.

We write a similar expression for the distribution of the RSE under the normal law:

$$\Delta_{0.95} = \frac{t_{0.95;(n-1)}s/\sqrt{n} + 1.96 s_\theta}{s/\sqrt{n} + s_\theta}\sqrt{s^2/n + s_\theta^2},$$

where s_θ is the SD of the RSE.

We equate the confidence limits of error $\Delta_{0.95}$ to the estimates of expanded uncertainty U_{GOST} [6], and then the expression for the Bayesian coverage factor, taking into account the equality $s_\theta = u_B$ and earlier introduced designations, will have the form:

$$k^*_{GOST} = \frac{U_{GOST}\sqrt{n}}{s\sqrt{\alpha^2+\gamma^2}} = \frac{t_{0.95;(n-1)} + \gamma\beta}{1+\gamma}\sqrt{\frac{1+\gamma^2}{\alpha^2+\gamma^2}}, \tag{5}$$

where $\beta = 3^{1/2}$ and 1.96 for the uniform and normal laws of distribution of standard type B uncertainty, respectively.

Distribution law of expanded uncertainty. A formula is presented in [8] for estimation of expanded uncertainty, called the distribution law of expanded uncertainty:

$$U_e = \sqrt{\left[t_{0.95;(n-1)}s/\sqrt{n}\right]^2 + (k_B u_B)^2}, \tag{6}$$

where the coverage factor $k_B = 1.65$ and 1.96, respectively, for the uniform and normal distribution laws that attribute type B uncertainty.

Then the Bayesian coverage factor is determined by the formula

$$k^*_e = \frac{U_e\sqrt{n}}{s\sqrt{\alpha^2+\gamma^2}} = \sqrt{\frac{t^2_{0.95;(n-1)} + (k_B\gamma)^2}{\alpha^2+\gamma^2}}. \tag{7}$$

Appendix 1 to the GUM. The Monte Carlo method implementation for finding the coverage factor was carried out in accordance with the following algorithm [3, 9]:

1) a random number X_i is generated, subject to unbiased and unscaled Student distribution with the set number of degrees of freedom $\nu = n - 1$;

2) a random number Y_i is generated with a mean of zero and a specified SD γ, subject to the normal (uniform) distribution law;

3) the summation $Z_i = X_i + Y_i$ is carried out;

4) steps 1 to 3 are repeated $M = 10^6$ times;

5) the set of numbers thus obtained Z_i (i = 1, ..., M) is arranged by increased value, and the expanded uncertainty is estimated by the formula

$$U = (Z_{975000} - Z_{25000})/2;$$

6) steps 1 to 5 are repeated 10 times, and the mean $\bar{U}$ and the relative SD are calculated:

$$\tilde{S}(U_i) = \frac{100}{\bar{U}}\sqrt{\frac{1}{9}\sum_{i=1}^{10}(U_i - \bar{U})^2};$$

7) from the value $\bar{U}$ derived, the coverage factor when using the MCM is calculated:

$$k_{MCM} = \bar{U}\Big/\sqrt{\alpha^2+\gamma^2}.$$

The relative SD k_{MCM} of the obtained estimates did not exceed 0.2%, and here the derived values of k_{MCM} completely coincided with the values of the coverage factor obtained in [5] by means of a Bayesian conclusion.

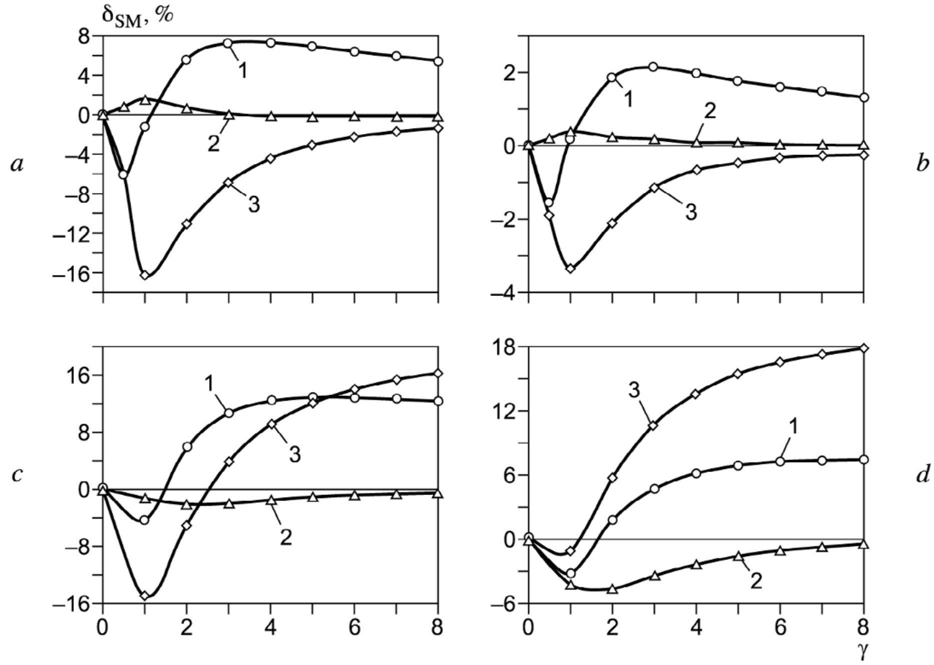

Fig. 1. Dependences $\delta_{SM}(\gamma)$ for normal (a, b) and uniform (c, d) distribution laws attributed to type B uncertainty, calculated for $n = 4$ (a, c) and 11 (b, d) measurements for various Bayesian factors of coverage: *1)* k^*_{GOST} per (5); *2)* k^*_e per (7); *3)* k^*_{GUM} per (3).

Comparison of derived results. Figure 1 presents the dependences of the relative deviations $\delta_{SM}(\gamma)$ of the coverage factors found by formulas (3), (5), and (7) for different n, under the normal and uniform laws of distribution of type B uncertainty. The smallest deviation from the values of k_{MCM} is observed for the coefficient k^*_e and does not exceed 4.5%. The greatest deviations are characteristic for k_{NewGUM} (up to 81%) and k^*_{GUM} (up to ±16%). The relative deviation of k^*_{GOST} from k_{MCM} is no greater than 12%. Taking into account the equality of formulas (1) and (2), the conclusions for the coverage factors of all SM can be extended to the corresponding expanded uncertainties U_{SM}.

Conclusion. Introduction of the concept of uncertainty in measurement as a product of the process of international standardization of the estimation of quality of measurements must ensure obtaining not only uniform, but also the most authentic estimates of uncertainty.

The maximum deviations from U_{MCM} are observed for U_{NewGUM} (up to 81%) and U_{GUM} (up to ±16%). The expanded uncertainty U_{GOST} has a relative deviation from U_{MCM} no greater than 12%. The most reliable estimate of expanded uncertainty can be derived by formula (6), and the relative deviation of U_e from U_{MCM} does not exceed ±4.5% throughout the range of modification of γ for the normal and uniform distribution laws of type B uncertainty.

It is necessary to continue studying the methodologies for calculating expanded uncertainty in which several uncertainties of types A and B are considered, and where the distribution laws of type B uncertainty that differ from normal and uniform are examined.

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