



# Accounting for the distributions of input quantities in the procedure for the measurement uncertainty evaluation when calibrating the goniometer

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## Abstract

The discords concerning the measurement uncertainty evaluation in the *Guide to the Expressing of Uncertainty in Measurement* (GUM) and its Supplement 1 are considered. To overcome these discords, the authors of the paper propose to use the kurtosis method and the law of the propagation of the expanded uncertainty. Using the example of the goniometer calibration, the features of accounting for the distribution laws of input quantities in the procedure for the measurement uncertainty evaluation are shown. A model for direct measurements of the value of a reference measure of the angle using a goniometer is written, the procedures for the measurement uncertainty evaluation are described, and uncertainty budgets for each of the methods are given. An example of the measurement uncertainty evaluation when calibrating a digital goniometer using a 24-sided reference prism is described. An estimate of the expanded measurement uncertainty for this example was made based on the web-based software application *NIST Uncertainty Machine*, which showed a good agreement with the estimates obtained by the considered methods. The technology of applying this software application for the confidence level of 0.9545, which the software lacks, is shown. The estimates of the measurement uncertainty obtained by the proposed methods, Monte Carlo method and methodology of the Guide to the Expressing of Uncertainty in Measurement are compared.

**Keywords:** goniometer; calibration; measurement uncertainty; uncertainty budget; kurtosis method; law of propagation of expanded uncertainty; Monte Carlo method.

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## 1. Introduction

The standard ISO 17025:20017 [1] prescribes the measurement uncertainty evaluation during tests and calibrations. To accomplish this task, [1] recommends using the methods described in the *Guide to the Expression of Uncertainty in Measurement* (GUM) [2]. However, the expanded uncertainty estimates obtained using the GUM methods do not depend on the probability density functions (PDF) of the input quantities. This shortcoming of the GUM is eliminated in its Supplement 1 [3] based on the Monte Carlo method (MCM). However, it is known that the measurement uncertainty estimates obtained using [2] and [3] do not match even for the linear model equations and the Gaussian PDF of all input quantities. Therefore, when evaluating the measurement uncertainty, it is advisable to rely on methods that lead to results that are compatible with the results obtained

using the MCM. Such approaches are described in [4] and in the Recommendation [5] by the NSC “Institute of Metrology”. Unfortunately, in both publications, there are no examples of using the proposed approaches to measuring angular values. Filling this gap, this paper discusses the application of the kurtosis method and the law of the propagation of the expanded uncertainty when calibrating the goniometer.

## 2. Basic theoretical relations

Goniometers are used to accurately measure angles and are widely used in optical laboratories. Using a goniometer, the refractive indices and refractive angles of prisms and crystals are determined, the parameters of diffraction gratings are studied, the wavelengths of spectral lines are measured, etc.

When calibrating the goniometer, the given angle of the reference multifaceted prism  $\alpha_s$  is repeatedly

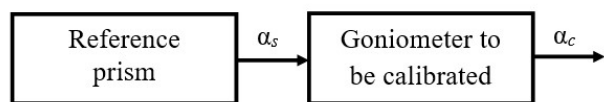


Fig. 1. Goniometer calibration scheme

measured. The measurement scheme in this case corresponds to the scheme “Direct measurement by a calibrated measuring device of a value reproduced by a reference measure” [6] and is shown in Fig. 1.

In this case, the bias of the value of the angle  $\alpha_c$ , which is measured by the calibrated goniometer from the actual angle  $\alpha_s$  reproduced by the reference measure, can be written in the form of a model [6]:

$$\Delta = (\alpha_c + \Delta_c) - (\alpha_s + \Delta_s), \quad (1)$$

where  $\Delta_c$  is the correction for the resolution of the goniometer reading;  $\Delta_s$  is the correction for the error in the basing of the reference measure.

Since the average values of both corrections  $\hat{\Delta}_c$  and  $\hat{\Delta}_s$  are equal to zero, the calibration result is taken as the estimate

$$\hat{\Delta} = \bar{\alpha}_c - \hat{\alpha}_s, \quad (2)$$

where  $\hat{\alpha}_s$  is the prism angle value taken from the calibration certificate;  $\bar{\alpha}_c$  is the arithmetic mean of the results of  $n$ -fold measurements of the polyhedral prism angle:

$$\bar{\alpha}_c = \frac{1}{n} \sum_{q=1}^n \alpha_{cq}. \quad (3)$$

The standard uncertainty of the measurand  $u(\hat{\Delta})$  is found by the formula:

$$u(\hat{\Delta}) = \sqrt{u^2(\bar{\alpha}_c) + u_B^2(\hat{\Delta}_c) + u_B^2(\hat{\alpha}_s) + u_B^2(\hat{\Delta}_s)}, \quad (4)$$

where  $u(\bar{\alpha}_c)$  is the standard uncertainty of the scattering of the goniometer readings, which is equal to:

$$u(\bar{\alpha}_c) = \frac{s(\alpha_c)}{\sqrt{n}}, \quad (5.1)$$

in the case of using the methods in [2] and

$$u(\bar{\alpha}_c) = \frac{s(\alpha_c)}{\sqrt{n}} \sqrt{\frac{n-1}{n-3}}, \quad (5.2)$$

in the case of using the methods in [4, 5], the standard deviation of the random variability of individual readings of the goniometer  $s(\alpha_c)$  is found by the formula:

$$s(\alpha_c) = \sqrt{\frac{1}{n-1} \sum_{q=1}^n (\alpha_{cq} - \bar{\alpha}_c)^2}; \quad (6)$$

$u_B(\hat{\Delta}_c)$  is the standard uncertainty of type  $B$  due to the resolution  $d$  of the goniometer reading:

$$u(\hat{\Delta}_c) = \frac{d}{2\sqrt{3}}; \quad (7)$$

$u(\hat{\alpha}_s)$  is the standard uncertainty of the reproduction of an angle by the reference prism, which is expressed in terms of the expanded instrumental uncertainty  $U_s$  of the prism at the calibration point assuming a Gaussian PDF (coverage factor  $k_s=2$  for the confidence level  $p=0.9545$ ) according to the formula:

$$u(\hat{\alpha}_s) = \frac{U_s}{k_s}; \quad (8)$$

$u_B(\hat{\Delta}_s)$  is the standard uncertainty of type  $B$  of the correction for the error in the basing of the reference measure:

$$u(\hat{\Delta}_s) = \frac{\theta_s}{\sqrt{3}}, \quad (9)$$

where  $\pm\theta_s$  are the limits of the error in the basing of the reference measure.

### 3. Calculation of the expanded uncertainty

According to [4, 5], the expanded uncertainty can be calculated in two ways: by the kurtosis method and using the law of the propagation of the expanded uncertainty.

The kurtosis method [4, 5] involves calculating the expanded uncertainty according to the formula:

$$U(\Delta) = k(\eta)u(\hat{\Delta}), \quad (10)$$

where  $k(\eta)$  is the coverage factor, which depends on the kurtosis  $\eta$  of the measurand PDF.

For the confidence level of 0.9545 [4, 5]:

$$k(\eta) = \begin{cases} 0.12 \cdot \eta^3 + 0.1 \cdot \eta + 2.0, & \text{for } \eta \leq 0; \\ t_{0.9545; (6/\eta)+4} \cdot \sqrt{\frac{3+\eta}{3+2\eta}}, & \text{for } \eta > 0, \end{cases} \quad (11)$$

where  $t_{0.9545; (6/\eta)+4}$  is the Student's coefficient for the probability of 0.9545 and the number of degrees of freedom  $\nu=(6/\eta)+4$ .

The kurtosis of the measurand is calculated by the formula:

$$\eta = \frac{\eta(\bar{\alpha}_c) \cdot u^4(\bar{\alpha}_c) + \eta(\Delta_c) \cdot u_B^4(\hat{\Delta}_c) + \eta(\alpha_s) u_B^4(\hat{\alpha}_s) + \eta(\Delta_s) \cdot u_B^4(\hat{\Delta}_s)}{u^4(\hat{\Delta})}, \quad (12)$$

in which the kurtosis of the input quantities are taken in accordance with their distribution laws and are equal, respectively,  $\eta(\bar{\alpha}_c) = \frac{6}{n-5}$ ;  $\eta(\Delta_c) = -1.2$ ;  $\eta_s = 0$ ;  $\eta(\Delta_s) = -1.2$ , and the standard uncertainty of the measurand is calculated by the formula:

$$u(\hat{\Delta}) = \sqrt{u^2(\bar{\alpha}_c) + u_B^2(\hat{\Delta}_c) + u_B^2(\hat{\alpha}_s) + u_B^2(\hat{\Delta}_s)}. \quad (13)$$

The uncertainty budget for this case is given in Table 1.

Table 1

The measurement uncertainty budget for the goniometer calibration when implementing the kurtosis method

$X_i$	$x_i$	$u(x_i)$	$\eta_i$	$c_i$	$u_i(y)$
$\alpha_c$	$\bar{\alpha}_c$ , (3)	$u(\bar{\alpha}_c)$ , (5.2, 6)	$\eta(\bar{\alpha}_c)$	1	$u(\bar{\alpha}_c)$
$\Delta_c$	0	$u(\hat{\Delta}_c)$ , (7)	$\eta(\Delta_c)$	1	$u(\Delta_c)$
$\alpha_s$	$\hat{\alpha}_s$	$u(\hat{\alpha}_s)$ , (8)	$\eta(\alpha_s)$	-1	$-u(\alpha_s)$
$\Delta_s$	0	$u(\hat{\Delta}_s)$ , (9)	$\eta(\Delta_s)$	-1	$-u(\hat{\Delta}_s)$
$Y$	$y$	$u(y)$	$\eta$	$k(\eta)$	$U(\Delta)$
$\Delta$	(2)	(13)	(12)	(11)	(10)

The law of the propagation of the expanded uncertainty [4, 5] involves a separate calculation of the expanded uncertainty for non-random  $U_B$  and random  $U_A$  input quantities, followed by their combination according to the formula:

$$U = \sqrt{U_B^2 + U_A^2}. \quad (14)$$

The expanded uncertainty  $U_B$  is calculated by the kurtosis method according to the formula:

$$U_B = k(\eta_B)u_B(\hat{\Delta}); \quad (15)$$

where the coverage factor  $k(\eta_B)$  is calculated by formula (11) for  $\eta \leq 0$ , and the kurtosis  $\eta_B$  is calculated as

$$\eta_B = \frac{\eta(\Delta_c) \cdot u^4(\hat{\Delta}_c) + \eta(\alpha_s)u^4(\hat{\alpha}_s) + \eta(\Delta_s) \cdot u^4(\hat{\Delta}_s)}{u_B^4(\hat{\Delta})}, \quad (16)$$

where  $u_B(\hat{\Delta})$  is type B standard uncertainty of the measurand:

$$u_B(\hat{\Delta}) = \sqrt{u^2(\hat{\Delta}_c) + u^2(\hat{\alpha}_s) + u^2(\hat{\Delta}_s)}. \quad (17)$$

The uncertainty budget for type B components is given in Table 2.

The expanded uncertainty  $U_A$  is calculated by the formula

$$U_A = t_{0.9545; (n-1)} \frac{s(\alpha_c)}{\sqrt{n}}, \quad (18)$$

where  $s(\alpha_c)$  is calculated by formula (6), and  $t_{0.9545; (n-1)}$  is the Student's coefficient for the probability of 0.9545 and the number of degrees of freedom  $n-1$ .

After calculating the combined expanded uncertainty  $U$  according to formula (14), the combined standard uncertainty of the measurand  $u(\hat{\Delta})$  is determined according to formula (4), followed by the calculation of the coverage factor according to the formula:

$$k = \frac{U}{u(\hat{\Delta})}. \quad (19)$$

#### 4. Example

Calibrating a digital static goniometer CG-1H using a 24-sided reference prism. The nominal value of the measure is  $30^\circ$ . The actual value  $30^\circ 00' 01.15''$  is determined with the expanded uncertainty of  $0.3''$ .

The results of 10 measurements of this angle using a goniometer are shown in Table 3.

Table 2

The measurement uncertainty budget for type B components

$X_i$	$x_i$	$u(x_i)$	$\eta_i$	$c_i$	$u_i(y)$
$\alpha_c$	$\bar{\alpha}_c$ , (3)	-	-	-	-
$\Delta_c$	0	$u(\hat{\Delta}_c)$ , (7)	$\eta(\Delta_c)$	1	$u(\Delta_c)$
$\alpha_s$	$\hat{\alpha}_s$	$u(\hat{\alpha}_s)$ , (8)	$\eta(\alpha_s)$	-1	$-u(\alpha_s)$
$\Delta_s$	0	$u(\hat{\Delta}_s)$ , (9)	$\eta(\Delta_s)$	-1	$-u(\hat{\Delta}_s)$
$Y$	$y$	$u(y)$	$\eta$	$k(\eta)$	$U_B(\Delta)$
$\Delta$	(2)	(17)	(16)	(11)	(15)

Table 3

The results of measuring the reference measure with a goniometer

29° 59' 55.8"	29° 59' 54.8"	29° 59' 55.8"	29° 59' 54.9"	29° 59' 55.3"
29° 59' 54.6"	29° 59' 54.8"	29° 59' 54.8"	29° 59' 55.3"	29° 59' 55.3"

Table 4

The measurement uncertainty budget for the goniometer calibration using the kurtosis method

$X_i$	$x_i$	$u(x_i)$	$\eta_i$	$c_i$	$u_i(y)$
$\alpha_c$	29°59' 55.14"	0.153"	1.2	1	0.153"
$\Delta_c$	0	0.0289"	-1.2	1	0.0289"
$\alpha_s$	30° 00' 01.15"	0.15"	0	1	-0.15"
$\Delta_s$	0	0.0577"	-1.2	-1	-0.0577"
$Y$	$y$	$u(y)$	$\eta$	$k(\eta)$	$U(\Delta)$
$\Delta$	-6.01"	0.2239"	0.258	2.019	0.452"

Table 5

The measurement uncertainty budget for type B components

$X_i$	$x_i$	$u(x_i)$	$\eta_i$	$c_i$	$u_i(y)$
$\alpha_c$	29°59' 55.14"	-	-	-	-
$\Delta_c$	0	0.0289"	0	1	0.0289"
$\alpha_s$	30° 00' 01.15"	0.15"	-1.2	-1	-0.15"
$\Delta_s$	0	0.0577"	-1.2	-1	-0.0577"
$Y$	$y$	$u(y)$	$\eta$	$k(\eta)$	$U_B(\Delta)$
$\Delta$	-6.01"	0.1633"	-0.0199	1.998	0.3263"

The arithmetic mean value of the measurement results is  $\bar{\alpha}_c = 29^\circ 59' 55.14''$ , the standard deviation of individual measurements is  $s(\alpha_c) = 0.4274''$ .

The goniometer resolution,  $d$ , is 0.1". The boundary of the error in the basing of the prism is  $\theta_s = 0.1''$ .

The measurement uncertainty budget using the kurtosis method is given in Table 4.

The measurement uncertainty budget for type B components using the law of the propagation of the expanded uncertainty is given in Table 5.

The expanded uncertainty  $U_A$  calculated by formula (18) is equal to:

$$U_A = 2.3198 \frac{0.4274''}{\sqrt{10}} = 0.3135''.$$

The combined expanded uncertainty  $U$  calculated by formula (14) will be equal to:

$$U = \sqrt{(0.3263'')^2 + (0.3135'')^2} = 0.4525''.$$

The combined standard uncertainty  $u(\hat{\Delta})$  of the measurand determined by formula (4) will be equal to:

$$u(\hat{\Delta}) = \sqrt{(0.153'')^2 + (0.0289'')^2 + (0.15'')^2 + (0.0577'')^2} = 0.2239'',$$

and the coverage factor determined by formula (19) will be equal to:

$$k = \frac{0.4525''}{0.2239''} = 2.02.$$

The measurement uncertainty evaluation for this example based on the *NIST Uncertainty Machine* web software application [7] resulted as follows:

- numerical value: -6.01";
- standard uncertainty: 0.224";
- 99% coverage interval: (-6.603", -5.417");
- 95% coverage interval: (-6.45", -5.57");
- 90% coverage interval: (-6.376", -5.644").

For the given coverage intervals the method of the least squares in the range of confidence levels

[0.9; 0.99], an interpolating formula for the expanded uncertainty was obtained:

$$U(p) = 26.056 \cdot p^2 - 46.723 \cdot p + 21.312,$$

whence for  $p=0.9545$  the value  $U_{0.9545}=0.4537''$  was obtained, for which the coverage factor was  $k=0.4537''/0.224''=2.03$ .

Thus, when evaluating measurement uncertainty with both of the proposed methods, there is almost perfect agreement with the results obtained by the Monte Carlo method.

It should be noted that when the expanded uncertainty evaluation according to the GUM method [2], the standard uncertainty  $u(\bar{x}_s)$  calculated by formula (5.1) will be equal to  $0.135''$ , therefore the standard uncertainty of the measurand  $u(\hat{\Delta})$  is  $0.212''$ , and the expanded uncertainty for the confidence level of  $0.9545$  and the coverage factor of  $2$  will be equal to  $0.424''$ , which is  $7\%$  less than the expanded uncertainty calculated using the MCM.

## Урахування розподілів вхідних величин у процедурі оцінки невизначеності вимірювання при калібруванні гоніометра

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### Анотація

Розглянуто розбіжності в оцінках невизначеності вимірювань у Настанові з подання невизначеності вимірювань та її Додатку 1. Показано, що можливими шляхами подолання цих суперечностей є застосування методу ексцесів та закону поширення розширеної невизначеності. На прикладі калібрування гоніометра показано особливості урахування законів розподілу вхідних величин у процедурі оцінювання невизначеності вимірювань. Наведено модель прямого вимірювання значення еталонної міри кута за допомогою гоніометра, описано процедури оцінювання невизначеності вимірювань, наводяться бюджети невизначеності для кожного з методів. Описано приклад оцінювання невизначеності вимірювань при калібруванні цифрового гоніометра за допомогою 24-гранної еталонної призми. Оцінено розширену невизначеність вимірювання для цього прикладу на основі вебзастосунку *NIST Uncertainty Machine*. Наведено технологію застосування цього застосунку для відсутнього в ньому рівня довіри  $0,9545$ . Порівняння результатів оцінювання невизначеності вимірювань, отриманих обома запропонованими методами, з результатами, отриманими за допомогою методу Монте-Карло, показало практично їхній повний збіг. При цьому розширена невизначеність, отримана за методикою GUM, виявилася на  $7\%$  меншою від розширеної невизначеності, розрахованої за допомогою методу Монте-Карло.

**Ключові слова:** гоніометр; калібрування; невизначеність вимірювань; бюджет невизначеності; метод ексцесів; закон поширення розширеної невизначеності; метод Монте-Карло.

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