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Uncertainty type A evaluation of autocorrelated measurement observations

ZYGMUNT LECH WARSZA, MYKHAYLO DOROZHOVETS*

Polish Metrological Society, (adres koresp.) 05-540 Zalesie Górne, ul. Szmaragdowych Żuków 32
*Rzeszow University of Technology PL, 35-959 Rzeszów, ul. W. Pola 2,
*Lviv University of Technology, UA

Abstract. This paper briefly discusses the limitations of the international Guide ISO GUM framework, and proposes improving the type A method of uncertainty evaluation of regularly sampled observations. The proposal demonstrates the influence of autocorrelation on measurement resultants and for correlated observations, the calculation of their effective number, smaller than the real value, is presented. Numerical example from the computer simulation is given. Results obtained by the proposed method and classical GUM method are compared and discussed.
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1. Introduction

International Guide ISO GUM [1] recommends to calculate the measured result as the mean value and its accuracy depends on the standard deviation evaluated by statistical method type A as the uncertainty u_A.

With the practice of a measurement there may exist serious inadequacies of the u_A value. Even after removal of all known systematic components from the raw observations, this corrected set of observations may not constitute a sample of purely random and normal population. There still may remain unknown components of regular systematic nature such as a trend or harmonics. If more information is known of the observations, such as how the collection took place as a series of time, e.g. by regular sampling, then some of the undesirable components can be eliminated using input filtration of a proper digital algorithm, e.g. by Least Square Method, FFT. This was described in detail in Ref. 5 by the authors and Korczyński.

The following problem is discussed in this paper with a proposal for solving it:

Corrected observations are not always statistically independent and they may be autocorrelated especially, if the observations are sampled with high density, that is if they are inside the equivalent diameter of the autocorrelation function. In this case a different formula than this recommended by the GUM for standard deviation has to be used.

2. Influence of autocorrelation of regularly sampled observations

2.1. Autocorrelation function

Let us consider a series of n uniformly sampled the corrected observations q_i of the constant value x. The estimator r_k of the normalized autocorrelation function ρ_k for the whole population is calculated [2-4, 7-9] as

$$r_k = \frac{1}{n-1-k} \frac{\sum_{i=1}^{n-k} (q_i - \overline{q})(q_{i+k} - \overline{q})}{s^2(q_i)}, \tag{1}$$

where k is the number of the periods between observations, $\overline{q}$ is the mean value of the sample, and $s(q_i)$ is the standard deviation of the single observation.

The functionρ_k is symmetrical for stationary processes, and its calculated accuracy decreases as k increases therefore $k < n/4$ in order to maintain accurate results [2].

2.2. Standard uncertainty of the sample of n correlated observations q_i

The variance D of the mean value of a linear function of n correlated random variables [7 (chapt.18.5-22)] is

$$D\left(a_0 + \sum_{i=1}^{n} a_i q_i\right) = \sum_{i=1}^{n} \sum_{j=1}^{n} a_i a_j \rho_{ij} \sigma_i \sigma_j . \tag{2}$$

If $a_0 = 0$ and weight coefficients of observations in the sample are equal, i.e. $a_i = 1/n$, then the mean value equals

$$\bar{x} = \sum_{i=1}^{n} a_i q_i = \frac{1}{n}\sum_{i=1}^{n} q_i. \tag{3}$$

Equation (2) can be transformed as follows

$$D\left(\bar{x} = \frac{1}{n}\sum_{i=1}^{n} q_i\right) = \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\rho_{ij}\sigma_i\sigma_j. \tag{4}$$

If all the observations of the sample are taken from the same general population then their standard deviations are also equal, i.e. $\sigma_i = \sigma_j = \sigma$, ($i = 1, 2,\ldots, n$) and

$$D\left(\bar{x}\right) = \frac{\sigma^2}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\rho_{ij}. \tag{5}$$

The double sum can be transformed in this way,

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\rho_{ij} = n + 2\sum_{k=1}^{n-1}(n-k)\rho_k = n\left[1 + \frac{2}{n}\sum_{k=1}^{n-1}(n-k)\rho_k\right]. \tag{6}$$

Equations (5) and (6) are used to form the theoretical variance of the population mean value

$$D\left(\bar{x}\right) = \frac{\sigma^2}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\rho_{ij} = \frac{\sigma^2}{n}\left(1 + \frac{2}{n}\sum_{k=1}^{n-1}(n-k)\rho_k\right). \tag{7}$$

In the practice of measurement, the standard deviation of the population mean value σ is estimated from the experimental standard deviation of the sample $s(q_i)$, where

$$s(q_i) = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}\left(q_i - \bar{q}\right)^2}. \tag{8}$$

Then, the standard deviation $s\left(\bar{x}\right)$ of the mean value for a sample of the autocorrelated observations q_i is

$$s\left(\bar{x}\right) = \sqrt{s^2\left(\bar{q}\right)} = \frac{s(q_i)}{\sqrt{n}}\sqrt{1 + \frac{2}{n}\sum_{k=1}^{n-1}(n-k)\rho_k} = \frac{s(q_i)}{\sqrt{n}}\sqrt{1 + D_\rho}. \tag{9}$$

where k is the number of sampling periods between observations and D_ρ is the component dependent on the autocorrelation function ρ_k,

$$D_\rho \equiv \frac{2}{n}\sum_{k=1}^{n-1}(n-k)\rho_k. \tag{10}$$

The GUM recommendation is

$$s\left(\bar{q}\right)_{GUM} = \frac{s(q_i)}{\sqrt{n}} = \sqrt{\frac{1}{n(n-1)}\sum_{i=1}^{n}\left(q_i-\bar{q}\right)^2}. \tag{11}$$

From Eqs. (10) and (11)

$$s\left(\bar{x}\right) = s\left(\bar{q}\right)_{GUM}\sqrt{1+D_\rho}. \tag{12}$$

Therefore the real value of the mean standard deviation of correlated observations is $\sqrt{1+D_\rho}$ times larger then the estimate using only the GUM recommendations.

Using the GUM definition of the uncertainty, u_A, as estimated by the type A evaluation to be valid then it must also be valid in the case of regularly sampled correlated observations q_i, i.e. if $u_A(x) \equiv s\left(\bar{x}\right)$, otherwise the more general Eq. (10) has to be used in the form

$$u_A(x) = \sqrt{\frac{s^2(q_i)}{n}\left(1+D_\rho\right)} = \frac{s(q_i)}{\sqrt{\frac{n}{1+D_\rho}}}. \tag{13}$$

If the observations are very strongly correlated (deterministically dependent), then $\rho_k \to 1$ and from (10)

$$D_\rho \to \frac{2}{n}\sum_{k=1}^{n-1}\left(n-k\right)\cdot 1 = n-1. \tag{14}$$

If observations are not correlated (statistically independent), then $\rho_k \to 0$ and

$$D_\rho \to \frac{2}{n}\sum_{k=1}^{n-1}\left(n-k\right)\cdot 0 = 0. \tag{15}$$

2.3. Effective number of autocorrelated observations

The last term of Eq. (13) can be transformed into a form similar to the uncertainty u_A in GUM,

$$s(\bar{x}) = \frac{s(q_i)}{\sqrt{\frac{n}{1+D_\rho}}} = \frac{s(q_i)}{\sqrt{n_{eff}}}, \tag{16}$$

where, $\frac{n}{1+D_\rho} = n_{eff}$ **is the effective number of uncorrelated observations equal to correlated ones.**

If the observations are uncorrelated $\rho_k = 0$, $D_\rho = 0$ and $n_{eff} = n$, and if they are strongly joined $n_{eff} = 1$.

In practice, uncorrelated observations can be classified as the ones taken from a random process during the minimal period ΔT of their sampling, and they are higher than half of the width of a rectangle with height 1 and the field equivalent to the integral of the autocorrelation function ρ_k. This means that during the collection of all observations, the related units have to be known. For regular sampling it is sufficient to know the number of the observations.

If a signal is considered with practically no limit in time and has a frequency range 0-B, then due to the Nyquist condition it has to be sampled at least twice during the period of the highest frequency. In this case, the maximum number of regularly sampled statistically independent observations during the entire collection period T is given in Ref. [6] as

$$n_{eff\,\max} = 2B\,T. \tag{17}$$

The number of independent observations does not increase even if the sampling frequency becomes higher.

Table 1 lists the new procedure for u_A, the uncertainty estimation of the sample of correlated observations which was used to determine the values in Example 1.

Example 1

Below there are given values of "clean" observations q_i, obtained after elimination of the trend and oscillations from the regularly sampled raw observations v_i, by the Least Square Method, as described in Ref. [5].

Cleaned results of observations of Example 1.

1.1742	1.1653	1.1787	1.1886	1.2137	1.2376	1.2637
1.2386	1.2149	1.1924	1.1804	1.1789	1.1750	1.1818
1.1807	1.1649	1.1940	1.2056	1.2224	1.2111	1.1944
1.1866	1.1931	1.2181	1.2100	1.2064	1.1925	1.1678
1.1848	1.1916	1.2049	1.2102	1.2102	1.2037	1.1972
1.2046	1.2056	1.2112	1.2230	1.2340	1.2228	1.2102
1.2014	1.2115	1.2251	1.2459	1.2192	1.2065	1.1696
1.1940	1.2131	1.2367	1.2351	1.2278	1.2327	1.2427
1.2281	1.2175	1.2159	1.2169	1.2154	1.2095	1.2102
1.1997	1.2112	1.2148	1.2291	1.2257	1.2060	1.1919
1.1789	1.1706	1.1592	1.1759	1.1965	1.2184	1.2033
1.1972	1.1827	1.1993	1.2154	1.2135	1.2132	1.2011
1.1886	1.2072	1.2151	1.2193	1.2211	1.2314	1.2351
1.2396	1.2365	1.2376	1.2254	1.2053	1.1807	1.1982
1.2336	1.2428	1.2378	1.2171	1.2045	1.2019	1.2008
1.2011	1.2262	1.2405	1.2629	1.2431	1.2281	1.2116
1.1855	1.1549	1.1307	1.1472	1.1600	1.1805	1.1838
1.1815	1.1926					

Values of q_i are presented in Fig. 1.

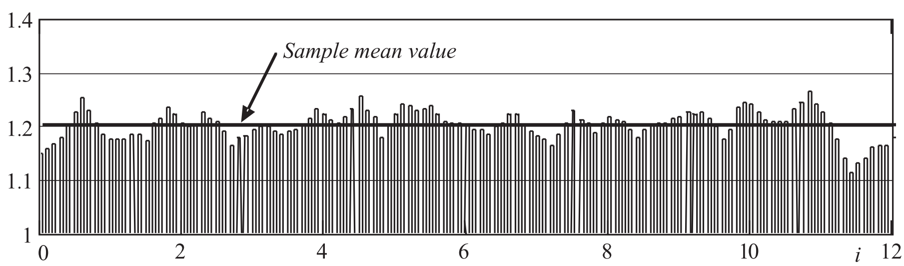

Fig. 1. The corrected values q_i of the regularly sampled rough observations v_i

Table 1 shows the steps to determine the calculated results. Systematic disturbances are eliminated from the sample data and their uncertainty u_A, is estimated by standard GUM method as the standard deviation of the mean value for corrected observations. As the model of the sample distribution Normal (Gauss) one is checked by the criterion χ^2 and a positive result is obtained.

TABLE 1

Parameters of the sample of correlated observations normally distributed (Example 1)

1	Cleaning rough results of observations (elimination of known systematic components, unknown: non periodic trend, oscillations and outliers)
2	Mean value of cleaned observations: $\overline{V} = \overline{q} = \frac{1}{121}\sum_{i=1}^{121} q_i \approx 1.2027$
3	Sample experimental standard deviation (calculated due to GUM recommendations) $s(q_i) = \sqrt{\frac{1}{121-1}\sum_{i=1}^{121}\left(q_i - \overline{q}\right)^2} \approx 0.0264$
4	GUM uncertainty $u_A(\overline{q}) = \frac{s(q_i)}{\sqrt{n}} \approx 0.0024$
5	Criterion χ^2 for normal (Gauss) distribution $\chi^2 = 4.888 < \chi^2_{5,\,0.05} = 11.1$ positive result
6	Normalized autocorrelation function: $r_k = \frac{1}{n-k-1}\frac{\sum_{i=1}^{n-k}\left(q_i - \overline{q}\right)\left(q_{i+k} - \overline{q}\right)}{s^2(q_i)}$ Values r_k (for $k = 0, 1\ldots m = 8 << n = 121$): 1; 0.7757; 0.4612; 0.1934; 0.0869; 0.0478; 0.0353; 0.0259
7	Term for correction of autocorrelation: $D_\rho = \frac{2}{n}\sum_{k=1}^{n-1}\left(n-k\right)\rho_k$
8	Effective number of observations $n_{eff} = \frac{n}{1+D_\rho} = \frac{121}{1+3.212} \approx 29$
9	Degrees of freedom $\nu_{eff} = n_{eff} - 1 = 28$
10	Standard uncertainty of the mean value (of the sample of autocorrelated observations) $s(\overline{q}) \equiv \frac{s(q_i)}{\sqrt{n_{eff}}} = \frac{0.02636}{\sqrt{29}} \approx 0.0049$
11	Result of measurements (if $u_B << u_A$, $k_P = 2$) $x = 1.2027 \pm 0,0098$

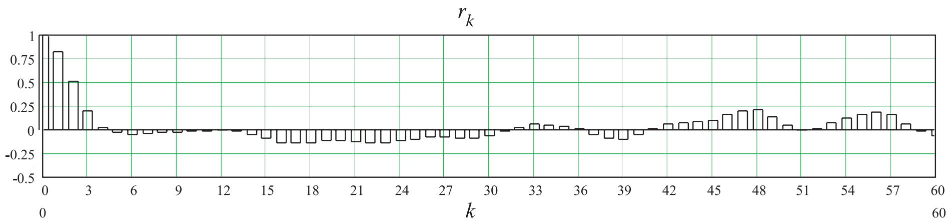

Fig. 2. Normalized autocorrelation function r_k of half of observations of the cleaned sample 1

Their normalized autocorrelation function r_k as the estimator of ρ_k for whole population is calculated from Eq. (1) for half of the observations and is shown in Fig. 2.

Then, the uncertainty, $u_{Aeff} \equiv s(\overline{q})$, is estimated again for effective number, n_{eff}, of observations q_i. One can see that n = 121 autocorrelated observations are equal to 29 ones. The ratio of uncertainties for both numbers is

$$u_{A\,eff}(\overline{q})/u_A(\overline{q}) = \sqrt{n/n_{eff}} = 2.04.$$

The real uncertainty $u_{A\,eff}$ of the sample is more than 2 times higher then u_A calculated by GUM recommendations. Then before evaluating the accuracy it is very important to test if the sample observations are correlated and to take into account the calculation of their effective number n_{eff}.

The effective equivalent number n_{eff} as used in Ref. [4] for such measurements was first proposed by Dorozhovetz at the 14th International Seminar on Metrology in Poland, Oct. 2006. This seminar is annually organized by Rzeszow and Lviv Technical Universities.

In accordance to the authors' work [4], the type A uncertainty evaluation of autocorrelated regularly sampled observations was also considered in the same time on slightly other way by Zhang in Ref. [2] and later used by Witt [3].

Summary

In this paper, and in the Refs. 4 and 6, recommendations for the improvement in the ISO GUM regarding the procedure of the type A uncertainty evaluation are introduced. Results of the classical GUM recommendation were provided as reference also in Table 1 and in example 1.

We proposed two additional steps to improve the current GUM procedure:

1. One should investigate a recorded series of raw observations apart from the random component to determine if any regular components exist, such as progressive (trend) or harmonics and try to eliminate them, by LSM method [5, 10].
2. For a collection of measurement observations taken within a time limit, the method often used to increase accuracy is to increase the sampling frequency of n observations. However, the higher sampling frequency is limited by autocorrelation of nearer observations. Because of this, the effective number of observations $n_{eff} < n$ and real uncertainty is higher than that calculated according to the GUM recommendation. The formula for n_{eff} is based on the autocorrelation function and it is possible only to calculate n_{eff} if the relative sampling positions of all observations are known, i.e. when the sample results are in a regular series of time or of the another variable, e.g. the coordinate of the position changed in space. Calculations are simplified if the sampling process is regular.

The effective number n_{eff} of the correlated observations sample can be very simply adapted to uncertainty estimations by GUM recommended type A method.

Furthermore, it has to be noticed that for any sample distribution the parameter of the highest probability (of the lowest standard deviation) should be always applied. The mean value is the best statistical parameter only for normal distribution type and others like a triangular type. For a uniform distribution the midrange and for double-exponential type (Laplace) the median are the best parameters. These estimators and their standard deviations can be used in the same way as mean value and the uncertainty u_A recommended by GUM. More details about that are in Refs. 4, 8, and 9.

There are additional proposals in [4] to upgrade also the type B uncertainty evaluation.

The proposal in this paper and all proposals in the previous papers [4, 5] offer better estimation methods for measurement accuracy. They should be applied to the practice of measurement in order to gain the needed experience for background material maybe of the next Supplement to ISO Guide [1].

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Z. L. WARSZA, M. DOROZHOVETS

Wyznaczanie niepewności typu A pomiarów o skorelowanych obserwacjach

Streszczenie. Krótko omówiono ograniczenia zasad wyznaczania niepewności wg zaleceń międzynarodowego Przewodnika ISO o angielskim akronimie GUM i zaproponowano udoskonalenie metody typu A szacowania niepewności pomiarów o regularnie próbkowanych obserwacjach. Przedstawiono wpływ autokorelacji na ocenę dokładności wyniku pomiarów i dla skorelowanych obserwacji zaproponowano obliczanie efektywnej ich liczby, mniejszej niż rzeczywista. Na symulowanym komputerowo przykładzie liczbowym porównano rezultaty otrzymywane metodą proponowaną i klasyczną wg GUM.

Słowa kluczowe: pomiar, niepewność typu A, autokorelacja, rozkład prawdopodobieństwa
Symbole UKD: 53.08