Methods of upgrading the uncertainty of type A evaluation (2)
Elimination of the influence of autocorrelation of observations and choosing the adequate distribution

Dorozhovets Mykhaylo[1], Warsza Zygmunt Lech[2]

[1]Rzeszow University of Technology, Poland,
[2]Polish Metrological Society Warsaw, Poland

Abstract. It is the continuation of the previous paper [4], in which limitations of uncertainty type A estimation due international guide GUM [1], are shortly discussed and method of elimination of influence of unknown systematic components: trend and oscillation, are introduced. Below two next proposals of development and upgrading of the method type A are presented, i.e. taking in estimation the influence of autocorrelation of observation resultants and choosing the adequate type of their probability distribution by $\chi 2$ criterion, if is different that normal one, are considered. It is illustrated by numerical examples of normal, rectangular and Laplace distribution. Results are compared to parameters calculated by the actual GUM method. Conclusions and background literature are included.

Key words: measurement type A uncertainty, trend, autocorrelation, random distributions.

I. Introduction

In the measurement praxis some serious inadequacies of ISO GUM statistical method type A are met. Due it result is evaluated as the mean value and accuracy depends on its standard deflection as uncertainty u_A. But:

- Even after removal all known systematic components from "rough" observations set of their corrected values still may be not the sample of the pure random and normal population.
- In the most of corrected probes of observations still remain some unknown components of the regular systematic nature. If additional information about observations is known, e.g. how they are collected as series of time or of other parameter, some of undesirable components could be eliminated by input filtration and others as trend or harmonics, after their identification, by special digital algorithms, e.g.: as ones described in the part 1.
- Corrected observations are not always statistically independent; they also may be autocorrelated, especially if observations are sampled with the high density, i.e. inside the equivalent diameter of autocorrelation function.
- The best distribution for observations could be different that of normal one. The mean value of the sample of such observations is not always the most likelihood parameter of their distribution and other ones should be used, e.g.: midrange of rectangular distribution and MED of double-exponential (Laplace) one.

Last two problems are shortly discussed in this paper and some proposals of solving it are given.

II. Influence of correlation between observations in the sample

Let us consider series of n uniformly sampled observations q_i. The normalized autocorrelation function $\rho(k) \equiv \rho_k$ of them is [2, 3, 8, 9]:

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

where: k – number of samples equal value periods between observations.

For stationary processes function ρ_k is symmetrical one. Accuracy of its calculations decreases for increasing k and because of that should be: $k<n/4$ [6].

Standard uncertainty of the sample of n correlated observations q_i could be fund from variance D of mean value of the linear function of n correlated random variables [9 (18.5-22)].

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

If mean value a_0=0, weight of sample observations are equal a_i=1 and for all observations of the same general population their standard deviations are also, i.e. $\sigma_i = \sigma_j = \sigma$. In measurement practice standard deviation of the population mean value σ is estimated from the sample ones $s(q_i)$ –see e.g. lines column b) of Table 3. Standard deviation of the mean value of n uniformly sampled in time and correlated random observations q_i is:

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

where: $\frac{2}{n} \sum_{k=1}^{n-1} (n-k)\rho_k \equiv D_\rho$; k – number of sampling periods between observations.

From (2): $$s(\bar{x}) = s(\bar{q})_{GUM} \cdot \sqrt{1 + D_\rho} \qquad (3)$$

It is larger then one before calculated due GUM method by $\sqrt{1 + D_\rho}$ times.

Last term of (2) could be transformed to similar form as has uncertainty u_A in GUM

$$s(\bar{x}) = \frac{s(q_i)}{\sqrt{\frac{n}{1 + D_\rho}}} = \frac{s(q_i)}{\sqrt{n_{eff}}} \qquad (4)$$

where: $\frac{n}{1 + D_\rho} = n_{eff}$ - number of uncorrelated observations equal to correlated ones.

From (2) and (4) follow written together few proposed forms of new generalized formula of standard uncertainty type A $u_A(x) \equiv s(\bar{x})$ of correlated observations q_i: If observations are uncorrelated $\rho_k = 0$, $D_\rho = 0$ and $n_{eff}=n$. Schedule of the new procedure of uncertainty $u_A(x)$ estimation of the sample of correlated observations is given in column b) of Table 1 and are illustrated by calculations of the numerical example 1. In parallel to authors' works [2, 3] the uncertainty A evaluation of autocorrelated sample was described in [6, 7].

Example 1

On Fig 1 are shown values q_i obtained after elimination of the trend and oscillations from regularly sampled rough observations V_i by the method described in [4]. Their numerical values are taken from [2-4]. Its normalized autocorrelation function ρ_k is calculated from (1) and for half number of observations is shown on Fig 2. The standard deviation of this sample is estimated as its uncertainty u_A by standard GUM method for rough and corrected observations and additionally for effective number n_{eff} of observations of the corrected sample. Steps of procedure and results are put together in the Table 1. One could see that n=121 autocorrelated observations are equal to only n_{eff}=29 uncorrelated ones and ratio of uncertainties for both numbers is $u_{A\,eff}(\bar{q})/u_A(\bar{q}) = \sqrt{n/n_{eff}} = 2.04$. Then before the evaluation of the accuracy it is very important to test the sample if its observations are correlated and to take in calculations their effective number n_{eff}.

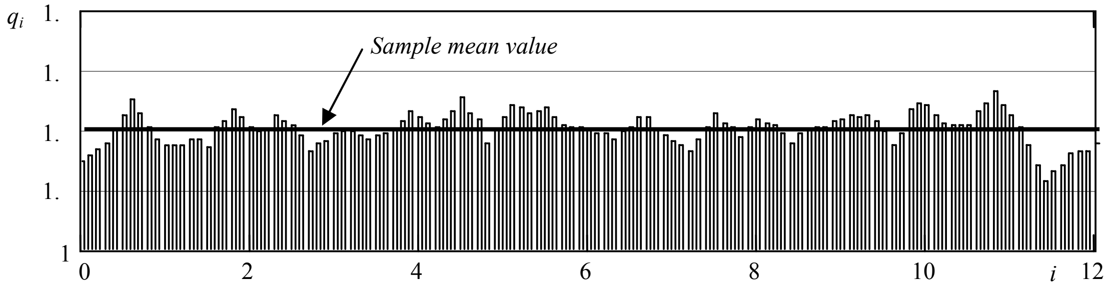

Fig. 1. Corrected values q_i of the regular series of rough observations V_i.

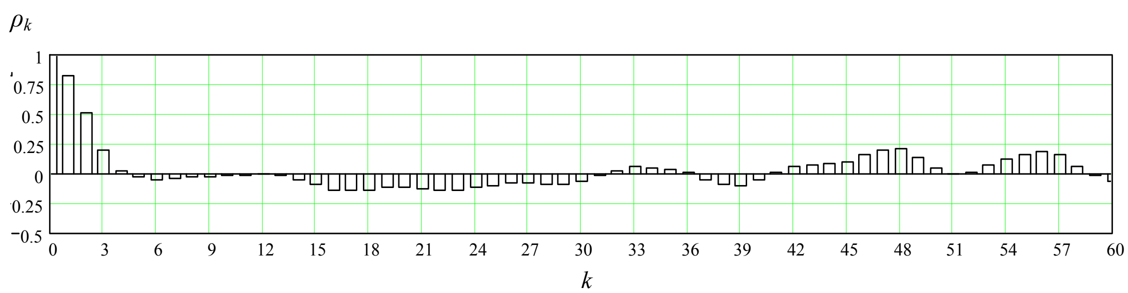

Fig 2 Normalized autocorrelation function of half of corrected observations of the sample of Fig 1.

Lp	Table 1 Parameters of the sample of correlated observations (p. 2.3)	
Lp	a) **„Rough" results**	b) **corrected sample** (without trend and oscillations)
1	**Criterion χ^2 for normal (Gauss) distribution**	
	$\chi^2 = 34.36 > \chi^2_{5,\ 0.05} = 11.1$ negative result	$\chi^2 = 4.888 < \chi^2_{5,\ 0.05} = 11.1$ **positive result**
2	**Mean value of observations:** $\overline{V} = \frac{1}{121}\sum_{i=1}^{121} V_i \approx 1.2027$	
3	**Standard deviation due GUM (without considering correlation)**	
	$s(V_i) = \sqrt{\frac{1}{121-1}\sum_{i=1}^{121}\left(V_i - \overline{V}\right)^2} \approx 0.0395$	$s(q_i) = \sqrt{\frac{1}{121-1}\sum_{i=1}^{121}\left(q_i - \overline{q}\right)^2} \approx 0.0264$
4	**Ratio of standard deviations:** $s(V_i)/s(q_i) = 0.0395/\ 0.0264 \approx 1.5$	
5	**Normalized autocorrelation function:** $\rho_k = \frac{1}{n-k}\frac{\sum_{i=1}^{n-k}\left(q_i - \overline{q}\right)\left(q_{i+k} - \overline{q}\right)}{s^2(q_i)}$	
6	**Values ρ_k (for k=0, 1… 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:** $D_\rho = \frac{2}{n}\sum_{k=1}^{n-1}(n-k)\rho_k$	$D_\rho \approx \frac{2}{121}\sum_{k=1}^{121-1}(121-k)\cdot\rho_k \approx 3.2118$
8	**Effective number of observation and freedom degree** $n_{eff} = \frac{n}{1+D_\rho},\ \nu_{eff} = n_{eff} - 1$	$n_{eff} = \frac{121}{1+3.21175} \approx 29,\ \nu_{eff} = 28$
9	**Standard GUM uncertainty $u_A(x)$ of „rough" results** ($s_S(\overline{V})$ of mean value)	**Standard uncertainty of the sample $u_{A\ \mathrm{eff}}(x)$** (after correction of the trend and autocorrelation)
	$u_A(\overline{V}) \equiv s(\overline{V}) = \frac{s(V_i)}{\sqrt{n}} \approx 0.00359$ where: $s(V_i)$, $s(\overline{V})$ - standard deviations of sample uncorrected and of its mean value - due GUM	$s_{eff}(\overline{q}) \equiv \frac{s(q_i)}{\sqrt{n_{eff}}} = \frac{0.02636}{\sqrt{29}} \approx 0.0049$ where: $s(q_i)$ - standard deviation of the corrected sample calculated due GUM recommendations.
10	**Ratio of standard deviations** $u_{A\ eff}(\overline{q})/u_A(\overline{V}) \approx 1.36$	**Ratio of stand. deviations** $s_{eff}(\overline{q})/u_A(\overline{q}) = \sqrt{n/n_{eff}} = 2.04$

III. Uncertainty estimation of the uniform distributed sample

From the statistic literature [10, 11] the best estimator of the sample with number of observations n taken from population of uniform distribution is the midrange. After Cramer [10] formulas for this unbiased estimator of population with the range R, midrange R/2 and its variance D are:

Range of the sample: $V = q_{i\max} - q_{i\min}$ (5a)	Midrange: $q_{V/2} = \frac{q_{i\min} + q_{i\max}}{2}$ (5b)
Expectation of V: $E(V) \approx \frac{n-1}{n+1}R$ (6a)	Variance: $D\left(q_{V/2}\right) \approx \frac{R^2}{2(n+1)(n+2)}$ (6b)
Standard deviation of midrange for $R \approx \frac{n+1}{n-1}V$: $s(q_{V/2}) \equiv s_{V/2} = \frac{R}{\sqrt{2(n+1)(n+2)}} \approx \frac{V}{\sqrt{2}\,(n-1)}\sqrt{\frac{n+1}{n+2}}$ (7)	

The midrange $q_{V/2}$ depends only on two extreme observations. Standard deviation of midrange depends also on their values and on number of observations. Each of extremes, if is lying to far from the rest ones should be canceled. It is important to be sure and checks by χ^2 criterion with needed high enough level of confidence that rectangular distribution is the best for particular sample observations including its borders. If not, trapezoidal distribution has to be recommended for considerations.

Example 2 (sample with negligible correlation)

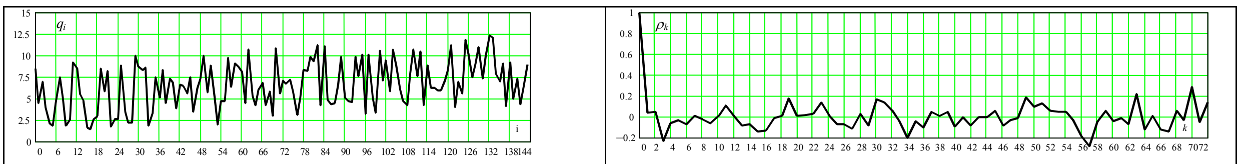

Fig.3: a) Values of rough observations of the example 2 b) Their autocorrelation function

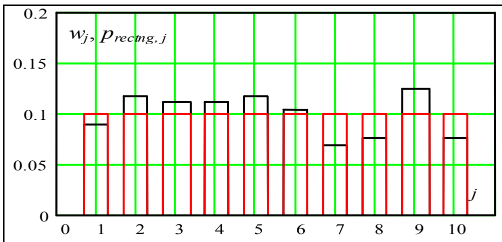

Fig..4. Histogram of the example 2 observations: black - w_i of sampled observations; red – $p_{rectg.,j}$ of rectangular distribution. The smallest and highest observations: 2.469…1.105 Number of histogram classes: m=10 of 0.864 width

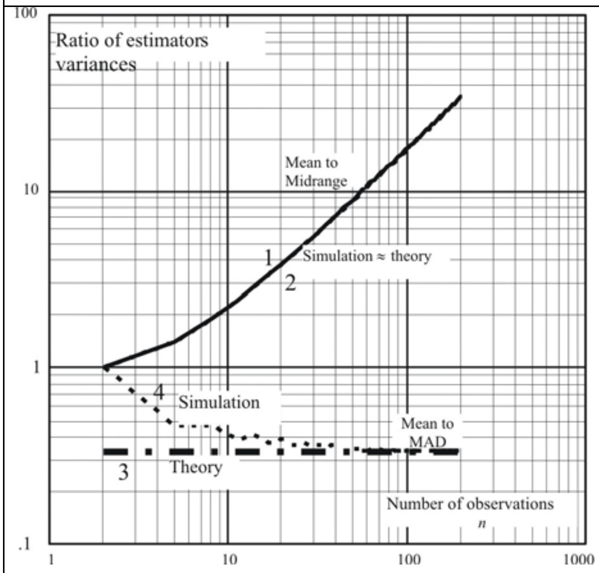

Fig. 5a Efficiency of rectangular distribution: estimators as functions of number n of observations (Monte Carlo simulation by 200×2^{20} random numbers [5]). Ratio of mean value and midrange variances $s^2(\bar{x})/s^2_{v/2}$: (1) ≈(2) - theoretical function (n+1)(n+2)/6n from [9] and curve from simulation. Ratio of mean value and of median MAD variances $s^2(\bar{x})/s^2_{MAD}$: (3) - theoretical function = 1/3, (4) - curve from simulation.

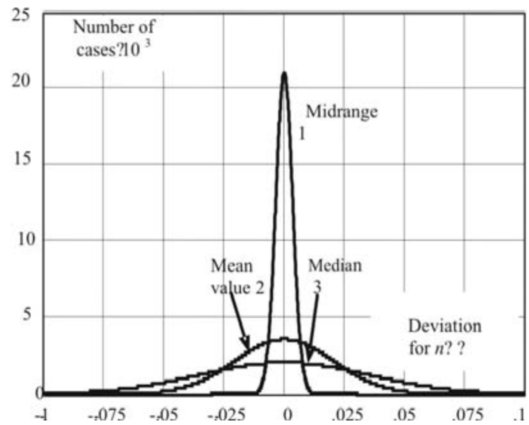

Fig. 5b Histograms of estimators of the rectangular distribution (-0.5…+0.5) simulated by 200×2^{20} random numbers [5]: 1 - midrange; 2 - mean value; 3 - median.

Table 2 Estimation procedure of measurement result – example 2

No	**Rough results of observations q_i – Fig 3a**	
	a) Mean value - GUM	b) **Midrange**
1	Parameters of rough observations	
	Mean value: $\bar{q} = \frac{1}{n}\sum_{i=1}^{n} q_i = 6.604$	
	Standard deflection: $s(q_i) = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(q_i-\bar{q})^2}$ =2.684	
2	**Elimination of a priori unknown regular components:** Linear trend of slope $A = 0.02491$is only found	
	Correction of observations in relation to mean values $\bar{q}$: $q_{kor,i} = q_i - A\cdot\left(i-\frac{n+1}{2}\right)$ (3)	
3	**Normalized autocorrelation function ρ_k after correction** $\rho_k = \frac{1}{n-k}\frac{\sum_{i=1}^{n-k}(q_{kor\,i}-\bar{q})(q_{kor\,i+k}-\bar{q})}{s^2(q_i)}$ (4)	
4	**Number of observations** and number of freedom	
	Real	**Effective**
	n	$n_{eff} = \frac{n}{1+\frac{2}{n}\sum_{k=1}^{n-1}(n-k)\rho_k}$ (5)
	$\nu = n-1$	$\nu_{eff} = n-1$ (6)
5	**Histogram of the sample after correction**	
	Boundary values:	$q_{s,1}$= 2.469…$q_{s,144}$=11.105
	Sample range:	$V = q_{s,144} - q_{s,1} = 8.636$
	Number of classes:	m=10 (of width 0,864)
6	**Selection of the distribution type - by criterion: χ^2**	
	Level of confidence	$\alpha = 0.05$
	Number of freedom	$\nu = m-2-1 = 7$
	Value of $\chi^2_{\nu,\alpha}$ (from table of χ^2):	$\chi^2_{7,\ 0.05} = 14.11$
	Normal (Gauss) distribution	**Uniform distribution**
	$\chi^2 = n\sum_{j=1}^{m}\frac{(w_j - p_{norm\,j})^2}{p_{norm\,j}}$	$\chi^2 = n\sum_{j=1}^{m}\frac{(w_j - p_{rectg,j})^2}{p_{rectg,j}}$ (7)
	$\chi^2 = 18.898 > \chi^2_{7,0.05} = 14.11$	$\chi^2 = 5.306 < \chi^2_{7,0.05} = 14.11$
	Negative result	**Positive result**
7	**Mean value** (corrected)	**Midrange**
	$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} q_{cor\,i} = \bar{q}_{cor} = 6.617$	$q_{V/2} = \frac{q_{s,1}+q_{s,144}}{2} = 6.8095$
8	Standard uncertainty $u_A(x)$	**Standard deflection: $q_{ś.r}$**
	$s(\bar{q}_{kor}) = \frac{s(q_{kor})}{\sqrt{n}} = \frac{2.475}{\sqrt{144}} = 0.207$	$s_{ś.r} = \frac{V}{\sqrt{2}\,(n-1)}\sqrt{\frac{n+1}{n+2}} = 0.0424$
	Ratio of standard deflections: $u_A(\bar{x})/s_{ś.r} \approx 4.93$	
9	**For quintile k_p of confidence level p (of normal distribution)**	
	Expanded uncertainty of mean value $\bar{x}$	**Expanded deflection of midrange $q_{ś.r}$**
	$U_p(\bar{q}_{kor}) = k_p\ s(\bar{q}_{kor})$	$U_p(q_{V/2}) = k_p\ s(q_{V/2})$
	when p=0,95, $k_{0.95} = 1.96$	when p=0.95, $k_{0.95} = 1.96$
	$U_{0.95}(\bar{q}) = 0.406$	$U_{0.95}(q_{V/2}) = 0.0831$
10	**Measurement results**	
	$x_{GUM} = 6.617 \pm 0.406$	$x_{\nu/2} = 6.810 \pm 0.083$

IV. Efficiency of rectangular distribution estimators

Comparison of standard deviations ratios and probability distributions of values of estimators of the rectangular distribution are given on Fig 5a and 5b. They show that its midrange is statistically the best one.

V. Double exponential (Laplace) distribution

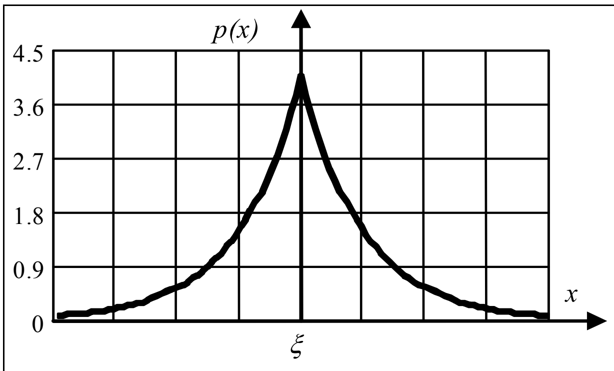

Fig. 6 Double-exponential Laplace distribution

$$p(x) = \frac{1}{2\lambda} e^{-\frac{|x-\xi|}{\lambda}}, \quad -\infty < x < \infty \tag{8}$$

where: ξ -, λ - distribution parameters

Ordered observations: $q_{s,1} \le q_{s,2} \le q_{s,3} \le \ldots \le q_{s,n}$

Median: $$q_{med} = q_{s,(n+1)/2} \quad q_{med} = \frac{q_{s,n/2} + q_{s,n/2+1}}{2} \tag{9}$$

Standard experimental deviation of median:

$$s_{med} \approx \sqrt{\frac{s^2}{2n}} = \frac{\bar{s}}{\sqrt{2}} = \frac{u_A(\bar{q})}{\sqrt{2}} \tag{10}$$

Standard deviation $u_A(\bar{q})$ of the mean value $\bar{q}$ is here about 1.41 times higher then s_{med} of median.

VI. Summary

In this and papers [2 - 4] some upgrading procedure of the uncertainty type A evaluation by the ISO GUM method is introduced. It is presented in the column b) of Table 3 and the classical GUM recommendation as reference is given in the column a). Proposed procedure has three steps additional :

1. One should firstly investigated if in results of rough observations recorded as random series existing are any regular, i.e. progressive (trend) [2, 3] and harmonic components [4] and tries to eliminate them.
2. In limited time for collection of measurement observations the commonly used method of increasing accuracy by higher number n of observations taken for the sample due the higher sampling frequency is limited by autocorrelation of nearer observations. Because of that effective number of observations $n_{eff} < n$ and u_A is higher. Formula for n_{eff} is based on the autocorrelation function, possible to calculate only if relative sampling times of all observations are known, i.e. when the sample results are the series of time or of the other quantity, e.g. coordinate of the position in space. Calculations are simplified if the sampling process is regular.
3. In the case when the type of the probability distribution of corrected observation results is a priori unknown or information is not reliable enough the sample histogram should be made. Hypothesis is tested by χ^2 criterion with needed level of confidence and the nearest to reality distribution has to be chosen. If distribution is not enough adequate then obtained result of measurement is not proper and its estimated measure of accuracy is too high – see numerical examples 1 and 2. To any distribution of the sample the most likelihood parameter (of the lowest standard deflection) should be applied. The mean value as the statistically best parameter is valid only for normal and some other distributions as triangle one. For uniform distribution it is the midrange and for double-exponential (Laplace) one – median MED. They and their standard deviations could be used in the same way as mean value and uncertainty u_A recommended by GUM.

All proposals of this and previous paper [4] are new, very actual and allow obtaining better accuracy estimation of measurements. They should be applied even immediately in the measurement practice to accumulate experience needed as the background material in elaboration of next Supplements to ISO Guide [1].
Some authors' proposal of upgrading evaluation of the uncertainty type B is described in paper [2].

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Table 3 Evaluation procedure of the statistical measure of the measurement result inaccuracy		
No	**a) Method recommended by ISO GUM**	**b) Upgraded method**
1	**Sample of corrected values of *n* observations**	
	$q_1, q_2, q_3, ..., q_n$	$q_1(t_1), q_2(t_2), q_3(t_3), ..., q_n(t_n)$
2	**'A priori' predicted normal distribution**	**Selection the distribution by test χ^2**
3	**Value of measurement result** x: the most likelihood parameter of the sample distribution	
	Mean value $\bar{q}=\frac{1}{n}\sum_{i=1}^{n} q_i$ (1)	e.g.: 1) normal distribution - **mean value** as in GUM $\bar{q}=\frac{1}{n}\sum_{i=1}^{n} q_i$ (1)
4	**Experimental sample variance** $s^2(q_i)=\frac{1}{n-1}\sum_{i=1}^{n}(q_i-\bar{q})^2$ (2)	2) uniform distribution - **midrange** $q_{V/2}=\frac{q_{i\min}+q_{i\max}}{2}$
5	**Experimental standard deviation** $s(q_i)=\sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(q_i-\bar{q})^2}$ (3)	3) Laplace distribution – **median**: even n: $q_{med}=q_{s,(n+1)/2}$; odd *n:* $q_{med}=\frac{q_{s,n/2}+q_{s,n/2+1}}{2}$
6	**Standard deviation of the most likelihood parameter**	
	$s(\bar{q})=\frac{s(q_i)}{\sqrt{n}}=\sqrt{\frac{1}{n(n-1)}\sum_{i=1}^{n}(q_i-\bar{q})^2}$ (4)	e.g.: 1) $s(\bar{q})=\frac{s(q_i)}{\sqrt{n}}$ (as in GUM) 2) $s(q_{V/2})\equiv s_{V/2}=\frac{q_{\max}-q_{\min}}{\sqrt{2}\,(n-1)}\sqrt{\frac{n+1}{n+2}}$ 3) $s(q_{med})\equiv s_{med}\approx\sqrt{\frac{s^2}{2n}}=\frac{\bar{s}}{\sqrt{2}}=\frac{u_A(\bar{q})}{\sqrt{2}}$
7	**Effective number of observations and of degrees of freedom**	
	Statistically independent (as of the primary sample) n $\nu=n-1$	**Autocorrelated** for regular sampling: $t_i=t_1+(i-1)\Delta T$ $n_{eff}\equiv\frac{n}{1+\frac{2}{n}\sum_{k=1}^{n-1}(n-k)\rho_k}$ (9) $\nu_{eff}=n_{eff}-1$ (11) where: ρ_k - normalized autocorrelation function $\rho_k=\frac{1}{n-k}\frac{\sum_{i=1}^{n-k}(q_i-\bar{q})(q_{i+k}-\bar{q})}{s^2(q_i)}$ (5) k – number of periods ΔT (distance) between any two regularly sampled observations
8	**Statistical measure of the measurement result inaccuracy**	
	Standard uncertainty type A $u_A(x)\equiv s(\bar{q})=\sqrt{\frac{1}{n(n-1)}\sum_{i=1}^{n}(q_i-\bar{q})^2}$ (4)	**Effective standard deviation of m. l. parameter *x*** e.g.: 1) $u_{A\,eff}(\bar{x})\equiv s_{eff}(\bar{x})=\frac{s(q_i)}{\sqrt{n_{eff}}}$ (10) 2) $s_{eff}(q_{V/2})=s_{V/2}(n_{eff})$ 3) $s_{eff}(q_{med})=s_{med}(n_{eff})$
	Continuation by procedure recommended by ISO GUM for type B and expanded uncertainties	

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