Evaluation of the type A uncertainty in measurements with autocorrelated observations

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Abstract. Described is the proposal of application of the GUM uncertainty type A evaluation to measurements with auto-correlated observations. The first step to it is the identification and cleaning of the raw sample data from the regularly variable components. Then formulas for standard deviation of the sample and of the mean value are expressed with the use correction coefficients or the so-called "effective number" of observations. These quantities depend on number of observations and on the sample autocorrelation function and allow to calculate the expanded uncertainty due to the GUM recommendations. The method of estimation of autocorrelation function for the sample data is also given. Considerations are illustrated by examples.

1. Introduction

The international guide about evaluation of uncertainty in measurement known under acronym GUM covers only measurement of the variable which data is randomly distributed but no related statistically (i.e. without autocorrelation of their data). Then use of GUM is limited in many types of measurements. In particular, it was not established how to estimate uncertainty in measurements of the processes variable in time or space.

This paper will synthetically discuss the results of some Polish work on the determination of measurement uncertainty of regularly sampled measurand, covered in detail in publications [1] - [6] and their bibliographies. This includes preparing of the raw data sample to further calculations by removal from it regularly variable components (i.e. "cleaning of the raw sample"). Then the estimation of sample proper uncertainty type A for known autocorrelation function \( \rho \) is given. Method how to find from the sample data the estimator \( r \) of the a priori unknown autocorrelation function is also presented.

2. "Cleaning" the raw data

The process of collecting measurement observations is now usually automated. The values of the measurement signal or the output readings are discrete as a result of sampling of the input analog signal with properly chosen frequency and A/D conversion.
The dispersion of the "raw" values of measurement observations is caused by reason of both random and determined type, and also as a result of changes of measurand itself, and changes of the internal parameters of the measuring circuit and environmental conditions. It is different for each of the samples taken at different times, measured by different instruments, and even by the same device over its lifetime. Random changes of the observations can be stationary or no stationary. There are short-term noise (called outliers), which prior to the assignment of values and the uncertainty of the measurements should be identified and eliminated from the raw data. Changes in the form of a regular (non periodic) component, i.e. the trend and periodic components affect the shape of the histogram of the sample, the mean value and uncertainty of type A. And there are also undesirable.

Calculations of the result and accuracy of measurement are made usually with the following assumptions:
- time $T_n$ to collect the sample of $n$ observations (width of the measurement window) was chosen properly, i.e. the random component of the sample can be assumed stationary,
- the sampling is uniform with the constant frequency $n/T_n$, and
- the random component is additive only, i.e. independent from the measurand value, and is described by the normal probability distribution.

Then values $y(i)$ of the discrete output signal obtained by sampling are

$$y(i) = f(i) + f_R(i) + N(0,\sigma)$$

(1)

where: $i \in (1,n)$ - the current number of the sample observation obtained in time $t_i$, $f(i)$ - values (estimated from measurements) of the known a priori measurand function at times $t_i$, $f_R(i)$ - the values of other unwanted regular components in time $t_i$, and $N(0,\sigma)$ - normal random component with standard deviation $\sigma$.

The statistical uncertainty $\sigma_A$ of measurements should be estimated only from values of last random component $N(0,\sigma)$. The values of function $f(i)$ estimating the measurand and of the residual signal contains the unwanted non-known a priori regular component $f_R(i)$ should be subtracted.

**Example 1**

Figure 1a shows a series of successive $n=121$ "raw" results of measurement observations (black squares), obtained by regular sampling of the tested process [3]. You can see that the sample contains non-linear decreasing trend, there are not noticeable periodic components, and rather a small laceration of the data graph indicates that this data can be autocorrelated. After removing one outlier, using LSM (least squares) the polynomial was determined:

$$y(i) = (-7.65 \cdot 10^{-7}) i^2 + (6.6 \cdot 10^{-7}) i + 0.034.$$

**Figure 1.** An example of the measurement data sample collected sequentially by regular sampling: a) deviations from the mean value of the raw data and their systematic regularly variable component - drift identified by the least squares method; b) distributions: of the raw data (1), after subtraction of the drift (2) and Gaussian pdf curve fitted to that data (3).
Trend is modeled and removed from the sample data, assuming that it passes through the average value. In Figure 1b a histogram of the raw sample is given - (1) and histogram after removal of the trend - (2) and a matching criterion $\chi^2$ its normal (Gaussian) probability density function (pdf) - (3). Trend causing asymmetry and the existence of a large "tail" on the left of histogram (1), which does not meet the criterion of $\chi^2$, and with trend uncertainty $u_A$ is about 64% higher than $u_A=0.00219$ without it. Purification of the raw data significantly reduced $u_A$. For $n=120$ the relative standard deviation $s(u_A)/s\approx8.5\%$.

3. The uncertainty of mean value for correlated observations
Presented is a brief description of the problem. The sequence of measurement data obtained from the sampling process and purified from the deterministic component can be described by a stationary time series. Statistical correlations between realizations $X_i$, $X_{i+k}$ of such series is characterized by the autocorrelation function

$$\rho_k = \frac{\text{cov}(X_i, X_{i+k})}{\sigma_x \sigma_x}$$

(2)

Function $\rho_k$ depends on the frequency spectrum of the test process and is known or its estimate $r_k$ should be found from the measurement data. In measurement of physical quantities the correlation function is positive.

The relationship between standard deviation $\sigma(\bar{x})$ of the mean value and $\sigma$ of the individual correlated observation $x_i$ results from the variance of the sum of random variables [1, 2, 4]

$$\sigma(\bar{x}) = \frac{\sigma}{\sqrt{n_{\text{eff}}}}$$

(3)

Where

$$n_{\text{eff}} = \frac{n}{1 + 2 \sum_{k=1}^{\infty} (1 - k/n) \rho_k} = \frac{n}{1 + D_\rho}$$

(3a)

For the statistically independent observations $\rho_k \to 0$ (for $k \geq 0$), consequently $D_\rho = 0$ and formula (2) passes to the commonly known relation

$$\sigma(\bar{x}) = \frac{\sigma}{\sqrt{n}}.$$  

In opposite, when the observations are fully correlated (closely linked), i.e. $\rho_k \to 1$, with (3a) results

$$D_\rho \to \frac{2}{n} \sum_{k=1}^{n-1} (n-k) \cdot 1 = n-1$$

(4)

Then the standard deviation of the mean is the same as for a single observation of the sample because in the limit $\rho_k \to 1$ all subsequently repeated observations will be the same.

The value of $n_{\text{eff}}$ is needed to proper estimation of the standard deviations $s_a(\bar{x})$ , $s_a(\bar{x})$ of sample of autocorrelated observations [4 -6]. Their relations to the GUM parameters $s(x_i)$, $s(\bar{x})$ are

$$s_a(\bar{x}) = s_a(x_i) = \left[ \frac{1}{n(n_{\text{eff}}-1)} \sum_{i=1}^{n_{\text{eff}}}(x_i - \bar{x})^2 \right]^{1/2}$$

(5)

or

$$s_a(\bar{x}) = k_{\rho, n_{\text{eff}}} s(\bar{x})$$

(5a)

where:

$$s(\bar{x}) = \frac{s(x_i)}{\sqrt{n}}, \quad k_{\rho, n_{\text{eff}}} = \left[ 1 - \frac{n_{\text{eff}}-1}{n(n_{\text{eff}}-1)} \right]^{1/2}$$

(5b), (5c)
\( s^2(x_i) = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})^2 , \) \hspace{2cm} (5d)

\( s_a(x_i) = k_a s(x_i) \) \hspace{2cm} (5e)

where:

\( k_a = \left[ \frac{n_{eff}(n-1)}{n(n_{eff}-1)} \right]^{1/2} \approx 1 ; \) \hspace{2cm} (5f)

For the autocorrelation data the effective number degrees of freedom \( \nu_{eff} \) can also be used. Value of \( \nu_{eff} \) is defined approximately [4-6] as

\[ \nu_{eff} = \frac{n}{1 + 2 \sum_{k=1}^{n-1} \rho_k^2} - 1 \] \hspace{2cm} (6)

But \( \nu_{eff} \neq n_{eff} - 1 \) [4, 5]. The relative dispersion of the standard deviation is:

\[ u(s_a) = u(s_a(\bar{x})) \approx \frac{1}{(2 \nu_{eff})^{1/2}} \] \hspace{2cm} (7)

4. Estimator of the autocorrelation function of measurement data sample

The autocorrelation function is usually not known and needs to be estimated from the measurement data. The most commonly used and implemented in computer programs has form

\[ r_k = \frac{\sum_{i=1}^{n-k} (x_i - \bar{x})(x_{i+k} - \bar{x})}{s^2(q_i)} \] \hspace{2cm} (8)

Estimate \( n_\ell \) (Figure 2a) has two qualitatively different parts. For small distances \( k \) is the falling edge, in which contains real information about the autocorrelation function. The remainder tail is the image of a rather large fluctuations of the correlated noise.

Replacement of the function \( \rho_k \) by its estimate \( r_k \) in formula (3) gives an estimate of the effective number of observations \( n_{eff} \) not of the satisfied properties. The reason is the influence of autocorrelation function of the tail. According Zięba [4, 5] summation in (8) can be reduced to only a few initial estimates of \( r_k \) elements, i.e.

\[ \hat{n}_{eff} = \frac{n}{1 + 2 \sum_{k=1}^{n_{eff} \ell} \left( 1 - \frac{k}{n} \right) r_k} \] \hspace{2cm} (9)

The border value \( n_\ell \) is determined by the last non-zero element of the \( r_k \) estimate before its first passage through zero (FTZ method – so called from the first transit through zero). For example, this value for the curve on Figure 2a is \( n_\ell = 3 \). FTZ method is valid only for positive correlations.

Figure 2b [6], [4] shows two examples of probability distributions of the estimators obtained by Monte Carlo method. The distribution marked as teor on figure 2.b is calculated from the formula for uncorrelated observations of the standard deviation \( z = s / \sigma \) resulting from the distribution of \( \chi^2 \), where \( v \) was substituted by the effective number of degrees of freedom \( \nu_{eff} \).

The simulation studies using MC [5] show that in this case estimator \( \hat{n}_{eff} \) reduce the negative bias of the mean value \( \bar{x} \). Obtained value of \( \hat{n}_{eff} \) is used for calculations of \( s_a(x_i) \) and \( s_a(\bar{x}) \) by (5e) and (5).
a) The initial part of the estimate \( \rho_k \) of autocorrelation function computed from data of Figure 1a (after removing the trend from the raw data); b) Probability density functions for normalized estimators of the standard deviation by the first order autoregressive model AR(1) and the random sample size \( n=60 \) [5, 6]. Curves 1 and 2 are derived from MC simulations and relate, respectively, \( \sigma / \sigma_s \) and \( \sigma_s (\bar{x}) / \sigma (\bar{x}) \). Theoretical curve 'teor' has been calculated theoretically using the model (9) for \( \nu_{\text{eff}} = 22.7 \).

**Example 2**

Let us calculate the standard deviation of single measurement \( s_a(q_i) \) and of the mean value \( s_a (\bar{q}) \) of 120 data of observations \( q_i \) from Example 1 after withdrawal trend. The estimator \( r_k \) of their autocorrelation function is taken for \( n_c=3 \) according to Figure 2a. The large obtained value \( r_k=0.81 \) confirms autocorrelation of these data. Standard deviation without considering the autocorrelation is \( s(q_i) = 0.0241 \). At this value of \( r_k \) the formula (9) implies the estimate \( \nu_{\text{eff}} = 32.1 \) and from (5f) and (5c) the coefficient \( k_a = 1.012 \) and \( k_b = 1.96 \). Correlation do not significantly affect the \( s_a (\bar{q}) = 0.0244 \), and much more the \( u_A \), which increases about 2 times from \( s(\bar{q}) = 0.00219 \) to \( s_a (\bar{q}) = 0.00472 \). From (6) and (7): \( u(s_a)/s \approx 11\% \).

**5. Summary and conclusions**

Discussed issues aroused from the purpose of determining the measurement uncertainty for the measurement data obtained by sampling. This paper summarizes the research results of cleaning such raw data from their regular components [3] and the extension of calculating the uncertainty by the method type A of GUM to the autocorrelated data [1, 2] -[4-7]. The developed method is easy to use in the practice of measurement and can provide a basis to adopting it into the GUM upgrading.

Conclusions:

• For a limited time to collect measurement observations, a reduction of measurement uncertainty by increasing the sample size (by increasing the sampling rate) is unreliable, because it leads to the necessity to reflect the impact of autocorrelation function of observation.
• Before calculating the uncertainty \( u_A (x) \) appropriate computational methods must first be used to identify and remove from the raw results the systematic (non periodic and periodic) components.
• For such a cleaned values of the observations one needs to know or estimate the autocorrelation function. This function causes a significant increase in uncertainty \( u_A \) compared to the calculated according to GUM. It corresponds to the lower effective number of independent measurements to be taken into account in estimating the standard uncertainty. The content specified adjusted formulas.

\(^1\) Model AR (1) - autoregressive time series of the first order, for which \( r_k = a^k \) [4]
• Programs for the calculation of uncertainty should be supplemented by algorithms for the identification and elimination from the "raw" data the regular components and to obtain estimators of the autocorrelation function from such cleaned measured data.

• Evaluation of the uncertainty \( u_A \) for autocorrelated data discussed here, is valid, as in GUM, for the model of normal distribution. For other distributions, this method requires further investigation.

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