Uncertainty analysis for measurement of measurand

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ABSTRACT

For measuring the true value of a measurand, vague statistical concept of measurand results in inefficient uncertainty analysis of measurement. The vagueness is caused by the fact that true value of the measurand is an unknown parameter such as population mean or median and the measurement of this true value is a random variable. Generally a parameter may be estimated remarkably more efficiently than the prediction of the random variable. The classical uncertainty analysis in the literature has been developed based on the structure that a measurand is a random variable. This misspecification of statistical concept costs serious price of sacrificing efficiency in terms of length of the uncertainty interval. The purpose of present study is to formally formulate a statistical model for the true value of measurand and provide an uncertainty analysis for the measurement of this true value.

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1. Introduction

An experiment for measuring a measurand is a method through a process that tries to gain or discover knowledge of the measurand. Measurements always have errors and therefore uncertainties. General rules for evaluating and reporting uncertainty in measurement has been published by the most important and internationally widespread metrological publication-ISO (the International Standards Organisation) *Guide to the Expression of Uncertainty in Measurement* [2]. According to the GUM, the measurement result should be reported with a specified confidence as an uncertainty interval defining the range of values that could reasonably be attributed to the measurand. Unfortunately, techniques for uncertainty analysis of measurement guided by the GUM do not, in our opinion, gain appropriate knowledge of measurand due to conflicting views of statistical concepts on measurand.

In GUM B.2.9, the measurand is defined as a particular quantity subject to measurement, and Baratto [1] proposed a precise and comprehensive definition of measurand guiding that it is a specific quantity that one intends to measure. These interpretations of measurand indicate that the interest of measurement for the measurand is to gain the knowledge of the true value, denoted by θ_y, of measurand while GUM 3.1.1 stated that the objective of a measurement is to determine the true value of the measurand. However, it is known that an estimate of this unknown true value is subject to measurement error and then it needs to perform an uncertainty analysis. For uncertainty analysis, GUM 3.3.1 guided that uncertainty should reflect the lack of exact knowledge of the true value. Hence, an uncertainty interval is supposed defining the range of measurement values that could reasonably be attributed to the true value of measurand. Unfortunately, the uncertainty analysis in the guideline of GUM is generally done by formulating the measurand as the random variable, denoted by Y, of measurement and constructing the uncertainty interval representing a coverage interval for this random variable Y with a fixed coverage probability 0.95. This uncertainty interval ensures that in a long run of experiments there is a proportion 0.95 of measurement observations of variable Y being contained in the interval. This is generally done in the literature and introduced in college courses of measurement science and introductory laboratory (see, for examples, Dunn [5] and Taylor [6]), but it does not provide direct information for knowledge of the true value θ_y. In this paper, we

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clarify the differences between uncertainty analyses of estimation of true measurand value θ_y and the measurement of variable Y. We also introduce the uncertainty interval for true value estimation.

2. A simple description of two uncertainty analyses

Our interest is to investigate uncertainty interval that truly defines the range of values that could reasonably be attributed to the true value of measurand. An uncertainty interval (called confidence interval in the literature of Statistics) of θ_y matches this need. A random interval (T_1, T_2), constructed from observations of Y, is a 95% uncertainty interval for true value θ_y if it satisfies

$$0.95 = P_{\theta_y}\{T_1 \leqslant \theta_y \leqslant T_2\}.$$

This random interval (T_1, T_2) ensures that in a long run of experiments there are observed intervals (t_1, t_2) with proportion 0.95 that covers the true value θ_y. The direct information provided by such experiment about the true value of the measurand seems to be more interesting to the metrologist than the information about the measurement variable Y itself. Let us consider an example for interpretation of this uncertainty interval and the classical one in problem of measurement of a measurand.

Example 1. Suppose that there is a pencil on a table and we like to measure its length. The knowledge we want to develop is the true length of the pencil with pencil as, from the view of GUM, the particular quantity to be measured. Hence, parameter θ_y represents this unknown true length. To measure the true length θ_y of the pencil, the measurement of true length is a random variable Y that follows some probability distribution with mean θ_y and repeated measurements can be done. Suppose that we have random variables $Y_1, \ldots, Y_n$ representing n repeated measurements of θ_y. We also assume that the instrument for measurement reveals that these random variables are independent and identically distributed with normal distribution $N(\theta_y, \sigma^2)$. The best estimate of true value θ_y is $\overline{Y} = \frac{1}{n}\sum Y_i$. With symmetric distribution, the 0.95 uncertainty interval for future observation Y is appropriately set as $(\theta_y - z_{0.025}\sigma, \theta_y + z_{0.025}\sigma)$, where $z_{0.025}$ is the coverage factor representing the 0.975 quantile of the standard normal (Gaussian) distribution $N(0, 1)$. Hence, a 95% uncertainty interval for Y is $(\overline{Y} - z_{0.025}S, \overline{Y} + z_{0.025}S)$, where S is the sample standard deviation with $S^2 = \frac{1}{n-1}\sum(Y_i - \overline{Y})^2$.

Suppose that we have a sequence of five measurements, in unit mm, as

$$41.12, \quad 41.08, \quad 41.10, \quad 41.14, \quad 41.06.$$

These observations are the sample realization of the repeated measurements $Y_1, \ldots, Y_5$. The average of these measurements is $\bar{y} = 41.10$ mm and sample standard deviation is $s = 0.032$ mm. The 95% uncertainty interval for the variable Y is

$$41.10 \pm 1.96 \times 0.032 \text{ mm} = 41.10 \pm 0.063 \text{ mm}.$$

From the sense of probability, the next realization of measurement Y will be between 41.037 mm and 41.163 mm with probability 0.95.

By letting $\hat{\theta}_y = \overline{Y}$, a 95% uncertainty interval for θ_y, derived from the fact that $\frac{\overline{Y} - \theta_y}{S/\sqrt{n}}$ has a t-distribution $t(n-1)$, where $n-1$ is the degrees of freedom, is $\hat{\theta}_y \pm t_{0.025}(n-1)\frac{s}{\sqrt{n}}$, where $t_{0.025}(n-1)$ is the coverage factor in this uncertainty interval representing the 0.975 quantile of t-distribution $t(n-1)$. In this case, it is

$$41.10 \pm 2.045 \times \frac{0.032}{\sqrt{5}} \text{ mm} = 41.10 \pm 0.029 \text{ mm}.$$

The uncertainty intervals of measurement Y and true value θ_y are with the same center point $\hat{y} = \hat{\theta}_y = 41.10$ mm. However, the expanded uncertainty for the true value θ_y is 0.029 mm which is significantly smaller than 0.063 mm, the expanded uncertainty for the measurement variable Y. This uncertainty interval indicates that we have 95% confidence with true length of the pencil to be between 41.071 mm and 41.129 mm. This conclusion gains more practical information about the true value of measurand, the true length of the pencil.

For large sample size, coverage factor $t_{0.025}(n-1)$ may be replaced by $z_{0.025}$. In this example, this replacement results expanded uncertainty 0.029 mm, revealing a very good approximation.

3. Models for measurement variable and true value of measurand

For general study of uncertainty analysis, the GUM was considered with the assumption that the true value of measurand cannot be measured directly, but is determined from several input (influence) quantities. We assume that there are fixed values $\theta_1, \ldots, \theta_k$ representing true but unknown values for input quantities such that the true value θ_y of measurand may be formulated through a known functional relation as

$$\theta_y = h(\theta_1, \ldots, \theta_k). \tag{1}$$

This relation between true value of measurand and true values of input quantities is not, except for very special cases, considered in GUM and literature. This reflects a conceptual confusion that classical statistical theory treats problems where parameters themselves are not measurable but metrology deals with problems where parameters themselves are measurable.

Any measurement for quantity θ_j is subject to errors, random errors such as short-term fluctuations in temperature, humidity or variability in the performance of the measurer and systematic errors such as offset of a measuring instrument, drift in its characteristics, personal bias in reading. This random effect reflects the variation of repeated measurement values. Hence, this measurement function represents a relationship for measurand not only a physical law but also a measurement process.

In measuring the true values $\theta_1, \ldots, \theta_k$, let us denote the corresponding measurement (input) quantities as $X_1, \ldots, X_k$. GUM formulates the measurement of measurand Y as the function h of input quantities $X_1, \ldots, X_k$ as

$$Y = h(X_1, \ldots, X_k). \tag{2}$$

Since $X_1,\ldots,X_k$ are random variables, this measurand Y is also a random variable. This formulation of measurand is the basis for developing uncertainty analysis as has been introduced in GUM and literature of uncertainty analysis. We, in next section, review the uncertainty analysis for measurement of variable Y and introduce the uncertainty analysis for true value estimation of measurand.

4. Uncertainty intervals for two models of measurand

For each j, it is assumed that there is a sample $X_{ji}, i = 1,\ldots,n_j$ available drawn from distribution of input quantity X_j. Let the realizations of this sample be x_{ji}, $i = 1,\ldots,n_j$. The classical uncertainty analysis following the GUM proposes to use sample mean $\hat{x}_j = \bar{x}_j$ as predicted value of input quantity X_j. Then, the predicted value (estimate) of measurement variable Y is

$$\hat{y} = h(\hat{x}_1,\ldots,\hat{x}_k).$$

(In GUM or literature, $\hat{y}$ is called the estimate of measurand.) For presenting the uncertainty in this prediction, the GUM defines variance of X_j as $\sigma_j^2 = E[(X_j - \hat{x}_j)^2]$ and covariance of X_j and X_ℓ as $\sigma_{j\ell} = E[(X_j - \hat{x}_j)(X_\ell - \hat{x}_\ell)]$, assuming that $\hat{x}_j$ and $\hat{x}_\ell$ are, respectively, the means of the distributions of input variables X_j and X_ℓ. With predicted value $\hat{y} = h(\hat{x}_1,\ldots,\hat{x}_k)$, the first-order Taylor series approximation to the measurement variable Y about the estimates $(\hat{x}_1,\ldots,\hat{x}_k)$ gives

$$Y \approx \hat{y} + \sum_{j=1}^{k} b_j(X_j - \hat{x}_j), \tag{3}$$

where $b_j = \frac{\partial h(x_1,\ldots,x_k)}{\partial x_j}\big|_{x_h=\hat{x}_h, h=1,\ldots,k}$, called the uncertainty coefficient with respect to influence quantity X_j. The combined standard uncertainty is defined as the estimated standard deviation of measurement variable Y, where the variance of Y is $\sigma_y^2 = E[(Y - E(Y))^2]$. From formulation (3), the variance σ_y^2 is approximated as

$$\sigma_y^2 \approx \sum_{j=1}^{k} b_j^2 \sigma_j^2 + \sum_{j\neq\ell} b_j b_\ell \sigma_{j\ell}. \tag{4}$$

The uncertainty interval introduced in GUM is defined as

$$Y = \hat{y} \pm kU, \tag{5}$$

with $U = \hat{\sigma}_y$, an estimate of σ_y, and k being the coverage factor so that this uncertainty interval may cover the possible values of measurement variable Y with a fixed probability such as 0.95. According to GUM, the coverage factor k may be determined as quantile of the t-distribution or normal distribution. Interpreted by Willink [10], this uncertainty interval in a potential series of equally-reliable independently-determined intervals encloses the value of the measurement variable Y averagely in 95 out of every 100 measurements. This violates the objective of GUM 3.3.1 that an uncertainty interval represents a range of measurement values that could reasonably be attributed to the true value of measurand. We then propose uncertainty analysis for true value θ_y of (1).

Let $\hat{\theta}_j = \hat{\theta}_j(x_{j1},\ldots,x_{jn_j})$ be appropriate estimate of θ_j based on observations $\{x_{ji}, i = 1,\ldots,n_j\}$, for $j = 1,\ldots,k$. The estimate of the true value of measurand is defined as

$$\hat{\theta}_y = h(\hat{\theta}_1,\ldots,\hat{\theta}_k).$$

By letting $\hat{\theta}_j = \hat{x}_j$, it is appropriate to set the estimate of true value θ_y to be identical to the predicted value of variable Y. We may make analogous assumption in GUM that estimate $\hat{\theta}_y$ satisfies $E[\hat{\theta}_y] = \theta_y$. Then the variance of $\hat{\theta}_y$ is

$$\sigma_{\theta_y}^2 = E[(\hat{\theta}_y - \theta_y)^2],$$

while an estimate $\hat{\sigma}_{\theta_y}$ represents the standard uncertainty in concern of estimation of true value θ_y. The first-order Taylor's expansion for function h of $\hat{\theta}_y$ on estimate $(\hat{\theta}_1,\ldots,\hat{\theta}_k)$ yields

$$\hat{\theta}_y = \theta_y + \sum_{j=1}^{k} c_j(\hat{\theta}_j - \theta_j) + R_{\hat{\theta}_y}, \tag{6}$$

where we let $c_j = \frac{\partial h(\hat{\theta}_1,\ldots,\hat{\theta}_k)}{\partial \hat{\theta}_j}\big|_{\hat{\theta}_i=\theta_i, i=1,\ldots,k}$, the sensitivity coefficient with respect to influence parameter θ_j, and $R_{\hat{\theta}_y}$ is the remainder expressed by

$$R_{\hat{\theta}_y} = \frac{1}{2}\left[\sum_{j=1}^{k} \frac{\partial^2 h(\hat{\theta}_1,\ldots,\hat{\theta}_k)}{\partial\hat{\theta}_j^2}\bigg|_{\hat{\theta}_i=\theta_i+\delta(\hat{\theta}_i-\theta_i)} (\hat{\theta}_j - \theta_j)^2 \right.$$
$$\left. + \sum_{j\neq\ell} \frac{\partial^2 h(\hat{\theta}_1,\ldots,\hat{\theta}_k)}{\partial\hat{\theta}_j\partial\hat{\theta}_\ell}\bigg|_{\hat{\theta}_i=\theta_i+\delta(\hat{\theta}_i-\theta_i)} (\hat{\theta}_j - \theta_j)(\hat{\theta}_\ell - \theta_\ell)\right],$$

with $0 < \delta < 1$. When $\hat{\theta}_j \to \theta_j$, for all j, the remainder term approaches zero more quickly than the first-order terms in (6) and all the higher terms are generally neglected.

The variance $\sigma_{\theta_y}^2$ can be substituted into Eq. (6) to yield

$$\sigma_{\theta_y}^2 \approx E\left\{\left[\sum_{j=1}^{k} c_j(\hat{\theta}_j - \theta_j)\right]^2\right\}$$
$$= E\left\{\sum_{j=1}^{k} c_j^2(\hat{\theta}_j - \theta_j)^2 + \sum_{j\neq\ell} c_j c_\ell(\hat{\theta}_j - \theta_j)(\hat{\theta}_\ell - \theta_\ell)\right\}$$
$$= \sum_{j=1}^{k} c_j^2 \sigma_{\theta_j}^2 + \sum_{j\neq\ell} c_j c_\ell \sigma_{\theta_j\theta_\ell},$$

where $\sigma_{\theta_j}^2 = E[(\hat{\theta}_j - \theta_j)^2]$, the variance of $\hat{\theta}_j$, and $\sigma_{\theta_j\theta_\ell} = E[(\hat{\theta}_j - \theta_j)(\hat{\theta}_\ell - \theta_\ell)]$, the covariance between estimates $\hat{\theta}_j$ and $\hat{\theta}_\ell$. The combined standard uncertainty $\hat{\sigma}_{\theta_y}$ is contributed from the estimates of variances and covariances of parameter estimators $\hat{\theta}_j$'s. We remind that when the function h of (1) is highly nonlinear, then higher-order terms in the Taylor series expansion of h should be included in (6).

Defining the uncertainty quantities $\hat{\sigma}_{\theta_j}^2$, $\hat{\sigma}_{\theta_j\theta_\ell}$ and $\hat{c}_j^2$ as, respectively, estimates of $\sigma_{\theta_j}^2$, $\sigma_{\theta_j\theta_\ell}$ and c_j^2, the combined standard uncertainty for measurement of true value θ_y is $\hat{\sigma}_{\theta_y}$ with

$$\hat{\sigma}_{\theta_y}^2 = \sum_{j=1}^{k} \hat{c}_j^2 \hat{\sigma}_{\theta_j}^2 + \sum_{j\neq\ell} \hat{c}_j \hat{c}_\ell \hat{\sigma}_{\theta_j\theta_\ell}.$$

The uncertainty interval for the estimation of true value of measurand is

$$\theta_y = \hat{\theta}_y \pm U_{\theta_y}, \tag{7}$$

where U_{θ_y} is the expanded uncertainty defined by

$$U_{\theta_y} = k_{\theta_y}\hat{\sigma}_{\theta_y}, \tag{8}$$

where k_{θ_y} is a coverage factor chosen to produce the uncertainty interval having a level of confidence such as 0.95. This uncertainty interval does match the objective of GUM 3.3.1 that it defines a range of measurement values that could reasonably be attributed to the true value of measurand.

Proposing uncertainty analysis for estimation of true value θ_y is not new. Willink and Hall [9] considered a multivariate model $Y = \mu + \epsilon$ with ϵ having multivariate normal distribution with zero mean vector and an unknown covariance matrix. Also, Wang and Iyer [8] considered the same but univariate model. These models which define parameter μ as true value of measurand are too simple that they have very limited applications in science of measurement from the view of the GUM.

5. Efficiency property for uncertainty interval of true value estimation of measurand

We may expect to gain efficiency in using the expanded uncertainty U_{θ_y} for estimation of true value θ_y rather than the expanded uncertainty for prediction of variable Y. The standard uncertainty for prediction of variable Y is based on a linear combination of σ_j's and $\sigma_{j\ell}$'s, where σ_j^2's are variances of input quantities X_j's and $\sigma_{j\ell}$'s are covariances between these quantities. On the other hand, the standard uncertainty for estimation of true value θ_y is based on a linear combination of σ_{θ_j}'s and $\sigma_{\theta_j\theta_\ell}$'s, where $\sigma_{\theta_j}^2$'s are variances of estimates $\hat{x}_j$'s and $\sigma_{\theta_j\theta_\ell}$'s are covariances between these estimates. With X_j being measurement of θ_j, statistical theory indicates that prediction of X_j is generally with larger uncertainty than the estimation of θ_j is, resulting in σ_j^2 being larger than $\sigma_{\theta_j}^2$. This leads to the desired results that combined standard uncertainty for estimation of true value is significantly smaller than that for the prediction of measurement of variable.

To provide a theoretical support for this indication, we consider the model that $(X_{1i}, X_{2i}, \ldots, X_{mi})$, $i = 1, \ldots, n$ are a random sample with mean $(\theta_1, \ldots, \theta_k)$ and covariance matrix

$$\Sigma = \begin{pmatrix} \sigma_1^2 & \sigma_{12} & \ldots & \sigma_{1m} \\ \sigma_{21} & \sigma_2^2 & \ldots & \sigma_{2m} \\ \vdots & \vdots & \vdots & \vdots \\ \sigma_{m1} & \sigma_{m2} & \ldots & \sigma_m^2 \end{pmatrix}.$$

In this model, we let $\hat{\theta}_j = \hat{x}_j = \bar{x}_j$, $j = 1, \ldots, m$. This indicates that $c_j = b_j$ and $\sigma_{\theta_j}^2 = \frac{\sigma_j^2}{n} = \frac{Var(X_j)}{n}$ and covariance $\sigma_{\theta_j\theta_\ell} = \frac{\sigma_{j\ell}}{n} = \frac{Cov(X_j X_\ell)}{n}$. Hence, we have

$$\sigma_{\theta_y}^2 \approx \frac{1}{n}\left\{ \sum_{j=1}^k b_j^2 \sigma_j^2 + \sum_{j\neq\ell} b_j b_\ell \sigma_{j\ell} \right\} = \frac{1}{n}\sigma_y^2.$$

This implies that the uncertainty interval for estimation of true value θ_y is $\hat{\theta}_y \pm k\frac{U}{\sqrt{n}}$. The combined standard uncertainty U_{θ_y} for estimation of true value θ_y is proportion $\frac{1}{\sqrt{n}}$

of the combined standard uncertainty U for prediction of measurement variable Y. This is the main contribution of using uncertainty interval for estimation of true value θ_y instead of using it for prediction of measurement variable Y. We summarized the differences between the classical and our proposed uncertainty analyses for the measurand as shown in Table 1.

Let us consider another example for interpretation.

Example 2. Sim and Lim [7] and Willink [10] considered random measurand Y as the velocity of a type of wave in some medium and measurement function as

$$Y = \frac{X_1}{X_2},$$

where X_1 is the distance from a transmitter to a receiver, X_2 is the time of flight and they are independent. Physically there are true but unknown values of distance and time of flight. The concerned velocity is appropriately formulated as

$$\theta_y = \frac{\theta_1}{\theta_2},$$

where θ_1 is the true distance from a transmitter to a receiver and θ_2 is the true time of flight. It is supposed that $\hat{\theta}_1 - \theta_1$ is distributed as $-2 \times 10^{-4}\theta_1 V_1$, where V_1 follows a chi-square distribution; $\hat{\theta}_2 - \theta_2$ is distributed as UV_2, where U follows the uniform distribution $U(-4.5 \times 10^{-6}, -5.5 \times 10^{-6})$ and V_2 follows an exponential distribution with mean 1. Furthermore, there estimates $\hat{\theta}_1 = 4.931$ mm, and $\hat{\theta}_2 = 10.9 \times 10^{-3}$ s.

According to the independence, we can see that the combined standard uncertainty for measurement of true value θ_y is

$$\hat{\sigma}_{\theta_y}^2 = \frac{1}{\hat{\theta}_2^2}\frac{\hat{\sigma}_{\theta_1}^2}{n} + \left(\frac{\hat{\theta}_1}{\hat{\theta}_2^2}\right)^2\frac{\hat{\sigma}_{\theta_2}^2}{n}.$$

Hence, a 95% uncertainty interval for the true measurand θ_y is

$$\left(\frac{\hat{\theta}_1}{\hat{\theta}_2} - z_{0.025}\hat{\sigma}_{\theta_y}, \frac{\hat{\theta}_1}{\hat{\theta}_2} + z_{0.025}\hat{\sigma}_{\theta_y}\right).$$

We list this 95% uncertainty interval with several sample sizes in Table 2.

The 95% uncertainty interval based on GUM for the random measurand is

$$(451.91, 452.86). \tag{9}$$

Sim and Lim has computed some other types 95% uncertainty intervals that are very close to (9). Comparing this with the obtained uncertainty intervals for the true

Table 1
Comparisons of two uncertainty intervals.

Approach	Measurand	UI[*] length
Classical	Variable	$2kU$
Proposed	Parameter	$2k\frac{U}{\sqrt{n}}$

[*] Uncertainty interval.

Table 2
Ninety-five percent uncertainty intervals for the true measurand θ_y.

Sample size	95% Uncertainty interval
$n = 1$	(451.91, 452.86)
$n = 5$	(452.17, 452.60)
$n = 10$	(452.23, 452.54)
$n = 30$	(452.30, 452.47)
$n = 50$	(452.32, 452.45)

measurand, we may be more efficient in prediction of true measurand than in prediction of future observation of random measurement.

In the last we need to illustrate the determination of coverage factor k_{θ_y}. The coverage factor k of (5) in the GUM for the uncertainty interval for prediction of measurement variable Y is obtained by assuming that the measurements X_j's follow, respectively, normal distributions $N(\theta_j, \sigma_j^2)$ as the design mentioned above. This is generally not true in practice. In fact, X_j's often follow asymmetric distributions. A supplement [3] to GUM and some authors, for examples, Cox and Siebert [4] and Willink [10], have devoted to develop the uncertainty analysis for measurement quantities of asymmetric distributions. There is another benefit for the development of uncertainty analysis for estimation of true value θ_y. It is that $\hat{\theta}_y$ of (6) is approximately normal, no matter how the input quantities are distributed, if we let $\hat{\theta}_j = \overline{X}_j$, since, from the central limit theorem, $\overline{X}_j$ is asymptotically normal. This benefit of asymptotic normality is not shared by the uncertainty interval for prediction of mea-

surement variable Y since Taylor expansion of (3) of Y depends on distribution of X_j, and asymptotic property cannot be applied on X_j since variable X_j is not a function of a sample. Hence, the coverage factor k_{θ_y} of (8) can be generally determined as quantile of the t-distribution or normal distribution.

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