Measurement 44 (2011) 1526–1530

Contents lists available at ScienceDirect

Measurement

journal homepage: www.elsevier.com/locate/measurement

Generalized expressions of second and third order for the evaluation of standard measurement uncertainty

M.A.F. Martins *, R. Requião, R.A. Kalid

Programa de Pós-Graduação em Engenharia Industrial, Universidade Federal da Bahia, Rua Aristides Novis, 02, Federação, 40210-630 Salvador, Bahia, Brazil

ARTICLE INFO

Article history:
Received 21 October 2010
Received in revised form 6 May 2011
Accepted 9 June 2011
Available online 16 June 2011

Keywords:
Measurement uncertainty
Higher order uncertainties
Propagation of uncertainties
Monte Carlo method
Non-linear models

ABSTRACT

The Guide to the Expression of Uncertainty in Measurement (GUM) requires the use of a first-order Taylor series expansion for propagating uncertainties. However, when the measurement function is strongly non-linear the use of this linear approximation may be inadequate and therefore higher order terms from the Taylor series cannot be neglected. The present paper aims to derive generalized expressions of second and third order for the evaluation of the estimate of a measurand and its associated standard uncertainty. A case study is given to illustrate an application of the proposed methods and the results obtained with the GUM method are compared to the corresponding ones when applying the method proposed in GUM Supplement 1.

1. Introduction

The Guide to the Expression of Uncertainty in Measurement (GUM) [1] is internationally recognized for the evaluation of measurement uncertainty. The GUM method uses a first-order Taylor series approximation for evaluating the estimate of a measurand and its associated standard uncertainty, via the law of propagation of uncertainties (LPU). In most practical cases that conventional LPU approach is enough to characterize the measurement uncertainty even in non-linear measurement functions. Nevertheless, its use is inappropriate when the non-linearities of the measurement function are significant. In these specific cases, GUM recommends that the estimate of the measurand should be calculated distinctly when the models are non-linear ([1], clause 4.1.4), which has advantages and disadvantages according to Bich et al. [2]. GUM also advises the use of some higher order terms to be added to the standard uncertainty, as will be presented later.

A more general approach is adopted by GUM Supplement 1 (GUM S1) [3] which treats the numerical evaluation of measurement uncertainty with a Monte Carlo method as an implementation of the propagation of probability density functions (PDFs). The GUM S1 method is expected to provide a more valid uncertainty evaluation than that given by GUM when: the measurement function is strongly non-linear; PDFs for the values of any quantities are asymmetric or non-Gaussian. Nevertheless, it requires considerable computational effort and can also accumulate numerical errors if the computational algorithm of the random numbers generator is not carefully developed [4,5].

As result of the preceding discussion on the GUM and GUM S1 approaches, alternative methods can be developed to overcome the limitations imposed by these approaches, i.e. new methods characterizing the non-linearities of the measurement functions with negligible computational costs. At present, some works in the literature have taken into account these issues. For example, Lira [6] presented the second order expression for standard uncertainty based on the third and fourth statistical moments for measurement functions with only one input quantity; Wang and Iyer [7] proposed a generalized expression of second order for standard uncertainty in measurement functions

* Corresponding author.
E-mail addresses: marcio.engquimica@gmail.com (M.A.F. Martins), reinereng@gmail.com (R. Requião), kalid@ufba.br (R.A. Kalid).

0263-2241/$ - see front matter © 2011 Elsevier Ltd. All rights reserved.
doi:10.1016/j.measurement.2011.06.008

with all input quantities to be mutually independent and Gaussian; Mekid and Vaja [8] developed expressions of second and third order for both the estimate and standard uncertainty of the measurand for measurement functions composed of one and two input quantities.

Inspired by Mekid and Vaja's work we have developed generalized expressions of second and third order for both the estimate and the standard uncertainty of a measurand based on the LPU approach. These expressions can be used for N mutually independent input quantities which make up the measurement function.

2. Review of GUM

A major achievement of GUM consists of an approach for combining uncertainty from frequentist statistics (Type A evaluation of measurement uncertainty) and Bayesian statistics (Type B evaluation of measurement uncertainty). In this approach, GUM considers that all the quantities are characterized by a PDF which describes the possible values of these quantities. PDF can usually be summarized in terms of parameters such as mean and variance (and standard deviation) which are used in the evaluation of measurement uncertainty. Such summaries are stated as

$$x_i = \mathrm{E}[X_i] \triangleq \int_{-\infty}^{+\infty} \xi_i g_{X_i}(\xi_i) d\xi_i \tag{1}$$

and

$$u^2(x_i) = \mathrm{Var}[X_i] = \mathrm{E}[(\xi_i - x_i)^2] \triangleq \int_{-\infty}^{+\infty} (\xi_i - x_i)^2 g_{X_i}(\xi_i) d\xi_i, \tag{2}$$

where ξ_i represents the possible values of the random variable X_i and g_{X_i} represents the PDF for X_i. Eq. (1) represents the first statistical moment which denotes the expectation of X_i, the so-called expectation operator. Eq. (2) represents the second central moment and, therefore, it denotes the variance of X_i, the so-called variance operator. According to GUM, Eqs. (1) and (2) represent the estimate (x_i) of a quantity X_i and the square of the standard uncertainty ($u^2(x_i)$) associated with the estimate x_i, respectively.

In most practical cases, the measurand Y is not measured directly but is determined from N other input quantities (X_i) which are related through a known functional relationship of the form

$$Y = f(X_1, \ldots, X_i, \ldots, X_N), \tag{3}$$

where the function f is generally determined from phenomenological or empiric modeling and may or may not be explicit and may be solved analytically or numerically. Furthermore, this function should include all known corrections, such as systematic effects that require modeling.

From Eq. (3) we can evaluate the estimate of the output quantity (measurand) and consequently its standard uncertainty. Therefore, the measurement function is fundamental for the evaluation of measurement uncertainty as any mistake made in its modeling will lead to quite misleading results. A detailed study [9] addresses the importance of the influence quantities for the careful development of a measurement function.

The GUM method consists of propagating the estimates, the standard uncertainties and the covariances of the N input quantities X_i through a linear approximation of the measurement function determined from the first-order Taylor series expansion around the estimates x_i. Therefore, the measurement function (Eq. (3)) may be rewritten as

$$Y \approx Y_{1\mathrm{ord}} = f(x_1, \ldots, x_i, \ldots, x_N) + \sum_{i=1}^{N} \left(\frac{\partial f}{\partial X_i}\right)(X_i - x_i), \tag{4}$$

where the partial derivatives $\frac{\partial f}{\partial X_i}$, called *sensitivity coefficients*, are evaluated at estimates x_i.

The estimate of the measurand (y) is obtained by evaluating the expectation operator on either side of Eq. (4), i.e.

$$y \approx y_{1\mathrm{ord}} = f(x_1, \ldots, x_i, \ldots, x_N). \tag{5}$$

The standard uncertainty associated with the estimate $y_{1\mathrm{ord}}$($u(y_{1\mathrm{ord}})$) is obtained by subtracting Eq. (4) from Eq. (5), squaring both sides and taking the expectation operator from either side

$$u^2(y_{1\mathrm{ord}}) = \sum_{i=1}^{N} \left(\frac{\partial f}{\partial X_i}\right)^2 u^2(x_i) + 2\sum_{i=1}^{N-1} \times \sum_{j=i+1}^{N} \left(\frac{\partial f}{\partial X_i}\right)\left(\frac{\partial f}{\partial X_j}\right) u(x_i, x_j). \tag{6}$$

As we are assuming that the input quantities are mutually independent in this work, i.e. the covariances are null ($u(x_i,x_j) = 0, \forall i \neq j$), therefore Eq. (6) reduces to

$$u^2(y_{1\mathrm{ord}}) = \sum_{i=1}^{N} \left(\frac{\partial f}{\partial X_i}\right)^2 u^2(x_i). \tag{7}$$

Eq. (7) represents a good estimate for the standard uncertainty when the measurement function is linear or weakly non-linear. But when the non-linearities in this function are significant, GUM ([1], note at clause 5.1.2) recommends the use of some higher order terms in combination with Eq. (7) for the evaluation of the standard measurement uncertainty, namely

$$\sum_{i=1}^{N}\sum_{j=1}^{N} \left\{ \frac{1}{2}\left(\frac{\partial^2 f}{\partial X_i \partial X_j}\right)^2 + \left(\frac{\partial f}{\partial X_i}\right)\left(\frac{\partial^3 f}{\partial X_i \partial X_j^2}\right) \right\} u^2(x_i) u^2(x_j). \tag{8}$$

However, there are restrictions on the use of these terms: all input quantities X_i must be independent and Gaussian, see [10] for further clarification.

3. Higher order methods

The evaluation of the standard uncertainty based on higher order expressions (e.g. second and third) through the LPU approach requires the second and third order Taylor series approximation for a measurement function. This procedure also requires higher order statistical moments, such as the third, fourth, fifth and sixth moments. In the GUM context, the third and fourth moments may be related to the variance (standard uncertainty squared) through parameters such as skewness and kurtosis, respectively.

Skewness is a measure of the asymmetry of a PDF. It is defined from the third central moment:

$$\mathrm{E}[(\xi_i - x_i)^3] \triangleq \int_{-\infty}^{+\infty} (\xi_i - x_i)^3 g_{X_i}(\xi_i) d\xi_i. \tag{9}$$

The parameter skewness is defined in the following equation:

$$\gamma \triangleq \frac{\mathrm{E}[(\xi_i - x_i)^3]}{\{\mathrm{E}[(\xi_i - x_i)^2]\}^{3/2}}. \tag{10}$$

Therefore, if we put the skewness γ in terms of standard uncertainty, it can be written as

$$\mathrm{E}[(\xi_i - x_i)^3] = \gamma u^3(x_i). \tag{11}$$

Kurtosis is a measure of concentration about the expectation of a PDF. It is defined from the fourth central moment:

$$\mathrm{E}[(\xi_i - x_i)^4] \triangleq \int_{-\infty}^{+\infty} (\xi_i - x_i)^4 g_{X_i}(\xi_i) d\xi_i. \tag{12}$$

The parameter kurtosis is defined in the following equation:

$$\kappa \triangleq \frac{\mathrm{E}[(\xi_i - x_i)^4]}{\{\mathrm{E}[(\xi_i - x_i)^2]\}^{2}}. \tag{13}$$

Therefore, if we put the kurtosis κ in terms of the standard uncertainty, it can be written as

$$\mathrm{E}[(\xi_i - x_i)^4] = \kappa u^4(x_i). \tag{14}$$

3.1. Second order method

To evaluate the standard uncertainty using the second order method, first we expand the measurement function from the second order truncation of the Taylor's series. Thus, the expression obtained is

$$Y \approx Y_{2\mathrm{ord}} = f(x_1, \ldots, x_i, \ldots, x_N) + \sum_{i=1}^{N} \left(\frac{\partial f}{\partial X_i}\right)(X_i - x_i) + \frac{1}{2}\sum_{i=1}^{N}\left(\frac{\partial^2 f}{\partial X_i^2}\right)(X_i - x_i)^2 + \frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N}\left(\frac{\partial^2 f}{\partial X_i \partial X_j}\right) \times (X_i - x_i)(X_j - x_j). \tag{15}$$

As previously stated we consider that all input quantities are statistically independent, i.e. all the terms that have $\mathrm{E}[(X_i - x_i)(X_j - x_j)]$ may be written as $\mathrm{E}[(X_i - x_i)]\ \mathrm{E}[(X_j - x_j)]$. Furthermore, all terms with $\mathrm{E}[(X_i - x_i)]$ are equal to zero because $x_i = \mathrm{E}[X_i]$. Therefore, evaluating the expectation on both sides of Eq. (15)\

$$y \approx y_{2\mathrm{ord}} = f(x_1, \ldots, x_i, \ldots, x_N) + \frac{1}{2}\sum_{i=1}^{N}\left(\frac{\partial^2 f}{\partial X_i^2}\right)u^2(x_i). \tag{16}$$

Now, if we subtract Eq. (15) from Eq. (16), squaring both sides and taking the expectation from either side we finally obtain

$$u^2(y) \approx u^2(y_{2\mathrm{ord}}) = \sum_{i=1}^{N} \underbrace{\left(\frac{\partial f}{\partial X_i}\right)^2 u^2(x_i)}_{\text{first order}} + \gamma_i \left(\frac{\partial f}{\partial X_i}\right)\left(\frac{\partial^2 f}{\partial X_i^2}\right)u^3(x_i) + \sum_{i=1}^{N}\left(\frac{\kappa_i - 1}{4}\right)\left(\frac{\partial^2 f}{\partial X_i^2}\right)^2 u^4(x_i) + \frac{1}{2}\sum_{i=1}^{N} \times \sum_{\substack{j=1\\ j\neq i}}^{N}\left(\frac{\partial^2 f}{\partial X_i \partial X_j}\right)^2 u^2(x_i)u^2(x_j). \tag{17}$$

The second order method, proposed in Eqs. (16) and (17), encompasses the expressions proposed by the GUM method (linear method). Therefore, this method may be more suitable than the GUM method for the evaluation of standard uncertainty mainly when the non-linearities of the measurement functions are significant.

3.2. Third order method

In order to increase the accuracy for the standard uncertainty, we must expand the measurement function from the third order truncation of the Taylor's series. Hence, the expression obtained is given by

$$Y \approx Y_{3\mathrm{ord}} = f(x_1, \ldots, x_i, \ldots, x_N) + \sum_{i=1}^{N}\left(\frac{\partial f}{\partial X_i}\right)(X_i - x_i) + \frac{1}{2} \times \sum_{i=1}^{N}\left(\frac{\partial^2 f}{\partial X_i^2}\right)(X_i - x_i)^2 + \frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N}\left(\frac{\partial^2 f}{\partial X_i \partial X_j}\right) \times (X_i - x_i)(X_j - x_j) + \frac{1}{6}\sum_{i=1}^{N}\left(\frac{\partial^3 f}{\partial X_i^3}\right)(X_i - x_i)^3 + \frac{1}{6}\sum_{i=1}^{N} \times \sum_{\substack{j=1\\ j\neq i}}^{N}\left(\frac{\partial^3 f}{\partial X_i^2 \partial X_j}\right)(X_i - x_i)^2(X_j - x_j) + \frac{1}{6}\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N} \times \sum_{\substack{k=1\\ k\neq i,j}}^{N}\left(\frac{\partial^3 f}{\partial X_i \partial X_j \partial X_k}\right)(X_i - x_i)(X_j - x_j)(X_k - x_k). \tag{18}$$

Considering all suppositions and following reasoning that led to the second order expressions, it is easy to verify that the third order expression of the estimate of the measurand turns out to be

$$y \approx y_{3\mathrm{ord}} = f(x_1, \ldots, x_i, \ldots, x_N) + \sum_{i=1}^{N}\left\{\frac{1}{2}\left(\frac{\partial^2 f}{\partial X_i^2}\right)u^2(x_i) + \frac{\gamma_i}{6}\left(\frac{\partial^3 f}{\partial X_i^3}\right)u^3(x_i)\right\}, \tag{19}$$

whereas its standard uncertainty is given by:

$$u^2(y) \approx u^2(y_{3\mathrm{ord}}) = u^2(y_{2\mathrm{ord}}) + \sum_{i=1}^{N}\frac{\kappa_i}{3}\left(\frac{\partial f}{\partial X_i}\right)\left(\frac{\partial^3 f}{\partial X_i^3}\right)u^4(x_i) + \frac{1}{6}\sum_{i=1}^{N}\left(\frac{\partial^2 f}{\partial X_i^2}\right)\left(\frac{\partial^3 f}{\partial X_i^3}\right)\left\{\mathrm{E}[(X_i - x_i)^5] - \gamma_i u^5(x_i)\right\}$$

$$+\frac{1}{36}\sum_{i=1}^{N}\left(\frac{\partial^3 f}{\partial X_i^3}\right)^2\left\{\mathrm{E}[(X_i-x_i)^6]-\gamma_i^2 u^6(x_i)\right\}$$
$$+\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N}\left(\frac{\partial f}{\partial X_i}\right)\left(\frac{\partial^3 f}{\partial X_i\partial X_j^2}\right)u^2(x_i)u^2(x_j)$$
$$+\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N}\gamma_i\left\{\frac{1}{2}\left(\frac{\partial^2 f}{\partial X_i\partial X_j}\right)\left(\frac{\partial^3 f}{\partial X_i^2\partial X_j}\right)\right.$$
$$\left.+\frac{1}{4}\left(\frac{\partial^2 f}{\partial X_i^2}\right)\left(\frac{\partial^3 f}{\partial X_i\partial X_j^2}\right)\right\}u^3(x_i)u^2(x_j)$$
$$+\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N}\kappa_i\left\{\frac{1}{4}\left(\frac{\partial^3 f}{\partial X_i^2\partial X_j}\right)^2+\frac{1}{6}\left(\frac{\partial^3 f}{\partial X_i^3}\right)\left(\frac{\partial^3 f}{\partial X_i\partial X_j^2}\right)\right\}$$
$$\times u^4(x_i)u^2(x_j)+\frac{1}{4}\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N}\gamma_i\gamma_j\left(\frac{\partial^3 f}{\partial X_i\partial X_j^2}\right)\left(\frac{\partial^3 f}{\partial X_i^2\partial X_j}\right)$$
$$\times u^3(x_i)u^3(x_j)+\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N}\sum_{\substack{k=1\\ k\neq i,j}}^{N}\left\{\frac{1}{6}\left(\frac{\partial^3 f}{\partial X_i\partial X_j\partial X_k}\right)^2\right.$$
$$\left.+\frac{1}{4}\left(\frac{\partial^3 f}{\partial X_i^2\partial X_j}\right)\left(\frac{\partial^3 f}{\partial X_j\partial X_k^2}\right)\right\}u^2(x_i)u^2(x_j)u^2(x_k). \quad (20)$$

The inclusion of the third order terms from the Taylor series expansion of the measurement function results in a more comprehensive method than the GUM and the second order methods. Thus, the evaluation of measurement uncertainty using this method can be considered more appropriate and robust than the latter methods.

Additional issues in the proposed methods of second and third order should also be addressed, for example: if Type A input quantities are only available these expressions require a large number of observations (e.g. $\geqslant 30$) to suitably evaluate the higher order moments; the expressions of higher order derivatives can be easily implemented by computer software which can handle algebraic differentiation [7] or automatic differentiation [11,12].

4. Results and discussion

A case study will be presented in this section to illustrate the proposed methods for the evaluation of the estimate of the measurand and its associated standard uncertainty. The results obtained by the GUM and the GUM S1 approaches are also given for comparative purposes.

The present case study emphasizes the implications of a non-linear measurement function which is given by

$$Y = X_1\exp(X_2X_3). \quad (21)$$

A derivation of this type of model might occur in several knowledge areas such as chemistry, materials and chemical engineering. Independent observations have been made for each of the input quantities and the treatment of these current data in terms of estimate, standard uncertainty, skewness, kurtosis, fifth and sixth moments is given in Table 1.

Table 1
Statistical parameters of the set of observations concerning the input quantities.

Parameters	X_1	X_2	X_3
Estimate (unit of X_i)	0.9891	1.6153	1.2019
Standard uncertainty (unit of X_i)	0.2615	0.1091	0.3532
Skewness (dimensionless)	0.1258	0.1831	0.1024
Kurtosis (dimensionless)	2.7638	2.6626	2.3149
Fifth moment (unit corresponding to X_i)	0.0004	0.0002	0.0030
Sixth moment (unit corresponding to X_i)	0.0031	0.0001	0.0121

As seen earlier, the application of the methods based on LPU approach (GUM, second and third order) requires the partial derivatives, which were computed by algebraic differentiation here. With respect to the GUM S1 method, for each of the three input quantities a Gaussian distribution was assigned with expectation equal to the given estimate and standard deviation equal to the given standard uncertainty.

Fig. 1 shows the resulting (empirical) PDF for the measurand Y obtained by the GUM S1 method using $M = 2 \times 10^7$ Monte Carlo trials, which was found to be sufficiently large in this case study. This method was implemented using the computational platform ®MATLAB under the operational system LINUX (Ubuntu 9.04 distribution), using a machine operating with 2.10 GHz Intel Core 2 Duo processor and 3 GB RAM. The values for the estimate of the measurand and its standard uncertainty as well as the CPU time required by the four methods are given in the inset of Fig. 1.

As can be seen for the given case study, the results of the GUM S1 method differ slightly from those obtained by the GUM method. These differences may be explained by the non-linearity of the measurement function. On the other hand, the results from the proposed methods have approximated the GUM S1 results through much simpler programming and lower computational cost than the lat-

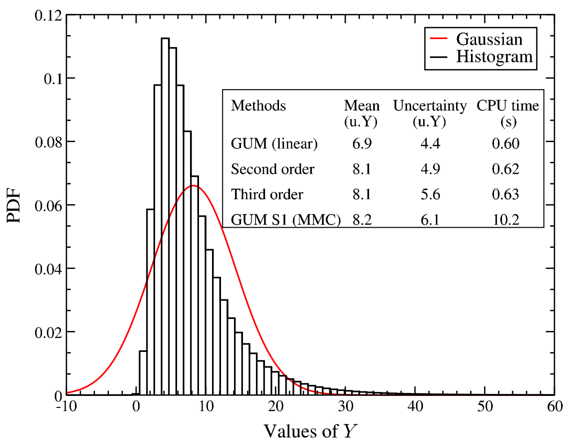

Fig. 1. Evaluation of the standard uncertainty for the measurand Y based on the four methods: GUM, second and third order and GUM S1.

ter. Although the CPU time of the GUM S1 method is negligible in this example, the runtime for this method can be very long when the models are complex, such as those with several input quantities.

The proposed methods of second and third order can be used as a reliable tool for evaluating the estimate of a measurand and its associated standard uncertainty in situations where the conditions for the applicability of the GUM method are not fulfilled and, therefore, these could be a useful companion to the GUM S1 method for this task.

5. Conclusions

As seen in this paper, the methods of second and third order can be useful for the evaluation of measurement uncertainty when the measurement functions present significant non-linearities. Nevertheless, the GUM method is useful only for linear or linearized measurement functions.

The results of the second and third order methods presented here approximate the results of the GUM S1 method and when the measurement functions are polynomials of second and third order the results of these higher order methods are closer to the GUM S1 method. The computational cost of the latter, however, increases with increasing complexity and non-linearity of the measurement function. It can be therefore concluded that these proposed methods can be easily used and implemented to evaluate the measurement uncertainty in non-linear measurement functions in order to give the GUM method wider applicability.

When the need to express measurement uncertainty as an interval (coverage interval) arises, the proposed methods are limited with respect to the GUM and GUM S1 methods. However, the standard uncertainty is universally used to express the measurement uncertainty of a quantity, see ([1], clause 6.1.2) [6,13]. A way to overcome this limitation consists of developing expressions of second and third order of the Welch–Satterthwaite formula to estimate the effective degrees of freedom, so that the coverage factor and interval could be evaluated. This is currently being investigated by the authors.

Acknowledgment

The authors gratefully acknowledge the financial support given by FAPESB (Foundation for Support for Research of Bahia).

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