GUIDE 98-3/Suppl.2

Uncertainty of measurement —

Part 3:

Guide to the expression of uncertainty in measurement (GUM:1995)

Supplement 2:

Extension to any number of output quantities

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ISO/IEC Foreword

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ISO/IEC Guide 98-3/Suppl.2 was prepared by Working Group 1 of the Joint Committee for Guides in Metrology (as JCGM 102:2011), and was adopted by the national bodies of ISO and IEC.

ISO/IEC Guide 98 consists of the following parts, under the general title *Uncertainty of measurement*:

— *Part 1: Introduction to the expression of uncertainty in measurement*

— *Part 3: Guide to the expression of uncertainty in measurement (GUM:1995)*

— *Part 4: Role of measurement uncertainty in conformity assessment*

The following parts are planned:

— *Part 2: Concepts and basic principles*

— *Part 5: Applications of the least-squares method*

ISO/IEC Guide 98-3 has three supplements:

— *Supplement 1: Propagation of distributions using a Monte Carlo method*

— *Supplement 2: Models with any number of output quantities*

— *Supplement 3: Modelling*

Given that ISO/IEC Guide 98-3:2008/Suppl.2:2011 is identical in content to JCGM 102:2011, the decimal symbol is a point on the line in the English version.

Annex ZZ has been appended to provide a list of corresponding ISO/IEC Guides and JCGM guidance documents for which equivalents are not given in the text.

Joint Committee for Guides in Metrology

JCGM
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Evaluation of measurement data — Supplement 2 to the "Guide to the expression of uncertainty in measurement" — Extension to any number of output quantities

Évaluation des données de mesure — Supplément 2 du "Guide pour l'expression de l'incertitude de mesure" — Extension à un nombre quelconque de grandeurs de sortie

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Foreword

In 1997 a Joint Committee for Guides in Metrology (JCGM), chaired by the Director of the Bureau International des Poids et Mesures (BIPM), was created by the seven international organizations that had originally in 1993 prepared the "Guide to the expression of uncertainty in measurement" (GUM) and the "International vocabulary of basic and general terms in metrology" (VIM). The JCGM assumed responsibility for these two documents from the ISO Technical Advisory Group 4 (TAG4).

The Joint Committee is formed by the BIPM with the International Electrotechnical Commission (IEC), the International Federation of Clinical Chemistry and Laboratory Medicine (IFCC), the International Laboratory Accreditation Cooperation (ILAC), the International Organization for Standardization (ISO), the International Union of Pure and Applied Chemistry (IUPAC), the International Union of Pure and Applied Physics (IUPAP), and the International Organization of Legal Metrology (OIML).

JCGM has two Working Groups. Working Group 1, "Expression of uncertainty in measurement", has the task to promote the use of the GUM and to prepare Supplements and other documents for its broad application. Working Group 2, "Working Group on International vocabulary of basic and general terms in metrology (VIM)", has the task to revise and promote the use of the VIM.

Supplements such as this one are intended to give added value to the GUM by providing guidance on aspects of uncertainty evaluation that are not explicitly treated in the GUM. The guidance will, however, be as consistent as possible with the general probabilistic basis of the GUM.

The present Supplement 2 to the GUM has been prepared by Working Group 1 of the JCGM, and has benefited from detailed reviews undertaken by member organizations of the JCGM and National Metrology Institutes.

Introduction

The "Guide to the expression of uncertainty in measurement" (GUM) [JCGM 100:2008] is mainly concerned with univariate measurement models, namely models having a single scalar output quantity. However, models with more than one output quantity arise across metrology. The GUM includes examples, from electrical metrology, with three output quantities [JCGM 100:2008 H.2], and thermal metrology, with two output quantities [JCGM 100:2008 H.3]. This Supplement to the GUM treats multivariate measurement models, namely models with any number of output quantities. Such quantities are generally mutually correlated because they depend on common input quantities. A generalization of the GUM uncertainty framework [JCGM 100:2008 5] is used to provide estimates of the output quantities, the standard uncertainties associated with the estimates, and covariances associated with pairs of estimates. The input or output quantities in the measurement model may be real or complex.

Supplement 1 to the GUM [JCGM 101:2008] is concerned with the propagation of probability distributions [JCGM 101:2008 5] through a measurement model as a basis for the evaluation of measurement uncertainty, and its implementation by a Monte Carlo method [JCGM 101:2008 7]. Like the GUM, it is only concerned with models having a single scalar output quantity [JCGM 101:2008 1]. This Supplement describes a generalization of that Monte Carlo method to obtain a discrete representation of the joint probability distribution for the output quantities of a multivariate model. The discrete representation is then used to provide estimates of the output quantities, and standard uncertainties and covariances associated with those estimates. Appropriate use of the Monte Carlo method would be expected to provide valid results when the applicability of the GUM uncertainty framework is questionable, namely when (a) linearization of the model provides an inadequate representation, or (b) the probability distribution for the output quantity (or quantities) departs appreciably from a (multivariate) Gaussian distribution.

Guidance is also given on the determination of a coverage region for the output quantities of a multivariate model, the counterpart of a coverage interval for a single scalar output quantity, corresponding to a stipulated coverage probability. The guidance includes the provision of coverage regions that take the form of hyper-ellipsoids and hyper-rectangles. A calculation procedure that uses results provided by the Monte Carlo method is also described for obtaining an approximation to the smallest coverage region.

Evaluation of measurement data — Supplement 2 to the "Guide to the expression of uncertainty in measurement" — Extension to any number of output quantities

1 Scope

This Supplement to the "Guide to the expression of uncertainty in measurement" (GUM) is concerned with measurement models having any number of input quantities (as in the GUM and GUM Supplement 1) and any number of output quantities. The quantities involved might be real or complex. Two approaches are considered for treating such models. The first approach is a generalization of the GUM uncertainty framework. The second is a Monte Carlo method as an implementation of the propagation of distributions. Appropriate use of the Monte Carlo method would be expected to provide valid results when the applicability of the GUM uncertainty framework is questionable.

The approach based on the GUM uncertainty framework is applicable when the input quantities are summarized (as in the GUM) in terms of estimates (for instance, measured values) and standard uncertainties associated with these estimates and, when appropriate, covariances associated with pairs of these estimates. Formulæ and procedures are provided for obtaining estimates of the output quantities and for evaluating the associated standard uncertainties and covariances. Variants of the formulæ and procedures relate to models for which the output quantities (a) can be expressed directly in terms of the input quantities as measurement functions, and (b) are obtained through solving a measurement model, which links implicitly the input and output quantities.

The counterparts of the formulæ in the GUM for the standard uncertainty associated with an estimate of the output quantity would be algebraically cumbersome. Such formulæ are provided in a more compact form in terms of matrices and vectors, the elements of which contain variances (squared standard uncertainties), covariances and sensitivity coefficients. An advantage of this form of presentation is that these formulæ can readily be implemented in the many computer languages and systems that support matrix algebra.

The Monte Carlo method is based on (i) the assignment of probability distributions to the input quantities in the measurement model [JCGM 101:2008 6], (ii) the determination of a discrete representation of the (joint) probability distribution for the output quantities, and (iii) the determination from this discrete representation of estimates of the output quantities and the evaluation of the associated standard uncertainties and covariances. This approach constitutes a generalization of the Monte Carlo method in Supplement 1 to the GUM, which applies to a single scalar output quantity.

For a prescribed coverage probability, this Supplement can be used to provide a coverage region for the output quantities of a multivariate model, the counterpart of a coverage interval for a single scalar output quantity. The provision of coverage regions includes those taking the form of a hyper-ellipsoid or a hyper-rectangle. These coverage regions are produced from the results of the two approaches described here. A procedure for providing an approximation to the smallest coverage region, obtained from results provided by the Monte Carlo method, is also given.

This Supplement contains detailed examples to illustrate the guidance provided.

This document is a Supplement to the GUM and is to be used in conjunction with it and GUM Supplement 1. The audience of this Supplement is that of the GUM and its Supplements. Also see JCGM 104.

2 Normative references

The following referenced documents are indispensable for the application of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

JCGM 100:2008. Guide to the expression of uncertainty in measurement (GUM).

JCGM 101:2008. Evaluation of measurement data — Supplement 1 to the "Guide to the expression of uncertainty in measurement" — Propagation of distributions using a Monte Carlo method.

JCGM 104:2009. Evaluation of measurement data — An introduction to the "Guide to the expression of uncertainty in measurement" and related documents.

JCGM 200:2008. International Vocabulary of Metrology—Basic and General Concepts and Associated Terms (VIM).

3 Terms and definitions

For the purposes of this Supplement, the definitions of the GUM and the VIM apply unless otherwise indicated. Some of the most relevant definitions, adapted or generalized where necessary from these documents, are given below. Further definitions are given, including definitions taken or adapted from other sources, that are especially important for this Supplement.

A glossary of principal symbols used is given in annex D.

3.1
real quantity
quantity whose numerical value is a real number

3.2
complex quantity
quantity whose numerical value is a complex number

NOTE A complex quantity $\boldsymbol{Z}$ can be represented by two real quantities in Cartesian form

$$\boldsymbol{Z} \equiv (Z_{\mathrm{R}}, Z_{\mathrm{I}})^{\top} = Z_{\mathrm{R}} + \mathrm{i}Z_{\mathrm{I}},$$

where $\top$ denotes "transpose", $\mathrm{i}^2 = -1$ and Z_{R} and Z_{I} are, respectively, the real and imaginary parts of $\boldsymbol{Z}$, or in polar form

$$\boldsymbol{Z} \equiv (Z_r, Z_\theta)^{\top} = Z_r(\cos Z_\theta + \mathrm{i}\sin Z_\theta) = Z_r \mathrm{e}^{\mathrm{i}Z_\theta},$$

where Z_r and Z_θ are, respectively, the magnitude (amplitude) and phase of $\boldsymbol{Z}$.

3.3
vector quantity
set of quantities arranged as a matrix having a single column

3.4
real vector quantity
vector quantity with real components

EXAMPLE A real vector quantity $\boldsymbol{X}$ containing N real quantities $X_1, \ldots, X_N$ expressed as a matrix of dimension $N \times 1$:

$$\boldsymbol{X} = \begin{bmatrix} X_1 \\ \vdots \\ X_N \end{bmatrix} = (X_1, \ldots, X_N)^{\top}.$$

3.5
complex vector quantity
vector quantity with complex components

EXAMPLE A complex vector quantity $\boldsymbol{Z}$ containing N complex quantities $\boldsymbol{Z}_1, \ldots, \boldsymbol{Z}_N$ expressed as a matrix of dimension $N \times 1$:

$$\boldsymbol{Z} = \begin{bmatrix} \boldsymbol{Z}_1 \\ \vdots \\ \boldsymbol{Z}_N \end{bmatrix} = (\boldsymbol{Z}_1, \ldots, \boldsymbol{Z}_N)^\top.$$

3.6
vector measurand
vector quantity intended to be measured

NOTE Generalized from JCGM 200:2008 definition 2.3.

3.7
measurement model
model of measurement
model
mathematical relation among all quantities known to be involved in a measurement

NOTE 1 Adapted from JCGM 200:2008 definition 2.48.

NOTE 2 A general form of a measurement model is the equation $h(Y, X_1, \ldots, X_N) = 0$, where Y, the output quantity in the measurement model, is the measurand, the quantity value of which is to be inferred from information about input quantities $X_1, \ldots, X_N$ in the measurement model.

NOTE 3 In cases where there are two or more output quantities in a measurement model, the measurement model consists of more than one equation.

3.8
multivariate measurement model
multivariate model
measurement model in which there is any number of output quantities

NOTE 1 The general form of a multivariate measurement model is the equations

$$h_1(Y_1, \ldots, Y_m, X_1, \ldots, X_N) = 0, \quad \ldots, \quad h_m(Y_1, \ldots, Y_m, X_1, \ldots, X_N) = 0,$$

where $Y_1, \ldots, Y_m$, the output quantities, m in number, in the multivariate measurement model, constitute the measurand, the quantity values of which are to be inferred from information about input quantities $X_1, \ldots, X_N$ in the multivariate measurement model.

NOTE 2 A vector representation of the general form of multivariate measurement model is

$$\boldsymbol{h}(\boldsymbol{Y}, \boldsymbol{X}) = \boldsymbol{0},$$

where $\boldsymbol{Y} = (Y_1, \ldots, Y_m)^\top$ and $\boldsymbol{h} = (h_1, \ldots, h_m)^\top$ are matrices of dimension $m \times 1$.

NOTE 3 If, in note 1, m, the number of output quantities, is unity, the model is known as a univariate measurement model.

3.9
multivariate measurement function
multivariate function
function in a multivariate measurement model for which the output quantities are expressed in terms of the input quantities

NOTE 1 Generalized from JCGM 200:2008 definition 2.49.

NOTE 2 If a measurement model $\boldsymbol{h}(\boldsymbol{Y}, \boldsymbol{X}) = \boldsymbol{0}$ can explicitly be written as $\boldsymbol{Y} = \boldsymbol{f}(\boldsymbol{X})$, where $\boldsymbol{X} = (X_1, \ldots, X_N)^\top$ are the input quantities, and $\boldsymbol{Y} = (Y_1, \ldots, Y_m)^\top$ are the output quantities, $\boldsymbol{f} = (f_1, \ldots, f_m)^\top$ is the multivariate measurement function. More generally, $\boldsymbol{f}$ may symbolize an algorithm, yielding for input quantity values $\boldsymbol{x} = (x_1, \ldots, x_N)^\top$ a corresponding unique set of output quantity values $y_1 = f_1(\boldsymbol{x}), \ldots, y_m = f_m(\boldsymbol{x})$.

NOTE 3 If, in note 2, m, the number of output quantities, is unity, the function is known as a univariate measurement function.

3.10
real measurement model
real model
measurement model, generally multivariate, involving real quantities

3.11
complex measurement model
complex model
measurement model, generally multivariate, involving complex quantities

3.12
multistage measurement model
multistage model
measurement model, generally multivariate, consisting of a sequence of sub-models, in which output quantities from one sub-model become input quantities to a subsequent sub-model

NOTE Only at the final stage of a multistage measurement model might it be necessary to consider a coverage region for the output quantities based on the joint probability density function for those quantities.

EXAMPLE A common instance in metrology is the following pair of measurement sub-models in the context of calibration. The first sub-model has input quantities whose measured values are provided by measurement standards and corresponding indication values, and as output quantities the parameters in a calibration function. This sub-model specifies the manner in which the output quantities are obtained from the input quantities, for example by solving a least-squares problem. The second sub-model has as input quantities the parameters in the calibration function and a quantity realized by a further indication value and as output quantity the quantity corresponding to that input quantity.

3.13
joint distribution function
distribution function
function giving, for every value $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_N)^\top$, the probability that each element X_i of the random variable $\boldsymbol{X}$ be less than or equal to ξ_i

NOTE The joint distribution for the random variable $\boldsymbol{X}$ is denoted by $G_{\boldsymbol{X}}(\boldsymbol{\xi})$, where

$$G_{\boldsymbol{X}}(\boldsymbol{\xi}) = \Pr(X_1 \le \xi_1, \ldots, X_N \le \xi_N).$$

3.14
joint probability density function
probability density function
non-negative function $g_{\boldsymbol{X}}(\boldsymbol{\xi})$ satisfying

$$G_{\boldsymbol{X}}(\boldsymbol{\xi}) = \int_{-\infty}^{\xi_1} \cdots \int_{-\infty}^{\xi_N} g_{\boldsymbol{X}}(\boldsymbol{z})\, \mathrm{d}z_N \cdots \mathrm{d}z_1$$

3.15
marginal probability density function
for a random variable X_i, a component of $\boldsymbol{X}$ having probability density function $g_{\boldsymbol{X}}(\boldsymbol{\xi})$, the probability density function for X_i alone:

$$g_{X_i}(\xi_i) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} g_{\boldsymbol{X}}(\boldsymbol{\xi})\, \mathrm{d}\xi_N \cdots \mathrm{d}\xi_{i+1} \mathrm{d}\xi_{i-1} \cdots \mathrm{d}\xi_1$$

NOTE When the components X_i of $\boldsymbol{X}$ are independent, $g_{\boldsymbol{X}}(\boldsymbol{\xi}) = g_{X_1}(\xi_1)g_{X_2}(\xi_2)\cdots g_{X_N}(\xi_N)$.

3.16
expectation
property of a random variable X_i, a component of $\boldsymbol{X}$ having probability density function $g_{\boldsymbol{X}}(\boldsymbol{\xi})$, given by

$$E(X_i) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \xi_i g_{\boldsymbol{X}}(\boldsymbol{\xi})\,\mathrm{d}\xi_N \cdots \mathrm{d}\xi_1 = \int_{-\infty}^{\infty} \xi_i g_{X_i}(\xi_i)\,\mathrm{d}\xi_i$$

NOTE 1 Generalized from JCGM 101:2008 definition 3.6.

NOTE 2 The expectation of the random variable $\boldsymbol{X}$ is $\boldsymbol{E}(\boldsymbol{X}) = (E(X_1), \ldots, E(X_N))^\top$, a matrix of dimension $N \times 1$.

3.17
variance
property of a random variable X_i, a component of $\boldsymbol{X}$ having probability density function $g_{\boldsymbol{X}}(\boldsymbol{\xi})$, given by

$$V(X_i) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} [\xi_i - E(X_i)]^2 g_{\boldsymbol{X}}(\boldsymbol{\xi})\,\mathrm{d}\xi_N \cdots \mathrm{d}\xi_1 = \int_{-\infty}^{\infty} [\xi_i - E(X_i)]^2 g_{X_i}(\xi_i)\,\mathrm{d}\xi_i$$

NOTE Generalized from JCGM 101:2008 definition 3.7.

3.18
covariance
property of a pair of random variables X_i and X_j, components of $\boldsymbol{X}$ having probability density function $g_{\boldsymbol{X}}(\boldsymbol{\xi})$, given by

$$\begin{aligned}\mathrm{Cov}(X_i, X_j) = \mathrm{Cov}(X_j, X_i) &= \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} [\xi_i - E(X_i)][\xi_j - E(X_j)] g_{\boldsymbol{X}}(\boldsymbol{\xi})\,\mathrm{d}\xi_N \cdots \mathrm{d}\xi_1 \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} [\xi_i - E(X_i)][\xi_j - E(X_j)] g_{X_i,X_j}(\xi_i, \xi_j)\,\mathrm{d}\xi_i \mathrm{d}\xi_j,\end{aligned}$$

where $g_{X_i,X_j}(\xi_i, \xi_j)$ is the joint PDF for the two random variables X_i and X_j

NOTE 1 Generalized from JCGM 101:2008 definition 3.10.

NOTE 2 The covariance matrix of the random variable $\boldsymbol{X}$ is $\boldsymbol{V}(\boldsymbol{X})$, a symmetric positive semi-definite matrix of dimension $N \times N$ containing the covariances $\mathrm{Cov}(X_i, X_j)$. Certain operations involving $\boldsymbol{V}(\boldsymbol{X})$ require positive definiteness.

3.19
correlation
property of a pair of random variables X_i and X_j, components of $\boldsymbol{X}$ having probability density function $g_{\boldsymbol{X}}(\boldsymbol{\xi})$, given by

$$\mathrm{Corr}(X_i, X_j) = \mathrm{Corr}(X_j, X_i) = \frac{\mathrm{Cov}(X_i, X_j)}{\sqrt{V(X_i)V(X_j)}}$$

NOTE $\mathrm{Corr}(X_i, X_j)$ is a quantity of dimension one.

3.20
measurement covariance matrix
covariance matrix
symmetric positive semi-definite matrix of dimension $N \times N$ associated with an estimate of a real vector quantity of dimension $N \times 1$, containing on its diagonal the squares of the standard uncertainties associated with the respective components of the estimate of the quantity, and, in its off-diagonal positions, the covariances associated with pairs of components of that estimate