



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**

First edition 2011

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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

102

2011

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
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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. Formulae and procedures are provided for obtaining estimates of the output quantities and for evaluating the associated standard uncertainties and covariances. Variants of the formulae 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 formulae in the GUM for the standard uncertainty associated with an estimate of the output quantity would be algebraically cumbersome. Such formulae 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 formulae 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 $\mathbf{Z}$ can be represented by two real quantities in Cartesian form

$$\mathbf{Z} \equiv (Z_R, Z_I)^\top = Z_R + iZ_I,$$

where $\top$ denotes “transpose”, $i^2 = -1$ and Z_R and Z_I are, respectively, the real and imaginary parts of $\mathbf{Z}$, or in polar form

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

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

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 $\mathbf{X}$ containing N real quantities $X_1, \dots, X_N$ expressed as a matrix of dimension $N \times 1$:

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

3.5**complex vector quantity**

vector quantity with complex components

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

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

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 $h(Y, X_1, \dots, X_N) = 0$, 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 $X_1, \dots, X_N$ 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

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

where $Y_1, \dots, Y_m$, 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 $X_1, \dots, X_N$ in the multivariate measurement model.

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

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

where $\mathbf{Y} = (Y_1, \dots, Y_m)^\top$ and $\mathbf{h} = (h_1, \dots, h_m)^\top$ 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 $h(\mathbf{Y}, \mathbf{X}) = \mathbf{0}$ can explicitly be written as $\mathbf{Y} = \mathbf{f}(\mathbf{X})$, where $\mathbf{X} = (X_1, \dots, X_N)^\top$ are the input quantities, and $\mathbf{Y} = (Y_1, \dots, Y_m)^\top$ are the output quantities, $\mathbf{f} = (f_1, \dots, f_m)^\top$ is the multivariate measurement function. More generally, $\mathbf{f}$ may symbolize an algorithm, yielding for input quantity values $\mathbf{x} = (x_1, \dots, x_N)^\top$ a corresponding unique set of output quantity values $y_1 = f_1(\mathbf{x}), \dots, y_m = f_m(\mathbf{x})$.

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 $\boldsymbol{\xi} = (\xi_1, \dots, \xi_N)^\top$, the probability that each element X_i of the random variable $\mathbf{X}$ be less than or equal to ξ_i

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

$$G_{\mathbf{X}}(\boldsymbol{\xi}) = \Pr(X_1 \leq \xi_1, \dots, X_N \leq \xi_N).$$

3.14

joint probability density function

probability density function

non-negative function $g_{\mathbf{X}}(\boldsymbol{\xi})$ satisfying

$$G_{\mathbf{X}}(\boldsymbol{\xi}) = \int_{-\infty}^{\xi_1} \cdots \int_{-\infty}^{\xi_N} g_{\mathbf{X}}(\mathbf{z}) \, dz_N \cdots dz_1$$

3.15

marginal probability density function

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

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

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

3.16

expectation

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

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

NOTE 1 Generalized from JCGM 101:2008 definition 3.6.

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

3.17

variance

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

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

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 $\mathbf{X}$ having probability density function $g_{\mathbf{X}}(\boldsymbol{\xi})$, given by

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

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 $\mathbf{X}$ is $\mathbf{V}(\mathbf{X})$, a symmetric positive semi-definite matrix of dimension $N \times N$ containing the covariances $\text{Cov}(X_i, X_j)$. Certain operations involving $\mathbf{V}(\mathbf{X})$ require positive definiteness.

3.19

correlation

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

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

NOTE $\text{Corr}(X_i, X_j)$ 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

NOTE 1 Adapted from JCGM 101:2008 definition 3.11.

NOTE 2 A covariance matrix $\mathbf{U}_{\mathbf{x}}$ of dimension $N \times N$ associated with the estimate $\mathbf{x}$ of a quantity $\mathbf{X}$ has the representation

$$\mathbf{U}_{\mathbf{x}} = \begin{bmatrix} u(x_1, x_1) & \cdots & u(x_1, x_N) \\ \vdots & \ddots & \vdots \\ u(x_N, x_1) & \cdots & u(x_N, x_N) \end{bmatrix} = \begin{bmatrix} u^2(x_1) & \cdots & u(x_1, x_N) \\ \vdots & \ddots & \vdots \\ u(x_N, x_1) & \cdots & u^2(x_N) \end{bmatrix},$$

where $u(x_i, x_i) = u^2(x_i)$ is the variance (squared standard uncertainty) associated with x_i and $u(x_i, x_j)$ is the covariance associated with x_i and x_j . When elements X_i and X_j of $\mathbf{X}$ are uncorrelated, $u(x_i, x_j) = 0$.

NOTE 3 In GUM Supplement 1 [JCGM 101:2008], the measurement covariance matrix is termed uncertainty matrix.

NOTE 4 Some numerical difficulties can occasionally arise when working with covariance matrices. For instance, a covariance matrix $\mathbf{U}_{\mathbf{x}}$ associated with a vector estimate $\mathbf{x}$ may not be positive definite. That possibility can be a result of the way $\mathbf{U}_{\mathbf{x}}$ has been calculated. As a consequence, the Cholesky factor of $\mathbf{U}_{\mathbf{x}}$ may not exist. The Cholesky factor is used in working numerically with $\mathbf{U}_{\mathbf{x}}$ [7]; also see annex B. Moreover, the variance associated with a linear combination of the elements of $\mathbf{x}$ could be negative, when otherwise it would be expected to be small and positive. In such a situation procedures exist for “repairing” $\mathbf{U}_{\mathbf{x}}$ such that the repaired covariance matrix is positive definite. As a result, the Cholesky factor would exist, and variances of such linear combinations would be positive as expected. Such a procedure is given by the following variant of that in reference [27]. Form the eigendecomposition

$$\mathbf{U}_{\mathbf{x}} = \mathbf{Q} \mathbf{D} \mathbf{Q}^{\top},$$

where $\mathbf{Q}$ is orthonormal and $\mathbf{D}$ is the diagonal matrix of eigenvalues of $\mathbf{U}_{\mathbf{x}}$. Construct a new diagonal matrix, $\mathbf{D}'$ say, which equals $\mathbf{D}$, but with elements that are smaller than $d_{\min}$ replaced by $d_{\min}$. Here, $d_{\min}$ equals the product of the unit roundoff of the computer used and the largest element of $\mathbf{D}$. Subsequent calculations would use a repaired covariance matrix $\mathbf{U}'_{\mathbf{x}}$ formed from

$$\mathbf{U}'_{\mathbf{x}} = \mathbf{Q} \mathbf{D}' \mathbf{Q}^{\top}.$$

NOTE 5 Certain operations involving $\mathbf{U}_{\mathbf{x}}$ require positive definiteness.

3.21

correlation 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 the correlations associated with pairs of components of the estimate

NOTE 1 A correlation matrix $\mathbf{R}_{\mathbf{x}}$ of dimension $N \times N$ associated with the estimate $\mathbf{x}$ of a quantity $\mathbf{X}$ has the representation

$$\mathbf{R}_{\mathbf{x}} = \begin{bmatrix} r(x_1, x_1) & \cdots & r(x_1, x_N) \\ \vdots & \ddots & \vdots \\ r(x_N, x_1) & \cdots & r(x_N, x_N) \end{bmatrix},$$

where $r(x_i, x_i) = 1$ and $r(x_i, x_j)$ is the correlation associated with x_i and x_j . When elements X_i and X_j of $\mathbf{X}$ are uncorrelated, $r(x_i, x_j) = 0$.

NOTE 2 Correlations are also known as correlation coefficients.

NOTE 3 $\mathbf{R}_{\mathbf{x}}$ is related to $\mathbf{U}_{\mathbf{x}}$ (see 3.20) by

$$\mathbf{U}_{\mathbf{x}} = \mathbf{D}_{\mathbf{x}} \mathbf{R}_{\mathbf{x}} \mathbf{D}_{\mathbf{x}},$$

where $\mathbf{D}_{\mathbf{x}}$ is a diagonal matrix of dimension $N \times N$ with diagonal elements $u(x_1), \dots, u(x_N)$. Element (i, j) of $\mathbf{U}_{\mathbf{x}}$ is given by

$$u(x_i, x_j) = r(x_i, x_j) u(x_i) u(x_j).$$

NOTE 4 A correlation matrix $\mathbf{R}_{\mathbf{x}}$ is positive definite or singular, if and only if the corresponding covariance matrix $\mathbf{U}_{\mathbf{x}}$ is positive definite or singular, respectively. Certain operations involving $\mathbf{R}_{\mathbf{x}}$ require positive definiteness.

NOTE 5 When presenting numerical values of the off-diagonal elements of a correlation matrix, rounding to three places of decimals is often sufficient. However, if the correlation matrix is close to being singular, more decimal digits need to be retained in order to avoid numerical difficulties when using the correlation matrix as input to an uncertainty evaluation. The number of decimal digits to be retained depends on the nature of the subsequent calculation, but as a guide can be taken as the number of decimal digits needed to represent the smallest eigenvalue of the correlation matrix with two significant decimal digits. For a correlation matrix of dimension 2×2 , the eigenvalues $\lambda_{\max}$ and $\lambda_{\min}$ are $1 \pm |r|$, the smaller, $\lambda_{\min}$, being $1 - |r|$, where r is the off-diagonal element of the matrix. If a correlation matrix is known to be singular prior to rounding, rounding towards zero reduces the risk that the rounded matrix is not positive semi-definite.

3.22

sensitivity matrix

matrix of partial derivatives of first order for a real measurement model with respect to either the input quantities or the output quantities evaluated at estimates of those quantities

NOTE For N input quantities and m output quantities, the sensitivity matrix with respect to $\mathbf{X}$ has dimension $m \times N$ and that with respect to $\mathbf{Y}$ has dimension $m \times m$.

3.23

coverage interval

interval containing the true quantity value with a stated probability, based on the information available

NOTE 1 Adapted from JCGM 101:2008 definition 3.12.

NOTE 2 The probabilistically symmetric coverage interval for a scalar quantity is the interval such that the probability that the true quantity value is less than the smallest value in the interval is equal to the probability that the true quantity value is greater than the largest value in the interval [adapted from JCGM 101:2008 3.15].

NOTE 3 The shortest coverage interval for a quantity is the interval of shortest length among all coverage intervals for that quantity having the same coverage probability [adapted from JCGM 101:2008 3.16].

3.24

coverage region

region containing the true vector quantity value with a stated probability, based on the information available

3.25

coverage probability

probability that the true quantity value is contained within a specified coverage interval or coverage region

NOTE 1 Adapted from JCGM 101:2008 definition 3.13.

NOTE 2 The coverage probability is sometimes termed “level of confidence” [JCGM 100:2008 6.2.2].

3.26

smallest coverage region

coverage region for a vector quantity with minimum (hyper-)volume among all coverage regions for that quantity having the same coverage probability

NOTE For a single scalar quantity, the smallest coverage region is the shortest coverage interval for the quantity. For a bivariate quantity, it is the coverage region with the smallest area among all coverage regions for that quantity having the same coverage probability.

3.27

multivariate Gaussian distribution

probability distribution of a random variable $\mathbf{X}$ of dimension $N \times 1$ having the joint probability density function

$$g_{\mathbf{X}}(\boldsymbol{\xi}) = \frac{1}{(2\pi)^{N/2} [\det(\mathbf{V})]^{1/2}} \exp \left(-\frac{1}{2} (\boldsymbol{\xi} - \boldsymbol{\mu})^{\top} \mathbf{V}^{-1} (\boldsymbol{\xi} - \boldsymbol{\mu}) \right)$$

NOTE $\boldsymbol{\mu}$ is the expectation and $\mathbf{V}$ is the covariance matrix of $\mathbf{X}$, which must be positive definite.

3.28

multivariate t -distribution

probability distribution of a random variable $\mathbf{X}$ of dimension $N \times 1$ having the joint probability density function

$$g_{\mathbf{X}}(\boldsymbol{\xi}) = \frac{\Gamma(\frac{\nu+N}{2})}{\Gamma(\frac{\nu}{2})(\pi\nu)^{N/2}} \times \frac{1}{[\det(\mathbf{V})]^{1/2}} \left[1 + \frac{1}{\nu}(\boldsymbol{\xi} - \boldsymbol{\mu})^{\top} \mathbf{V}^{-1}(\boldsymbol{\xi} - \boldsymbol{\mu}) \right]^{-(\nu+N)/2},$$

with parameters $\boldsymbol{\mu}$, $\mathbf{V}$ and ν , where $\mathbf{V}$ is symmetric positive definite and

$$\Gamma(z) = \int_0^{\infty} t^{z-1} e^{-t} dt, \quad z > 0,$$

is the gamma function

NOTE 1 The multivariate t -distribution is based on the observation that if a vector random variable $\mathbf{Q}$ of dimension $N \times 1$ and a scalar random variable W are independent and have respectively a Gaussian distribution with zero expectation and positive definite covariance matrix $\mathbf{V}$ of dimension $N \times N$, and a chi-squared distribution with ν degrees of freedom, and $(\nu/W)^{1/2} \mathbf{Q} = \mathbf{X} - \boldsymbol{\mu}$, then $\mathbf{X}$ has the given probability distribution.

NOTE 2 $g_{\mathbf{X}}(\boldsymbol{\xi})$ does not factorize into the product of N probability density functions even when $\mathbf{V}$ is a diagonal matrix. Generally, the components of $\mathbf{X}$ are statistically dependent random variables.

EXAMPLE When $N = 2$, $\nu = 5$, and $\mathbf{V}$ is the identity matrix of dimension 2×2 , the probability that $X_1 > 1$ is 18 %, while the conditional probability that $X_1 > 1$ given that $X_2 > 2$ is 26 %.

4 Conventions and notation

For the purposes of this Supplement the following conventions and notation are adopted.

4.1 In the GUM [JCGM 100:2008 4.1.1 note 1], for economy of notation the same (upper case) symbol is used for

- (i) the (physical) quantity, which is assumed to have an essentially unique true value, and
- (ii) the corresponding random variable.

NOTE The random variable has different roles in Type A and Type B uncertainty evaluations. In a Type A uncertainty evaluation, the random variable represents "...the possible outcome of an observation of the quantity". In a Type B uncertainty evaluation, the probability distribution for the random variable describes the state of knowledge about the quantity.

This ambiguity in the symbol is harmless in most circumstances.

In this Supplement, as well as in Supplement 1, for the input quantities subjected to a Type A uncertainty evaluation, the same (uppercase) symbol is used for three concepts, namely

- a) the quantity,
- b) the random variable representing the possible outcome of an observation of the quantity, and
- c) the random variable whose probability distribution describes the state of knowledge about the quantity.

This further ambiguity between two distinct random variables is not present in the GUM and is a potential source of misunderstanding. In particular, it might be believed that the Monte Carlo procedure adopted in this Supplement, as well as in Supplement 1, complies with the procedure suggested in GUM 4.1.4 note. Although the two procedures are analogous in principle, in that both are based on repeatedly evaluating the model for individual input quantity values drawn from a probability distribution, they are different in practice, in that draws are made from different distributions. In GUM 4.1.4 note, draws are made from the frequency distribution for the random variable b). In the Supplements, draws are made from the probability distribution for the random variable c). The former approach is not recommended in most experimental situations [2].

4.2 The input quantities in a measurement model are generically denoted by $X_1, \dots, X_N$, and collectively by $\mathbf{X} = (X_1, \dots, X_N)^\top$, a matrix of dimension $N \times 1$, $\top$ denoting “transpose”.

4.3 Likewise the output quantities in a measurement model are generically denoted by $Y_1, \dots, Y_m$, and collectively by $\mathbf{Y} = (Y_1, \dots, Y_m)^\top$, a matrix of dimension $m \times 1$.

4.4 When the Y_i are expressed directly as formulæ in $\mathbf{X}$, the measurement model can be written as

$$\mathbf{Y} = \mathbf{f}(\mathbf{X}), \quad (1)$$

where $\mathbf{f}$ is the multivariate measurement function. Equivalently (see 3.9), the measurement model can be expressed as

$$Y_1 = f_1(\mathbf{X}), \quad \dots, \quad Y_m = f_m(\mathbf{X}),$$

where $f_1(\mathbf{X}), \dots, f_m(\mathbf{X})$ are components of $\mathbf{f}(\mathbf{X})$.

4.5 When the Y_i are not expressed directly as formulæ in $\mathbf{X}$, the measurement model is represented by the equation

$$\mathbf{h}(\mathbf{Y}, \mathbf{X}) = \mathbf{0}, \quad (2)$$

or, equivalently (see 3.8), by

$$h_1(\mathbf{Y}, \mathbf{X}) = 0, \quad \dots, \quad h_m(\mathbf{Y}, \mathbf{X}) = 0.$$

4.6 An estimate of $\mathbf{X}$ is denoted by $\mathbf{x} = (x_1, \dots, x_N)^\top$, a matrix of dimension $N \times 1$. The covariance matrix associated with $\mathbf{x}$ is denoted by $\mathbf{U}_\mathbf{x}$, a matrix of dimension $N \times N$ (see 3.20).

4.7 An estimate of $\mathbf{Y}$ is denoted by $\mathbf{y} = (y_1, \dots, y_m)^\top$, a matrix of dimension $m \times 1$. The covariance matrix associated with $\mathbf{y}$ is denoted by $\mathbf{U}_\mathbf{y}$, a matrix of dimension $m \times m$.

NOTE $\mathbf{U}_\mathbf{y}$ is the counterpart, for m output quantities, of the variance $u^2(y)$ associated with y in the context of the univariate measurement models of the GUM and GUM Supplement 1. In the GUM, $u(y)$ is denoted by $u_c(y)$, the subscript “c” denoting combined. As in Supplement 1, the use of “c” in this context is considered superfluous for the reasons stated in 4.10 of that Supplement. Accordingly, “c” is similarly not used in this Supplement.

4.8 When estimates of the output quantities in a measurement model are to be used individually, each of these quantities may be considered as the output quantity in the corresponding univariate (scalar) measurement model. When the output quantities are to be considered together, for instance used in a subsequent calculation, any correlations associated with pairs of estimates of the output quantities need to be taken into account.

4.9 The symbol adopted for the standard uncertainty associated with a quantity value x is $u(x)$. When the context is such that there is no possibility of misunderstanding, the alternative notation u_x can be adopted. The alternative notation is not recommended when a quantity value is indexed or otherwise adorned, for example x_i or $\hat{x}$.

4.10 $\mathbf{x}$ may be described as either “estimates of the input quantities”, or “an estimate of the (vector) input quantity”. The latter description is mainly used in this Supplement (and similarly for the output quantities).

4.11 As in subclauses 4.2 to 4.10, a quantity is generally denoted by an upper case letter and an estimate or some fixed value of the quantity (such as the expectation) by the corresponding lower case letter. Although valuable for generic considerations, such a notation is largely inappropriate for physical quantities, because of the established use of specific symbols, for example T for thermodynamic temperature and t for time. Therefore, in some of the examples, a different notation is used, in which a quantity is denoted by its conventional symbol and its expectation or an estimate of it by that symbol hatted. For instance, the quantity representing the amplitude of an alternating current (example 1 of 6.2.2) is denoted by I and an estimate of I by $\hat{I}$ [JCGM 101:2008 4.8].

4.12 A departure is made from the symbols often used for a probability density function (PDF) and distribution function. The GUM uses the generic symbol f to refer to a model and a PDF. Little confusion arises in the GUM as a consequence of this usage. The situation in this Supplement is different. The concepts of measurement function, PDF, and distribution function are central to following and implementing the guidance provided. Therefore, in place of the symbols f and F to denote a PDF and a distribution function, respectively, the symbols g and G are used. These symbols are indexed appropriately to denote the quantity concerned. The symbol f is reserved for a measurement function. Vector counterparts of these symbols are also used.

4.13 A PDF is assigned to a quantity, which might be a single scalar quantity X or a vector quantity $\mathbf{X}$. In the scalar case, the PDF for X is denoted by $g_X(\xi)$, where ξ is a variable describing the possible values of X . This X is considered as a random variable with expectation $E(X)$ and variance $V(X)$.

4.14 In the vector case, the PDF for $\mathbf{X}$ is denoted by $g_{\mathbf{X}}(\boldsymbol{\xi})$, where $\boldsymbol{\xi} = (\xi_1, \dots, \xi_N)^\top$ is a variable describing the possible values of the quantity $\mathbf{X}$. This $\mathbf{X}$ is considered as a random variable with expectation $\mathbf{E}(\mathbf{X})$ and covariance matrix $\mathbf{V}(\mathbf{X})$.

4.15 Analogously, in the scalar case, the PDF for Y is denoted by $g_Y(\eta)$ and, in the vector case, the PDF for $\mathbf{Y}$ is denoted by $g_{\mathbf{Y}}(\boldsymbol{\eta})$.

4.16 According to Resolution 10 of the 22nd CGPM (2003) "... the symbol for the decimal marker shall be either the point on the line or the comma on the line ...". The JCGM has decided to adopt, in its documents in English, the point on the line.

5 Basic principles

5.1 General

5.1.1 In the GUM [JCGM 100:2008 4.1], a measuring system is modelled in terms of a function involving real input quantities $X_1, \dots, X_N$ and a real output quantity Y in the form of expression (1), namely $Y = f(\mathbf{X})$, where $\mathbf{X} \equiv (X_1, \dots, X_N)^\top$ is referred to as the real vector input quantity. This function is known as a real univariate measurement function (see 3.9 note 3).

5.1.2 In practice, not all measuring systems encountered can be modelled as a measurement function in a single scalar output quantity. Such systems might instead involve either

- a) a number of output quantities $Y_1, \dots, Y_m$ (denoted collectively by the real vector output quantity $\mathbf{Y} \equiv (Y_1, \dots, Y_m)^\top$), taking the form (1), namely $\mathbf{Y} = \mathbf{f}(\mathbf{X})$, or
- b) the more general form of measurement model, taking the form (2), namely $\mathbf{h}(\mathbf{Y}, \mathbf{X}) = \mathbf{0}$.

5.1.3 Further, some or all of the components of $\mathbf{X}$ and $\mathbf{Y}$ might correspond to components (real part and imaginary part, or magnitude and phase) of complex input quantities. Therefore, all measurement models can be considered (without loss of generality) as real. However, a treatment that is simpler than the corresponding treatment involving real and imaginary parts applies for the complex case [14]. The treatment gives succinct matrix expressions for the law of propagation of uncertainty when applied to measurement models with complex quantities (complex models). See 6.4 and annex A.

5.1.4 This GUM Supplement considers the more general measurement models in 5.1.2 and 5.1.3.

5.2 Main stages of uncertainty evaluation

5.2.1 The main stages of uncertainty evaluation constitute formulation, propagation, and summarizing:

a) *Formulation:*

- 1) define the output quantity $\mathbf{Y}$, the quantity intended to be measured (the vector measurand);
- 2) determine the input quantity $\mathbf{X}$ upon which $\mathbf{Y}$ depends;
- 3) develop a measurement function [f in (1)] or measurement model (2) relating $\mathbf{X}$ and $\mathbf{Y}$;
- 4) on the basis of available knowledge assign PDFs — Gaussian (normal), rectangular (uniform), etc. — to the components of $\mathbf{X}$. Assign instead a joint PDF to the components of $\mathbf{X}$ that are not pairwise independent;

b) *Propagation:*

propagate the PDFs for the components of $\mathbf{X}$ through the model to obtain the (joint) PDF for $\mathbf{Y}$;

c) *Summarizing:*

use the PDF for $\mathbf{Y}$ to obtain

- 1) the expectation of $\mathbf{Y}$, taken as an estimate $\mathbf{y}$ of $\mathbf{Y}$,
- 2) the covariance matrix of $\mathbf{Y}$, taken as the covariance matrix $\mathbf{U}_y$ associated with $\mathbf{y}$, and
- 3) a coverage region containing $\mathbf{Y}$ with a specified probability p (the coverage probability).

5.2.2 The steps in the formulation stage are carried out by the metrologist. Guidance on the assignment of PDFs (step 4 of stage a) in 5.2.1) is given in GUM Supplement 1 for some common cases and in 5.3. The propagation and summarizing stages, b) and c), for which detailed guidance is provided here, require no further metrological information, and in principle can be carried out to any required numerical tolerance for the problem specified in the formulation stage.

NOTE Once the formulation stage a) in 5.2.1 has been carried out, the PDF for $\mathbf{Y}$ is completely specified mathematically, but generally the calculation of the expectation, covariance matrix and coverage regions require numerical methods that involve a degree of approximation.

5.3 Probability density functions for the input quantities

5.3.1 General

GUM Supplement 1 gives guidance on the assignment, in some common circumstances, of PDFs to the input quantities X_i in the formulation stage of uncertainty evaluation [JCGM 101:2008 6]. The only multivariate distribution considered in GUM Supplement 1 is the multivariate Gaussian [JCGM 101:2008 6.4.8]. This distribution is assigned to the input quantity $\mathbf{X}$ when the estimate $\mathbf{x}$ and associated covariance matrix $\mathbf{U}_x$ constitute the only information available about $\mathbf{X}$. A further multivariate distribution, the multivariate t -distribution, is described in 5.3.2. This distribution arises when a series of indication values, regarded as being obtained independently from a vector quantity with unknown expectation and unknown covariance matrix having a multivariate Gaussian distribution, is the only information available about $\mathbf{X}$. Also see 6.5.4.

5.3.2 Multivariate t -distribution

5.3.2.1 Suppose that a series of n indication values $\mathbf{x}_1, \dots, \mathbf{x}_n$, each of dimension $N \times 1$, is available, with $n > N$, regarded as being obtained independently from a quantity with unknown expectation $\boldsymbol{\mu}$ and covariance matrix $\boldsymbol{\Sigma}$ of dimension $N \times N$ having the multivariate Gaussian distribution $N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$. The desired input quantity $\mathbf{X}$ of dimension $N \times 1$ is taken to be equal to $\boldsymbol{\mu}$. Then, assigning a non-informative

joint prior distribution to $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$, and using Bayes' theorem, the marginal (joint) PDF for $\mathbf{X}$ is a multivariate t -distribution $t_\nu(\bar{\mathbf{x}}, \mathbf{S}/n)$ with $\nu = n - N$ degrees of freedom [11], where

$$\bar{\mathbf{x}} = \frac{1}{n}(\mathbf{x}_1 + \cdots + \mathbf{x}_n), \quad \mathbf{S} = \frac{1}{\nu}[(\mathbf{x}_1 - \bar{\mathbf{x}})(\mathbf{x}_1 - \bar{\mathbf{x}})^\top + \cdots + (\mathbf{x}_n - \bar{\mathbf{x}})(\mathbf{x}_n - \bar{\mathbf{x}})^\top].$$

NOTE The prior can be assigned in other ways, which would influence the degrees of freedom or even the distribution.

5.3.2.2 The PDF for $\mathbf{X}$ is

$$g_{\mathbf{X}}(\boldsymbol{\xi}) = \frac{\Gamma(n/2)}{\Gamma(\nu/2)(\pi\nu)^{N/2}} \times [\det(\mathbf{S}/n)]^{-1/2} \left[1 + \frac{1}{\nu}(\boldsymbol{\xi} - \bar{\mathbf{x}})^\top \left(\frac{\mathbf{S}}{n} \right)^{-1} (\boldsymbol{\xi} - \bar{\mathbf{x}}) \right]^{-n/2},$$

where $\Gamma(z)$ is the gamma function with argument z .

5.3.2.3 $\mathbf{X}$ has expectation and covariance matrix

$$\mathbf{E}(\mathbf{X}) = \bar{\mathbf{x}}, \quad \mathbf{V}(\mathbf{X}) = \frac{\nu}{\nu - 2} \frac{\mathbf{S}}{n},$$

where $\mathbf{E}(\mathbf{X})$ is defined only for $\nu > 1$ (that is for $n > N + 1$) and $\mathbf{V}(\mathbf{X})$ only for $\nu > 2$ (that is for $n > N + 2$).

5.3.2.4 To make a random draw from $t_\nu(\bar{\mathbf{x}}, \mathbf{S}/n)$, make N random draws z_i , $i = 1, \dots, N$, from the standard Gaussian distribution $N(0, 1)$ and a single random draw w from χ_ν^2 , the chi-squared distribution with ν degrees of freedom, and form

$$\boldsymbol{\xi} = \bar{\mathbf{x}} + \mathbf{L}\mathbf{z}\sqrt{\frac{\nu}{w}}, \quad \mathbf{z} = (z_1, \dots, z_N)^\top,$$

where $\mathbf{L}$ is the lower triangular matrix of dimension $N \times N$ given by the Cholesky decomposition $\mathbf{S}/n = \mathbf{L}\mathbf{L}^\top$ [13].

NOTE The matrix $\mathbf{L}$ can be determined as in reference [13], for example.

5.3.3 Construction of multivariate probability density functions

When the input quantities $X_1, \dots, X_N$ are correlated, the information that typically is available about them are the forms of their PDFs (say, that one is Gaussian, another is rectangular, etc.), estimates $x_1, \dots, x_N$, used as their expectations, associated standard uncertainties $u(x_1), \dots, u(x_N)$, used as their standard deviations, and covariances associated with pairs of the x_i . A mathematical device known as a *copula* [20] can be used to produce a PDF for $\mathbf{X}$ consistent with such information. Such a PDF is not unique.

5.4 Propagation of distributions

5.4.1 Figure 1 (left) shows an instance of a measurement model in which there are $N = 3$ mutually independent input quantities $\mathbf{X} = (X_1, X_2, X_3)^\top$ and $m = 2$ output quantities $\mathbf{Y} = (Y_1, Y_2)^\top$. The measurement function is $\mathbf{f} = (f_1, f_2)^\top$. For $i = 1, 2, 3$, X_i is assigned the PDF $g_{X_i}(\xi_i)$, and $\mathbf{Y}$ is characterized by the joint PDF $g_{\mathbf{Y}}(\boldsymbol{\eta}) \equiv g_{Y_1, Y_2}(\eta_1, \eta_2)$. Figure 1 (right) adapts this instance to where X_1 and X_2 are mutually dependent and characterized by the joint PDF $g_{X_1, X_2}(\xi_1, \xi_2)$.

5.4.2 There might be an additional output quantity, $\mathbf{Q}$ say, depending on $\mathbf{Y}$. $\mathbf{Y}$ would be regarded as an input quantity to a further measurement model represented in terms of a measurement function $\mathbf{t}$, say:

$$\mathbf{Q} = \mathbf{t}(\mathbf{Y}).$$

For example, $\mathbf{Y}$ might be the vector of masses in a set of mass standards, and $\mathbf{Q}$ the sums of some of them.

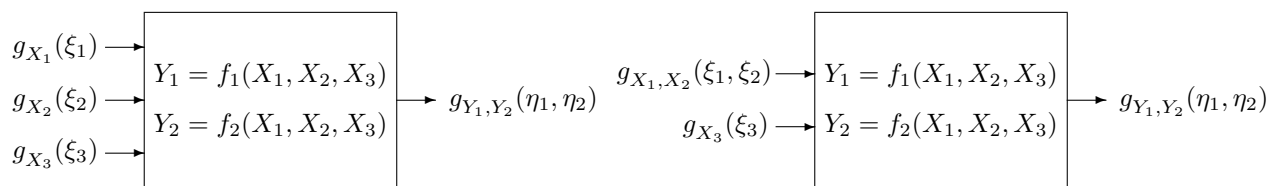


Figure 1 — Propagation of distributions for $N = 3$ input quantities and $m = 2$ output quantities when the input quantities X_1 , X_2 and X_3 are mutually independent and (right) when X_1 and X_2 are mutually dependent (5.4.1)

5.4.3 Composition of the measurement functions f and t , which are regarded as sub-models, gives Q as a function of X . It can, however, be desirable to retain the individual sub-models when they relate to functionally distinct stages. These two sub-models constitute an instance of a multistage model (see 3.12).

5.4.4 The case when the final stage of a multistage model has an output quantity that is a single scalar quantity, and that quantity is the only output quantity of interest, can be handled using GUM Supplement 1.

5.5 Obtaining summary information

5.5.1 An estimate y of the output quantity Y is the expectation $E(Y)$. The covariance matrix U_y associated with y is the covariance matrix $V(Y)$.

5.5.2 For a coverage probability p , a coverage region R_Y for Y satisfies

$$\int_{R_Y} g_Y(\eta) d\eta = p.$$

NOTE 1 Although random variables corresponding to some quantities might be characterized by distributions having no expectation or covariance matrix (see, for example, 5.3.2), a coverage region for Y always exists.

NOTE 2 Generally there is more than one coverage region for a stated coverage probability p .

5.5.3 There is no direct multivariate counterpart of the probabilistically symmetric $100p\%$ coverage interval considered in GUM Supplement 1. There is, however, a counterpart of the shortest $100p\%$ coverage interval. It is the $100p\%$ coverage region for Y of smallest hyper-volume.

5.6 Implementations of the propagation of distributions

5.6.1 The propagation of distributions can be implemented in several ways:

- analytical methods, that is methods that provide a mathematical representation of the PDF for Y ;
- uncertainty propagation based on replacing the model by a first-order Taylor series approximation (a generalization of the treatment in the GUM [JCGM 100:2008 5.1.2]) — the (generalized) law of propagation of uncertainty;
- numerical methods [JCGM 100:2008 G.1.5] that implement the propagation of distributions, specifically using a Monte Carlo method (MCM).

NOTE 1 Solutions expressible analytically are ideal in that they do not introduce any approximation. They are applicable in simple cases only, however. These methods are not considered further in this Supplement, apart from in the examples for comparison purposes.

NOTE 2 MCM as considered here is regarded as a means for providing a numerical representation of the distribution for the vector output quantity, rather than a simulation method *per se*. In the context of the propagation stage of uncertainty evaluation, the problem to be solved is deterministic, there being no random physical process to be simulated.

5.6.2 In uncertainty propagation, the estimate $\mathbf{x} = \mathbf{E}(\mathbf{X})$ of $\mathbf{X}$ and the associated covariance matrix $\mathbf{U}_x = \mathbf{V}(\mathbf{X})$ are propagated through (a linearization of) the measurement model. This Supplement provides procedures for doing so for the various types of model considered.

5.6.3 Figure 2 (left) illustrates the (generalized) law of propagation of uncertainty for a measurement model with $N = 3$ mutually independent input quantities $\mathbf{X} = (X_1, X_2, X_3)^\top$ and $m = 2$ output quantities $\mathbf{Y} = (Y_1, Y_2)^\top$. $\mathbf{X}$ is estimated by $\mathbf{x} = (x_1, x_2, x_3)^\top$ with associated standard uncertainties $u(x_1)$, $u(x_2)$ and $u(x_3)$. $\mathbf{Y}$ is estimated by $\mathbf{y} = (y_1, y_2)^\top$ with associated covariance matrix $\mathbf{U}_y$. Figure 2 (right) applies when X_1 and X_2 are mutually dependent with covariance $u(x_1, x_2)$ associated with the estimates x_1 and x_2 .

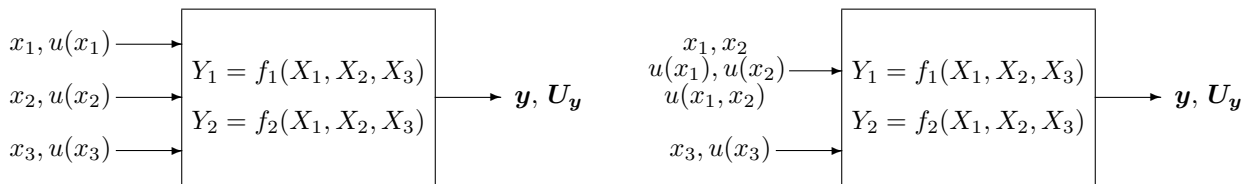


Figure 2 — Generalized law of propagation of uncertainty for $N = 3$ mutually independent input quantities X_1 , X_2 and X_3 , and $m = 2$ (almost invariably) mutually dependent output quantities, and (right) as left, but for mutually dependent X_1 and X_2 (5.6.3)

5.6.4 In MCM, a discrete representation of the (joint) probability distribution for $\mathbf{X}$ is propagated through the measurement model to obtain a discrete representation of the (joint) probability distribution for $\mathbf{Y}$ from which the required summary information is determined.

6 GUM uncertainty framework

6.1 General

6.1.1 The propagation of uncertainty for measurement models that are more general than the form $Y = f(\mathbf{X})$ in the GUM is described (see 6.2 and 6.3). Although such measurement models are not directly considered in the GUM, the same underlying principles may be used to propagate estimates of the input quantities and the uncertainties associated with the estimates through the measurement model to obtain estimates of the output quantities and the associated uncertainties. Mathematical expressions for the evaluation of uncertainty are stated using matrix-vector notation, rather than the subscripted summations given in the GUM, because generally such expressions are more compact and more naturally implemented within modern software packages and computer languages.

6.1.2 For the application of the law of propagation of uncertainty, the same information concerning the input quantities as for the univariate measurement model treated in the GUM is used:

- an estimate $\mathbf{x} = (x_1, \dots, x_N)^\top$ of the input quantity $\mathbf{X}$;
- the covariance matrix $\mathbf{U}_x$ associated with $\mathbf{x}$ containing the covariances $u(x_i, x_j)$, $i = 1, \dots, N$, $j = 1, \dots, N$, associated with x_i and x_j .

6.1.3 The description of the propagation of uncertainty given in 6.2 and 6.3 is for real measurement models, including complex measurement models that are expressed in terms of real quantities. A treatment for complex measurement models is given in 6.4. Also see 5.1.3.

6.1.4 Obtaining a coverage region for a vector output quantity is described in 6.5.

6.2 Propagation of uncertainty for explicit multivariate measurement models

6.2.1 General

6.2.1.1 An explicit multivariate measurement model specifies a relationship between an output quantity $\mathbf{Y} = (Y_1, \dots, Y_m)^\top$ and an input quantity $\mathbf{X} = (X_1, \dots, X_N)^\top$, and takes the form

$$\mathbf{Y} = \mathbf{f}(\mathbf{X}), \quad \mathbf{f} = (f_1, \dots, f_m)^\top,$$

where $\mathbf{f}$ denotes the multivariate measurement function.

NOTE Any particular function $f_j(\mathbf{X})$ may depend only on a subset of $\mathbf{X}$, with each X_i appearing in at least one function.

6.2.1.2 Given an estimate $\mathbf{x}$ of $\mathbf{X}$, an estimate of $\mathbf{Y}$ is

$$\mathbf{y} = \mathbf{f}(\mathbf{x}).$$

6.2.1.3 The covariance matrix of dimension $m \times m$ associated with $\mathbf{y}$ is

$$\mathbf{U}_{\mathbf{y}} = \begin{bmatrix} u(y_1, y_1) & \cdots & u(y_1, y_m) \\ \vdots & \ddots & \vdots \\ u(y_m, y_1) & \cdots & u(y_m, y_m) \end{bmatrix},$$

where $\text{cov}(y_j, y_j) = u^2(y_j)$, and is given by

$$\mathbf{U}_{\mathbf{y}} = \mathbf{C}_{\mathbf{x}} \mathbf{U}_{\mathbf{x}} \mathbf{C}_{\mathbf{x}}^\top, \quad (3)$$

where $\mathbf{C}_{\mathbf{x}}$ is the sensitivity matrix of dimension $m \times N$ given by evaluating

$$\mathbf{C}_{\mathbf{x}} = \begin{bmatrix} \frac{\partial f_1}{\partial X_1} & \cdots & \frac{\partial f_1}{\partial X_N} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial X_1} & \cdots & \frac{\partial f_m}{\partial X_N} \end{bmatrix}$$

at $\mathbf{X} = \mathbf{x}$ [19, page 29].

6.2.2 Examples

EXAMPLE 1 *Resistance and reactance of a circuit element* [JCGM 100:2008 H.2]

The resistance R and reactance X of a circuit element are determined by measuring the amplitude V of a sinusoidal alternating potential difference applied to it, the amplitude I of the alternating current passed through it, and the phase angle ϕ between the two. The bivariate measurement model for R and X in terms of V , I and ϕ is

$$R = f_1(V, I, \phi) = \frac{V}{I} \cos \phi, \quad X = f_2(V, I, \phi) = \frac{V}{I} \sin \phi. \quad (4)$$

In terms of the general notation, $N = 3$, $m = 2$, $\mathbf{X} \equiv (V, I, \phi)^\top$ and $\mathbf{Y} \equiv (R, X)^\top$.

An estimate $\mathbf{y} \equiv (\hat{R}, \hat{X})^\top$ of resistance and reactance is obtained by evaluating expressions (4) at an estimate $\mathbf{x} \equiv (\hat{V}, \hat{I}, \hat{\phi})^\top$ of the input quantity $\mathbf{X}$.

The covariance matrix $\mathbf{U}_{\mathbf{y}}$ of dimension 2×2 associated with $\mathbf{y}$ is given by formula (3), where $\mathbf{C}_{\mathbf{x}}$ is the sensitivity matrix of dimension 2×3 given by evaluating

$$\begin{bmatrix} \frac{\partial f_1}{\partial V} & \frac{\partial f_1}{\partial I} & \frac{\partial f_1}{\partial \phi} \\ \frac{\partial f_2}{\partial V} & \frac{\partial f_2}{\partial I} & \frac{\partial f_2}{\partial \phi} \end{bmatrix} = \begin{bmatrix} \frac{\cos \phi}{I} & -\frac{V \cos \phi}{I^2} & -\frac{V \sin \phi}{I} \\ \frac{\sin \phi}{I} & -\frac{V \sin \phi}{I^2} & \frac{V \cos \phi}{I} \end{bmatrix}$$

at $\mathbf{X} = \mathbf{x}$, and $\mathbf{U}_x$ is the covariance matrix of dimension 3×3 associated with $\mathbf{x}$.

NOTE In the GUM, reactance is denoted by X , which is the notation used here. The reactance X , a component of the vector output quantity $\mathbf{Y}$, is not to be confused with $\mathbf{X}$, the vector input quantity.

EXAMPLE 2 *Reflection coefficient measured by a microwave reflectometer (approach 1)*

The (complex) reflection coefficient Γ measured by a calibrated microwave reflectometer, such as an automatic network analyser, is given by the complex measurement model

$$\Gamma = \frac{\mathbf{a}\mathbf{W} + \mathbf{b}}{\mathbf{c}\mathbf{W} + 1}, \quad (5)$$

where $\mathbf{W}$ is the (complex) uncorrected reflection coefficient and $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ are (complex) calibration coefficients characterizing the reflectometer [10, 16, 26].

In terms of the general notation, and working with real and imaginary parts of the quantities involved, $N = 8$, $m = 2$, $\mathbf{X} \equiv (a_R, a_I, b_R, b_I, c_R, c_I, W_R, W_I)^\top$ and $\mathbf{Y} \equiv (\Gamma_R, \Gamma_I)^\top$.

An estimate $\mathbf{y} \equiv (\hat{\Gamma}_R, \hat{\Gamma}_I)^\top$ of the (complex) reflection coefficient is given by the real and imaginary parts of the right-hand side of expression (5) evaluated at the estimate $\mathbf{x}$ of the input quantity $\mathbf{X}$.

The covariance matrix $\mathbf{U}_y$ of dimension 2×2 associated with $\mathbf{y}$ is given by formula (3), where $\mathbf{C}_x$ is the sensitivity matrix of dimension 2×8 given by evaluating

$$\begin{bmatrix} \frac{\partial \Gamma_R}{\partial a_R} & \frac{\partial \Gamma_R}{\partial a_I} & \frac{\partial \Gamma_R}{\partial b_R} & \frac{\partial \Gamma_R}{\partial b_I} & \frac{\partial \Gamma_R}{\partial c_R} & \frac{\partial \Gamma_R}{\partial c_I} & \frac{\partial \Gamma_R}{\partial W_R} & \frac{\partial \Gamma_R}{\partial W_I} \\ \frac{\partial \Gamma_I}{\partial a_R} & \frac{\partial \Gamma_I}{\partial a_I} & \frac{\partial \Gamma_I}{\partial b_R} & \frac{\partial \Gamma_I}{\partial b_I} & \frac{\partial \Gamma_I}{\partial c_R} & \frac{\partial \Gamma_I}{\partial c_I} & \frac{\partial \Gamma_I}{\partial W_R} & \frac{\partial \Gamma_I}{\partial W_I} \end{bmatrix}$$

at $\mathbf{X} = \mathbf{x}$, and $\mathbf{U}_x$ is the covariance matrix of dimension 8×8 associated with $\mathbf{x}$.

EXAMPLE 3 *Calibration of mass standards*

This example constitutes an instance of a multistage model (see 3.12, 5.4.2 and 5.4.3).

A set of q mass standards of unknown mass values $\mathbf{m} = (m_1, \dots, m_q)^\top$ is calibrated by comparison with a reference kilogram, using a mass comparator, a sensitivity weight for determining the comparator sensitivity, and a number of ancillary instruments such as a thermometer, a barometer and a hygrometer for determining the correction due to air buoyancy. The reference kilogram and the sensitivity weight have masses m_R and m_S , respectively. The calibration is carried out by performing, according to a suitable measurement procedure, a sufficient number k of comparisons between groups of standards, yielding apparent, namely, in-air differences $\boldsymbol{\delta} = (\delta_1, \dots, \delta_k)^\top$. Corresponding buoyancy corrections $\mathbf{b} = (b_1, \dots, b_k)^\top$ are calculated. In-vacuo mass differences $\mathbf{X}$ are obtained from the sub-model $\mathbf{X} = \mathbf{f}(\mathbf{W})$, where $\mathbf{W} = (m_R, m_S, \boldsymbol{\delta}^\top, \mathbf{b}^\top)^\top$.

An estimate $\mathbf{y} \equiv (\hat{m}_1, \dots, \hat{m}_q)^\top$ of the masses $\mathbf{m}$ is typically given by the least-squares solution of the over-determined system of equations $\mathbf{A}\mathbf{m} = \mathbf{X}$, where $\mathbf{A}$ is a matrix of dimension $k \times q$ with elements equal to +1, -1 or zero, according to the mass standards involved in each comparison, and respecting the uncertainties associated with the estimate $\mathbf{x}$ of $\mathbf{X}$. With this choice, the estimate $\mathbf{y}$ is given by

$$\mathbf{y} = \mathbf{U}_y \mathbf{A}^\top \mathbf{U}_x^{-1} \mathbf{x}, \quad (6)$$

where the covariance matrix $\mathbf{U}_y$ of dimension $q \times q$ associated with $\mathbf{y}$ is given by $\mathbf{U}_y = (\mathbf{A}^\top \mathbf{U}_x^{-1} \mathbf{A})^{-1}$. $\mathbf{U}_x$ is the covariance matrix of dimension $k \times k$ associated with $\mathbf{x}$. A more detailed description of the sub-model, as well as a procedure for obtaining $\mathbf{U}_x$ in terms of $\mathbf{U}_w$, the covariance matrix associated with the estimate $\mathbf{w}$ of $\mathbf{W}$, is available [3].

The multivariate measurement model for this example can be expressed as

$$\mathbf{Y} = \mathbf{U}_y \mathbf{A}^\top \mathbf{U}_x^{-1} \mathbf{X},$$

where the measurement function is $\mathbf{U}_y \mathbf{A}^\top \mathbf{U}_x^{-1} \mathbf{X}$. In terms of the general notation, $N = k$, $m = q$ and $\mathbf{Y} \equiv \mathbf{m}$.

NOTE It is preferable computationally to obtain the estimate given by formula (6) by an algorithm based on orthogonal factorization [13], rather than use this explicit formula.