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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

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

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

NOTE 1 Adapted from JCGM 101:2008 definition 3.11.

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

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

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 $\boldsymbol{X}$ 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 $\boldsymbol{U}_{\boldsymbol{x}}$ associated with a vector estimate $\boldsymbol{x}$ may not be positive definite. That possibility can be a result of the way $\boldsymbol{U}_{\boldsymbol{x}}$ has been calculated. As a consequence, the Cholesky factor of $\boldsymbol{U}_{\boldsymbol{x}}$ may not exist. The Cholesky factor is used in working numerically with $\boldsymbol{U}_{\boldsymbol{x}}$ [7]; also see annex B. Moreover, the variance associated with a linear combination of the elements of $\boldsymbol{x}$ could be negative, when otherwise it would be expected to be small and positive. In such a situation procedures exist for "repairing" $\boldsymbol{U}_{\boldsymbol{x}}$ 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

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

where $\boldsymbol{Q}$ is orthonormal and $\boldsymbol{D}$ is the diagonal matrix of eigenvalues of $\boldsymbol{U}_{\boldsymbol{x}}$. Construct a new diagonal matrix, $\boldsymbol{D}'$ say, which equals $\boldsymbol{D}$, 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 $\boldsymbol{D}$. Subsequent calculations would use a repaired covariance matrix $\boldsymbol{U}'_{\boldsymbol{x}}$ formed from

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

NOTE 5 Certain operations involving $\boldsymbol{U}_{\boldsymbol{x}}$ 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 $\boldsymbol{R}_{\boldsymbol{x}}$ of dimension $N \times N$ associated with the estimate $\boldsymbol{x}$ of a quantity $\boldsymbol{X}$ has the representation

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

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 $\boldsymbol{X}$ are uncorrelated, $r(x_i, x_j) = 0$.

NOTE 2 Correlations are also known as correlation coefficients.

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

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

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

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

NOTE 4 A correlation matrix $\boldsymbol{R}_{\boldsymbol{x}}$ is positive definite or singular, if and only if the corresponding covariance matrix $\boldsymbol{U}_{\boldsymbol{x}}$ is positive definite or singular, respectively. Certain operations involving $\boldsymbol{R}_{\boldsymbol{x}}$ 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 $\boldsymbol{X}$ has dimension $m \times N$ and that with respect to $\boldsymbol{Y}$ 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 $\boldsymbol{X}$ of dimension $N \times 1$ having the joint probability density function

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

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

3.28
multivariate t-distribution
probability distribution of a random variable $\boldsymbol{X}$ of dimension $N \times 1$ having the joint probability density function

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

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

$$\Gamma(z) = \int_0^{\infty} t^{z-1} \mathrm{e}^{-t} \, \mathrm{d}t, \qquad z > 0,$$

is the gamma function

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

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

EXAMPLE When $N = 2$, $\nu = 5$, and $\boldsymbol{V}$ 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 $X_1, \ldots, X_N$, and collectively by $\boldsymbol{X} = (X_1, \ldots, X_N)^\top$, a matrix of dimension $N \times 1$, $\top$ denoting "transpose".

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

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

$$\boldsymbol{Y} = \boldsymbol{f}(\boldsymbol{X}), \tag{1}$$

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

$$Y_1 = f_1(\boldsymbol{X}), \quad \ldots, \quad Y_m = f_m(\boldsymbol{X}),$$

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

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

$$\boldsymbol{h}(\boldsymbol{Y}, \boldsymbol{X}) = \boldsymbol{0}, \tag{2}$$

or, equivalently (see 3.8), by

$$h_1(\boldsymbol{Y}, \boldsymbol{X}) = 0, \quad \ldots, \quad h_m(\boldsymbol{Y}, \boldsymbol{X}) = 0.$$

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

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

NOTE $\boldsymbol{U}_{\boldsymbol{y}}$ 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 $u_{\mathrm{c}}(y)$, 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 $\widehat{x}$.

4.10 $\boldsymbol{x}$ 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 $\widehat{I}$ [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 $\boldsymbol{X}$. 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 $\boldsymbol{X}$ is denoted by $g_{\boldsymbol{X}}(\boldsymbol{\xi})$, where $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_N)^\top$ is a variable describing the possible values of the quantity $\boldsymbol{X}$. This $\boldsymbol{X}$ is considered as a random variable with expectation $\boldsymbol{E}(\boldsymbol{X})$ and covariance matrix $\boldsymbol{V}(\boldsymbol{X})$.

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 $\boldsymbol{Y}$ is denoted by $g_{\boldsymbol{Y}}(\boldsymbol{\eta})$.

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 $X_1, \ldots, X_N$ and a real output quantity Y in the form of expression (1), namely $Y = f(\boldsymbol{X})$, where $\boldsymbol{X} \equiv (X_1, \ldots, X_N)^\top$ 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 $Y_1, \ldots, Y_m$ (denoted collectively by the real vector output quantity $\boldsymbol{Y} \equiv (Y_1, \ldots, Y_m)^\top$), taking the form (1), namely $\boldsymbol{Y} = \boldsymbol{f}(\boldsymbol{X})$, or

b) the more general form of measurement model, taking the form (2), namely $\boldsymbol{h}(\boldsymbol{Y}, \boldsymbol{X}) = \boldsymbol{0}$.

5.1.3 Further, some or all of the components of $\boldsymbol{X}$ and $\boldsymbol{Y}$ 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 $\boldsymbol{Y}$, the quantity intended to be measured (the vector measurand);

2) determine the input quantity $\boldsymbol{X}$ upon which $\boldsymbol{Y}$ depends;

3) develop a measurement function [$\boldsymbol{f}$ in (1)] or measurement model (2) relating $\boldsymbol{X}$ and $\boldsymbol{Y}$;

4) on the basis of available knowledge assign PDFs — Gaussian (normal), rectangular (uniform), etc. — to the components of $\boldsymbol{X}$. Assign instead a joint PDF to the components of $\boldsymbol{X}$ that are not pairwise independent;

b) *Propagation*:

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

c) *Summarizing*:

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

1) the expectation of $\boldsymbol{Y}$, taken as an estimate $\boldsymbol{y}$ of $\boldsymbol{Y}$,

2) the covariance matrix of $\boldsymbol{Y}$, taken as the covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$ associated with $\boldsymbol{y}$, and

3) a coverage region containing $\boldsymbol{Y}$ 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 $\boldsymbol{Y}$ 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 cirumstances, 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 $\boldsymbol{X}$ when the estimate $\boldsymbol{x}$ and associated covariance matrix $\boldsymbol{U}_{\boldsymbol{x}}$ constitute the only information available about $\boldsymbol{X}$. 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 $\boldsymbol{X}$. Also see 6.5.4.

5.3.2 Multivariate t-distribution

5.3.2.1 Suppose that a series of n indication values $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$, 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 $\mathrm{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$. The desired input quantity $\boldsymbol{X}$ 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 $\boldsymbol{X}$ is a multivariate t-distribution $t_\nu(\bar{\boldsymbol{x}}, \boldsymbol{S}/n)$ with $\nu = n - N$ degrees of freedom [11], where

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

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 $\boldsymbol{X}$ is

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

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

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

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

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

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

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

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

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

5.3.3 Construction of multivariate probability density functions

When the input quantities $X_1, \ldots, X_N$ 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 $x_1, \ldots, x_N$, used as their expectations, associated standard uncertainties $u(x_1), \ldots, u(x_N)$, 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 $\boldsymbol{X}$ 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 $\boldsymbol{X} = (X_1, X_2, X_3)^\top$ and $m = 2$ output quantities $\boldsymbol{Y} = (Y_1, Y_2)^\top$. The measurement function is $\boldsymbol{f} = (f_1, f_2)^\top$. For $i = 1, 2, 3$, X_i is assigned the PDF $g_{X_i}(\xi_i)$, and $\boldsymbol{Y}$ is characterized by the joint PDF $g_{\boldsymbol{Y}}(\boldsymbol{\eta}) \equiv g_{Y_1,Y_2}(\eta_1, \eta_2)$. 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, $\boldsymbol{Q}$ say, depending on $\boldsymbol{Y}$. $\boldsymbol{Y}$ would be regarded as an input quantity to a further measurement model represented in terms of a measurement function $\boldsymbol{t}$, say:

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

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

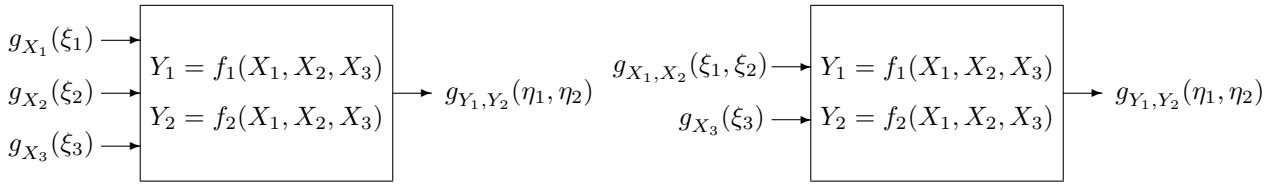

Figure 1 — Propagation of distributions for $N = 3$ input quantities and $m = 2$ output quantities when the input quantities X_1, X_2 and X_3 are mutually independent and (right) when X_1 and X_2 are mutually dependent (5.4.1)

5.4.3 Composition of the measurement functions $\boldsymbol{f}$ and $\boldsymbol{t}$, which are regarded as sub-models, gives $\boldsymbol{Q}$ as a function of $\boldsymbol{X}$. 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 $\boldsymbol{y}$ of the output quantity $\boldsymbol{Y}$ is the expectation $\boldsymbol{E}(\boldsymbol{Y})$. The covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$ associated with $\boldsymbol{y}$ is the covariance matrix $\boldsymbol{V}(\boldsymbol{Y})$.

5.5.2 For a coverage probability p, a coverage region $R_{\boldsymbol{Y}}$ for $\boldsymbol{Y}$ satisfies

$$\int_{R_{\boldsymbol{Y}}} g_{\boldsymbol{Y}}(\boldsymbol{\eta})\,\mathrm{d}\boldsymbol{\eta} = p.$$

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 $\boldsymbol{Y}$ 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 $\boldsymbol{Y}$ 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:

a) analytical methods, that is methods that provide a mathematical representation of the PDF for $\boldsymbol{Y}$;

b) 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;

c) 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 $\boldsymbol{x} = \boldsymbol{E}(\boldsymbol{X})$ of $\boldsymbol{X}$ and the associated covariance matrix $\boldsymbol{U}_{\boldsymbol{x}} = \boldsymbol{V}(\boldsymbol{X})$ 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 $\boldsymbol{X} = (X_1, X_2, X_3)^\top$ and $m = 2$ output quantities $\boldsymbol{Y} = (Y_1, Y_2)^\top$. $\boldsymbol{X}$ is estimated by $\boldsymbol{x} = (x_1, x_2, x_3)^\top$ with associated standard uncertainties $u(x_1)$, $u(x_2)$ and $u(x_3)$. $\boldsymbol{Y}$ is estimated by $\boldsymbol{y} = (y_1, y_2)^\top$ with associated covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$. 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.

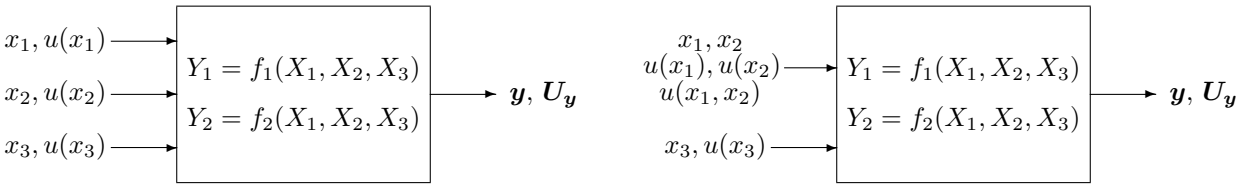

Figure 2 — Generalized law of propagation of uncertainty for $N = 3$ mutually independent input quantities X_1, X_2 and X_3, and $m = 2$ (almost invariably) mutually dependent output quantities, and (right) as left, but for mutually dependent X_1 and X_2 (5.6.3)

5.6.4 In MCM, a discrete representation of the (joint) probability distribution for $\boldsymbol{X}$ is propagated through the measurement model to obtain a discrete representation of the (joint) probability distribution for $\boldsymbol{Y}$ 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 $Y = f(\boldsymbol{X})$ 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:

a) an estimate $\boldsymbol{x} = (x_1, \ldots, x_N)^\top$ of the input quantity $\boldsymbol{X}$;

b) the covariance matrix $\boldsymbol{U}_{\boldsymbol{x}}$ associated with $\boldsymbol{x}$ containing the covariances $u(x_i, x_j)$, $i = 1, \ldots, N$, $j = 1, \ldots, N$, 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 $\boldsymbol{Y} = (Y_1, \ldots, Y_m)^\top$ and an input quantity $\boldsymbol{X} = (X_1, \ldots, X_N)^\top$, and takes the form

$$\boldsymbol{Y} = \boldsymbol{f}(\boldsymbol{X}), \qquad \boldsymbol{f} = (f_1, \ldots, f_m)^\top,$$

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

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

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

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

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

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

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

$$\boldsymbol{U}_{\boldsymbol{y}} = \boldsymbol{C}_{\boldsymbol{x}} \boldsymbol{U}_{\boldsymbol{x}} \boldsymbol{C}_{\boldsymbol{x}}^\top, \tag{3}$$

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

$$\boldsymbol{C}_{\boldsymbol{X}} = \begin{bmatrix} \dfrac{\partial f_1}{\partial X_1} & \cdots & \dfrac{\partial f_1}{\partial X_N} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial f_m}{\partial X_1} & \cdots & \dfrac{\partial f_m}{\partial X_N} \end{bmatrix}$$

at $\boldsymbol{X} = \boldsymbol{x}$ [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

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

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

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

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

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

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

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 $\boldsymbol{Y}$, is not to be confused with $\boldsymbol{X}$, the vector input quantity.

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

The (complex) reflection coefficient $\boldsymbol{\Gamma}$ measured by a calibrated microwave reflectometer, such as an automatic network analyser, is given by the complex measurement model

$$\boldsymbol{\Gamma} = \frac{\boldsymbol{a}\boldsymbol{W} + \boldsymbol{b}}{\boldsymbol{c}\boldsymbol{W} + 1}, \tag{5}$$

where $\boldsymbol{W}$ is the (complex) uncorrected reflection coefficient and $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$ 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, $N = 8$, $m = 2$, $\boldsymbol{X} \equiv (a_{\mathrm{R}}, a_{\mathrm{I}}, b_{\mathrm{R}}, b_{\mathrm{I}}, c_{\mathrm{R}}, c_{\mathrm{I}}, W_{\mathrm{R}}, W_{\mathrm{I}})^{\top}$ and $\boldsymbol{Y} \equiv (\Gamma_{\mathrm{R}}, \Gamma_{\mathrm{I}})^{\top}$.

An estimate $\boldsymbol{y} \equiv (\widehat{\Gamma}_{\mathrm{R}}, \widehat{\Gamma}_{\mathrm{I}})^{\top}$ 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 $\boldsymbol{x}$ of the input quantity $\boldsymbol{X}$.

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

$$\begin{bmatrix} \dfrac{\partial \Gamma_{\mathrm{R}}}{\partial a_{\mathrm{R}}} & \dfrac{\partial \Gamma_{\mathrm{R}}}{\partial a_{\mathrm{I}}} & \dfrac{\partial \Gamma_{\mathrm{R}}}{\partial b_{\mathrm{R}}} & \dfrac{\partial \Gamma_{\mathrm{R}}}{\partial b_{\mathrm{I}}} & \dfrac{\partial \Gamma_{\mathrm{R}}}{\partial c_{\mathrm{R}}} & \dfrac{\partial \Gamma_{\mathrm{R}}}{\partial c_{\mathrm{I}}} & \dfrac{\partial \Gamma_{\mathrm{R}}}{\partial W_{\mathrm{R}}} & \dfrac{\partial \Gamma_{\mathrm{R}}}{\partial W_{\mathrm{I}}} \\ \dfrac{\partial \Gamma_{\mathrm{I}}}{\partial a_{\mathrm{R}}} & \dfrac{\partial \Gamma_{\mathrm{I}}}{\partial a_{\mathrm{I}}} & \dfrac{\partial \Gamma_{\mathrm{I}}}{\partial b_{\mathrm{R}}} & \dfrac{\partial \Gamma_{\mathrm{I}}}{\partial b_{\mathrm{I}}} & \dfrac{\partial \Gamma_{\mathrm{I}}}{\partial c_{\mathrm{R}}} & \dfrac{\partial \Gamma_{\mathrm{I}}}{\partial c_{\mathrm{I}}} & \dfrac{\partial \Gamma_{\mathrm{I}}}{\partial W_{\mathrm{R}}} & \dfrac{\partial \Gamma_{\mathrm{I}}}{\partial W_{\mathrm{I}}} \end{bmatrix}$$

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

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 $\boldsymbol{m} = (m_1, \ldots, m_q)^{\top}$ 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 $\boldsymbol{\delta} = (\delta_1, \ldots, \delta_k)^{\top}$. Corresponding buoyancy corrections $\boldsymbol{b} = (b_1, \ldots, b_k)^{\top}$ are calculated. In-vacuo mass differences $\boldsymbol{X}$ are obtained from the sub-model $\boldsymbol{X} = \boldsymbol{f}(\boldsymbol{W})$, where $\boldsymbol{W} = \left(m_{\mathrm{R}},\ m_{\mathrm{S}},\ \boldsymbol{\delta}^{\top},\ \boldsymbol{b}^{\top}\right)^{\top}$.

An estimate $\boldsymbol{y} \equiv (\widehat{m}_1, \ldots, \widehat{m}_q)^{\top}$ of the masses $\boldsymbol{m}$ is typically given by the least-squares solution of the over-determined system of equations $\boldsymbol{A}\boldsymbol{m} = \boldsymbol{X}$, where $\boldsymbol{A}$ 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 $\boldsymbol{x}$ of $\boldsymbol{X}$. With this choice, the estimate $\boldsymbol{y}$ is given by

$$\boldsymbol{y} = \boldsymbol{U}_{\boldsymbol{y}} \boldsymbol{A}^{\top} {\boldsymbol{U}_{\boldsymbol{x}}}^{-1} \boldsymbol{x}, \tag{6}$$

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

The multivariate measurement model for this example can be expressed as

$$\boldsymbol{Y} = \boldsymbol{U}_{\boldsymbol{y}} \boldsymbol{A}^{\top} {\boldsymbol{U}_{\boldsymbol{x}}}^{-1} \boldsymbol{X},$$

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

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.

6.3 Propagation of uncertainty for implicit multivariate measurement models

6.3.1 General

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

$$\boldsymbol{h}(\boldsymbol{Y}, \boldsymbol{X}) = \boldsymbol{0}, \qquad \boldsymbol{h} = (h_1, \ldots, h_m)^\top.$$

6.3.1.2 Given an estimate $\boldsymbol{x}$ of $\boldsymbol{X}$, an estimate $\boldsymbol{y}$ of $\boldsymbol{Y}$ is given by the solution of the system of equations

$$\boldsymbol{h}(\boldsymbol{y}, \boldsymbol{x}) = \boldsymbol{0}. \tag{7}$$

NOTE The system of equations (7) has generally to be solved numerically for $\boldsymbol{y}$, using, for example, Newton's method [12] or a variant of that method, starting from an approximation $\boldsymbol{y}^{(0)}$ to the solution.

6.3.1.3 The covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$ of dimension $m \times m$ associated with $\boldsymbol{y}$ is evaluated from the system of equations

$$\boldsymbol{C}_{\boldsymbol{y}} \boldsymbol{U}_{\boldsymbol{y}} \boldsymbol{C}_{\boldsymbol{y}}^\top = \boldsymbol{C}_{\boldsymbol{x}} \boldsymbol{U}_{\boldsymbol{x}} \boldsymbol{C}_{\boldsymbol{x}}^\top, \tag{8}$$

where $\boldsymbol{C}_{\boldsymbol{y}}$ is the sensitivity matrix of dimension $m \times m$ containing the partial derivatives $\partial h_\ell / \partial Y_j$, $\ell = 1, \ldots, m$, $j = 1, \ldots, m$, and $\boldsymbol{C}_{\boldsymbol{x}}$ is the sensitivity matrix of dimension $m \times N$ containing the partial derivatives $\partial h_\ell / \partial X_i$, $\ell = 1, \ldots, m$, $i = 1, \ldots, N$, all derivatives being evaluated at $\boldsymbol{X} = \boldsymbol{x}$ and $\boldsymbol{Y} = \boldsymbol{y}$.

NOTE 1 The covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$ in expression (8) is not defined if $\boldsymbol{C}_{\boldsymbol{y}}$ is singular.

NOTE 2 Expression (8) is obtained in a similar way as expression (3), with the use of the implicit function theorem.

6.3.1.4 Formally, the covariance matrices $\boldsymbol{U}_{\boldsymbol{x}}$ and $\boldsymbol{U}_{\boldsymbol{y}}$ are related by

$$\boldsymbol{U}_{\boldsymbol{y}} = \boldsymbol{C} \boldsymbol{U}_{\boldsymbol{x}} \boldsymbol{C}^\top, \tag{9}$$

where

$$\boldsymbol{C} = \boldsymbol{C}_{\boldsymbol{y}}^{-1} \boldsymbol{C}_{\boldsymbol{x}}, \tag{10}$$

a matrix of sensitivity coefficients of dimension $m \times N$.

6.3.1.5 Annex B contains a procedure for forming $\boldsymbol{U}_{\boldsymbol{y}}$. It is not recommended that $\boldsymbol{U}_{\boldsymbol{y}}$ is obtained directly by evaluating expression (10) and then expression (9); such a procedure is less stable numerically.

6.3.2 Examples

EXAMPLE 1 *Set of pressures generated by a pressure balance*

The pressure p generated by a pressure balance is defined implicitly by the equation

$$p = \frac{m_{\mathrm{w}} \left(1 - \rho_{\mathrm{a}} / \rho_{\mathrm{w}}\right) g_\ell}{A_0 \left(1 + \lambda p\right) \left(1 + \alpha \delta\theta\right)}, \tag{11}$$

where m_{w} is the total applied mass, ρ_{a} and ρ_{w} are, respectively, the densities of air and the applied masses, g_ℓ is the local acceleration due to gravity, A_0 is the effective cross-sectional area of the balance at zero pressure, λ is the distortion coefficient of the piston-cylinder assembly, α is the coefficient of thermal expansion, and $\delta\theta$ is the deviation from a 20 °C reference Celsius temperature [17].

Let $p_1, \ldots, p_q$ denote the generated pressures for, respectively, applied masses $m_{\mathrm{w},1}, \ldots, m_{\mathrm{w},q}$ and temperature deviations $\delta\theta_1, \ldots, \delta\theta_q$.

In terms of the general notation, $N = 6 + 2q$, $m = q$, $\boldsymbol{X} \equiv (A_0, \lambda, \alpha, \delta\theta_1, m_{\mathrm{w},1}, \ldots, \delta\theta_q, m_{\mathrm{w},q}, \rho_\mathrm{a}, \rho_\mathrm{w}, g_\ell)^\top$ and $\boldsymbol{Y} \equiv (p_1, \ldots, p_q)^\top$.

$\boldsymbol{X}$ and $\boldsymbol{Y}$ are related by the measurement model

$$h_j(\boldsymbol{Y}, \boldsymbol{X}) = A_0 p_j \,(1 + \lambda p_j)\,(1 + \alpha\delta\theta_j) - m_{\mathrm{w},j}\,(1 - \rho_\mathrm{a}/\rho_\mathrm{w})\,g_\ell = 0, \qquad j = 1, \ldots, q. \tag{12}$$

An estimate $\widehat{p}_j$ of p_j is obtained by solving an equation of the form (12) given estimates of A_0, λ, α, $\delta\theta_j$, $m_{\mathrm{w},j}$, ρ_a, ρ_w and g_ℓ. However, the resulting estimates have associated covariances because they all depend on the measured quantities A_0, λ, α, ρ_a, ρ_w and g_ℓ.

The covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$ of dimension $q \times q$ associated with $\boldsymbol{y} \equiv (\widehat{p}_1, \ldots, \widehat{p}_q)^\top$ is evaluated from expression (8), where $\boldsymbol{C}_{\boldsymbol{y}}$ is the sensitivity matrix of dimension $q \times q$ containing the partial derivatives $\partial h_\ell/\partial Y_j$, $\ell = 1, \ldots, q$, $j = 1, \ldots, q$, and $\boldsymbol{C}_{\boldsymbol{x}}$ is the matrix of dimension $q \times (6 + 2q)$ containing the partial derivatives $\partial h_\ell/\partial X_i$, $\ell = 1, \ldots, q$, $i = 1, \ldots, 6 + 2q$, both evaluated at $\boldsymbol{X} = \boldsymbol{x}$ and $\boldsymbol{Y} = \boldsymbol{y}$, and $\boldsymbol{U}_{\boldsymbol{x}}$ is the covariance matrix of dimension $(6 + 2q) \times (6 + 2q)$ associated with $\boldsymbol{x}$.

NOTE 1 A measurement function [giving Y_j ($\equiv p_j$) explicitly as a function of $\boldsymbol{X}$] can be determined in this case as the solution of a quadratic equation. Such a form is not necessarily numerically stable. Moreover, measurement models involving additional, higher-order powers of p are sometimes used [9]. Determination of an explicit expression is not generally possible in such a case.

NOTE 2 There is more than one way to express the measurement model (12). For instance, in place of the form (12), the model based on equating to zero the difference between the left- and right-hand sides of model (11) could be used. The efficiency and stability of the numerical solution of the measurement model depends on the choice made.

NOTE 3 More complete models of the pressure generated by a pressure balance can also be considered [17], which include, for example, a correction to account for surface tension effects.

NOTE 4 Not all the input quantities appear in each equation, with the jth equation involving only A_0, λ, α, $\delta\theta_j$, $m_{\mathrm{w},j}$, ρ_a, ρ_w and g_ℓ.

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

Another approach to example 2 given in 6.2.2 is to relate the input quantity $\boldsymbol{X} \equiv (a_\mathrm{R}, a_\mathrm{I}, b_\mathrm{R}, b_\mathrm{I}, c_\mathrm{R}, c_\mathrm{I}, W_\mathrm{R}, W_\mathrm{I})^\top$ and the output quantity $\boldsymbol{Y} \equiv (\Gamma_\mathrm{R}, \Gamma_\mathrm{I})^\top$ using the bivariate measurement model

$$h_1(\boldsymbol{Y}, \boldsymbol{X}) = 0, \qquad h_2(\boldsymbol{Y}, \boldsymbol{X}) = 0, \tag{13}$$

where $h_1(\boldsymbol{Y}, \boldsymbol{X})$ and $h_2(\boldsymbol{Y}, \boldsymbol{X})$ are, respectively, the real and imaginary parts of

$$(\boldsymbol{c}\boldsymbol{W} + 1)\,\boldsymbol{\Gamma} - (\boldsymbol{a}\boldsymbol{W} + \boldsymbol{b})\,.$$

An advantage of this approach is that the calculation of derivatives and thence sensitivity coefficients is more straightforward.

An estimate $\boldsymbol{y} \equiv (\widehat{\Gamma}_\mathrm{R}, \widehat{\Gamma}_\mathrm{I})^\top$ of the (complex) reflection coefficient is given by setting $\boldsymbol{X} = \boldsymbol{x}$ in equations (13) and solving them numerically.

The covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$ of dimension 2×2 associated with $\boldsymbol{y}$ is evaluated from expression (8), where $\boldsymbol{C}_{\boldsymbol{y}}$ is the sensitivity matrix of dimension 2×2 containing the partial derivatives $\partial h_\ell/\partial Y_j$, $\ell = 1, 2$, $j = 1, 2$, and $\boldsymbol{C}_{\boldsymbol{x}}$ is the sensitivity matrix of dimension 2×8 containing the partial derivatives $\partial h_\ell/\partial X_i$, $\ell = 1, 2$, $i = 1, \ldots, 8$, both evaluated at $\boldsymbol{X} = \boldsymbol{x}$ and $\boldsymbol{Y} = \boldsymbol{y}$, and $\boldsymbol{U}_{\boldsymbol{x}}$ is the covariance matrix of dimension 8×8 associated with $\boldsymbol{x}$.

EXAMPLE 3 *Reflectometer calibration*

The calibration of a reflectometer (example 2 of 6.2.2) is typically undertaken by measuring values $\boldsymbol{W}$ of the uncorrected reflection coefficient corresponding to a number of standards with reflection coefficients $\boldsymbol{\Gamma}$. Often, three standards are used, giving the three (complex) simultaneous equations

$$(\boldsymbol{c}\boldsymbol{W}_j + 1)\,\boldsymbol{\Gamma}_j - (\boldsymbol{a}\boldsymbol{W}_j + \boldsymbol{b}) = 0, \tag{14}$$

for $j = 1, 2, 3$. Separation of these equations into real and imaginary parts gives rise to six simultaneous linear equations that are solved for estimates of the real and imaginary parts of the calibration coefficients $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$ given estimates of the real and imaginary parts of the uncorrected reflection coefficients $\boldsymbol{W}_j$ and of the reflection coefficients $\boldsymbol{\Gamma}_j$ for the standards.

In terms of the general notation, $N = 12$, $m = 6$, $\boldsymbol{X} \equiv (W_{1,\mathrm{R}}, W_{1,\mathrm{I}}, \Gamma_{1,\mathrm{R}}, \Gamma_{1,\mathrm{I}}, W_{2,\mathrm{R}}, W_{2,\mathrm{I}}, \Gamma_{2,\mathrm{R}}, \Gamma_{2,\mathrm{I}}, W_{3,\mathrm{R}}, W_{3,\mathrm{I}}, \Gamma_{3,\mathrm{R}}, \Gamma_{3,\mathrm{I}})^\top$ and $\boldsymbol{Y} \equiv (a_\mathrm{R}, a_\mathrm{I}, b_\mathrm{R}, b_\mathrm{I}, c_\mathrm{R}, c_\mathrm{I})^\top$.

The input and output quantities are related by a multivariate measurement model, where, for $j = 1, 2, 3$, $h_{2j-1}(\boldsymbol{Y}, \boldsymbol{X})$ and $h_{2j}(\boldsymbol{Y}, \boldsymbol{X})$ are, respectively, the real and imaginary parts of the left-hand side of expression (14).

An estimate $\boldsymbol{y} \equiv (\widehat{a}_{\mathrm{R}}, \widehat{a}_{\mathrm{I}}, \widehat{b}_{\mathrm{R}}, \widehat{b}_{\mathrm{I}}, \widehat{c}_{\mathrm{R}}, \widehat{c}_{\mathrm{I}})^{\top}$ of the (complex) calibration coefficients is given by using the estimates of $\boldsymbol{W}_j$ and $\boldsymbol{\Gamma}_j$ in equations (14) and solving these equations numerically.

The covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$ of dimension 6×6 associated with $\boldsymbol{y}$ is evaluated from expression (8), where $\boldsymbol{C}_{\boldsymbol{y}}$ is the sensitivity matrix of dimension 6×6 containing the partial derivatives $\partial h_\ell / \partial Y_j$, $\ell = 1, \ldots, 6$, $j = 1, \ldots, 6$, and $\boldsymbol{C}_{\boldsymbol{x}}$ is the sensitivity matrix of dimension 6×12 containing the partial derivatives $\partial h_\ell / \partial X_i$, $\ell = 1, \ldots, 6$, $i = 1, \ldots, 12$, both evaluated at $\boldsymbol{X} = \boldsymbol{x}$ and $\boldsymbol{Y} = \boldsymbol{y}$, and $\boldsymbol{U}_{\boldsymbol{x}}$ is the covariance matrix of dimension 12×12 associated with $\boldsymbol{x}$.

NOTE 1 If a computer system capable of operating with complex quantities is available, separation of these equations into real and imaginary parts is unnecessary. The equations can be solved "directly" for $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$.

NOTE 2 The jth equation involves only the four input quantities $W_{j,\mathrm{R}}$, $W_{j,\mathrm{I}}$, $\Gamma_{j,\mathrm{R}}$ and $\Gamma_{j,\mathrm{I}}$.

6.4 Propagation of uncertainty for models involving complex quantities

Annex A covers the algebraically efficient determination of the partial derivatives of first order of complex multivariate measurement functions. These derivatives are needed in a particularization of the law of propagation of uncertainty to such models. The treatment can be extended to complex multivariate measurement models in general.

EXAMPLE *Reflection coefficient measured by a microwave reflectometer (approach 3)*

Consider again example 2 given in 6.2.2.

The complex output quantity $\boldsymbol{Y} \equiv \boldsymbol{\Gamma}$ is related to the complex input quantity $\boldsymbol{X} = (\boldsymbol{X}_1, \ldots, \boldsymbol{X}_4)^{\top} \equiv (\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}, \boldsymbol{W})^{\top}$ by the measurement model (5). Using annex A, $\boldsymbol{C}_{\boldsymbol{x}}$, a sensitivity matrix of dimension 2×8, is given by evaluating

$$\boldsymbol{C}_{\boldsymbol{X}} = \left[\begin{array}{cccc} \boldsymbol{C}_{\boldsymbol{a}} & \boldsymbol{C}_{\boldsymbol{b}} & \boldsymbol{C}_{\boldsymbol{c}} & \boldsymbol{C}_{\boldsymbol{W}} \end{array} \right],$$

with

$$\boldsymbol{C}_{\boldsymbol{t}} = \boldsymbol{M}\left(\frac{\partial \boldsymbol{\Gamma}}{\partial \boldsymbol{t}}\right), \qquad \boldsymbol{t} \equiv \boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}, \boldsymbol{W},$$

at the estimate $\boldsymbol{x}$ of $\boldsymbol{X}$. For instance, since

$$\frac{\partial \boldsymbol{\Gamma}}{\partial \boldsymbol{b}} = \frac{1}{\boldsymbol{c}\boldsymbol{W} + 1}, \tag{15}$$

the further use of annex A gives

$$\boldsymbol{C}_{\boldsymbol{b}} = \left[\begin{array}{cc} Q_{\mathrm{R}} & -Q_{\mathrm{I}} \\ Q_{\mathrm{I}} & Q_{\mathrm{R}} \end{array} \right],$$

where Q_{R} and Q_{I} denote the real and imaginary parts, respectively, of the right-hand side of expression (15).

The covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$ of dimension 2×2 associated with $\boldsymbol{y} \equiv \widehat{\boldsymbol{\Gamma}}$, where

$$\boldsymbol{U}_{\boldsymbol{y}} = \left[\begin{array}{cc} u(\widehat{\Gamma}_{\mathrm{R}}, \widehat{\Gamma}_{\mathrm{R}}) & u(\widehat{\Gamma}_{\mathrm{R}}, \widehat{\Gamma}_{\mathrm{I}}) \\ u(\widehat{\Gamma}_{\mathrm{I}}, \widehat{\Gamma}_{\mathrm{R}}) & u(\widehat{\Gamma}_{\mathrm{I}}, \widehat{\Gamma}_{\mathrm{I}}) \end{array} \right] \equiv \left[\begin{array}{cc} u^2(\widehat{\Gamma}_{\mathrm{R}}) & u(\widehat{\Gamma}_{\mathrm{R}}, \widehat{\Gamma}_{\mathrm{I}}) \\ u(\widehat{\Gamma}_{\mathrm{I}}, \widehat{\Gamma}_{\mathrm{R}}) & u^2(\widehat{\Gamma}_{\mathrm{I}}) \end{array} \right],$$

is evaluated from expression (A.1) of annex A, where $\boldsymbol{U}_{\boldsymbol{x}}$ is the covariance matrix of dimension 8×8 associated with $\boldsymbol{x}$.

6.5 Coverage region for a vector output quantity

6.5.1 General

6.5.1.1 In electrical metrology, for example, it is appropriate to treat a vector output quantity as a single entity and in dealing with summaries of the joint probability distribution for this quantity to maintain as much information as possible.

6.5.1.2 Given an estimate $\boldsymbol{y}$ of the output quantity $\boldsymbol{Y} = (Y_1, \ldots, Y_m)^\top$, its associated covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$ and a coverage probability p, it is required to specify a region $R_{\boldsymbol{Y}}$ in m-dimensional space that contains $\boldsymbol{Y}$ with probability p.

6.5.1.3 If $\boldsymbol{y}$ and $\boldsymbol{U}_{\boldsymbol{y}}$ constitute the only available information about $\boldsymbol{Y}$, according to the principle of maximum entropy the Gaussian PDF $\mathrm{N}(\boldsymbol{y}, \boldsymbol{U}_{\boldsymbol{y}})$ is used to describe the state of knowledge of $\boldsymbol{Y}$ [JCGM 101:2008 6.4.8].

NOTE This choice of PDF is consistent, within the GUM uncertainty framework, with the characterization of a single scalar output quantity Y by a univariate Gaussian PDF when the associated degrees of freedom is infinite.

6.5.1.4 In general, once the PDF for $\boldsymbol{Y}$ is established, either the coverage probability for a specified coverage region or a coverage region for a specified coverage probability can be determined. Doing so is straightforward for a Gaussian PDF (see 6.5.2, 6.5.3 and 6.5.4). For other PDFs, a numerical method such as a Monte Carlo method (see 7) is helpful in obtaining approximate solutions that are acceptable for practical purposes.

6.5.1.5 The determination of a coverage region for a bivariate quantity (see 6.5.2) is used to motivate the treatment for the more general multivariate case (see 6.5.3). Consideration is also given to the determination of a coverage region for a quantity representing the average of a set of indication values regarded as random draws made independently from a multivariate Gaussian distribution (see 6.5.4).

6.5.2 Bivariate case

6.5.2.1 The problem of specifying bivariate coverage regions illustrates the aspects that distinguish the determination of multivariate coverage regions from the univariate case. Consider a point $\boldsymbol{Y} = (Y_1, Y_2)^\top$ in the plane with rectangular co-ordinates Y_1 (abscissa) and Y_2 (ordinate). Both co-ordinates of $\boldsymbol{Y}$ are measured with the same calibrated instrument. The information about $\boldsymbol{Y}$ constitutes estimates y_1 and y_2 of the co-ordinates, standard uncertainties $u(y_1)$ and $u(y_2)$ associated with the estimates, as well as the covariance $u(y_1, y_2)$ due to the use of the same instrument in obtaining the estimates.

6.5.2.2 In the context of the GUM uncertainty framework, as there is no other information, the joint PDF $g_{Y_1,Y_2}(\eta_1, \eta_2)$ characterizing $\boldsymbol{Y}$ is the bivariate Gaussian PDF $\mathrm{N}(\boldsymbol{y}, \boldsymbol{U}_{\boldsymbol{y}})$ (see 6.5.1.3) with

$$\boldsymbol{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}, \qquad \boldsymbol{U}_{\boldsymbol{y}} = \begin{bmatrix} u^2(y_1) & u(y_1, y_2) \\ u(y_2, y_1) & u^2(y_2) \end{bmatrix}.$$

6.5.2.3 Two particular coverage regions are considered:

a) An ellipse centred at $\boldsymbol{y}$ [19, page 38]:

$$(\boldsymbol{\eta} - \boldsymbol{y})^\top \boldsymbol{U}_{\boldsymbol{y}}{}^{-1} (\boldsymbol{\eta} - \boldsymbol{y}) = k_p^2, \tag{16}$$

with k_p a constant determined such that the area under the PDF over the elliptical region is equal to p. With this approach, the mutual dependence of Y_1 and Y_2 is taken into account.

When $\boldsymbol{Y}$ is characterized by a (bivariate) Gaussian probability distribution, the quantity

$$(\boldsymbol{Y} - \boldsymbol{y})^\top \boldsymbol{U}_{\boldsymbol{y}}{}^{-1} (\boldsymbol{Y} - \boldsymbol{y}) \tag{17}$$

is characterized by a chi-squared distribution with two degrees of freedom. It follows that k_p^2 is given by an upper percentage point of this chi-squared distribution, and satisfies

$$p = \Pr(\chi_2^2 \leq k_p^2),$$

where χ_2^2 has a chi-squared distribution with two degrees of freedom. For the coverage probability $p = 0.95$, $k_p = 2.45$ (see 6.5.3);

b) A rectangle centred at $\boldsymbol{y}$ with sides parallel to the axes and equal to the lengths of separately determined coverage intervals for Y_1 and Y_2. The coverage interval for Y_1 is determined from the PDF for Y_1 given by marginalization:

$$g_{Y_1}(\eta_1) = \int_{-\infty}^{\infty} g_{Y_1,Y_2}(\eta_1, \eta_2)\, \mathrm{d}\eta_2, \tag{18}$$

irrespective of the state of knowledge of Y_2, and similarly for the coverage interval for Y_2. The coverage intervals $y_j \pm k_q u(y_j)$ are determined for coverage probability

$$q = 1 - (1 - p)/2 = (1 + p)/2. \tag{19}$$

This rectangle constitutes a coverage region for $\boldsymbol{Y}$ corresponding to a coverage probability of at least p [5].

When $\boldsymbol{Y}$ is characterized by a (bivariate) Gaussian probability distribution, the marginal distribution (18) for Y_1 is Gaussian as is that for Y_2. It follows that k_q is given by an upper percentage point of the standard Gaussian distribution, and satisfies

$$q = \Pr(|Z| \leq k_q),$$

where Z has the standard Gaussian distribution $\mathrm{N}(0, 1)$. For the coverage probability $p = 0.95$, the coverage intervals are $y_j \pm k_q u(y_j)$, for $j = 1, 2$, with $q = 0.975$ and $k_q = 2.24$ (see 6.5.3).

NOTE 1 In the context of the GUM uncertainty framework, the elliptical coverage region given in a) is the smallest $100p\,\%$ coverage region.

NOTE 2 When Y_1 and Y_2 are mutually independent, q in expression (19) can be replaced by $q = p^{1/2}$.

EXAMPLE 1 Consider a bivariate quantity $\boldsymbol{Y}$ characterized by the Gaussian probability distribution $\mathrm{N}(\boldsymbol{y}, \boldsymbol{U}_{\boldsymbol{y}})$, where

$$\boldsymbol{y} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \qquad \boldsymbol{U}_{\boldsymbol{y}} = \begin{bmatrix} 2.0 & 0.0 \\ 0.0 & 1.0 \end{bmatrix}.$$

Figure 3 (left) shows 95 % elliptical and rectangular coverage regions for $\boldsymbol{Y}$, obtained as in a) and b). Also shown are 1 000 points representing random draws from this probability distribution. The ellipse is the smallest coverage region for the stipulated coverage probability. 950 of the 1 000 points are contained within the elliptical coverage region, which has area 26.6 unit^2, and 953 within the rectangular region, which has area 28.4 unit^2.

EXAMPLE 2 Consider a bivariate quantity $\boldsymbol{Y}$ characterized by the Gaussian probability distribution $\mathrm{N}(\boldsymbol{y}, \boldsymbol{U}_{\boldsymbol{y}})$, where

$$\boldsymbol{y} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \qquad \boldsymbol{U}_{\boldsymbol{y}} = \begin{bmatrix} 2.0 & 1.9 \\ 1.9 & 2.0 \end{bmatrix}.$$

Figure 3 (right) shows 95 % elliptical and rectangular coverage regions for $\boldsymbol{Y}$, obtained as in a) and b). Unlike example 1, the component quantities Y_1 and Y_2 of $\boldsymbol{Y}$ are (positively) correlated. 957 of the 1 000 points are contained within the elliptical coverage region, which has area 11.8 unit^2, and 972 within the rectangular region, which has area 40.1 unit^2, indicating that the coverage probability for the rectangular region exceeds 0.95. The rectangular region, whose shape does not reflect the correlated component quantities and the distribution of the randomly drawn points, might be considered inappropriate as a coverage region for $\boldsymbol{Y}$. A rectangle with sides parallel to the axes of the ellipse would have smaller area and might be considered more appropriate, but might be inconvenient since it would be expressed in terms of variables that would be artificial in terms of the application.

6.5.2.4 Further examples of coverage regions for the output quantities of bivariate measurement models are given in clause 9.

6.5.3 Multivariate case

For more than two quantities, coverage regions are no longer easily visualized, but can be constructed in an analogous manner to those described in a) and b) of 6.5.2.3 for the bivariate case. A region $R_{\boldsymbol{Y}}$ in the m-dimensional space of the output quantity $\boldsymbol{Y} = (Y_1, \ldots, Y_m)^\top$ is required such that the probability that $\boldsymbol{Y}$ lies in $R_{\boldsymbol{Y}}$ is equal to the stipulated coverage probability p. The following two forms of $R_{\boldsymbol{Y}}$, analogous to those described in a) and b) of 6.5.2.3, can be considered:

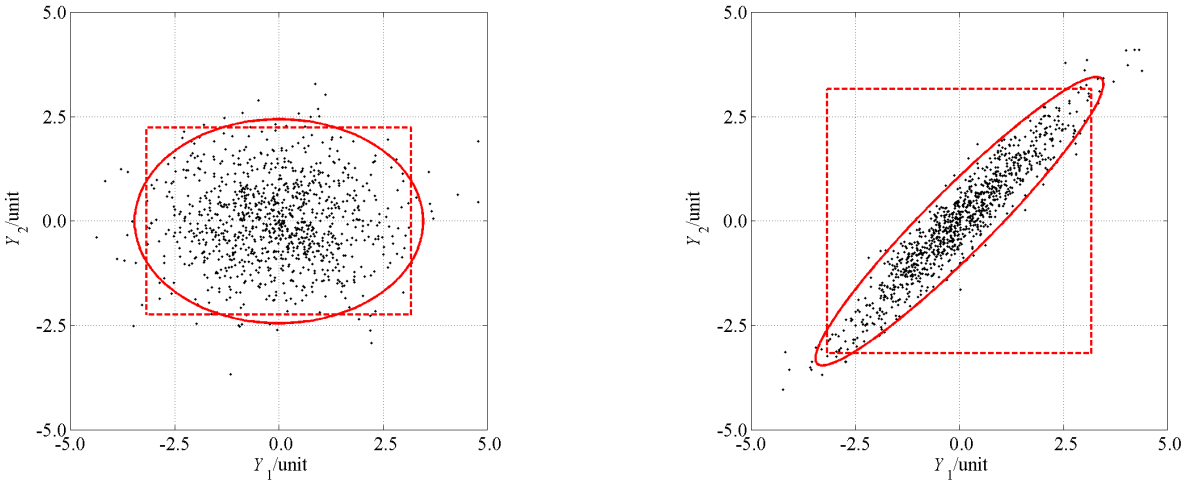

Figure 3 — Elliptical and rectangular coverage regions for a bivariate quantity $\boldsymbol{Y}$ characterized by a Gaussian probability distribution for which the component quantities Y_1 and Y_2 are mutually independent, and (right) correlated (6.5.2.3 examples 1 and 2)

a) A hyper-ellipsoid (or multivariate ellipse) in m dimensions given by expression (16).

When $\boldsymbol{Y}$ is characterized by a (multivariate) Gaussian probability distribution, the quantity (17) is characterized by a chi-squared distribution with m degrees of freedom. It follows that k_p^2 is given by an upper percentage point of this chi-squared distribution, and satisfies

$$p = \Pr(\chi_m^2 \leq k_p^2),$$

where χ_m^2 has a chi-squared distribution with m degrees of freedom. Table 1 gives values for the coverage factor k_p for the coverage probability $p = 0.95$ and m jointly evaluated Gaussian quantities for a selection of values of m.

b) A hyper-rectangle (or multivariate rectangle) in m dimensions centered at $\boldsymbol{y}$ with sides equal to the lengths of separately determined coverage intervals for Y_j, $j = 1, \ldots, m$. The coverage intervals are determined for coverage probability $q = 1 - (1 - p)/m$. This hyper-rectangle constitutes a coverage region for $\boldsymbol{Y}$ corresponding to a coverage probability of at least p [5]. The coverage interval for each Y_j is calculated following marginalization.

When $\boldsymbol{Y}$ is characterized by a (multivariate) Gaussian probability distribution, the marginal distribution for each Y_j is Gaussian. It follows that the coverage factor k_q is given by an upper percentage point of the standard Gaussian distribution as in b) of 6.5.2.3. Table 2 gives values for k_q for the coverage probability $p = 0.95$ and m jointly evaluated Gaussian quantities for a selection of values of m.

NOTE 1 For the univariate case ($m = 1$), expression (16) reduces to

$$(\eta - y)^2 = k_p^2 u_y^2,$$

giving

$$\eta = y \pm k_p u_y,$$

the endpoints of a coverage interval for Y. For the coverage probability $p = 0.95$, $k_p = 1.96$ (table 1).

NOTE 2 When the Y_j are mutually independent, q can be replaced by $q = p^{1/m}$.

6.5.4 Coverage region for the expectation of a multivariate Gaussian distribution

Consider n vectors $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_n$, each of dimension $m \times 1$, with $n > m$, corresponding to repeated indication values of a multivariate quantity $\boldsymbol{Y} = (Y_1, \ldots, Y_m)^\top$. Suppose $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_n$ can be regarded as realizations of

Table 1 — Coverage factors for hyper-ellipsoidal coverage regions corresponding to coverage probability $p = 0.95$ (6.5.2 and 6.5.3)

m	k_p	m	k_p	m	k_p	m	k_p
1	1.96	6	3.55	11	4.44	20	5.60
2	2.45	7	3.75	12	4.59	25	6.14
3	2.80	8	3.94	13	4.73	30	6.62
4	3.08	9	4.11	14	4.87	40	7.47
5	3.33	10	4.28	15	5.00	50	8.22

Table 2 — As table 1, but for hyper-rectangular coverage regions (6.5.2 and 6.5.3)

m	k_q	m	k_q	m	k_q	m	k_q
1	1.96	6	2.64	11	2.84	20	3.02
2	2.24	7	2.69	12	2.87	25	3.09
3	2.39	8	2.73	13	2.89	30	3.14
4	2.50	9	2.77	14	2.91	40	3.23
5	2.58	10	2.81	15	2.94	50	3.29

independent random vectors $\boldsymbol{Y}_1, \ldots, \boldsymbol{Y}_n$, each characterized by a multivariate Gaussian probability distribution with expectation $\boldsymbol{\mu}$ and covariance matrix $\boldsymbol{\Sigma}$. Define the average and covariance matrix

$$\boldsymbol{A} = \frac{1}{n}(\boldsymbol{Y}_1 + \cdots + \boldsymbol{Y}_n), \qquad \boldsymbol{V} = \frac{1}{n}[(\boldsymbol{Y}_1 - \boldsymbol{A})(\boldsymbol{Y}_1 - \boldsymbol{A})^\top + \cdots + (\boldsymbol{Y}_n - \boldsymbol{A})(\boldsymbol{Y}_n - \boldsymbol{A})^\top],$$

of dimensions $m \times 1$ and $m \times m$, respectively. Then, the random variable

$$\frac{n-m}{m}(\boldsymbol{A} - \boldsymbol{\mu})^\top \boldsymbol{V}^{-1}(\boldsymbol{A} - \boldsymbol{\mu})$$

has an $F_{m,n-m}$ distribution [19, Corollary 3.5.2.1], the so-called Fisher-Snedecor distribution with m and $n-m$ degrees of freedom.

NOTE The counterpart of this result for a univariate quantity is as follows: for independent random variables $Y_1, \ldots, Y_n$, each characterized by a univariate Gaussian probability distribution with expectation μ and variance σ^2, $(n-1)^{1/2}(A-\mu)/S$ has a t-distribution with $n-1$ degrees of freedom, where now

$$A = \frac{1}{n}(Y_1 + \cdots + Y_n), \qquad S^2 = \frac{1}{n}[(Y_1 - A)^2 + \cdots + (Y_n - A)^2].$$

EXAMPLE Consider $n = 12$ repeated indication values in the form of pairs, representing measured values of the volume fractions of microcline (A_1) and biotite (A_2) in one thin section cut from G–2 granite [4, 25]. Figure 4 shows these pairs as dots, together with a 95 % elliptical coverage region for the expectation of a quantity $\boldsymbol{A}$ of dimension 2×1. The expectation and covariance matrix for the indication values are

$$\boldsymbol{a} = \begin{bmatrix} 27.0 \\ 6.2 \end{bmatrix}, \qquad \boldsymbol{v} = \begin{bmatrix} 1.202 & -0.396 \\ -0.396 & 0.381 \end{bmatrix}.$$

The 95th percentile of the $F_{2,10}$ distribution is 4.10. A 95 % coverage region for $\boldsymbol{A}$ is the ellipse with equation

$$(\boldsymbol{A} - \boldsymbol{a})^\top \boldsymbol{v}^{-1}(\boldsymbol{A} - \boldsymbol{a}) = 4.10 \times \frac{2}{12-2}.$$

The small number of indication values prevents any meaningful, critical assessment of whether the assumptions hold to validate this coverage region.

7 Monte Carlo method

7.1 General

7.1.1 This clause gives information about the implementation of a Monte Carlo method (MCM) for the propagation of distributions: see the procedure given in 7.1.7, which is presented diagrammatically in figure 5.

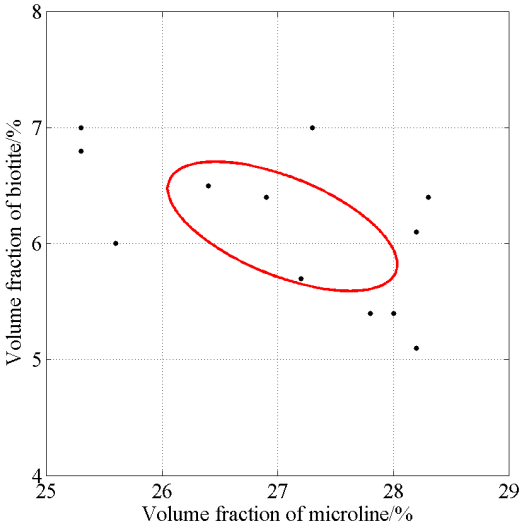

Figure 4 — Twelve indication values in the form of pairs and 95 % elliptical coverage region for the expectation taken as the average of these pairs (6.5.4 example)

7.1.2 MCM provides a general approach to obtain an approximate numerical representation $\boldsymbol{G}$, say, of the distribution function $G_{\boldsymbol{Y}}(\boldsymbol{\eta})$ for $\boldsymbol{Y}$ [18, page 75]. The heart of the approach is making repeated draws from the PDFs for the X_i (or joint PDF for $\boldsymbol{X}$) and the evaluation of the vector output quantity in each case.

7.1.3 Since $G_{\boldsymbol{Y}}(\boldsymbol{\eta})$ encodes all the information known about $\boldsymbol{Y}$, any property of $\boldsymbol{Y}$ such as expectation, variances and covariances, and coverage regions can be approximated using $\boldsymbol{G}$. The quality of these calculated results generally improves with the number of draws made.

7.1.4 The set of output quantity values obtained in 7.1.2 are taken as drawn independently from the joint probability distribution for $\boldsymbol{Y}$. Expectations, variances (and higher moments) and covariances can be determined directly from these values. The determination of coverage regions requires these values to be analyzed in an appropriate manner (see 7.7).

7.1.5 Let $\boldsymbol{y}_r$, for $r = 1, \ldots, M$, represent the output quantity values in 7.1.4. The expectation $\boldsymbol{E}(\boldsymbol{Y})$ and variance $\boldsymbol{V}(\boldsymbol{Y})$ of $\boldsymbol{Y}$ can be approximated using the $\boldsymbol{y}_r$. In general, the moments of $\boldsymbol{Y}$ (including $\boldsymbol{E}(\boldsymbol{Y})$ and $\boldsymbol{V}(\boldsymbol{Y})$) are approximated by the moments of these values. Let $M_{\boldsymbol{y}_0}$ denote the number of $\boldsymbol{y}_r$ for which each component is no greater than the corresponding component of $\boldsymbol{y}_0$, any prescribed numerical vector of dimension $m \times 1$. The probability $\Pr(\boldsymbol{Y} \leq \boldsymbol{y}_0)$ is approximated by $M_{\boldsymbol{y}_0}/M$. In this way, $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_M$ provide a discrete representation of the distribution function $G_{\boldsymbol{Y}}(\boldsymbol{\eta})$.

7.1.6 $\boldsymbol{G}$, the primary output from MCM, constitutes the matrix of dimension $m \times M$ given by

$$\boldsymbol{G} = (\boldsymbol{y}_1, \ldots, \boldsymbol{y}_M).$$

7.1.7 MCM as an implementation of the propagation of distributions when $\boldsymbol{Y}$ can be expressed explicitly in terms of $\boldsymbol{X}$, where M is provided in advance (see 7.8 otherwise), is shown diagrammatically in figure 5. MCM can be stated as a step-by-step procedure:

a) select the number M of Monte Carlo trials to be made. See 7.2;

b) generate M vectors, by drawing randomly from the PDFs assigned to the input quantities X_i (or the joint PDF for $\boldsymbol{X}$), as realizations of the (set of N) X_i. See 7.3;

c) for each such vector, form the corresponding value of $\boldsymbol{Y}$, yielding M vector output quantity values in all. See 7.4;

d) take the representation $\boldsymbol{G}$ of the distribution function for $\boldsymbol{Y}$ as the set of M vector output quantity values. See 7.5;

e) use $\boldsymbol{G}$ to form an estimate $\boldsymbol{y}$ of $\boldsymbol{Y}$ and the covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$ associated with $\boldsymbol{y}$. See 7.6;

f) use $\boldsymbol{G}$ to form an appropriate coverage region for $\boldsymbol{Y}$, for a stipulated coverage probability p. See 7.7.

NOTE Mathematically, the average of the M vector output quantity values is a realization of a random variable with expectation $\boldsymbol{E}(\boldsymbol{Y})$ and variance $\boldsymbol{V}(\boldsymbol{Y})/M$. Thus, the closeness of agreement between this average and $\boldsymbol{E}(\boldsymbol{Y})$ can be expected to be proportional to $M^{-1/2}$.

7.1.8 The effectiveness of MCM to determine $\boldsymbol{y}$, $\boldsymbol{U}_{\boldsymbol{y}}$ and a coverage region for $\boldsymbol{Y}$ depends on the use of an adequately large value of M (step a) in 7.1.7). Guidance on obtaining such a value and generally on implementing MCM is available [8]. Also see 7.2 and 7.8.

7.2 Number of Monte Carlo trials

7.2.1 A value of M, the number of Monte Carlo trials, i.e. the number of vector output quantity values, needs to be selected. It can be chosen *a priori*, in which case there will be no direct control over the quality of the numerical results provided by MCM. The reason is that the number of trials needed to provide these results to a prescribed numerical tolerance will depend on the "shape" of the PDF for the output quantity and on the coverage probability required. Also, the calculations are stochastic in nature, being based on random draws.

7.2.2 Because there is no guarantee that any specific pre-assigned number will suffice, a procedure that selects M adaptively, i.e. as the trials progress, can be used. Subclause 7.8 provides such a procedure, a property of which is that the number of trials taken is economically consistent with the expectation of achieving a required numerical tolerance.

NOTE If the model is complicated, e.g. involving the solution of a finite-element model, because of large computing times it may not be possible to use a sufficiently large value of M to obtain adequate distributional knowledge of the output quantity. In such a case an approximate approach would be to regard $g_{\boldsymbol{Y}}(\boldsymbol{\eta})$ as Gaussian (as in the GUM) and proceed as follows. A relatively small value of M, 50 or 100, for example, would be used. The average and covariance matrix of the resulting M values of $\boldsymbol{Y}$ would be taken as $\boldsymbol{y}$ and $\boldsymbol{U}_{\boldsymbol{y}}$, respectively. Given this information, a Gaussian PDF $\mathrm{N}(\boldsymbol{y}, \boldsymbol{U}_{\boldsymbol{y}})$ would be assigned to characterize the knowledge of $\boldsymbol{Y}$ [JCGM 101:2008 6.4.7] and a desired coverage region for $\boldsymbol{Y}$ calculated. Although this use of a small value of M is inevitably less reliable than that of a large value in that it does not provide an approximation to the PDF for $\boldsymbol{Y}$, it does take account of model non-linearity.

7.3 Making draws from probability distributions

7.3.1 In an implementation of MCM, M vectors $\boldsymbol{x}_r$, $r = 1, \ldots, M$, are drawn from the PDFs $g_{X_i}(\xi_i)$ for the input quantities $X_1, \ldots, X_N$. Draws would be made from the joint (multivariate) PDF $g_{\boldsymbol{X}}(\boldsymbol{\xi})$ if appropriate.

7.3.2 Recommendations concerning the manner in which these draws can be obtained for the commonest distributions, including the rectangular, Gaussian, t-distribution and multivariate Gaussian, are given in GUM Supplement 1 [JCGM 101:2008 6.4; JCGM 101:2008 annex C]. It is possible to draw at random from any other distribution [JCGM 101:2008 C.2]. Some such distributions could be approximations to distributions based on Monte Carlo results from a previous uncertainty calculation [JCGM 101:2008 6.5; JCGM 101:2008 D].

7.3.3 A procedure to make draws form a further multivariate distribution, the multivariate t-distribution, is described in 5.3.2.4.

NOTE For the results of MCM to be statistically valid, it is necessary that the pseudo-random number generators used to draw from the distributions required have appropriate properties. Some tests of randomness of the numbers produced by a generator are indicated in C.3.2 of GUM Supplement 1.

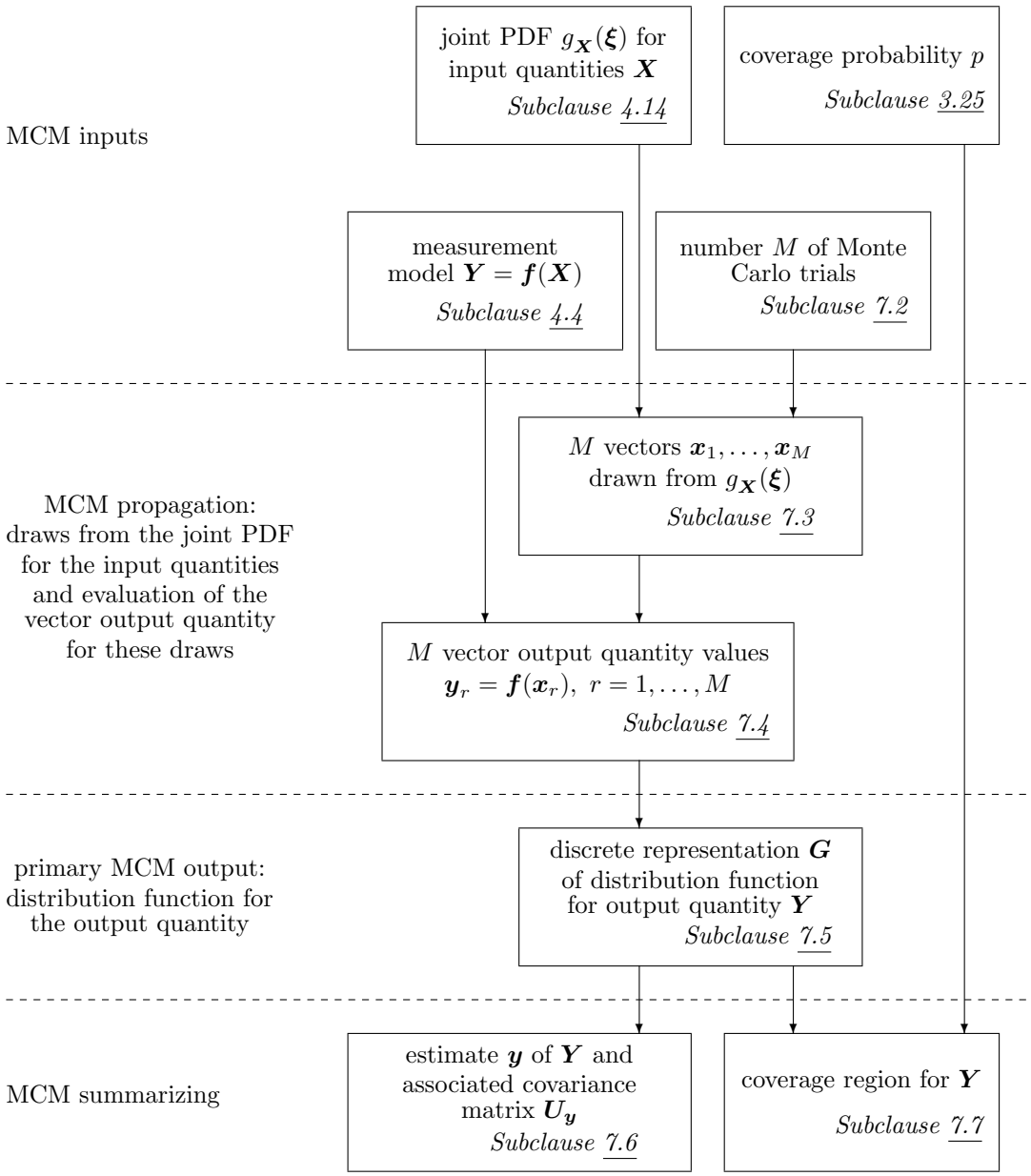

Figure 5 — Propagation and summarizing stages of uncertainty evaluation using MCM to implement the propagation of distributions when the vector output quantity can be expressed explicitly in terms of the input quantities (7.1.7)

7.4 Evaluation of the vector output quantity

7.4.1 The vector output quantity is evaluated for each of the M draws from the PDFs for the N input quantities. Specifically, denote the M draws by $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_M$, each of dimension $N \times 1$, where the rth draw $\boldsymbol{x}_r$ contains $x_{1,r}, \ldots, x_{N,r}$, with $x_{i,r}$ a draw from the PDF for X_i. When the measurement model is explicit the vector output quantity values are

$$\boldsymbol{y}_r = \boldsymbol{f}(\boldsymbol{x}_r),\ r = 1, \ldots, M.$$

NOTE Measurement function and derivative evaluations are made at the estimates of the input quantities when applying the law of propagation of uncertainty using exact derivatives. Measurement function evaluations only are made when applying the law of propagation of uncertainty using numerical (finite-difference) approximations to derivatives. These evaluations are made, if the GUM recommendation [JCGM 100:2008 5.1.3 note 2] is adopted, at the estimates of the input quantities and at points perturbed by $u(x_i)$ and $-u(x_i)$ from each individual estimate x_i in turn. With MCM, measurement function evaluations are made in the neighbourhood of these estimates, viz. at points that can be expected to be up to several standard uncertainties away from these estimates. The fact that measurement function evaluations are made at different points according to the approach used may raise issues regarding the numerical procedure used to evaluate the function, e.g. ensuring its convergence (where iterative schemes are used) and numerical stability. The user should ensure that, where appropriate, the numerical methods used to evaluate the measurement function are valid for a sufficiently large region containing these estimates. Only occasionally would it be expected that this aspect is critical.

7.4.2 The necessary modifications are made to 7.4.1 if the X_i are not independent and hence a joint PDF is assigned to them.

7.4.3 The necessary modifications are made to 7.4.1 if the measurement model is implicit. The vector output quantity values $\boldsymbol{y}_r$ are obtained as the solutions to the equations

$$\boldsymbol{h}(\boldsymbol{y}_r, \boldsymbol{x}_r) = \boldsymbol{0},\ r = 1, \ldots, M.$$

7.5 Discrete representation of the distribution function for the output quantity

A discrete representation of the distribution function for the vector output quantity is formed from the M values of the vector output quantity obtained in 7.4. In general, this representation is a matrix $\boldsymbol{G}$ of dimension $m \times M$ whose rth column is the rth value of the vector output quantity. For a univariate model, $\boldsymbol{G}$ is a row vector.

NOTE 1 The jth row of $\boldsymbol{G}$ provides a discrete representation of an approximation to the marginal distribution for Y_j.

NOTE 2 $\boldsymbol{G}$ has a graphical interpretation for $m = 1, 2, 3$. Consider $m = 2$ and, for $r = 1, \ldots, M$, plot a point in the Y_1, Y_2 plane having co-ordinates corresponding to the two elements in column r of $\boldsymbol{G}$. For M sufficiently large, the local density of points in any small region of the plane will be approximately proportional to the probability density there.

NOTE 3 A variety of information can be deduced from $\boldsymbol{G}$, such as higher-order moments. However, only the expectation and variance, used as an estimate of $\boldsymbol{Y}$ and an approximation to the associated covariance matrix, respectively, are to be used as the basis for uncertainty propagation in a further stage of uncertainty evaluation [JCGM 100:2008 0.4] in the context of the GUM uncertainty framework.

NOTE 4 If $\boldsymbol{Y}$ is to become a vector input quantity for a further uncertainty calculation, making random draws from its probability distribution is readily carried out by drawing randomly from the $\boldsymbol{y}_r$, $r = 1, \ldots, M$, (or equivalently from the columns of $\boldsymbol{G}$) with equal probability [JCGM 101:2008 6.5].

7.6 Estimate of the output quantity and the associated covariance matrix

The average and covariance matrix,

$$\widetilde{\boldsymbol{y}} = \frac{1}{M}(\boldsymbol{y}_1 + \cdots + \boldsymbol{y}_M), \qquad \boldsymbol{U}_{\widetilde{\boldsymbol{y}}} = \frac{1}{M-1}[(\boldsymbol{y}_1 - \widetilde{\boldsymbol{y}})(\boldsymbol{y}_1 - \widetilde{\boldsymbol{y}})^\top + \cdots + (\boldsymbol{y}_M - \widetilde{\boldsymbol{y}})(\boldsymbol{y}_M - \widetilde{\boldsymbol{y}})^\top],$$

are taken, respectively, as an estimate $\boldsymbol{y}$ of $\boldsymbol{Y}$ and the covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$ associated with $\boldsymbol{y}$.

NOTE Irrespective of whether the measurement model is linear or non-linear, in the limit as M tends to infinity, $\widetilde{\boldsymbol{y}}$ approaches in probability $\boldsymbol{E}(\boldsymbol{f}(\boldsymbol{X}))$ when the latter exists.

7.7 Coverage region for a vector output quantity

7.7.1 General

There are arbitrarily many $100p\,\%$ coverage regions for $\boldsymbol{Y}$. Three forms of coverage regions are given here. They are considered to have practical value, but other coverage regions might sometimes be useful in particular circumstances. Each form of coverage region addressed is based on $\boldsymbol{G}$, namely, a set of M points $\boldsymbol{y}_r$ randomly drawn from the PDF for $\boldsymbol{Y}$, such as obtained with a Monte Carlo method (see 7.5). The forms of coverage regions considered are as follows:

a) Hyper-ellipsoidal coverage region, which will be close to the smallest coverage region for $\boldsymbol{Y}$ when to a good approximation the PDF for $\boldsymbol{Y}$ is Gaussian;

b) Hyper-rectangular coverage region, which has a simple interpretation but is often pessimistically large;

c) Smallest coverage region, which in general does not have any particular geometric definition and is obtained to a degree of approximation that depends on M.

7.7.2 Hyper-ellipsoidal coverage region

A $100p\,\%$ hyper-ellipsoidal coverage region for $\boldsymbol{Y}$ is

$$(\boldsymbol{\eta} - \boldsymbol{y})^{\top} \boldsymbol{U}_{\boldsymbol{y}}{}^{-1} (\boldsymbol{\eta} - \boldsymbol{y}) = k_p^2, \tag{20}$$

where $\boldsymbol{y}$ specifies its location, $\boldsymbol{U}_{\boldsymbol{y}}$ specifies its shape, and k_p specifies its size. A procedure for determining such a coverage region is as follows:

a) Transform the points $\boldsymbol{y}_r$, denoting the transformed points by $\mathring{\boldsymbol{y}}_r$, according to

$$\mathring{\boldsymbol{y}}_r = \boldsymbol{L}^{-1}(\boldsymbol{y}_r - \boldsymbol{y}), \qquad r = 1, \ldots, M, \tag{21}$$

where $\boldsymbol{L}$ is the lower triangular matrix of dimension $m \times m$ given by the Cholesky decomposition $\boldsymbol{U}_{\boldsymbol{y}} = \boldsymbol{L}\boldsymbol{L}^{\top}$;

b) Sort the transformed points $\mathring{\boldsymbol{y}}_r$ according to increasing value of d_r, where

$$d_r^2 = \mathring{\boldsymbol{y}}_r^{\top} \mathring{\boldsymbol{y}}_r = \sum_{j=1}^{m} \mathring{y}_{j,r}^2, \qquad r = 1, \ldots, M;$$

c) Use the sorted $\mathring{\boldsymbol{y}}_r$ to determine the coverage factor k_p such that a fraction p of the $\mathring{\boldsymbol{y}}_r$ satisfies $d_r < k_p$;

d) Take the hyper-ellipsoid defined by equation (20) as the boundary of a $100p\,\%$ coverage region for $\boldsymbol{Y}$.

NOTE 1 This procedure is based on reference [1], where multidimensional data is sorted using the metric

$$(\boldsymbol{y}_r - \boldsymbol{a})^{\top} \boldsymbol{\Sigma}^{-1} (\boldsymbol{y}_r - \boldsymbol{a}),$$

with $\boldsymbol{a}$ denoting a location statistic and $\boldsymbol{\Sigma}$ a dispersion statistic. The choice made here is $\boldsymbol{a} = \boldsymbol{y}$ and $\boldsymbol{\Sigma} = \boldsymbol{U}_{\boldsymbol{y}}$. The procedure is also based on transforming the points so that the transformed points have a covariance matrix equal to the identity matrix, and hence there is no correlation associated with the transformed points. The points can then be sorted. The points $\boldsymbol{y}_r$, which can be regarded as a cluster of points centered on $\boldsymbol{y}$, approximate the distribution for $\boldsymbol{Y}$, as a consequence of the approach used to obtain them. A coverage region can be defined by the hyper-ellipsoid centred on $\boldsymbol{y}$ that (just) contains $100p\,\%$ of these $\boldsymbol{y}_r$.

NOTE 2 The extent to which the coverage region obtained is appropriate depends on the context. It might be inappropriate if the distribution of the points $\boldsymbol{y}_r$ differed appreciably from a multivariate Gaussian PDF.

NOTE 3 The matrix $\boldsymbol{L}$ in step a) can be determined as in reference [13], for instance. See example.

NOTE 4 This procedure takes into account the mutual dependence between pairs of components of $\boldsymbol{Y}$.

NOTE 5 For a complicated measurement model, for example, involving a finite-element calculation, because of large computing times it may not be possible to use a sufficiently large value of M to obtain adequate distributional knowledge of the output quantity. In such a case an approximate approach would be to regard the distribution for $\boldsymbol{Y}$ as Gaussian and proceed as follows. A relatively small value of M, say 50 or 100, would be used. The average and covariance matrix of the resulting M values of $\boldsymbol{Y}$ would be taken as $\boldsymbol{y}$ and $\boldsymbol{U}_{\boldsymbol{y}}$, respectively. Given this information, a Gaussian PDF with expectation $\boldsymbol{y}$ and covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$ would be used to characterize the knowledge of Y, and a coverage region for $\boldsymbol{Y}$ calculated accordingly. Although this use of a small value of M is inevitably less reliable than that of a large value in that it does not provide an approximation to the PDF for $\boldsymbol{Y}$, it does take account of model non-linearity. Table 1 gives values of k_p for coverage probability $p = 0.95$ as a function of m, the number of output quantities, under the assumption that $\boldsymbol{Y}$ is Gaussian.

EXAMPLE Consider the measurement model

$$Y_1 = X_1 + X_3, \qquad Y_2 = X_2 + X_3, \tag{22}$$

where the input quantities X_1 and X_2 are each assigned the Gaussian distribution $\mathrm{N}(0, 0.1)$, X_3 is assigned the rectangular distribution $\mathrm{R}(-(3 \times 1.9)^{1/2}, (3 \times 1.9)^{1/2})$, and the quantities are (pairwise) independent. The expectations of the input quantities X_i are $x_i = 0$, $i = 1, 2, 3$, with associated variances $u^2(x_i) = 0.1$, $i = 1, 2$, and $u^2(x_3) = 1.9$. Then, as in 6.5.2.3 example 2 , $\boldsymbol{Y} = (Y_1, Y_2)^{\top}$ has expectation and covariance matrix

$$\boldsymbol{y} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \qquad \boldsymbol{U}_{\boldsymbol{y}} = \begin{bmatrix} 2.0 & 1.9 \\ 1.9 & 2.0 \end{bmatrix}.$$

The $\mathring{\boldsymbol{y}}_r$ in step a) are formed using $\boldsymbol{L}^{-1}$, where to three decimal places,

$$\boldsymbol{L} = \begin{bmatrix} 1.414 & 1.344 \\ 0.000 & 0.442 \end{bmatrix}, \qquad \boldsymbol{L}^{-1} = \begin{bmatrix} 0.707 & -2.151 \\ 0.000 & 2.265 \end{bmatrix}.$$

Figure 6 (left) shows 1 000 points randomly drawn from the probability distribution for $\boldsymbol{Y}$ defined by the measurement model (22) and the above Gaussian probability distributions for the input quantities X_i, $i = 1, 2, 3$. The 95 % elliptical coverage region for $\boldsymbol{Y}$ based on characterizing $\boldsymbol{Y}$ by the bivariate Gaussian distribution $\mathrm{N}(\boldsymbol{y}, \boldsymbol{U}_{\boldsymbol{y}})$ (as in a) of 6.5.2.3) is shown by a broken line. This region has area 11.8 unit^2, $k_p = 2.45$ and contains 968 of the 1 000 points. The elliptical coverage region determined on the basis of the 1 000 draws (as in the above procedure) is shown by a solid line. This region has area 10.6 unit^2, $k_p = 2.33$, that is, it is slightly smaller than the region obtained under the Gaussian assumption, and, by construction, contains exactly 950 points.

The measurement model (22) is considered in more detail in clause 9, and further examples of coverage regions for the output quantities in bivariate measurement models are also given in clause 9.

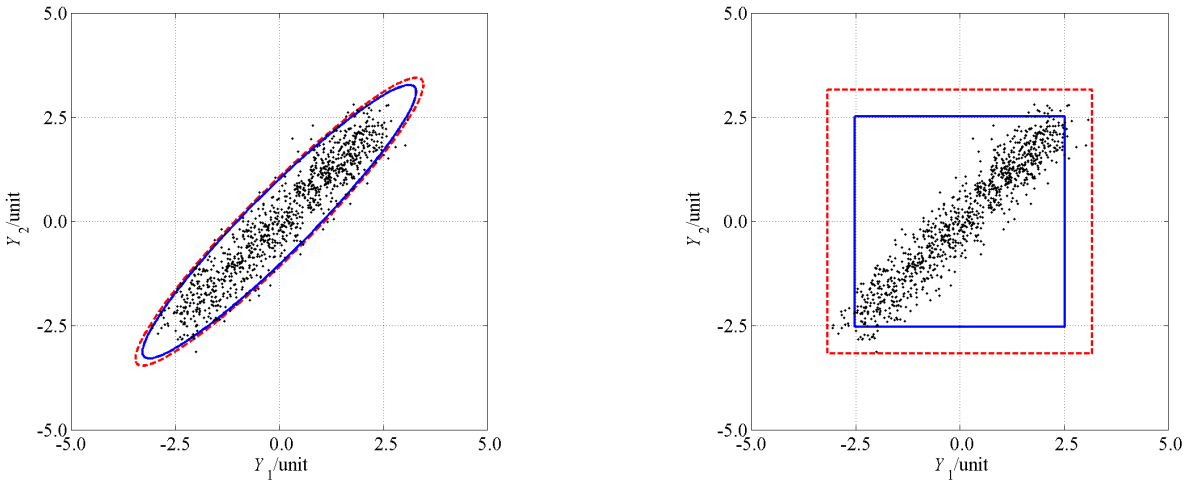

Figure 6 — Elliptical coverage regions based on 6.5.2.3 a) and 7.7.2, and (right) rectangular coverage regions based on 6.5.2.3 b) and 7.7.3 (7.7.2 example and 7.7.3 example)

7.7.3 Hyper-rectangular coverage region

A $100p\,\%$ hyper-rectangular coverage region for $\boldsymbol{Y}$ is

$$y_j \pm k_q u(y_j), \qquad j = 1, \ldots, m, \tag{23}$$

where $\boldsymbol{y} = (y_1, \ldots, y_m)^\top$ specifies its location, $\boldsymbol{u}(\boldsymbol{y}) = (u(y_1), \ldots, u(y_m))^\top$ specifies its shape, and k_q specifies its size. A procedure for determining such a coverage region is as follows:

a) Transform the points $\boldsymbol{y}_r$ according to expression (21), denoting the transformed points by $\mathring{\boldsymbol{y}}_r$, where $\boldsymbol{L}$ is now the diagonal matrix of dimension $m \times m$ with diagonal elements $u(y_1), \ldots, u(y_m)$;

b) Rank the transformed points $\mathring{\boldsymbol{y}}_r$ according to increasing value of d_r, where now

$$d_r = \max_{j=1,\ldots,m} |\mathring{y}_{j,r}|, \qquad r = 1, \ldots, M;$$

c) Use the ranked $\mathring{\boldsymbol{y}}_r$ to determine the coverage factor k_q such that a fraction p of the $\mathring{\boldsymbol{y}}_r$ satisfies $d_r < k_q$;

d) Take the hyper-rectangle defined by expression (23) as the boundary of a $100p\,\%$ coverage region for $\boldsymbol{Y}$.

NOTE With this approach, mutual dependence between pairs of components of $\boldsymbol{Y}$ is not taken into account.

EXAMPLE Figure 6 (right) shows the same 1 000 points as in figure 6 (left). The 95 % rectangular coverage region for $\boldsymbol{Y}$ based on characterizing Y_j, $j = 1, 2$, by the Gaussian distribution $\mathrm{N}(y_j, u^2(y_j))$, and ignoring the correlation associated with y_1 and y_2 (as in b) of 6.5.2.3), is shown by a broken line. This region has area 40.1 unit^2, $k_q = 2.24$ and contains all 1 000 points. The rectangular coverage region determined on the basis of the 1 000 draws (as in the above procedure) is shown by a solid line. This region has area 25.5 unit^2, $k_q = 1.78$, that is, it is smaller than the region obtained under the Gaussian assumption, and, by construction, contains exactly 950 points.

7.7.4 Smallest coverage region

A procedure that provides an approximation to the smallest $100p\,\%$ coverage region is as follows:

a) Construct a (hyper-)rectangular region in the space of the output quantities;

b) Subdivide this rectangular region into a mesh of small rectangles;

c) Assign each output quantity value to the small rectangle containing it;

d) Use the fraction of output quantity values assigned to each rectangle as the approximate probability that $\boldsymbol{Y}$ lies in that rectangle;

e) List the rectangles in terms of decreasing probability;

f) Form the cumulative sum of probabilities for these listed rectangles, stopping when this sum is no smaller than p;

g) Take the corresponding set of rectangles as defining the smallest coverage region.

NOTE 1 The procedure is based on reference [20] and consists of subdividing the space of the output quantities into a number of small (hyper-)rectangles, approximating the probability that $\boldsymbol{Y}$ lies in each small rectangle by the proportion of output quantity values assigned to that rectangle, and approximating the smallest coverage region by the smallest set of such rectangles that contain $100p\,\%$ of the M output quantity values.

NOTE 2 The rectangular region in step a) should just contain all the $\boldsymbol{y}_r$.

NOTE 3 The fineness of the mesh in b) influences the approximate coverage region produced.

NOTE 4 The quality of the approximation generally improves with M. To achieve a sufficiently good approximation, particularly for a number of output quantities larger than about two or three, might necessitate a very large value of M.

NOTE 5 The region so obtained might be disjointed, particularly if M is insufficiently large.

NOTE 6 Step d) sets the probability for each rectangle to be the relative frequency of output quantity values assigned to that rectangle. A coverage region that is less disjointed and having a smoother boundary would be expected to be obtained if step d) were replaced by the use of a more sophisticated approximation to the probability density [23].

NOTE 7 Some of the approximate probabilities in step d) may be equal in value. In such a case the order of the items in the list in step e) is not unique. As a consequence a different approximate coverage region might be obtained for each possible ordering.

NOTE 8 In the bivariate case ($m = 2$), steps a) to d) are also carried out in the initial stages of a typical contouring algorithm used in visualizing an approximation to the PDF for $\boldsymbol{Y}$ (see 9.1.6).

EXAMPLE Consider the same problem as in 7.7.2 example. Figure 7 shows approximations to the 95 % smallest coverage region, obtained using the procedure in this subclause, based on a set of small rectangles forming a 10×10 mesh and (right) a 100×100 mesh. The coverage region in figure 7 (left) relates to 1 000 points drawn randomly from the PDF for $\boldsymbol{Y}$, has area 11.3 unit^2 and contains 955 of the points. The coverage region in figure 7 (right) relates to 1 000 000 points drawn randomly from the PDF for $\boldsymbol{Y}$, has area 9.4 unit^2 and contains 950 074 of the points. For comparison, in each figure, the 95 % elliptical coverage region for $\boldsymbol{Y}$ based on the procedure in 7.7.2 is shown by a solid line.

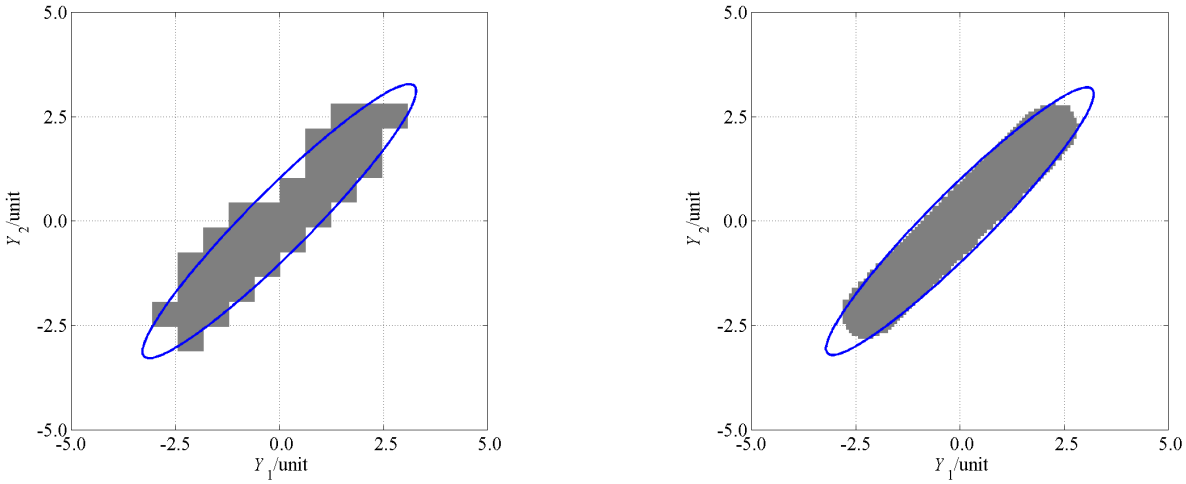

Figure 7 — Elliptical coverage regions based on 7.7.2 and approximations to the smallest coverage region based on 7.7.4 for a 10×10 mesh and 1 000 points drawn randomly from the PDF for $\boldsymbol{Y}$, and (right) for a 100×100 mesh and 1 000 000 points (7.7.4 example)

7.8 Adaptive Monte Carlo procedure

7.8.1 General

7.8.1.1 The effectiveness of MCM to determine estimates $\boldsymbol{y}$ of the output quantities $\boldsymbol{Y}$, the associated covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$ and a coverage region for $\boldsymbol{Y}$ depends on the use of an adequately large value for the number M of Monte Carlo trials. A value for M can be chosen *a priori* as in 7.2. Alternatively, an adaptive Monte Carlo procedure can be used that involves carrying out an increasing number of Monte Carlo trials until the various results of interest have stabilized in a statistical sense. A numerical result is deemed to have stabilized if twice the standard deviation associated with it is less than a stipulated numerical tolerance (see 7.8.2).

7.8.1.2 The objective of the adaptive procedure given in 7.8.3 is to provide

a) an estimate $\boldsymbol{y} = (y_1, \ldots, y_m)^{\top}$ of $\boldsymbol{Y}$,

b) a vector $\boldsymbol{u}(\boldsymbol{y}) = (u(y_1), \ldots, u(y_m))^{\top}$ of standard uncertainties associated with the estimates,

c) a positive definite matrix $\boldsymbol{R}_{\boldsymbol{y}}$ of dimension $m \times m$ of correlation coefficients $r_{ij} = r(y_i, y_j)$ associated with pairs of the estimates, and

d) a coverage factor k_p defining a $100p$ % coverage region for $\boldsymbol{Y}$ in the form of a hyper-ellipsoid in m dimensions,

such that each of these values can be expected to meet a stipulated numerical tolerance.

NOTE 1 By its stochastic nature, the procedure cannot be guaranteed to meet these tolerances.

NOTE 2 Generally, the larger is the coverage probability p, the larger is the number of Monte Carlo trials required to determine k_p for a given numerical tolerance.

NOTE 3 The standard uncertainties $\boldsymbol{u}(\boldsymbol{y})$ and correlation matrix $\boldsymbol{R_y}$ together determine the covariance matrix $\boldsymbol{U_y}$ associated with the estimates $\boldsymbol{y}$ (see 3.21 note 3 and 7.8.2.4).

NOTE 4 When a coverage region is to be determined that is not in the form of a hyper-ellipsoid in m dimensions, a test for stabilization can be made in terms of the parameters defining the region. For example, for a coverage region in the form of a hyper-rectangle in m dimensions, a test could be made in terms of the coverage factor k_q defining the region and a numerical tolerance associated with k_q. The procedure given in 7.8.3 is modified accordingly.

NOTE 5 When a coverage region is not required, an increasing number of Monte Carlo trials is undertaken until the estimates $\boldsymbol{y}$, associated standard uncertainties $\boldsymbol{u}(\boldsymbol{y})$ and correlation matrix $\boldsymbol{R_y}$ have stabilized.

NOTE 6 When dependencies exist among the output quantities, $\boldsymbol{R_y}$ may not be positive definite. See 9.4 (particularly 9.4.2.3 note 2) for an example.

7.8.2 Numerical tolerance associated with a numerical value

7.8.2.1 Let n_{dig} denote the number of significant decimal digits regarded as meaningful in a numerical value z. The numerical tolerance δ associated with z is given as follows:

a) express z in the form $c \times 10^{\ell}$, where c is an n_{dig} decimal digit integer and ℓ an integer;

b) take

$$\delta = \frac{1}{2} 10^{\ell}.$$

7.8.2.2 For $j = 1, \ldots, m$, the numerical tolerance δ_j used to test for stabilization of the estimate y_j of Y_j and the standard uncertainty $u(y_j)$ associated with y_j in the adaptive procedure of 7.8.3 is calculated in terms of a number of significant decimal digits regarded as meaningful in the value of $u(y_j)$.

7.8.2.3 The numerical tolerance ρ used to test for stabilization of the matrix $\boldsymbol{R_y}$ of correlation coefficients $r_{i,j}$ associated with the estimate $\boldsymbol{y}$ is calculated in terms of a number of significant decimal digits in $\lambda_{\max}$, the largest eigenvalue of $\boldsymbol{R_y}$ (see 3.21 note 3).

7.8.2.4 The matrix $\boldsymbol{R_y}$ would often be used in a subsequent uncertainty evaluation. Commonly, this evaluation would relate to a scalar quantity Q expressed as some linear combination

$$Q = c_1 Y_1 + \cdots + c_m Y_m = \boldsymbol{c}^{\top} \boldsymbol{Y}$$

of the Y_i. Using

$$\boldsymbol{U_y} = \boldsymbol{D_y} \boldsymbol{R_y} \boldsymbol{D_y}$$

(see 3.21 note 3), the standard uncertainty $u(q)$ associated with the estimate

$$q = \boldsymbol{c}^{\top} \boldsymbol{y}$$

of Q is given by

$$u^2(q) = \boldsymbol{c}^{\top} \boldsymbol{U_y} \boldsymbol{c} = \boldsymbol{d}^{\top} \boldsymbol{R_y} \boldsymbol{d},$$

where

$$\boldsymbol{d} = \boldsymbol{D_y} \boldsymbol{c}.$$

7.8.2.5 The numerical accuracy of $u(q)$ depends on that of $\boldsymbol{R_y}$ and $\boldsymbol{d}$, the latter depending on $\boldsymbol{D_y}$ and hence $\boldsymbol{u}(\boldsymbol{y}) = (u_1(y_1), \ldots, u_m(y_m))^\top$.

7.8.2.6 For subsequent uncertainty evaluations that are more complicated, such as involving a least squares calculation using explicitly or implicitly the inverse of $\boldsymbol{U_y}$, it would be necessary to utilize a different stabilization test. For a least squares calculation, it would be appropriate to calculate ρ in 7.8.2.3 in terms of a number of significant decimal digits in the smallest eigenvalue of $\boldsymbol{R_y}$ (also see 3.21 note 5): the sensitivity of the solution to the least squares problem depends on the condition number $\lambda_{\max}/\lambda_{\min}$ of $\boldsymbol{R_y}$. Hence, in order to reduce the number of Monte Carlo trials, a parametrization of that problem should be used that makes the condition number as small as reasonably possible.

7.8.2.7 The numerical tolerance κ_p used to test for stabilization of the coverage factor k_p is calculated in terms of a number of significant decimal digits regarded as meaningful in the value k_p.

7.8.2.8 For a subsequent uncertainty evaluation based on the use of $\boldsymbol{G}$ (see 7.5) as an approximation to the distribution function for $\boldsymbol{Y}$, it should be ensured that this discrete representation is adequate for the purpose, especially when a coverage region is to be provided. Detailed advice on this aspect is beyond the scope of this Supplement.

7.8.3 Adaptive procedure

A suggested practical approach, involving carrying out a sequence of applications of MCM, is as follows:

a) set n_{dig} to an appropriate small positive integer (see 7.8.2);

b) set $M = \max(J, 10^4)$, where J is the smallest integer greater than or equal to $100/(1-p)$;

c) set $h = 1$, denoting the first application of MCM in the sequence;

d) carry out M Monte Carlo trials, as in 7.3 and 7.4;

e) use the M vector output quantity values $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_M$ so obtained to calculate $\boldsymbol{y}^{(h)}$, $\boldsymbol{u}(\boldsymbol{y}^{(h)})$, $\boldsymbol{R_y}^{(h)}$ and $k_p^{(h)}$ as an estimate of $\boldsymbol{Y}$, the associated standard uncertainties, the associated correlation matrix and a coverage factor for a $100p\,\%$ coverage region, respectively, i.e. for the hth member of the sequence;

f) if $h \leq 10$, increase h by one and return to step d);

g) for $j = 1, \ldots, m$, calculate the standard deviation s_{y_j} associated with the average of the estimates $y_j^{(1)}, \ldots, y_j^{(h)}$ of Y_j, given by

$$s_{y_j}^2 = \frac{1}{h(h-1)} \sum_{r=1}^{h} (y_j^{(r)} - y_j)^2, \qquad y_j = \frac{1}{h} \sum_{r=1}^{h} y_j^{(r)};$$

h) calculate the counterpart of this statistic for the components of $\boldsymbol{u}(\boldsymbol{y}^{(h)})$ and for $\lambda_{\max}$ and $k_p^{(h)}$;

i) use all $h \times M$ model values available so far to form values for $\boldsymbol{u}(\boldsymbol{y})$, $\boldsymbol{R_y}$ and k_p;

j) for $j = 1, \ldots, m$, calculate the numerical tolerances δ_j associated with $u(y_j)$ as in 7.8.2.1 and 7.8.2.2;

k) calculate the numerical tolerance ρ associated with the matrix $\boldsymbol{R_y}$ of correlation coefficients as in 7.8.2.1 and 7.8.2.3;

l) calculate the numerical tolerance κ_p associated with k_p as in 7.8.2.1 and 7.8.2.7;

m) if for any $j = 1, \ldots, m$, $2s_{y_j}$ or $2s_{u(y_j)}$ exceeds δ_j, or $2s_{\lambda_{\max}}$ exceeds ρ, or $2s_{k_p}$ exceeds κ_p, increase h by one and return to step d);

n) regard the overall computation as having stabilized, and use all $h \times M$ vector output quantity values obtained to calculate $\boldsymbol{y}$, $\boldsymbol{U_y}$ and the coverage factor k_p for a $100p\,\%$ coverage region, as in 7.6 and 7.7.

NOTE 1 For (stochastic) convergence of the adaptive procedure, the expectation and covariance matrix of $\boldsymbol{Y}$ must exist.

NOTE 2 The choice of M in step b) is arbitrary, but has been found suitable in practice.

NOTE 3 The initial use of ten applications of MCM with M trials in steps d) to f) helps to prevent premature convergence of the procedure, and, moreover, makes the assumption, implied by note 6, more reasonable. A similar change to the counterpart of this procedure when there is a single scalar output quantity [JCGM 101:2008 7.9.4] would also improve the performance of the scheme there for some problems.

NOTE 4 In step g), y_j is regarded as a realization of a random variable with standard deviation s_{y_j}.

NOTE 5 The standard deviations formed in steps g) and h) tend to reduce in a manner proportional to $h^{-1/2}$ (see 7.1.7 note).

NOTE 6 The factor 2 used in step m) is based on regarding the averages as realizations of Gaussian variables, and corresponds to a coverage probability of approximately 95 %.

NOTE 7 Reference [28] considers improvements to the adaptive scheme of GUM Supplement 1 [JCGM 101:2008 7.9].

8 Validation of the GUM uncertainty framework using a Monte Carlo method

8.1 The (generalized) GUM uncertainty framework (GUF) can be expected to work well in many circumstances. However, it is not always straightforward to determine whether all the conditions for its application hold [JCGM 101:2008 5.7, JCGM 101:2008 5.8]. Indeed, the degree of difficulty of doing so would typically be considerably greater than that required to apply MCM, assuming suitable software were available [8]. Therefore, since these circumstances cannot readily be tested, any cases of doubt should be validated. Since the domain of validity for MCM is broader than that for the GUM uncertainty framework, it is recommended that both the GUM uncertainty framework and MCM be applied and the results compared. Should the comparison be favourable, the GUM uncertainty framework could be used on this occasion and for sufficiently similar problems in the future. Otherwise, consideration should be given to using MCM or another appropriate approach instead.

8.2 Specifically, it is recommended that steps a) and b) below and the comparison process in 8.3 be carried out:

a) apply the GUM uncertainty framework (see 6) to yield (i) an estimate $\boldsymbol{y}^{\mathrm{GUF}}$ of $\boldsymbol{Y}$, (ii) the standard uncertainties $\boldsymbol{u}(\boldsymbol{y}^{\mathrm{GUF}})$ associated with $\boldsymbol{y}^{\mathrm{GUF}}$, (iii) the correlation matrix $\boldsymbol{R_y}^{\mathrm{GUF}}$ associated with $\boldsymbol{y}^{\mathrm{GUF}}$, and (iv) the coverage factor k_p^{GUF} defining a $100p\,\%$ coverage region for $\boldsymbol{Y}$ in the form of a hyper-ellipsoid in m dimensions;

b) apply the adaptive Monte Carlo procedure (see 7.8.3) to provide, similarly, $\boldsymbol{y}^{\mathrm{MCM}}$, $\boldsymbol{u}(\boldsymbol{y}^{\mathrm{MCM}})$, $\boldsymbol{R_y}^{\mathrm{MCM}}$ and k_p^{MCM}.

8.3 The objective of the comparison procedure is to determine whether the results provided by the GUM uncertainty framework and MCM agree to within a stipulated numerical tolerance. The procedure is as follows:

a) set n_{dig} to an appropriate small positive integer (see 7.8.2);

b) for $j = 1, \ldots, m$, calculate the numerical tolerances δ_j associated with $u(y_j)$ as in 7.8.2.1 and 7.8.2.2;

c) calculate the numerical tolerance ρ associated with the matrix $\boldsymbol{R_y}$ of correlation coefficients as in 7.8.2.1 and 7.8.2.3;

d) calculate the numerical tolerance κ_p associated with k_p as in 7.8.2.1 and 7.8.2.7;

e) compare the estimates, associated standard uncertainties and correlation coefficients, and coverage factors obtained using the GUM uncertainty framework and MCM to determine whether the required number of correct decimal digits in the results provided by the GUM uncertainty framework has been obtained. Specifically, determine

$$\begin{aligned} d_{y_j} &= |y_j^{\mathrm{GUF}} - y_j^{\mathrm{MCM}}|, & j = 1, \ldots, m, \\ d_{u(y_j)} &= |u(y_j^{\mathrm{GUF}}) - u(y_j^{\mathrm{MCM}})|, & j = 1, \ldots, m, \\ d_{\lambda_{\max}} &= |\lambda_{\max}^{\mathrm{GUF}} - \lambda_{\max}^{\mathrm{MCM}}|, \\ d_{k_p} &= |k_p^{\mathrm{GUF}} - k_p^{\mathrm{MCM}}|, \end{aligned}$$

viz. the absolute differences of the respective numerical results. Then, if for all $j = 1, \ldots, m$, d_{y_j} and $d_{u(y_j)}$ are no larger than δ_j, $d_{\lambda_{\max}}$ is no larger than ρ, and d_{k_p} is no larger than κ_p, the comparison is favourable and the GUM uncertainty framework has been validated in this instance.

NOTE 1 The choice of $100p\,\%$ coverage region will influence the comparison. Therefore, the validation applies for the specified coverage probability p and coverage region only.

NOTE 2 In situations where a coverage region is not required, the test in step d) can be based instead on d_{y_j}, $d_{u(y_j)}$ and $d_{\lambda_{\max}}$ only. In cases where a coverage region is determined that is not in the form of a hyper-ellipsoid in m dimensions, a test can be made in terms of the parameters defining the region. For example, for a coverage region in the form of a hyper-rectangle in m dimensions, a test can be made in terms of the coverage factor k_q defining the region and a numerical tolerance κ_q associated with k_q.

NOTE 3 A sufficient number M of Monte Carlo trials should be performed in obtaining MCM results for the purpose of validating those from the GUM uncertainty framework. It is recommended that the numerical tolerances set in the adaptive procedure of 7.8 are no greater than one fifth of the respective numerical tolerances used in the validation procedure [JCGM 101:2008 8.2]. Alternatively, the number of significant decimal digits set in the adaptive procedure can be set to be one greater than the number of digits set in the validation procedure.

9 Examples

9.1 Illustrations of aspects of this Supplement

9.1.1 The first example (see 9.2) is a linear measurement model in which the output quantities of the measurement model depend on a common effect and on effects that are different for the output quantities. This is an example for which analytical solutions are available for some special cases.

9.1.2 The second example (see 9.3) is a non-linear measurement model concerning the transformation from a Cartesian representation (in terms of real and imaginary parts) of a complex quantity to a polar representation (in terms of magnitude and phase) of the quantity. This is an example for which analytical solutions are available for some special cases [6].

9.1.3 The third example (see 9.4), constituting a further non-linear measurement model, is that in the GUM concerned with the simultaneous measurement of resistance and reactance [JCGM 100:2008 H.2]. The example illustrates the treatment of a series of simultaneous indication values of a vector quantity that have been obtained independently.

9.1.4 The fourth example (see 9.5) is concerned with the measurement of Celsius temperature using a resistance thermometer. The example illustrates the treatment of a univariate measurement model and a multivariate measurement model.

9.1.5 Many of the figures used to illustrate the results for the examples are best viewed in colour. In the figures showing contours, contours with a common colour correspond to the same contour value. The correspondence between contours of the same colour for contour plots within the same figure is applied throughout this

Supplement unless a statement is made to the contrary. When two or more figures are used to compare results, such as those from the GUM uncertainty framework and a Monte Carlo method, the same axes are generally used. There are some exceptions when the PDFs, etc. for the methods are very different.

9.1.6 Since the primary output from MCM is the set of M values of the vector quantity $\boldsymbol{Y}$ gathered in the matrix $\boldsymbol{G}$ of dimension $m \times M$ (see 7.1.6), it is often desirable to summarize them by an approximation to the corresponding probability density function, and to depict this function by its contour lines. The figures in this clause show such contour lines in cases where the output quantity is of dimension $m = 2$. The contour lines should be drawn in ways that guarantee that, as the number M of draws from the probability distribution of the output quantity grows large, they converge to the contours of the corresponding probability density function: doing so requires appropriate smoothing [22, 24]. Some contour diagrams shown in this clause are computed directly from an approximation to the corresponding probability density function. For others an appropriate smoothing algorithm is applied and the resulting smoothed contours drawn. In one instance (figure 10) unsmoothed and smoothed contours are shown to indicate the effect of the smoothing algorithm.

9.2 Additive measurement model

9.2.1 Formulation

This example (compare 7.7.2 example) considers the additive (linear) bivariate measurement model

$$Y_1 = X_1 + X_3, \qquad Y_2 = X_2 + X_3 \tag{24}$$

for three different sets of PDFs $g_{X_i}(\xi_i)$ assigned to the input quantities X_i, regarded as independent. The measurement model has three input quantities X_1, X_2 and X_3, with X_3 representing an effect that is common to the output quantities Y_1 and Y_2, and X_1 and X_2 effects that are different for Y_1 and Y_2. For the first set of input PDFs (see 9.2.2), each $g_{X_i}(\xi_i)$ is chosen to be a standard Gaussian distribution with X_i having expectation zero and standard deviation unity. The second set of PDFs (see 9.2.3) is identical to the first, but $g_{X_3}(\xi_3)$ is a rectangular distribution, also with X_3 having expectation zero and standard deviation unity. The third set of PDFs (see 9.2.4) is identical to the second except that X_3 has standard deviation three, representing a dominant common effect.

9.2.2 Propagation and summarizing: case 1

9.2.2.1 Characterize each X_i by a standard Gaussian distribution. The estimates of the X_i are $x_i = 0$, $i = 1, 2, 3$, with associated standard uncertainties $u(x_i) = 1$. The results obtained from the application of the GUM uncertainty framework (see 6) and MCM (see 7) are summarized in table 3 and figures 8 to 10. Some results in the table are reported to four significant decimal digits in order to facilitate their comparison.

Table 3 — Application of the GUM uncertainty framework (GUF) and MCM to the additive model (24), with each X_i characterized by a standard Gaussian distribution (9.2.2)

Method	M	y_1	y_2	$u(y_1)$	$u(y_2)$	$r(y_1, y_2)$	k_p	k_q
GUF		0.000	0.000	1.414	1.414	0.500	2.45	2.24
MCM	1×10^5	0.003	0.005	1.412	1.408	0.498	2.45	2.22
MCM	1×10^6	0.000	0.000	1.416	1.415	0.500	2.45	2.21
MCM	1×10^7	0.000	0.000	1.414	1.414	0.500	2.45	2.21
Adaptive MCM	0.35×10^6	0.001	−0.001	1.417	1.417	0.502	2.45	2.22
Adaptive MCM	0.45×10^6	0.001	−0.001	1.416	1.414	0.501	2.45	2.21

9.2.2.2 The (generalized) GUM uncertainty framework gives the estimate $\boldsymbol{y} = (0, 0)^\top$ of $\boldsymbol{Y}$. The covariance matrix associated with this estimate is

$$\boldsymbol{U}_{\boldsymbol{y}} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix},$$

obtained by applying formula (3), namely $\boldsymbol{U}_{\boldsymbol{y}} = \boldsymbol{C}_{\boldsymbol{x}} \boldsymbol{U}_{\boldsymbol{x}} \boldsymbol{C}_{\boldsymbol{x}}^{\top}$, with

$$\boldsymbol{U}_{\boldsymbol{x}} = \begin{bmatrix} 1^2 & 0 & 0 \\ 0 & 1^2 & 0 \\ 0 & 0 & 1^2 \end{bmatrix}, \qquad \boldsymbol{C}_{\boldsymbol{x}} = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix}.$$

The correlation coefficient associated with the estimates y_1 and y_2 (see 3.21) is $r(y_1, y_2) = 0.5$. 95 % coverage regions for $\boldsymbol{Y}$ taking the forms of an ellipse and a rectangle are defined, respectively, by coverage factors $k_p = 2.45$ (table 1) and $k_q = 2.24$ (table 2). These results are summarized in row 1 (GUF) of table 3. In the context of the GUM uncertainty framework, given the information available, $\boldsymbol{Y}$ is characterized by the bivariate Gaussian PDF $\mathrm{N}(\boldsymbol{y}, \boldsymbol{U}_{\boldsymbol{y}})$.

9.2.2.3 The application of MCM with, respectively, $M = 10^5$, 10^6 and 10^7 trials gives the results summarized in rows 2 to 4 (MCM) of table 3. The fourth and fifth numerical values of M (0.35×10^6 and 0.45×10^6) given in rows 5 and 6 (Adaptive MCM) of the table are the numbers of trials taken by two applications of the adaptive Monte Carlo procedure (see 7.8.3) with n_{dig}, the number of significant decimal digits regarded as meaningful in the numerical value of a result, set equal to three (see note 3 of 8.3). For the applications of the adaptive procedure, it is required that all the results, i.e. y_1, y_2, $u(y_1)$, $u(y_2)$, $r(y_1, y_2)$, k_p and k_q, have stabilized in a statistical sense.

9.2.2.4 The PDF for $\boldsymbol{Y}$ obtained analytically is the bivariate Gaussian PDF $\mathrm{N}(\boldsymbol{y}, \boldsymbol{U}_{\boldsymbol{y}})$ with $\boldsymbol{y}$ and $\boldsymbol{U}_{\boldsymbol{y}}$ given in 9.2.2.2.

9.2.2.5 Figure 8 (left) shows contours of the bivariate Gaussian PDF for $\boldsymbol{Y}$ obtained from the GUM uncertainty framework (or obtained analytically). The contours take the form of ellipses with equations

$$(\boldsymbol{\eta} - \boldsymbol{y})^{\top} \boldsymbol{U}_{\boldsymbol{y}}{}^{-1} (\boldsymbol{\eta} - \boldsymbol{y}) = k^2$$

for various values of k. Figure 8 (right) shows contours of the approximation to the PDF for $\boldsymbol{Y}$ obtained from the application of MCM with $M = 10^7$ trials. The approximate PDF is described by the numbers of model values from the Monte Carlo calculation contained within each cell of a (suitably large) mesh defined on the domain of $\boldsymbol{Y}$, with each number scaled (by the same scaling factor) so that the volume under the PDF (regarded as constant over each cell) is unity. A contouring algorithm is used to determine contours from this description of the approximate PDF for the same values of k used to define the ellipses in figure 8 (left). The contours in figure 8 (right) are not smoothed (see 9.1.6).

NOTE Figure 8 and subsequent contour plots include a colour bar indicating the contour heights according to a colour code.

9.2.2.6 Figure 9 shows the marginal PDF $\mathrm{N}(y_1, u^2(y_1))$ for Y_1 resulting from the GUM uncertainty framework. It also shows the approximate PDF provided by MCM with $M = 10^7$ trials. The approximation is displayed as a scaled frequency distribution (histogram) of the model values for Y_1 from the Monte Carlo calculation. These two PDFs are almost indistinguishable by eye. Comparable results would be obtained for Y_2.

9.2.2.7 Figure 10 (left) shows the contours of the approximation to the PDF for $\boldsymbol{Y}$ provided by MCM with 0.45×10^6 trials. The contours are considerably less "smooth" than those in figure 8 (right) obtained from a much larger number of trials. Figure 10 (right) provides an instance of contour smoothing (see 9.1.6).

NOTE A large value for the number M of Monte Carlo trials, and a fine discretization of the domain of $\boldsymbol{Y}$, are generally needed to ensure that the contours in a graphical representation of the approximate PDF for $\boldsymbol{Y}$ obtained using MCM are smooth. A similar effect arises for a single scalar output quantity, where a large value for M and many classes (or bins), are generally needed to ensure that the approximate PDF displayed as a histogram (or scaled frequency distribution) is smooth.

9.2.2.8 The validation procedure of clause 8 is applied to validate the results obtained from the GUM uncertainty framework against those from the two applications of the adaptive Monte Carlo calculation. The procedure is applied with n_{dig}, the number of significant decimal digits regarded as meaningful in the numerical value of a result, set equal to two. In this case, the numerical tolerances associated with the results are, respectively,

$$\delta_1 = \delta_2 = 0.05, \qquad \rho = 0.05, \qquad \kappa_p = \kappa_q = 0.05.$$

The results obtained from the GUM uncertainty framework were validated in both instances. Excepting k_q, agreement between the results would be expected because all the conditions hold for the application of the GUM uncertainty framework. The evaluation of k_q in the GUM uncertainty framework does not take account of the mutual dependence between Y_1 and Y_2 (see 6.5.2.3). Nevertheless, the values for k_q obtained agree to the required number of significant decimal digits.

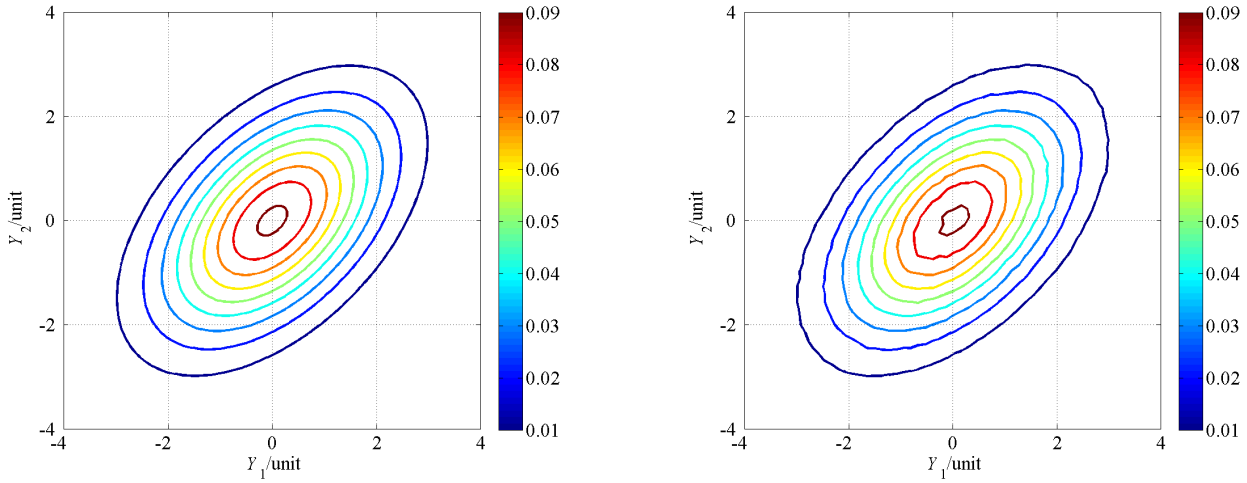

Figure 8 — Contours of the joint PDFs for the output quantities in the additive measurement model (24) provided by the GUM uncertainty framework and (right) MCM without contour smoothing, where the input quantities in the measurement model are characterized by standard Gaussian distributions (9.2.2)

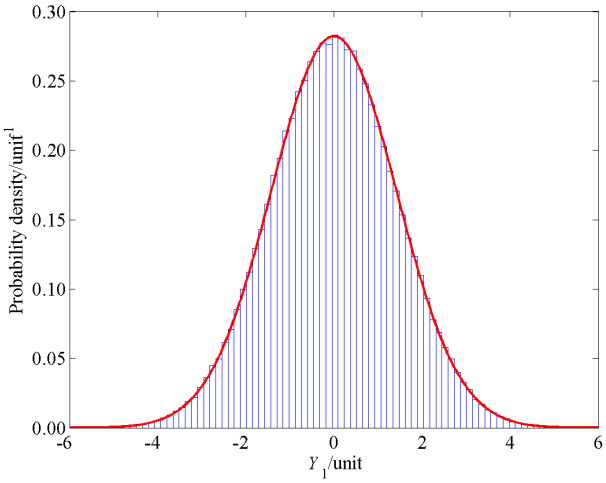

Figure 9 — As figure 8, but showing the marginal PDF for Y_1 (9.2.2)

9.2.3 Propagation and summarizing: case 2

9.2.3.1 This case is identical to that in 9.2.2 except that X_3 is characterized by a rectangular distribution so that X_3 has an expectation of zero and a standard deviation of unity. Again, the estimates of the X_i are $x_i = 0$, $i = 1, 2, 3$, with associated standard uncertainties $u(x_i) = 1$. The results from the application of the GUM uncertainty framework (see 6) and MCM (see 7) are summarized in table 4 and figures 11 and 12.

9.2.3.2 The GUM uncertainty framework provides exactly the same (bivariate Gaussian) PDF for $\boldsymbol{Y}$ (figure 11, left) when the PDF for X_3 is Gaussian (as in 9.2.2) or rectangular (as here), because the expec-

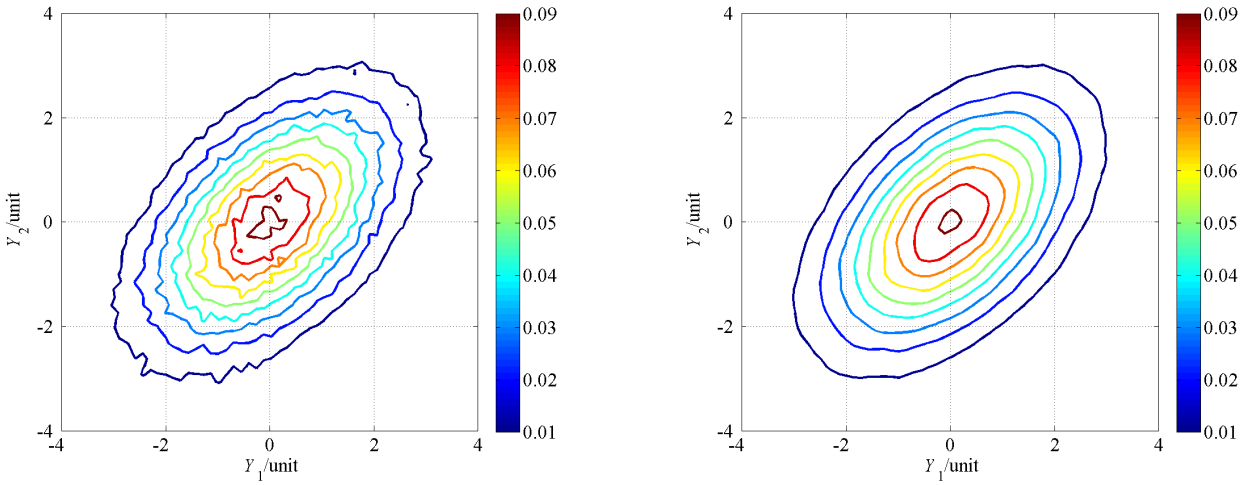

Figure 10 — Contours of the joint PDF for the output quantities in the additive measurement model (24) provided by the adaptive MCM procedure and (right) with contour smoothing, where the input quantities in the model are characterized by standard Gaussian distributions (9.2.2)

Table 4 — As table 3, except that X_3 is characterized by a rectangular distribution (9.2.3)

Method	M	y_1	y_2	$u(y_1)$	$u(y_2)$	$r(y_1, y_2)$	k_p	k_q
GUF		0.000	0.000	1.414	1.414	0.500	2.45	2.24
MCM	1×10^5	0.008	0.010	1.414	1.410	0.500	2.38	2.15
MCM	1×10^6	0.001	0.001	1.414	1.414	0.499	2.38	2.15
MCM	1×10^7	0.000	0.000	1.414	1.414	0.500	2.38	2.15
Adaptive MCM	0.36×10^6	0.000	−0.002	1.413	1.414	0.500	2.38	2.15
Adaptive MCM	0.35×10^6	0.002	−0.001	1.418	1.415	0.502	2.38	2.15

tations of the input quantities are identical, as are the standard deviations, in the two cases. Because the measurement model depends linearly on the input quantities, there is no approximation involved in the application of the law of propagation of uncertainty to obtain an estimate $\boldsymbol{y}$ of $\boldsymbol{Y}$ and the associated covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$. However, the PDF provided by the GUM uncertainty framework is not the same as the analytical solution, since the latter depends on the distribution used to characterize X_3, and not only the expectation and standard deviation of the quantity.

9.2.3.3 Figure 11 (right) and figure 12 show the influence of the distribution used to characterize X_3 on the approximations to, respectively, the PDF for $\boldsymbol{Y}$ and the marginal PDF for Y_1 obtained from MCM.

9.2.3.4 The validation procedure of clause 8 is again applied (see 9.2.2). In this case, values for y_1, y_2, $u(y_1)$, $u(y_2)$ and $r(y_1, y_2)$ obtained from the GUM uncertainty framework were validated against those obtained from the two applications of the adaptive Monte Carlo procedure, but the values for k_p and k_q were not validated.

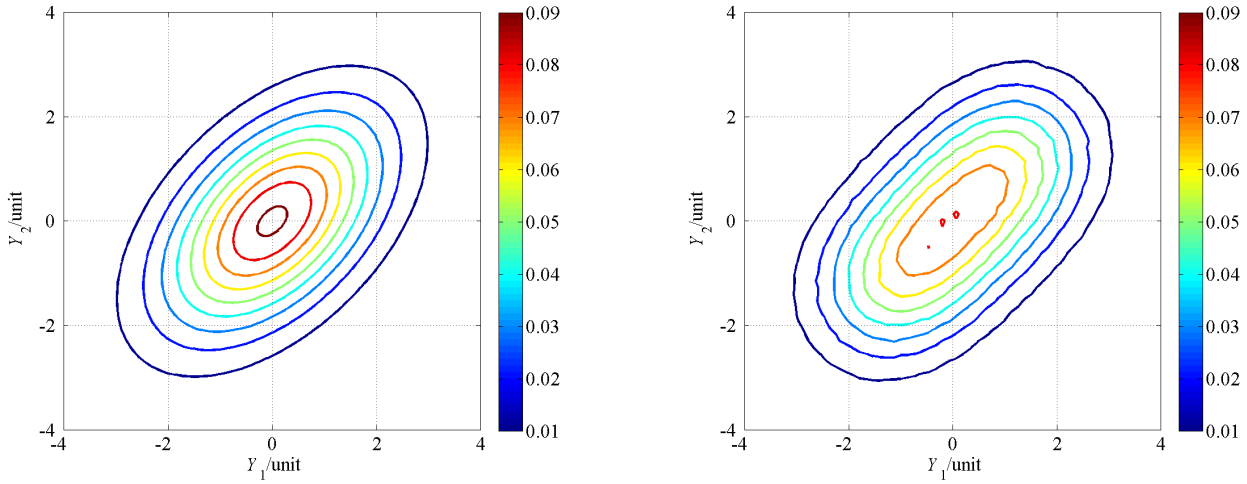

Figure 11 — Counterpart of figure 8 for an input quantity X_3 characterized by a rectangular distribution (9.2.3)

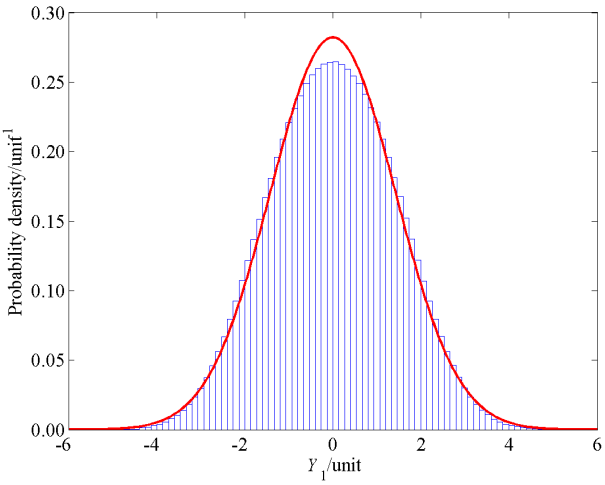

Figure 12 — Counterpart of figure 9 for an input quantity X_3 characterized by a rectangular distribution (9.2.3)

9.2.4 Propagation and summarizing: case 3

9.2.4.1 Consider the example of 9.2.3, except that X_3 now has a standard deviation of three rather than unity. The results from the application of the GUM uncertainty framework (see 6) and MCM (see 7) are summarized in table 5 and figures 13 and 14.

Table 5 — As table 4, except that X_3 has a standard deviation of three (9.2.4)

Method	M	y_1	y_2	$u(y_1)$	$u(y_2)$	$r(y_1, y_2)$	k_p	k_q
GUF		0.000	0.000	3.162	3.162	0.900	2.45	2.24
MCM	1×10^5	0.023	0.025	3.159	3.157	0.900	2.28	1.87
MCM	1×10^6	0.003	0.002	3.161	3.161	0.900	2.28	1.87
MCM	1×10^7	0.000	0.000	3.162	3.161	0.900	2.28	1.87
Adaptive MCM	1.49×10^6	0.002	0.002	3.163	3.162	0.900	2.28	1.87
Adaptive MCM	1.85×10^6	0.001	0.001	3.163	3.162	0.900	2.28	1.87

9.2.4.2 The GUM uncertainty framework gives the estimate $\boldsymbol{y} = (0, 0)^\top$ of $\boldsymbol{Y}$. The covariance matrix associated with this estimate is

$$\boldsymbol{U}_{\boldsymbol{y}} = \begin{bmatrix} 10 & 9 \\ 9 & 10 \end{bmatrix},$$

obtained by applying formula (3) with

$$\boldsymbol{U}_{\boldsymbol{x}} = \begin{bmatrix} 1^2 & 0 & 0 \\ 0 & 1^2 & 0 \\ 0 & 0 & 3^2 \end{bmatrix}, \qquad \boldsymbol{C}_{\boldsymbol{x}} = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix}.$$

The correlation coefficient associated with the estimates y_1 and y_2 is $r(y_1, y_2) = 0.9$. 95 % coverage regions for $\boldsymbol{Y}$ taking the forms of an ellipse and a rectangle are defined, respectively, by coverage factors $k_p = 2.45$ (table 1) and $k_q = 2.24$ (table 2). These results are summarized in row 1 (GUF) of table 5. In the context of the GUM uncertainty framework, given the information available about $\boldsymbol{Y}$, $\boldsymbol{Y}$ is characterized by the bivariate Gaussian PDF $\mathrm{N}(\boldsymbol{y}, \boldsymbol{U}_{\boldsymbol{y}})$, the contours for which are shown in figure 13 (left). There is a stronger correlation between Y_1 and Y_2 in this example compared to the earlier examples because the relative contribution of the common effect X_3 to the uncertainties associated with the estimates of Y_1 and Y_2 is greater.

9.2.4.3 Figure 13 (right) and figure 14 show the greater influence (compared to the results of 9.2.3) of the distribution used to characterize X_3 on the approximations to, respectively, the PDF for $\boldsymbol{Y}$ and the marginal PDF for Y_1 obtained from MCM.

9.2.4.4 The validation procedure of clause 8 is again applied (see 9.2.2 and 9.2.3). In this case, values for y_1, y_2, $u(y_1)$, $u(y_2)$ and $r(y_1, y_2)$ obtained from the GUM uncertainty framework were validated against those obtained from the two applications of the adaptive Monte Carlo procedure, but the values for k_p and k_q were not validated. The value of k_p obtained from the GUM uncertainty framework is about 7 % bigger than that obtained from MCM, and the value of k_q about 20 % bigger.

9.3 Co-ordinate system transformation

9.3.1 Formulation

9.3.1.1 Consider a complex quantity $\boldsymbol{Z}$ represented in Cartesian form

$$X_1 + \mathrm{i}X_2,$$

where $X_1 \equiv Z_\mathrm{R}$ and $X_2 \equiv Z_\mathrm{I}$ are, respectively, the real and imaginary parts of $\boldsymbol{Z}$, or in polar form

$$R(\cos\Theta + \mathrm{i}\sin\Theta) = Re^{\mathrm{i}\Theta},$$

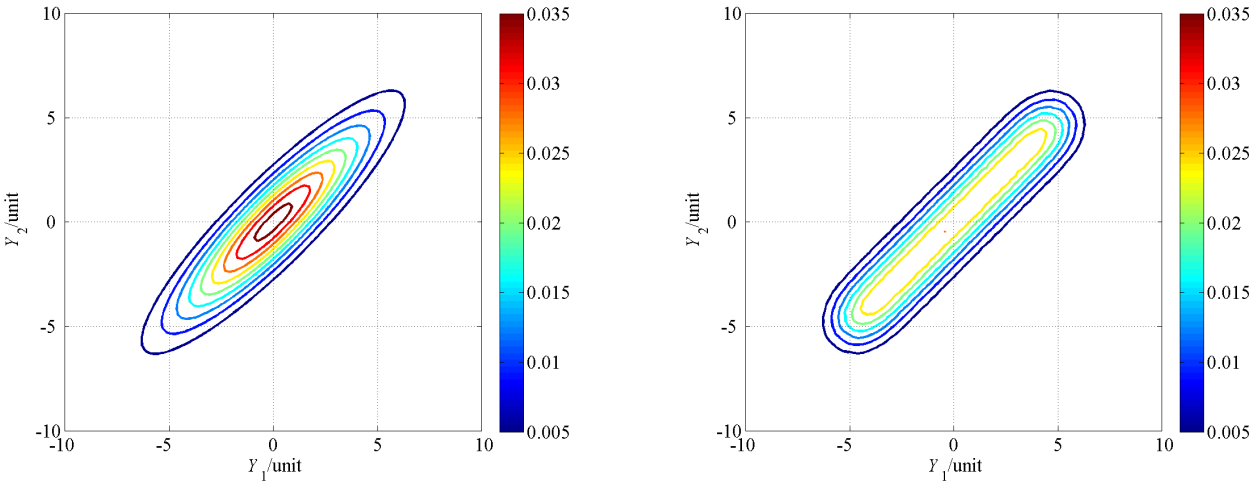

Figure 13 — Counterpart of figure 11 for an input quantity X_3 with a standard deviation of three (9.2.4)

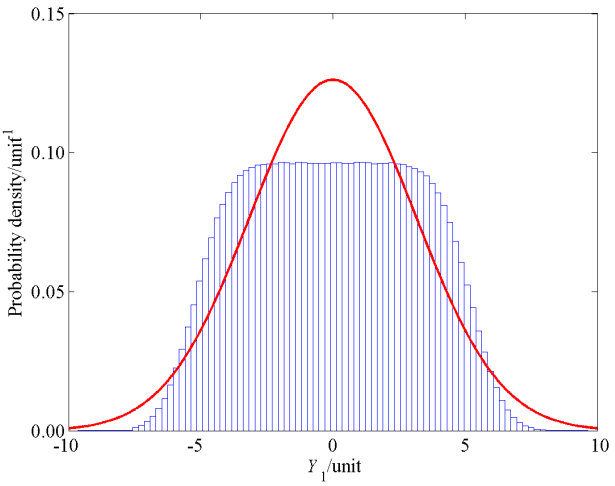

Figure 14 — Counterpart of figure 12 for an input quantity X_3 with a standard deviation of three (9.2.4)

where R and Θ are, respectively, the magnitude and phase of $\boldsymbol{Z}$. This example considers the transformation from Cartesian to polar representations of $\boldsymbol{Z}$ described by the bivariate measurement model

$$Y_1^2 = X_1^2 + X_2^2, \qquad \tan Y_2 = X_2/X_1, \tag{25}$$

with input quantity $\boldsymbol{X} = (X_1, X_2)^\top \equiv (Z_\mathrm{R}, Z_\mathrm{I})^\top$ and output quantity $\boldsymbol{Y} = (Y_1, Y_2)^\top \equiv (R, \Theta)^\top$.

NOTE Expressions (25) constitute a bivariate measurement model for R and Θ. Since R is a magnitude, and is known to be non-negative, it is determined uniquely by the positive square root of R^2. By using a "four quadrant inverse tangent function" (often denoted by "atan2") Θ is determined uniquely to satisfy $-\pi < \Theta \leq \pi$. Thus expressions (25) can be cast as a bivariate measurement model.

9.3.1.2 Given are estimates x_1 and x_2 of the quantities X_1 and X_2, obtained from a suitable measuring system, and associated standard uncertainties $u(x_1)$ and $u(x_2)$ and covariance $u(x_1, x_2) = ru(x_1)u(x_2)$, where $r = r(x_1, x_2)$ denotes the associated correlation coefficient [JCGM 100:2008 5.2.2]. On the basis of this information [JCGM 101:2008 6.4.8.1], $\boldsymbol{X}$ is assigned a bivariate Gaussian PDF, with expectation and covariance matrix

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \qquad \begin{bmatrix} u^2(x_1) & ru(x_1)u(x_2) \\ ru(x_1)u(x_2) & u^2(x_2) \end{bmatrix}.$$

The quantities X_1 and X_2 are assumed to have dimension one.

9.3.1.3 The determination of an estimate $\boldsymbol{y}$ of $\boldsymbol{Y}$ and the associated covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$ is considered for different choices of x_1, x_2, $u(x_1)$, $u(x_2)$ and $r(x_1, x_2)$.

9.3.1.4 Six cases are considered, in all of which x_2 is taken as zero and $u(x_1) = u(x_2) = u_x = 0.010$. The first three of these cases correspond to taking $x_1 = 0.001, 0.010$ and 0.100, each with $r(x_1, x_2) = 0$ (see 9.3.2). The second three cases correspond to taking the same x_1, but with $r(x_1, x_2) = 0.9$ (see 9.3.3). Figure 15 shows the contours of the joint PDFs assigned to the input quantities $\boldsymbol{X}$ for case 1 ($x_1 = 0.001$ and $r(x_1, x_2) = 0$) and case 4 ($x_1 = 0.001$ and $r(x_1, x_2) = 0.9$). (In this figure a common set of contour values is not used for the two contour plots.) The contours of the joint PDFs for the other cases are obtained by translating the contours shown along the X_1-axis so that they are centred on $x_1 = 0.010$ (cases 2 and 5) or $x_1 = 0.100$ (cases 3 and 6).

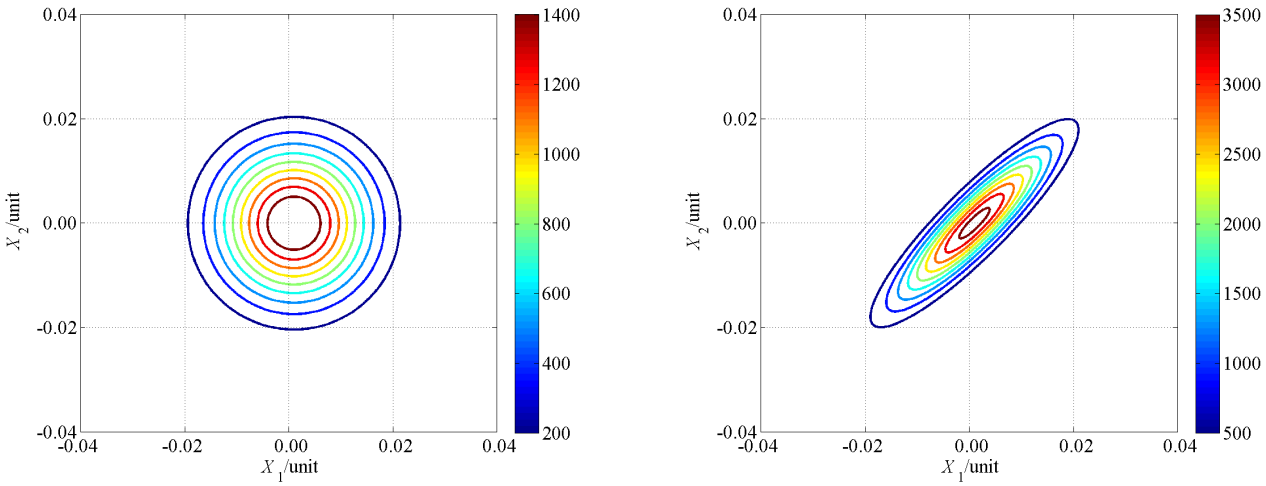

Figure 15 — Contours of the joint PDFs for the input quantities in the co-ordinate system transformation model for cases 1 and (right) 4 (9.3.1.4)

9.3.2 Propagation and summarizing: zero covariance

9.3.2.1 General

9.3.2.1.1 The evaluation of uncertainty is treated by applying the propagation of distributions (a) analytically (for purposes of comparison), (b) using the (generalized) GUM uncertainty framework, and (c) using MCM.

9.3.2.1.2 The (joint) PDF for $\boldsymbol{Y}$, and the marginal PDFs for Y_1 and Y_2, can be obtained analytically in the case that X_1 is described by the Gaussian distribution $\mathrm{N}(x_1, u_x^2)$ and X_2 by $\mathrm{N}(x_2, u_x^2)$, with X_1 and X_2 mutually independent. See C.2.

9.3.2.1.3 In the context of the GUM uncertainty framework, $\boldsymbol{Y}$ is characterized by the bivariate Gaussian distribution $\mathrm{N}(\boldsymbol{y}, \boldsymbol{U_y})$, where the estimate $\boldsymbol{y} = (y_1, y_2)^\top$ of $\boldsymbol{Y}$ is given by the solution to the equations

$$y_1^2 = x_1^2 + x_2^2, \qquad \tan y_2 = x_2/x_1,$$

with associated covariance matrix $\boldsymbol{U_y}$ obtained by applying a generalization of the law of propagation of uncertainty. See clause 6 and C.3.

9.3.2.1.4 MCM is applied with $M = 10^7$ trials. See clause 7.

9.3.2.2 Input estimate $x_1 = 0.001$

9.3.2.2.1 For the input estimate $x_1 = 0.001$, with correlation coefficient $r(x_1, x_2) = 0$, rows 1 to 3 of table 6 give the results obtained analytically, using the GUM uncertainty framework (GUF) and MCM.

NOTE The analytical results for y_1 and $u(y_1)$ given in table 6 are determined by calculating numerically, to a high degree of approximation, $E(Y_1)$ and $V(Y_1)$, which take the form of definite integrals involving the marginal distribution for Y_1 obtained analytically (see expression (C.2) in annex C). Similarly, the analytical results for y_2 and $u(y_2)$ are determined by calculating numerically $E(Y_2)$ and $V(Y_2)$, which involve the marginal distribution for Y_2 obtained analytically (see expression (C.3) in annex C). It is straightforward to show that $\mathrm{Cov}(Y_1, Y_2) = 0$ and, therefore, the analytical result $r(y_1, y_2) = 0$.

Table 6 — Co-ordinate system transformation results, for input estimates with associated zero covariance (9.3.2.2.1, 9.3.2.3.1 and 9.3.2.4.1)

x_1	**Method**	y_1	y_2	$u(y_1)$	$u(y_2)$	$r(y_1, y_2)$
0.001	Analytical	0.013	0.000	0.007	1.744	0.000
	GUF	0.001	0.000	0.010	10.000	0.000
	MCM	0.013	−0.001	0.007	1.744	0.000
0.010	Analytical	0.015	0.000	0.008	1.118	0.000
	GUF	0.010	0.000	0.010	1.000	0.000
	MCM	0.015	0.000	0.008	1.117	0.000
0.100	Analytical	0.101	0.000	0.010	0.101	0.000
	GUF	0.100	0.000	0.010	0.100	0.000
	MCM	0.101	0.000	0.010	0.101	0.000

9.3.2.2.2 Figure 16 shows in the top three graphs the contours of the joint PDFs for $\boldsymbol{Y}$ obtained analytically, using the GUM uncertainty framework and using MCM. The PDF provided by MCM is consistent with the analytic solution. However, the PDF provided by the GUM uncertainty framework is very different from the analytic solution, and it is necessary to use a different set of contour values to illustrate this PDF (see 9.1.5). Furthermore, the PDF provided by the GUM uncertainty framework takes positive values for infeasible values of the output quantities, i.e. for values $\eta_1 < 0$, $\eta_2 \leq -\pi$ and $\eta_2 > \pi$, erroneously implying a non-zero probability density for such infeasible values.

9.3.2.2.3 Figure 16 shows in the bottom two graphs the marginal PDFs for the output quantities Y_1 and Y_2 obtained from the joint distribution for $\boldsymbol{Y}$. The marginal PDFs provided by MCM (shown as histograms or

scaled frequency distributions) are consistent with the analytic solutions (shown as dashed lines). However, the marginal distributions provided by the GUM uncertainty framework (shown as solid lines) are very different from the analytic solutions. For convenience of presentation, the graph of the marginal PDF for Y_2 provided by the GUM uncertainty interval is only shown for (feasible) values of η_2 satisfying $-\pi < \eta_2 \leq \pi$, although the PDF, which is the Gaussian $\mathrm{N}(0, 10^2)$, extends well beyond this interval. The marginal PDFs provided by the GUM uncertainty framework imply a non-zero probability density for infeasible values of the output quantities (see also 9.3.2.2.2).

9.3.2.3 Input estimate $x_1 = 0.010$

9.3.2.3.1 For the input estimate $x_1 = 0.010$, with correlation coefficient $r(x_1, x_2) = 0$, rows 4 to 6 of table 6 give the results obtained analytically, using the GUM uncertainty framework (GUF) and MCM. Figure 17 shows the contours of the joint PDFs for $\boldsymbol{Y}$ obtained using the three approaches and the marginal PDFs for Y_1 and Y_2 obtained from the respective joint PDFs.

9.3.2.3.2 It is seen that the results obtained using MCM are consistent with the analytic solution. However, the results obtained using the GUM uncertainty framework are different from the analytic solution, but not so different as for the case $x_1 = 0.001$. The relative differences between the standard uncertainties $u(y_1)$ and $u(y_2)$ determined using the GUM uncertainty framework and analytically are approximately 25 % and 10 % (compared with approximately 40 % and 470 % for the case $x_1 = 0.001$).

9.3.2.4 Input estimate $x_1 = 0.100$

9.3.2.4.1 For the input estimate $x_1 = 0.100$, with correlation coefficient $r(x_1, x_2) = 0$, the results obtained using the three aproaches are given in rows 7 to 9 of table 6 and figure 18.

9.3.2.4.2 It is seen that the results obtained using the GUM uncertainty framework and MCM are both consistent with the analytic solution. The marginal distributions provided by the three approaches shown in figure 18 are virtually indistinguishable. The estimates, associated standard uncertainties and associated correlation coefficient determined using the three approaches agree to two significant decimal digits.

9.3.3 Propagation and summarizing: non-zero covariance

9.3.3.1 The evaluation of uncertainty is treated by applying the propagation of distributions (a) using the (generalized) GUM uncertainty framework (see 6 and C.3), and (b) using MCM with $M = 10^7$ trials (see 7).

9.3.3.2 For the input estimates $x_1 = 0.001$, $x_1 = 0.010$ and $x_1 = 0.100$, with correlation coefficient $r(x_1, x_2) = 0.9$, table 7 gives the results obtained. The joint PDFs for $\boldsymbol{Y}$ and the marginal PDFs for Y_1 and Y_2 obtained from the two approaches are shown for the three cases in, respectively, figures 19, 20 and 21.

Table 7 — Co-ordinate system transformation results, for input estimates with associated covariance $r(x_1, x_2) = 0.9$ (9.3.3.2)

x_1	**Method**	y_1	y_2	$u(y_1)$	$u(y_2)$	$r(y_1, y_2)$
0.001	GUF	0.001	0.000	0.010	10.000	0.900
	MCM	0.012	−0.556	0.008	1.599	−0.070
0.010	GUF	0.010	0.000	0.010	1.000	0.900
	MCM	0.015	−0.343	0.008	0.903	0.352
0.100	GUF	0.100	0.000	0.010	0.100	0.900
	MCM	0.101	−0.009	0.010	0.102	0.882

9.3.3.3 For the cases $x_1 = 0.001$ and $x_1 = 0.010$ the results provided by the GUM uncertainty framework and MCM are very different. In particular, MCM gives marginal PDFs for Y_2 in these two cases

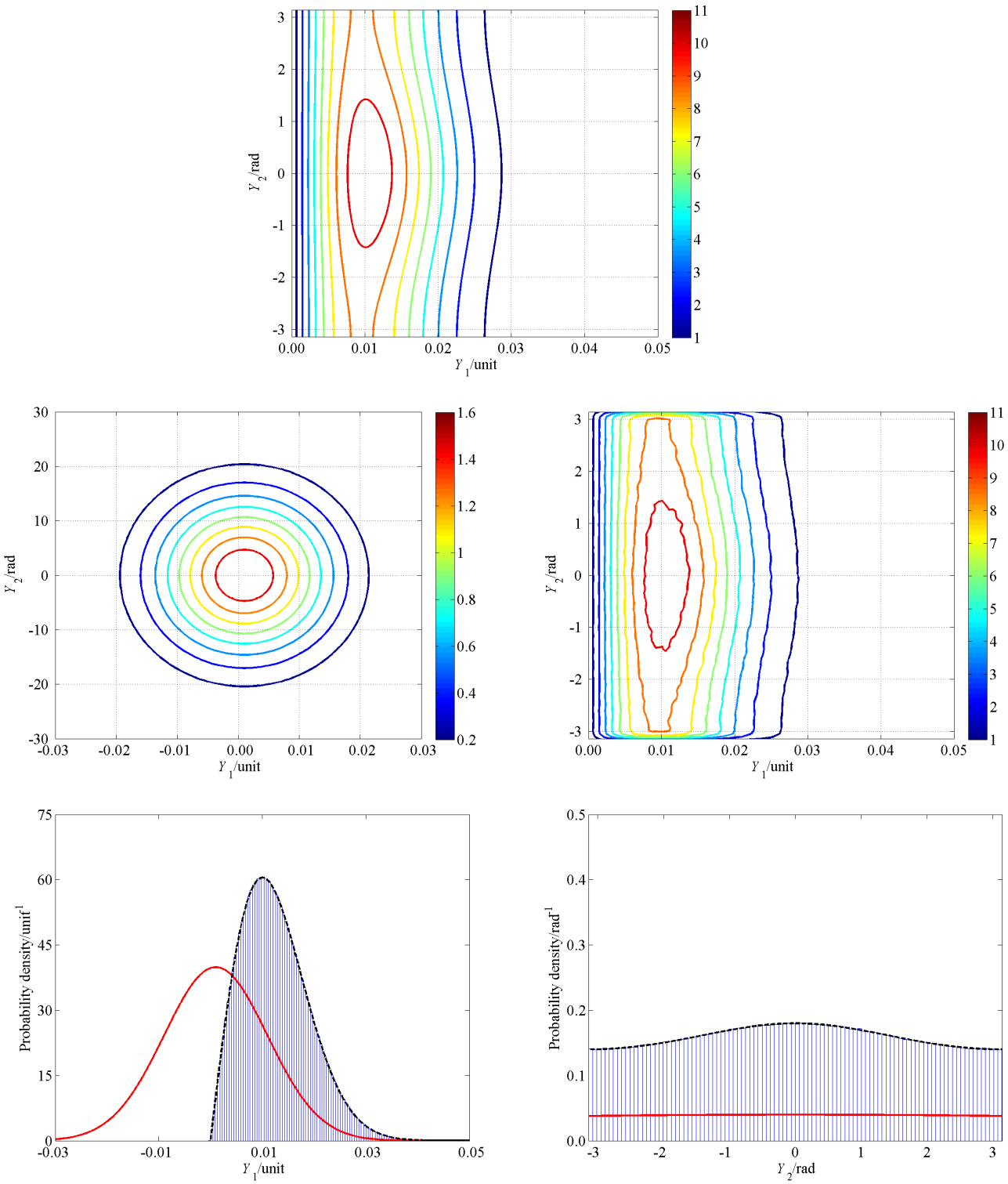

Figure 16 — Co-ordinate system transformation results, for input estimate $x_1 = 0.001$ and covariance $r(x_1, x_2) = 0$, showing (a) contours of the joint PDFs for $\boldsymbol{Y}$ obtained analytically (top), using the GUM uncertainty framework (middle left) and MCM (middle right), and (b) marginal PDFs for Y_1 (bottom left) and Y_2 (bottom right) obtained analytically (dashed line), using the GUM uncertainty framework (solid line) and MCM (histogram) (9.3.2.2.2 and 9.3.2.2.3)

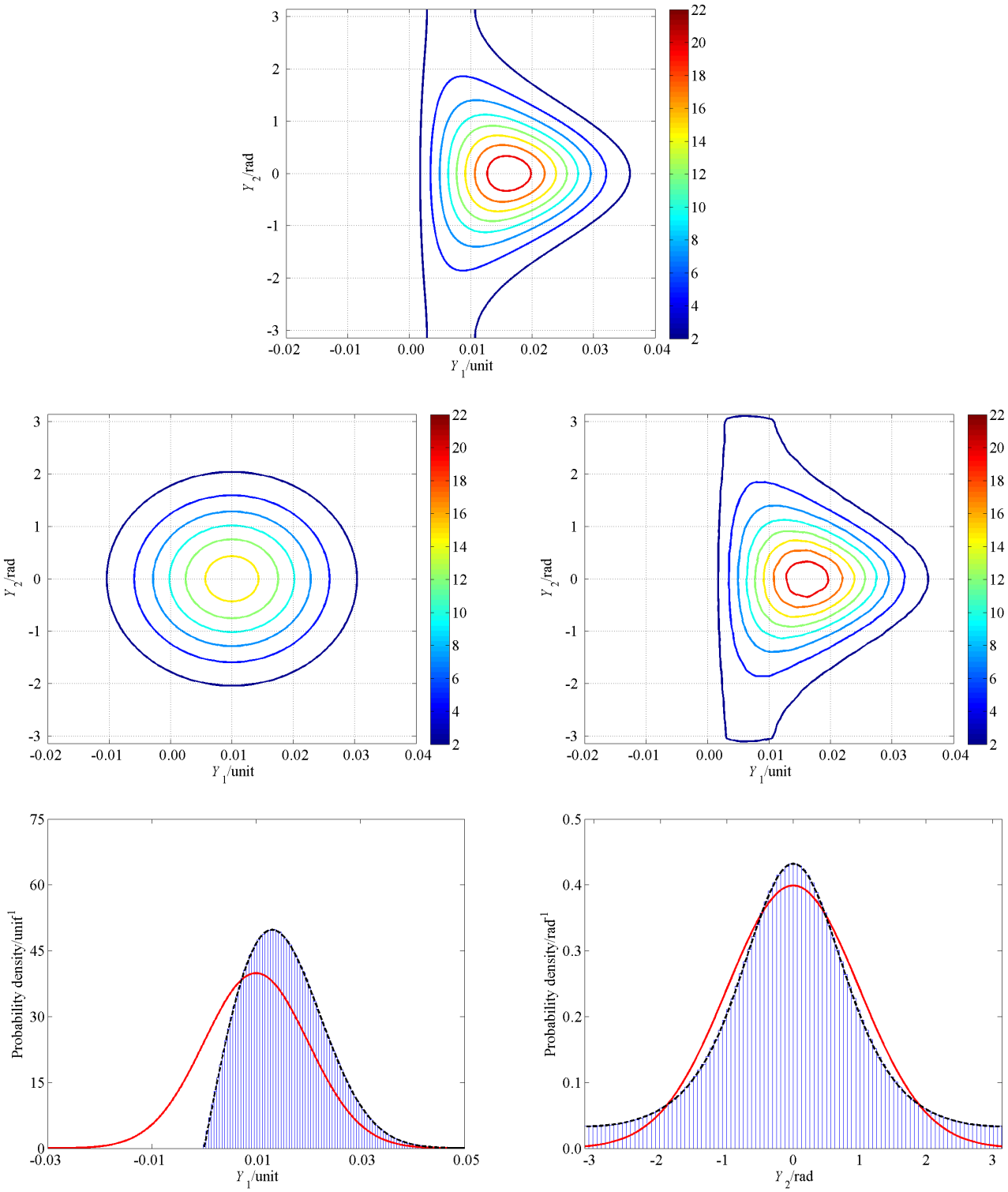

Figure 17 — As figure 16 except that $x_1 = 0.010$ (9.3.2.3.1)

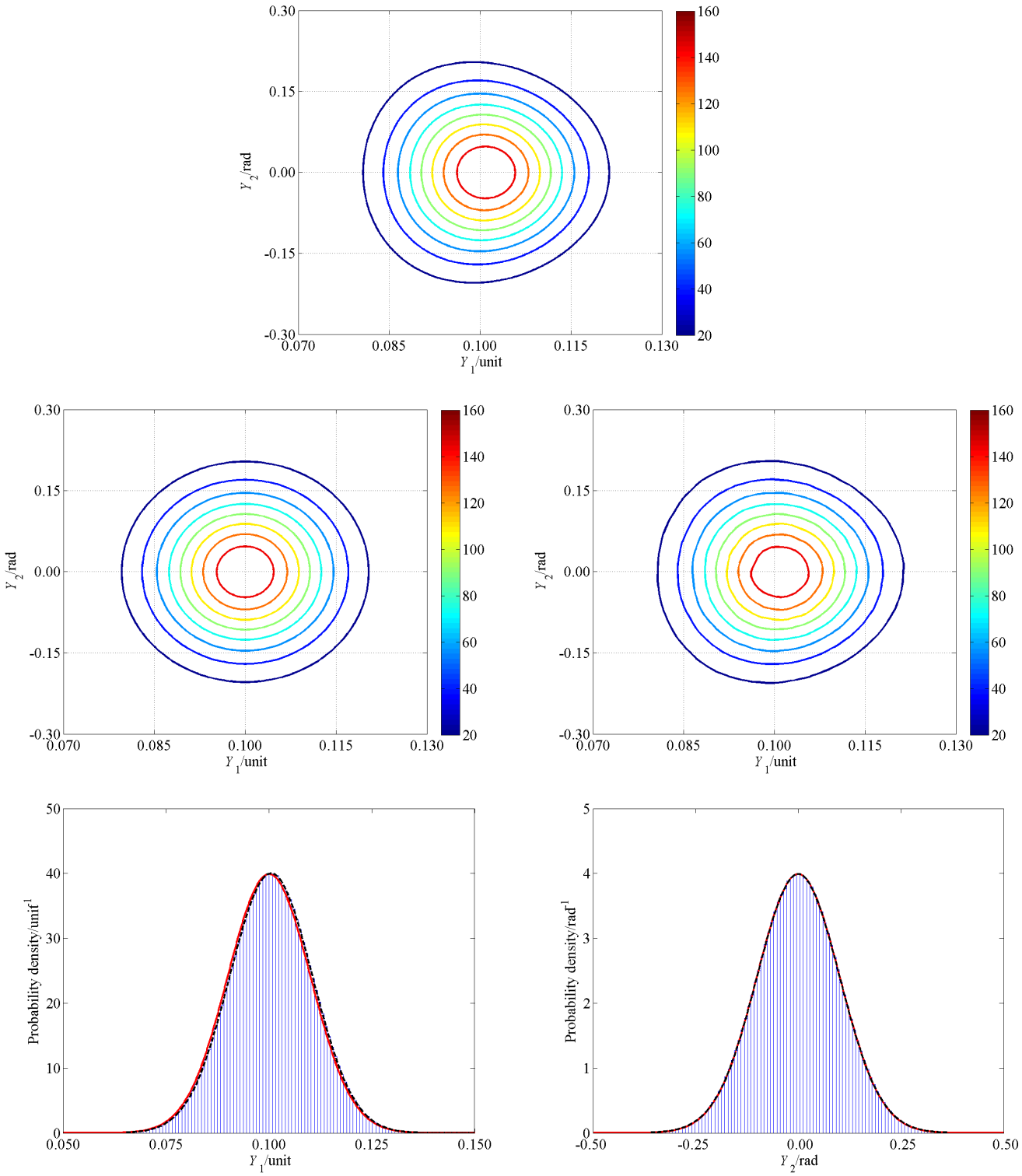

Figure 18 — As figure 16 except that $x_1 = 0.100$ (9.3.2.4.1)

that have two peaks, and which are very different from the Gaussian (unimodal) distributions provided by the GUM uncertainty framework. The positions of these peaks in the marginal PDFs are (approximately) at the values $\eta_2 = \pi/4 \approx 0.785$ and $\eta_2 = \pi/4 - \pi \approx -2.356$. These values are the polar angles that define the orientation of the major axis of the elliptical contours of the joint PDF for the input quantities $\boldsymbol{X}$ (see figure 15, right).

9.3.3.4 For the case $x_1 = 0.100$ there is much better agreement between the results provided by the GUM uncertainty framework and MCM.

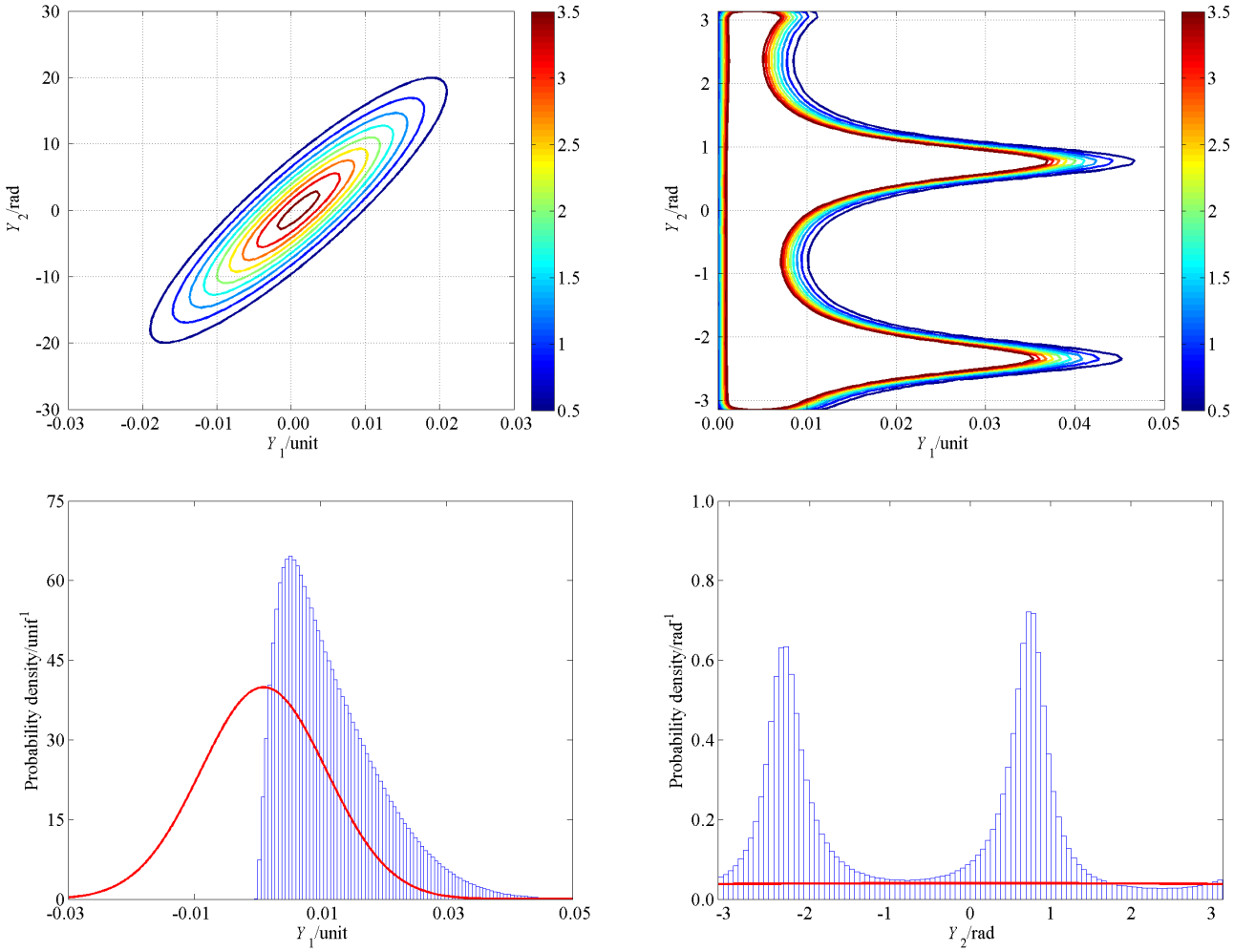

Figure 19 — Co-ordinate system transformation results, for input estimate $x_1 = 0.001$ and covariance $r(x_1, x_2) = 0.9$, showing (a) contours of the joint PDFs for $\boldsymbol{Y}$ obtained using the GUM uncertainty framework (GUF, top left) and MCM (top right), and (b) the marginal PDFs for Y_1 (bottom left) and Y_2 (bottom right) obtained using GUF (solid line) and MCM (histogram) (9.3.3.2)

9.3.4 Discussion

9.3.4.1 For both cases of zero and non-zero covariance, as x_1 becomes increasingly removed from zero, the results given by the GUM uncertainty framework and those for MCM become closer to each other.

9.3.4.2 For the input estimates $x_1 = 0.001$ and $x_1 = 0.010$, and generally for values of x_1 close to zero, the effect of the non-zero covariance is to change noticeably the results provided by MCM.

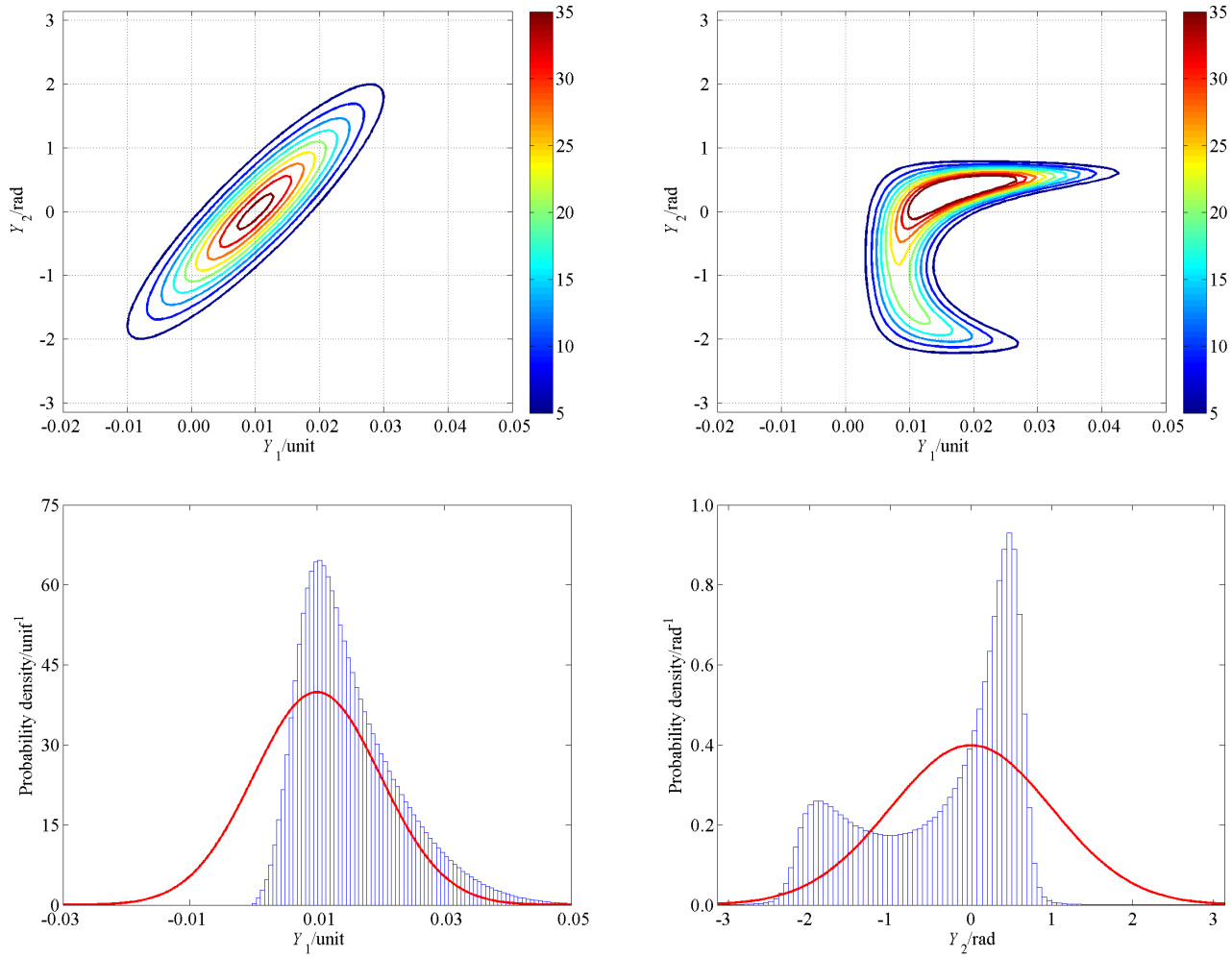

Figure 20 — As figure 19 except that $x_1 = 0.010$ (9.3.3.2)

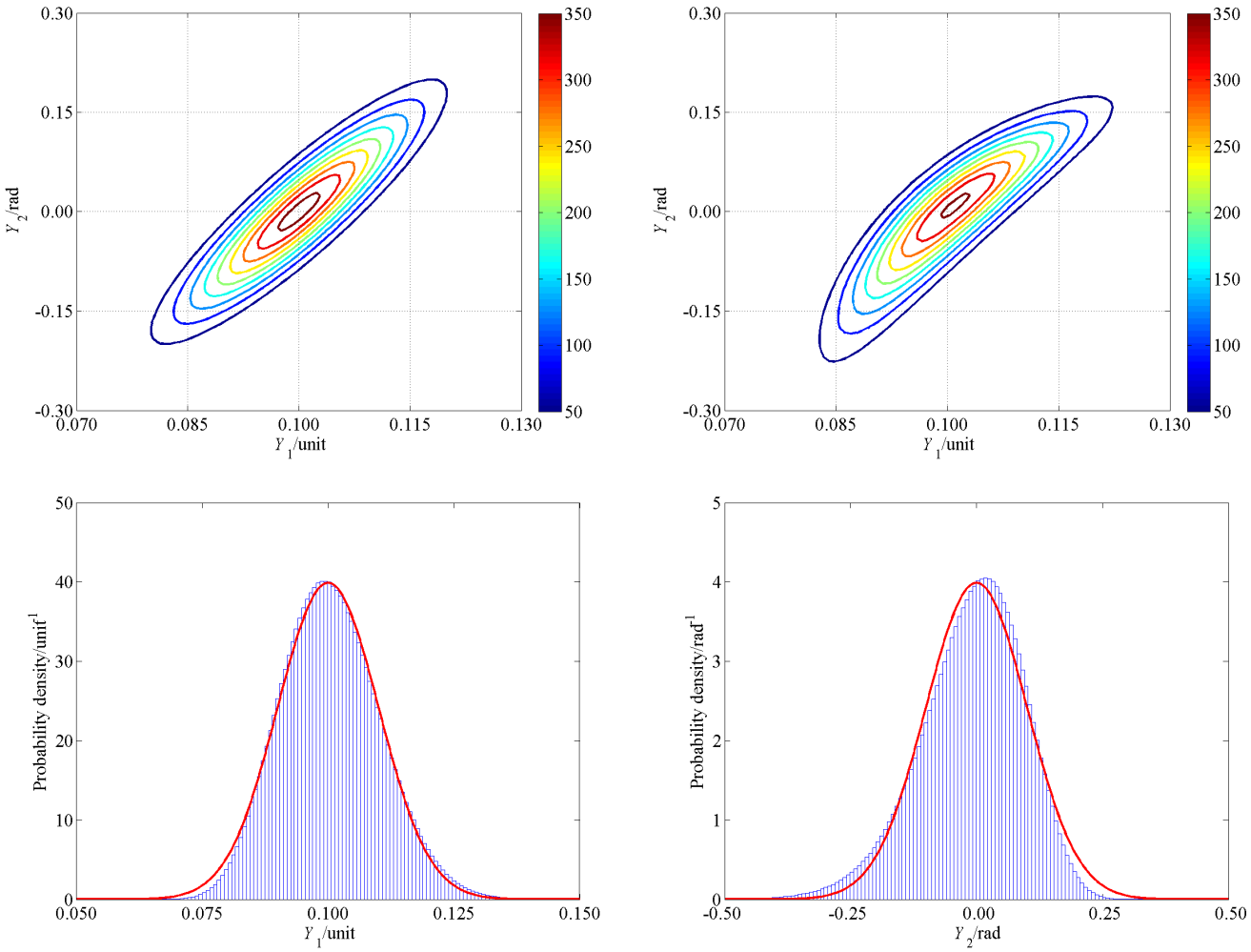

Figure 21 — As figure 19 except that $x_1 = 0.100$ (9.3.3.2)

9.3.4.3 The (numerical) results given in tables 6 and 7 provide summaries of the (joint and marginal) PDFs shown in the figures. In some circumstances such summaries may not be appropriate or may be insufficient to describe the nature of the PDF characterizing the output quantity. Consider the results for the case of the input estimate $x_1 = 0.001$ and non-zero covariance $r(x_1, x_2) = 0.9$ (figure 19). The marginal PDF for Y_2 obtained using MCM is essentially bimodal, and the estimate y_2 of Y_2 is midway between the modes of the distribution in an interval of values of Y_2 where the probability density is small.

NOTE For an output quantity characterized by a multivariate Gaussian distribution, the expectation vector and covariance matrix for the quantity completely describes the distribution.

9.3.4.4 For the input estimates $x_1 = 0.001$ and $x_1 = 0.010$, and generally for measured values of x_1 close to zero, the determination of coverage regions in the form of ellipses and rectangles is inappropriate.

9.4 Simultaneous measurement of resistance and reactance

9.4.1 Formulation

9.4.1.1 The resistance R and reactance X of a circuit element are determined by measuring the amplitude V of a sinusoidally-alternating potential difference across its terminals, the amplitude I of the alternating current passing through it, and the phase angle ϕ of the alternating potential difference relative to the alternating current. The input quantities are V, I and ϕ and the output quantities are the three impedance components R, X and Z, where $Z^2 = R^2 + X^2$.

9.4.1.2 The application of Ohm's law gives the trivariate measurement model

$$R = \frac{V}{I}\cos\phi, \qquad X = \frac{V}{I}\sin\phi, \qquad Z = \frac{V}{I}. \tag{26}$$

as the relationship between the input quantity $\boldsymbol{X} = (X_1, X_2, X_3)^\top \equiv (V, I, \phi)^\top$ and the output quantity $\boldsymbol{Y} = (Y_1, Y_2, Y_3)^\top \equiv (R, X, Z)^\top$.

NOTE 1 For reasons of simplicity, any systematic errors that may be present in V, I and ϕ are ignored.

NOTE 2 In the GUM, reactance is denoted by X, the notation also used here. The reactance X, a component of the vector output quantity $\boldsymbol{Y}$, is not to be confused with $\boldsymbol{X}$, the vector input quantity.

9.4.1.3 A series of $n = 6$ sets $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$ of simultaneous indication values of the input quantities are obtained independently under similar conditions resulting in the data given in table 8.

NOTE In the GUM, the data consists of a series of five sets of simultaneous indication values obtained independently (sets 1 to 5 of table 8). At least six sets are required for the covariance matrix in 9.4.2.5 to be defined. Set 6 in table 8 is therefore included, and is chosen to be the average of sets 1 to 5. This particular choice for set 6 is not essential, but has the consequence that its inclusion does not change the average of the series.

Table 8 — A series of $n = 6$ sets of simultaneous indication values, obtained independently, of the input quantities for the measurement of resistance and reactance (9.4.1.3)

Set	V/V	I/mA	ϕ/rad
1	5.007	19.663	1.045 6
2	4.994	19.639	1.043 8
3	5.005	19.640	1.046 8
4	4.990	19.685	1.042 8
5	4.999	19.678	1.043 3
6	4.999	19.661	1.044 5

9.4.2 Propagation and summarizing

9.4.2.1 The determination of an estimate $\boldsymbol{y}$ of $\boldsymbol{Y}$ and the associated covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$ is considered. The approach here treats the problem defined by the measurement model (26) and information about the input

quantities in that model in the form of the sets $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$ of indication values obtained independently given in table 8. The GUM addresses this problem using the GUM uncertainty framework [JCGM 100:2008 H.2.3]. The treatment here is extended to include MCM and an approach involving a multivariate t-distribution (see 5.3.2).

9.4.2.2 For the purpose of applying the (generalized) GUM uncertainty framework, estimates $\boldsymbol{x} \equiv (\widehat{V}, \widehat{I}, \widehat{\phi})^\top$ of the input quantities $\boldsymbol{X} \equiv (V, I, \phi)^\top$ are determined as the averages of the indication values given in table 8 [JCGM 100:2008 4.2]:

$$\boldsymbol{x} = \frac{1}{n}(\boldsymbol{x}_1 + \cdots + \boldsymbol{x}_n).$$

The covariance matrix $\boldsymbol{U}_{\boldsymbol{x}}$ associated with $\boldsymbol{x}$ contains the variances associated with the averages [JCGM 100:2008 4.2] and the covariances associated with each pair of averages [JCGM 100:2008 5.2.3], and is evaluated from

$$\boldsymbol{U}_{\boldsymbol{x}} = \frac{1}{n(n-1)}\boldsymbol{M}, \qquad \boldsymbol{M} = (\boldsymbol{x}_1 - \boldsymbol{x})(\boldsymbol{x}_1 - \boldsymbol{x})^\top + \cdots + (\boldsymbol{x}_n - \boldsymbol{x})(\boldsymbol{x}_n - \boldsymbol{x})^\top.$$

$\boldsymbol{M}$ is the matrix of sums of squares and products. The estimates $\boldsymbol{x}$ and the associated standard uncertainties determined in this way are given in table 9, and the correlation coefficients associated with pairs of the estimates in table 10.

NOTE In the GUM, an approach 2 is presented for this example, based on GUM 4.1.4 note. This approach is not followed here, for the reason given in 4.1.

Table 9 — Estimates of the input quantities $\boldsymbol{X} \equiv (V, I, \phi)^\top$ for the simultaneous measurement of resistance and reactance and the associated standard uncertainties (9.4.2.2)

	V/V	I/mA	ϕ/rad
Estimate	4.999 0	19.661 0	1.044 46
Std unc	0.002 6	0.007 7	0.000 61

Table 10 — Correlation coefficients associated with pairs of estimates of the input quantities $\boldsymbol{X} \equiv (V, I, \phi)^\top$ for the simultaneous measurement of resistance and reactance (9.4.2.2)

	V	I	ϕ
V	1	−0.355	0.858
I		1	−0.645
ϕ			1

9.4.2.3 In the GUM uncertainty framework, estimates $\boldsymbol{y} \equiv (\widehat{R}, \widehat{X}, \widehat{Z})^\top$ of the output quantities $\boldsymbol{Y} \equiv (R, X, Z)^\top$ are obtained by evaluating the measurement model (26) for the estimates $\boldsymbol{x}$ of the input quantities:

$$\boldsymbol{y} = \left[\begin{array}{ccc} \dfrac{\widehat{V}}{\widehat{I}}\cos\widehat{\phi}, & \dfrac{\widehat{V}}{\widehat{I}}\sin\widehat{\phi}, & \dfrac{\widehat{V}}{\widehat{I}} \end{array} \right]^\top.$$

The covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$ associated with $\boldsymbol{y}$ is evaluated using formula (3) in 6.2.1.3, namely $\boldsymbol{U}_{\boldsymbol{y}} = \boldsymbol{C}_{\boldsymbol{x}}\boldsymbol{U}_{\boldsymbol{x}}\boldsymbol{C}_{\boldsymbol{x}}^\top$, where $\boldsymbol{C}_{\boldsymbol{x}}$ is the sensitivity matrix given by

$$\boldsymbol{C}_{\boldsymbol{x}} = \left[\begin{array}{ccc} \dfrac{\cos\widehat{\phi}}{\widehat{I}} & -\dfrac{\widehat{V}\cos\widehat{\phi}}{\widehat{I}^2} & -\dfrac{\widehat{V}\sin\widehat{\phi}}{\widehat{I}} \\ \dfrac{\sin\widehat{\phi}}{\widehat{I}} & -\dfrac{\widehat{V}\sin\widehat{\phi}}{\widehat{I}^2} & \dfrac{\widehat{V}\cos\widehat{\phi}}{\widehat{I}} \\ \dfrac{1}{\widehat{I}} & -\dfrac{\widehat{V}}{\widehat{I}^2} & 0 \end{array} \right]. \tag{27}$$

The results obtained from the application of the GUM uncertainty framework are summarized in row 1 (GUF) of table 11.

NOTE 1 The right-most column in table 11 is expressed as $1 - r(X, Z)$ because the correlation coefficient $r(X, Z)$ is close to unity (see 3.21 note 5).

NOTE 2 The covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$ is singular as a result of dependencies in the trivariate measurement model (26):

$$Z^2 = R^2 + X^2. \tag{28}$$

Because of relation (28), the correlation matrix associated with the best estimates of R, X and Z is singular. However, due to rounding, the correlation matrix given in line 1 of table 11 is neither singular nor positive definite. Owing to the smallness of the standard uncertainties associated with the estimates of the input quantities, this singularity has no practical influence on the results obtained [20, section 4].

Table 11 — Results for the simultaneous measurement of resistance and reactance (9.4.2.3, 9.4.2.4 and 9.4.2.5)

Method	R/Ω	X/Ω	Z/Ω	$u(R)/\Omega$	$u(X)/\Omega$	$u(Z)/\Omega$	$r(R, X)$	$r(R, Z)$	$1 - r(X, Z)$
GUF	127.732	219.847	254.260	0.058	0.241	0.193	−0.588	−0.485	0.749×10^{-2}
MCM	127.732	219.847	254.260	0.130	0.536	0.429	−0.587	−0.482	0.770×10^{-2}
Alt. GUF	127.732	219.847	254.260	0.130	0.540	0.431	−0.588	−0.485	0.749×10^{-2}

9.4.2.4 Consider that the only information available about the input quantities is the series of indication values listed in table 8, and that the three such values in each set can be regarded as a realization of the same multivariate Gaussian distribution. Then $\boldsymbol{X}$ is characterized by the multivariate t-distribution $t_\nu(\boldsymbol{x}, \boldsymbol{M}/(\nu n))$ with $\nu = n - N = 3$ degrees of freedom, where $\boldsymbol{x}$ contains the averages of the indication values (as in 9.4.2.2). See 5.3.2. The results obtained from an application of MCM with $M = 10^6$ trials are summarized in row 2 (MCM) of table 11.

9.4.2.5 The quantity $\boldsymbol{X}$ characterized by the multivariate t-distribution given in 9.4.2.4 has covariance matrix

$$\boldsymbol{V}(\boldsymbol{X}) = \frac{1}{(\nu - 2)n}\boldsymbol{M}.$$

An alternative approach that is preferred to the treatment in 9.4.2.3 is to evaluate formula (3), namely $\boldsymbol{U}_{\boldsymbol{y}} = \boldsymbol{C}_{\boldsymbol{x}}\boldsymbol{U}_{\boldsymbol{x}}\boldsymbol{C}_{\boldsymbol{x}}^{\top}$, with $\boldsymbol{C}_{\boldsymbol{x}}$ the sensitivity matrix (27) and $\boldsymbol{U}_{\boldsymbol{x}}$ replaced by $\boldsymbol{V}(\boldsymbol{X})$. The results obtained from this alternative approach are summarized in row 3 (Alt. GUF) of table 11. Also see reference [15].

NOTE 1 $\boldsymbol{V}(\boldsymbol{X})$ is the covariance matrix corresponding to the additional information considered in 9.4.2.4.

NOTE 2 The covariance matrix for $\boldsymbol{X}$ obtained in this way is only defined if $\nu = n - N > 2$. It is for this reason that, in this example, at least $n = 6$ simultaneous indication values of the $N = 3$ input quantities are required.

9.4.2.6 The covariance matrix $\boldsymbol{V}(\boldsymbol{X})$ obtained from the distribution used to characterize $\boldsymbol{X}$ is related to the covariance matrix $\boldsymbol{U}_{\boldsymbol{x}}$ used in the application of the GUM uncertainty framework by

$$\boldsymbol{V}(\boldsymbol{X}) = \frac{n - 1}{n - N - 2}\boldsymbol{U}_{\boldsymbol{x}}.$$

9.4.2.7 The results obtained from the application of MCM and the alternative application of the GUM uncertainty framework are negligibly different, which indicates that the measurement functions in the measurement model (26) can be linearized, to a good degree of approximation, about the estimates of the input quantities.

9.4.2.8 In this example, the conditions for the application of the Welch-Satterthwaite formula [JCGM 100:2008 formula (G.2b)] of the GUM uncertainty framework to calculate an effective degrees of freedom are not valid because there are quantities for which the standard uncertainties have associated degrees of freedom that are finite and those quantities are not independent.

9.5 Measurement of Celsius temperature using a resistance thermometer

9.5.1 General

The example described in this subclause is concerned with the measurement of Celsius temperature by comparing the resistance of an industrial platinum resistance thermometer with that of a standard resistor using a resistance bridge. The measurement of a single Celsius temperature is described by a univariate measurement model (see 9.5.2), and that of several temperatures by a multivariate measurement model (see 9.5.3). The example illustrates the treatment of these (univariate and multivariate) measurement models using the (generalized) GUM uncertainty framework.

9.5.2 Measurement of a single Celsius temperature

9.5.2.1 The Celsius temperature θ is measured by comparing the resistance $R(\theta)$ of a resistance thermometer with the resistance R_S of a standard resistor using a resistance bridge. In the temperature interval from 0 °C to 30 °C, the resistance of the thermometer is approximated by a parabolic function of its Celsius temperature θ:

$$R(\theta) = \left(1 + A\theta + B\theta^2\right) R_0, \tag{29}$$

where R_0, A and B are determined from a calibration of the thermometer. Estimates of R_0, A and B and the associated standard uncertainties are given in table 12, and the non-zero correlation coefficients associated with pairs of the estimates in table 13.

Table 12 — Estimates of the input quantities $\boldsymbol{X} \equiv (R_0, A, B, R_S, r)^\top$ for the measurement of a single Celsius temperature and the associated standard uncertainties (9.5.2.1, 9.5.2.2 and 9.5.2.3)

	R_0/Ω	$A/°C^{-1}$	$B/°C^{-2}$	R_S/Ω	$r/1$
Estimate	99.996 10	0.003 909 6	-6.0×10^{-7}	99.999 47	1.078 005 7
Std unc	0.000 50	0.000 002 7	1.1×10^{-7}	0.000 10	0.000 005 0

Table 13 — Non-zero correlation coefficients associated with pairs of estimates of the input quantities for the measurement of a single Celsius temperature (9.5.2.1, 9.5.2.2 and 9.5.2.3)

	R_0	A	B
R_0	1	−0.155	0.092
A		1	−0.959
B			1

9.5.2.2 The estimate of R_S and the associated standard uncertainty, determined by calibration, are given in table 12. R_S is independent of the parameters R_0, A and B.

9.5.2.3 The quantity measured with the resistance bridge is the resistance ratio

$$r = \frac{R(\theta)}{R_S}. \tag{30}$$

The measured value of r and the associated standard uncertainty are given in table 12. The resistance ratio is independent of the parameters R_0, A and B of the resistance thermometer and the resistance R_S of the standard resistor; there are thus no further non-zero correlation coefficients beyond those given in table 13.

9.5.2.4 By combining expressions (29) and (30), the following measurement model for the Celsius temperature θ is obtained:

$$\left(1 + A\theta + B\theta^2\right) R_0 - rR_S = 0. \tag{31}$$

In terms of the general notation, $N = 5$, $m = 1$, $\boldsymbol{X} \equiv (R_0, A, B, R_S, r)^\top$, $Y \equiv \theta$, and

$$h(Y, \boldsymbol{X}) = \left(1 + A\theta + B\theta^2\right) R_0 - rR_S.$$

NOTE By considering expressions for the roots of a quadratic equation, transformation of the measurement model (31) to explicit form is possible. However, the numerical evaluation of the transformed model can suffer from subtractive cancellation, and the evaluation of sensitivity coefficients is made more difficult by the transformation.

9.5.2.5 The estimate $y \equiv \widehat{\theta}$ of the Celsius temperature generating the measured resistance ratio r is found by inserting the estimates given in table 12 into equation (31) and solving this equation. The solution obtained is $\widehat{\theta} = 20.023\,2\,^{\circ}\mathrm{C}$.

9.5.2.6 The standard uncertainty $u_y \equiv u(\widehat{\theta})$ associated with the estimate y is evaluated using expression (8) in 6.3.1.3, namely $\boldsymbol{C_y U_y C_y^{\top}} = \boldsymbol{C_x U_x C_x^{\top}}$. Evaluating the matrices $\boldsymbol{C_y}$ and $\boldsymbol{C_x}$in 6.3.1.3, namely

$$\boldsymbol{C_Y} = \frac{\partial h}{\partial Y} \equiv \frac{\partial h}{\partial \theta} = (A + 2B\theta)R_0,$$
$$\boldsymbol{C_X} = \frac{\partial h}{\partial \boldsymbol{X}} \equiv \left[\frac{\partial h}{\partial R_0}, \frac{\partial h}{\partial A}, \frac{\partial h}{\partial B}, \frac{\partial h}{\partial R_{\mathrm{S}}}, \frac{\partial h}{\partial r}\right] = \left[1 + A\theta + B\theta^2, R_0\theta, R_0\theta^2, -r, -R_{\mathrm{S}}\right],$$

at the estimates of the input quantities given in table 12 and the corresponding estimate of the output quantity, gives the sensitivity matrices

$$c_y = 0.389\,\Omega\,^{\circ}\mathrm{C}^{-1}$$

and

$$\boldsymbol{C_x} = \left[\ 1.08, \quad 2.00 \times 10^3\,\Omega\,^{\circ}\mathrm{C}, \quad 4.01\,\Omega^{\circ}\mathrm{C}^2, \quad -1.08, \quad -1.00 \times 10^2\,\Omega\ \right].$$

The elements of the covariance matrix $\boldsymbol{U_x}$ associated with the estimates of the input quantities are calculated from the standard uncertainties in table 12 and the correlation coefficients in table 13. The result obtained is $u(\widehat{\theta}) = 0.004\,5\,^{\circ}\mathrm{C}$.

9.5.3 Measurement of several Celsius temperatures

9.5.3.1 The resistance thermometer, standard resistor and resistance bridge described in 9.5.2 are used to measure the resistance ratios $r_1, \ldots, r_{10}$ generated by ten Celsius temperatures $\theta_1, \ldots, \theta_{10}$.

9.5.3.2 The estimates of the input quantities, R_0, A, B and R_{S} and the associated standard uncertainties are given in table 12 and the estimates of $r_1, \ldots, r_{10}$ in table 14. The only non-zero correlation coefficients associated with pairs of the estimates remain those given in table 13. The resistance ratios are assumed to be independent, an assumption that is valid if the magnitudes of the random errors in the measured resistance ratios dominate.

Table 14 — Estimates of the resistance ratios for the measurement of several Celsius temperatures and the associated standard uncertainties (9.5.3.2)

	r_1	r_2	r_3	r_4	r_5
(**Estimate**−1)/10^{-7}	53	150 054	300 055	450 056	600 056
Std unc/10^{-7}	50	50	50	50	50
	r_6	r_7	r_8	r_9	r_{10}
(**Estimate**−1)/10^{-7}	780 057	900 058	1 050 059	1 200 060	780 057
Std unc/10^{-7}	50	50	50	50	50

9.5.3.3 Each resistance ratio r_j is related to the corresponding Celsius temperature θ_j by an equation of the form (31):

$$\left(1 + A\theta_j + B\theta_j^2\right) R_0 - r_j R_{\mathrm{S}} = 0, \qquad j = 1, \ldots, 10. \tag{32}$$

In terms of the general notation, $N = 14$, $m = 10$, $\boldsymbol{X} \equiv (R_0, A, B, R_{\mathrm{S}}, r_1, \ldots, r_{10})^{\top}$, $\boldsymbol{Y} \equiv (\theta_1, \ldots, \theta_{10})^{\top}$, and

$$\boldsymbol{h}(\boldsymbol{Y}, \boldsymbol{X}) = \begin{bmatrix} h_1(\boldsymbol{Y}, \boldsymbol{X}) \\ \vdots \\ h_{10}(\boldsymbol{Y}, \boldsymbol{X}) \end{bmatrix} = \begin{bmatrix} R_0\left(1 + A\theta_1 + B\theta_1^2\right) - r_1 R_{\mathrm{S}} \\ \vdots \\ R_0\left(1 + A\theta_{10} + B\theta_{10}^2\right) - r_{10} R_{\mathrm{S}} \end{bmatrix}.$$

NOTE Transformation of the measurement model (32) to explicit form is possible (see 9.5.2.4).

9.5.3.4 The estimates $\boldsymbol{y} \equiv (\widehat{\theta}_1, \ldots, \widehat{\theta}_{10})$ of the Celsius temperatures $\boldsymbol{Y}$ are given by inserting the estimates given in columns 1 to 4 of table 12 and in table 14 into equations (32) and solving these equations. These estimates are given in table 15.

Table 15 — Estimates of the output quantities $\boldsymbol{Y}$ and the associated standard uncertainties for the measurement of several Celsius temperatures (9.5.3.4 and 9.5.3.5)

	θ_1	θ_2	θ_3	θ_4	θ_5	θ_6	θ_6	θ_8	θ_9	θ_{10}
Estimate/°C	0.010 0	3.849 1	7.692 8	11.541 0	15.393 8	20.023 2	23.113 1	26.979 7	30.850 9	20.023 2
Std unc/°C	0.001 8	0.002 7	0.004 0	0.004 6	0.004 7	0.004 5	0.004 6	0.006 0	0.008 9	0.004 5

Table 16 — Correlation coefficients associated with pairs of estimates of the output quantities $\boldsymbol{Y}$ for the measurement of several Celsius temperatures (9.5.3.5)

	θ_1	θ_2	θ_3	θ_4	θ_5	θ_6	θ_7	θ_8	θ_9	θ_{10}
θ_1	1	0.252	0.127	0.079	0.059	0.054	0.056	0.054	0.050	0.054
θ_2		1	0.815	0.800	0.755	0.580	0.312	−0.092	−0.358	0.580
θ_3			1	0.902	0.868	0.691	0.400	−0.057	−0.365	0.691
θ_4				1	0.909	0.766	0.495	0.040	−0.281	0.766
θ_5					1	0.847	0.629	0.208	−0.115	0.847
θ_6						1	0.841	0.549	0.264	0.918
θ_7							1	0.812	0.613	0.841
θ_8								1	0.909	0.549
θ_9									1	0.264
θ_{10}										1

9.5.3.5 The covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$ associated with $\boldsymbol{y}$ is evaluated using expression (8) in 6.3.1.3, namely $\boldsymbol{C}_{\boldsymbol{y}}\boldsymbol{U}_{\boldsymbol{y}}\boldsymbol{C}_{\boldsymbol{y}}^{\top} = \boldsymbol{C}_{\boldsymbol{x}}\boldsymbol{U}_{\boldsymbol{x}}\boldsymbol{C}_{\boldsymbol{x}}^{\top}$. $\boldsymbol{C}_{\boldsymbol{y}}$ and $\boldsymbol{C}_{\boldsymbol{x}}$ are sensitivity matrices given by evaluating $\boldsymbol{C}_{\boldsymbol{Y}}$ and $\boldsymbol{C}_{\boldsymbol{X}}$, respectively, at the estimates of the input and output quantities. $\boldsymbol{C}_{\boldsymbol{Y}}$ is a diagonal matrix of dimension 10×10 with diagonal entries $R_0(A + 2B\theta_1), \ldots, R_0(A + 2B\theta_{10})$. $\boldsymbol{C}_{\boldsymbol{X}}$ is a matrix of dimension 10×14 given by

$$\boldsymbol{C}_{\boldsymbol{X}} = \left[\boldsymbol{C}_{\boldsymbol{X}}{}^{(1)} \quad \boldsymbol{C}_{\boldsymbol{X}}{}^{(2)}\right],$$

where

$$\boldsymbol{C}_{\boldsymbol{X}}{}^{(1)} = \begin{bmatrix} 1 + A\theta_1 + B\theta_1^2 & R_0\theta_1 & R_0\theta_1^2 & -r_1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 + A\theta_{10} + B\theta_{10}^2 & R_0\theta_{10} & R_0\theta_{10}^2 & -r_{10} \end{bmatrix}$$

is a matrix of dimension 10×4, and $\boldsymbol{C}_{\boldsymbol{X}}{}^{(2)}$ is a diagonal matrix of dimension 10×10 with diagonal elements all equal to $-R_{\mathrm{S}}$. The covariance matrix $\boldsymbol{U}_{\boldsymbol{x}}$ is calculated from the standard uncertainties given in columns 1 to 4 of table 12 and in table 13. The standard uncertainties associated with the estimates of the Celsius temperatures and the correlation coefficients associated with pairs of estimates, derived from the matrix $\boldsymbol{U}_{\boldsymbol{y}}$, are given in table 15 and table 16, respectively.

9.5.3.6 The results given in table 15 and figure 22 show how the standard uncertainty $u(\widehat{\theta}_j)$ varies with the estimate $\widehat{\theta}_j$ of Celsius temperature θ_j. The uncertainty is smallest around 0 °C and increases rapidly for temperatures greater than 25 °C. This effect is due to the fact that the resistance thermometer was calibrated at the temperatures 0 °C, 15 °C, 20 °C and 25 °C, and that the Celsius temperature 0 °C during calibration was generated using an ice bath with a standard uncertainty three times smaller than those associated with the other three temperatures, which were generated using an oil bath.

NOTE In figures 22 and 23 the straight-line segments joining the plotted points are included for purpose of visualization.

9.5.3.7 Using the results given in the final column of table 16, figure 23 shows how the correlation coefficient associated with the pair of estimates $\widehat{\theta}_j$ and $\widehat{\theta}_{10}$ of Celsius temperatures θ_j and $\theta_{10} = 20\,°\mathrm{C}$ varies with $\widehat{\theta}_j$,

$j = 1, \ldots, 9$. The correlation coefficient has a maximum for $\widehat{\theta}_j = \widehat{\theta}_6$ and approaches zero as the absolute difference $|\widehat{\theta}_j - \widehat{\theta}_{10}|$ becomes large. The example demonstrates that quantities measured with the same instrument can be highly correlated.

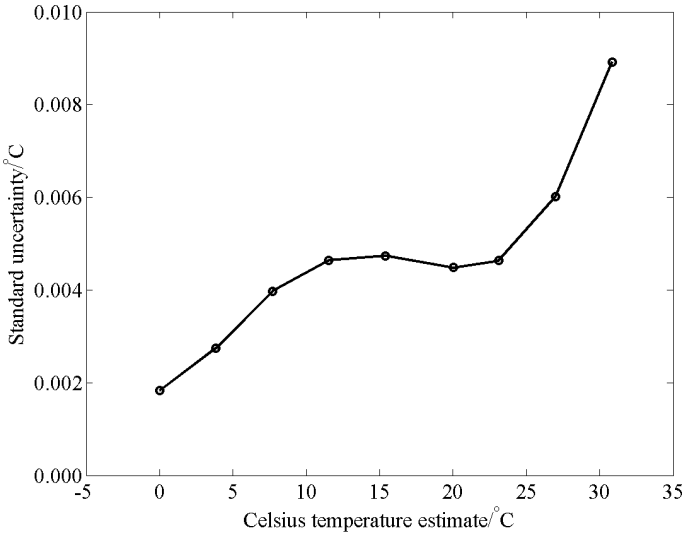

Figure 22 — Standard uncertainty $u(\widehat{\theta}_j)$ associated with the estimate $\widehat{\theta}_j$ of Celsius temperature θ_j (9.5.3.6)

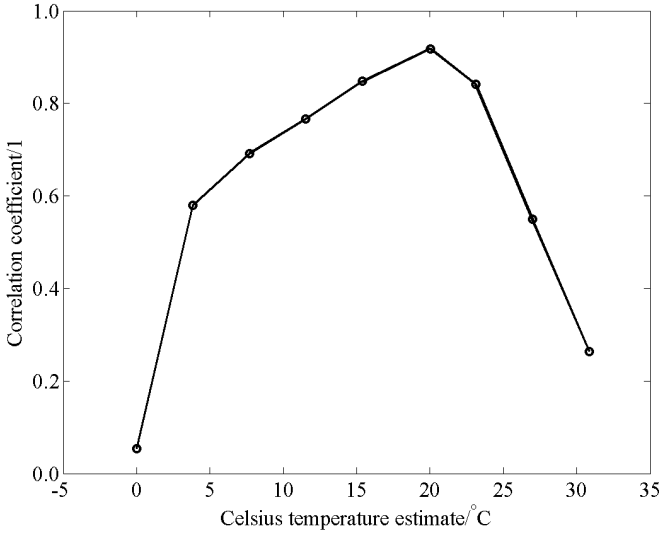

Figure 23 — Correlation coefficient associated with the pair of estimates $\widehat{\theta}_j$ and $\widehat{\theta}_{10}$ of Celsius temperatures θ_j and $\theta_{10} = 20\,°\mathrm{C}$ (9.5.3.7)

Annex A
(informative)
Derivatives of complex multivariate measurement functions

A.1 In this annex consideration is given to the algebraically efficient determination of the partial derivatives of first order of the measurement function $\boldsymbol{f}$ in a complex multivariate measurement model

$$\boldsymbol{Y} = \boldsymbol{f}(\boldsymbol{X}),$$

where

$$\boldsymbol{X} = (\boldsymbol{X}_1, \ldots, \boldsymbol{X}_N)^\top, \qquad \boldsymbol{Y} = (\boldsymbol{Y}_1, \ldots, \boldsymbol{Y}_m)^\top,$$

and

$$\boldsymbol{f} = (\boldsymbol{f}_1, \ldots, \boldsymbol{f}_m)^\top,$$

$\boldsymbol{X}_i$ denoting the complex quantity $X_{i,\mathrm{R}} + \mathrm{i}X_{i,\mathrm{I}}$, with $X_{i,\mathrm{R}}$ and $X_{i,\mathrm{I}}$ real scalar quantities, and $\mathrm{i}^2 = -1$, and similarly for $\boldsymbol{Y}_j$ and $\boldsymbol{f}_j$.

A.2 Let $\boldsymbol{U}_{\boldsymbol{x}}$ denote the covariance matrix of dimension $2N \times 2N$ associated with an estimate $\boldsymbol{x}$ of $\boldsymbol{X}$. $\boldsymbol{U}_{\boldsymbol{x}}$ takes the form

$$\boldsymbol{U}_{\boldsymbol{x}} = \begin{bmatrix} \boldsymbol{U}(\boldsymbol{x}_1, \boldsymbol{x}_1) & \cdots & \boldsymbol{U}(\boldsymbol{x}_1, \boldsymbol{x}_N) \\ \vdots & \ddots & \vdots \\ \boldsymbol{U}(\boldsymbol{x}_N, \boldsymbol{x}_1) & \cdots & \boldsymbol{U}(\boldsymbol{x}_N, \boldsymbol{x}_N) \end{bmatrix},$$

where

$$\boldsymbol{U}(\boldsymbol{x}_i, \boldsymbol{x}_j) = \begin{bmatrix} u(x_{i,\mathrm{R}}, x_{j,\mathrm{R}}) & u(x_{i,\mathrm{R}}, x_{j,\mathrm{I}}) \\ u(x_{i,\mathrm{I}}, x_{j,\mathrm{R}}) & u(x_{i,\mathrm{I}}, x_{j,\mathrm{I}}) \end{bmatrix}$$

is the covariance matrix of dimension 2×2 associated with the (complex) estimates $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ of $\boldsymbol{X}_i$ and $\boldsymbol{X}_j$, respectively.

A.3 The covariance matrix

$$\boldsymbol{U}_{\boldsymbol{y}} = \begin{bmatrix} \boldsymbol{U}(\boldsymbol{y}_1, \boldsymbol{y}_1) & \cdots & \boldsymbol{U}(\boldsymbol{y}_1, \boldsymbol{y}_m) \\ \vdots & \ddots & \vdots \\ \boldsymbol{U}(\boldsymbol{y}_m, \boldsymbol{y}_1) & \cdots & \boldsymbol{U}(\boldsymbol{y}_m, \boldsymbol{y}_m) \end{bmatrix},$$

of dimension $2m \times 2m$, where

$$\boldsymbol{U}(\boldsymbol{y}_\ell, \boldsymbol{y}_j) = \begin{bmatrix} u(y_{\ell,\mathrm{R}}, y_{j,\mathrm{R}}) & u(y_{\ell,\mathrm{R}}, y_{j,\mathrm{I}}) \\ u(y_{\ell,\mathrm{I}}, y_{j,\mathrm{R}}) & u(y_{\ell,\mathrm{I}}, y_{j,\mathrm{I}}) \end{bmatrix},$$

associated with the estimate

$$\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x})$$

of $\boldsymbol{Y}$ is given by the generalized law of propagation of uncertainty

$$\boldsymbol{U}_{\boldsymbol{y}} = \boldsymbol{C}_{\boldsymbol{x}} \boldsymbol{U}_{\boldsymbol{x}} \boldsymbol{C}_{\boldsymbol{x}}{}^\top. \tag{A.1}$$

A.4 $\boldsymbol{C}_{\boldsymbol{x}}$ is the sensitivity matrix of dimension $2m \times 2N$ given by evaluating

$$\boldsymbol{C}_{\boldsymbol{X}} = \begin{bmatrix} \boldsymbol{C}_{1,1} & \cdots & \boldsymbol{C}_{1,N} \\ \vdots & \ddots & \vdots \\ \boldsymbol{C}_{m,1} & \cdots & \boldsymbol{C}_{m,N} \end{bmatrix}$$

at $\boldsymbol{X} = \boldsymbol{x}$, where $\boldsymbol{C}_{j,i}$ is the matrix of dimension 2×2 of the partial derivatives of first order of the real and imaginary parts of $\boldsymbol{f}_j$ with respect to the real and imaginary parts of $\boldsymbol{X}_i$:

$$\boldsymbol{C}_{j,i} = \begin{bmatrix} \dfrac{\partial f_{j,\mathrm{R}}}{\partial X_{i,\mathrm{R}}} & \dfrac{\partial f_{j,\mathrm{R}}}{\partial X_{i,\mathrm{I}}} \\ \\ \dfrac{\partial f_{j,\mathrm{I}}}{\partial X_{i,\mathrm{R}}} & \dfrac{\partial f_{j,\mathrm{I}}}{\partial X_{i,\mathrm{I}}} \end{bmatrix}.$$

A.5 For any complex scalar quantity $\boldsymbol{Q} = Q_{\mathrm{R}} + \mathrm{i}Q_{\mathrm{I}}$, consider the matrix representation of dimension 2×2 for $\boldsymbol{Q}$ [14]:

$$\boldsymbol{M}(\boldsymbol{Q}) = \begin{bmatrix} Q_{\mathrm{R}} & -Q_{\mathrm{I}} \\ Q_{\mathrm{I}} & Q_{\mathrm{R}} \end{bmatrix}.$$

Then, $\boldsymbol{C}_{j,i}$ can be expressed as

$$\boldsymbol{C}_{j,i} = \boldsymbol{M}\left(\frac{\partial \boldsymbol{f}_j}{\partial \boldsymbol{X}_i}\right),$$

and provides the basis for an algebraically efficient means for forming the partial derivatives: only the complex derivatives of first order of the $\boldsymbol{f}_j$ with respect to the $\boldsymbol{X}_i$ need be formed.

Annex B
(informative)
Evaluation of sensitivity coefficients and covariance matrix for multivariate measurement models

B.1 When recognized concepts from numerical linear algebra [13] are used, a numerically stable way to form $\boldsymbol{U}_{\boldsymbol{y}}$, the solution of the linear system of equations (8) is as follows:

a) form the Cholesky factor $\boldsymbol{R}_{\boldsymbol{x}}$ of $\boldsymbol{U}_{\boldsymbol{x}}$, that is the upper triangular matrix such that $\boldsymbol{R}_{\boldsymbol{x}}^{\top}\boldsymbol{R}_{\boldsymbol{x}} = \boldsymbol{U}_{\boldsymbol{x}}$;

b) factorize $\boldsymbol{C}_{\boldsymbol{x}}$ as the product $\boldsymbol{C}_{\boldsymbol{x}} = \boldsymbol{Q}_{\boldsymbol{x}}\boldsymbol{W}_{\boldsymbol{x}}$, where $\boldsymbol{Q}_{\boldsymbol{x}}$ is an orthogonal matrix and $\boldsymbol{W}_{\boldsymbol{x}}$ is upper triangular;

c) factorize $\boldsymbol{C}_{\boldsymbol{y}}$ as the product $\boldsymbol{C}_{\boldsymbol{y}} = \boldsymbol{L}_{\boldsymbol{y}}\boldsymbol{W}_{\boldsymbol{y}}$, where $\boldsymbol{L}_{\boldsymbol{y}}$ is lower triangular and $\boldsymbol{W}_{\boldsymbol{y}}$ is upper triangular;

d) solve the matrix equation $\boldsymbol{W}_{\boldsymbol{y}}^{\top}\boldsymbol{M}_1 = \boldsymbol{I}$ for $\boldsymbol{M}_1$;

e) solve $\boldsymbol{L}_{\boldsymbol{y}}^{\top}\boldsymbol{M}_2 = \boldsymbol{M}_1$ for $\boldsymbol{M}_2$;

f) form $\boldsymbol{M}_3 = \boldsymbol{Q}_{\boldsymbol{x}}^{\top}\boldsymbol{M}_2$;

g) form $\boldsymbol{K} = \boldsymbol{W}_{\boldsymbol{x}}^{\top}\boldsymbol{M}_3$;

h) form $\boldsymbol{M} = \boldsymbol{R}_{\boldsymbol{x}}\boldsymbol{K}$;

i) orthogonally triangularize $\boldsymbol{M}$ to give the upper triangular matrix $\boldsymbol{R}$;

j) form $\boldsymbol{U}_{\boldsymbol{y}} = \boldsymbol{R}^{\top}\boldsymbol{R}$.

B.2 This procedure can be verified using elementary matrix algebra. Further details are available [7].

Annex C
(informative)
Co-ordinate system transformation

C.1 General

This annex is concerned with some deatils of the co-ordinate system transformation problem (see 9.3). Subclause C.2 provides the joint PDF for $\boldsymbol{Y}$ analytically for the case that X_1 is described by the Gaussian distribution $\mathrm{N}(x_1, u_x^2)$ and X_2 by $\mathrm{N}(x_2, u_x^2)$, with X_1 and X_2 mutually independent. Subclause C.3 applies the GUM uncertainty framework for correlated and uncorrelated input quantities.

C.2 Analytical solution for a special case

C.2.1 Suppose $\boldsymbol{X}$ has PDF $g_{\boldsymbol{X}}(\boldsymbol{\xi})$, and $\boldsymbol{\xi} = \boldsymbol{f}^{-1}(\boldsymbol{\eta})$ is a transformation from values $\boldsymbol{\eta} = (\eta_1, \ldots, \eta_N)^\top$ of $\boldsymbol{Y}$ to values $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_N)^\top$ of $\boldsymbol{X}$ that is one-to-one. Then [19, page 35], $\boldsymbol{Y}$ has PDF

$$g_{\boldsymbol{Y}}(\boldsymbol{\eta}) = g_{\boldsymbol{X}}(\boldsymbol{f}^{-1}(\boldsymbol{\eta}))|\det(\boldsymbol{J})|, \tag{C.1}$$

where $\det(\boldsymbol{J})$ is the determinant of the Jacobian matrix $\boldsymbol{J}$,

$$\boldsymbol{J} = \begin{bmatrix} \dfrac{\partial \xi_1}{\partial \eta_1} & \cdots & \dfrac{\partial \xi_1}{\partial \eta_N} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial \xi_N}{\partial \eta_1} & \cdots & \dfrac{\partial \xi_N}{\partial \eta_N} \end{bmatrix}$$

regarded as a function of $\boldsymbol{\eta}$, with $\det(\boldsymbol{J})$ assumed to be nowhere zero or infinite.

NOTE 1 The result (C.1) is sometimes known as the "Change of variables theorem".

NOTE 2 The result for the transformation of a single quantity ($N = 1$) is as follows [21, pages 57–61]: if $\eta = f(\xi)$ is differentiable and monotonic, Y has PDF

$$g_Y(\eta) = g_X\left(f^{-1}(\eta)\right)\left|\frac{\mathrm{d}f^{-1}(\eta)}{\mathrm{d}\eta}\right|.$$

C.2.2 For the co-ordinate system transformation problem considered in 9.3, $\boldsymbol{X} \equiv (X_1, X_2)^\top$ with values $\boldsymbol{\xi} = (\xi_1, \xi_2)^\top$, $\boldsymbol{Y} \equiv (R, \Theta)^\top$ with values $\boldsymbol{\eta} = (\eta_1, \eta_2)^\top$, and

$$\xi_1 = \eta_1 \cos\eta_2, \qquad \xi_2 = \eta_1 \sin\eta_2.$$

Therefore,

$$\boldsymbol{J} = \begin{bmatrix} \cos\eta_2 & -\eta_1 \sin\eta_2 \\ \sin\eta_2 & \eta_1 \cos\eta_2 \end{bmatrix},$$

and

$$\det(\boldsymbol{J}) = \eta_1.$$

It follows that, provided $\eta_1 > 0$,

$$g_{Y_1,Y_2}(\eta_1, \eta_2) = \eta_1 g_{X_1,X_2}(\eta_1 \cos\eta_2, \eta_1 \sin\eta_2).$$

C.2.3 Consider the case that X_1 is described by the Gaussian distribution $\mathrm{N}(x_1, u_x^2)$ and X_2 by $\mathrm{N}(x_2, u_x^2)$, with X_1 and X_2 mutually independent. Then,

$$g_{X_1,X_2}(\xi_1,\xi_2) = g_{X_1}(\xi_1)g_{X_2}(\xi_2) = \frac{1}{2\pi u_x^2}\exp\left(-\frac{(\xi_1 - x_1)^2 + (\xi_2 - x_2)^2}{2u_x^2}\right),$$

giving

$$g_{Y_1,Y_2}(\eta_1,\eta_2) = \frac{\eta_1}{2\pi u_x^2}\exp\left(-\frac{(\eta_1\cos\eta_2 - x_1)^2 + (\eta_1\sin\eta_2 - x_2)^2}{2u_x^2}\right).$$

C.2.4 The marginal distribution for $Y_1 \equiv R$ is

$$g_{Y_1}(\eta_1) = \int_{-\pi}^{\pi} g_{Y_1,Y_2}(\eta_1,\eta_2)\,\mathrm{d}\eta_2 = \frac{\eta_1}{u_x^2}\exp\left(-\frac{\eta_1^2 + y_1^2}{2u_x^2}\right) I_0\left(\frac{\eta_1 y_1}{u_x^2}\right), \tag{C.2}$$

where

$$y_1^2 = x_1^2 + x_2^2,$$

and I_0 is the modified Bessel function of the first kind of order zero.

NOTE 1 The distribution is the Rice distribution with parameters y_1 and u_x.

NOTE 2 If $y_1 = 0$, the distribution is the Rayleigh distribution with parameter u_x.

NOTE 3 If $u_x = 1$, the distribution is the non-central chi-squared distribution with two degrees of freedom and non-centrality parameter y_1^2.

C.2.5 The marginal distribution for $Y_2 \equiv \Theta$ is

$$g_{Y_2}(\eta_2) = \int_0^{\infty} g_{Y_1,Y_2}(\eta_1,\eta_2)\,\mathrm{d}\eta_1 = \frac{1}{2\pi}\exp\left(-\frac{y_1^2}{2u_x^2}\right)\left[1 + \sqrt{\pi}\tau\exp(\tau^2)\mathrm{erfc}(-\tau)\right], \tag{C.3}$$

where

$$\tau = \frac{x_1\cos\eta_2 + x_2\sin\eta_2}{\sqrt{2}u_x},$$

and

$$\mathrm{erfc}(z) = 1 - \frac{2}{\sqrt{\pi}}\int_0^x \exp(-t^2)\,\mathrm{d}t$$

is the complementary error function.

C.2.6 If also $x_1 = x_2 = 0$, then

$$g_{Y_1,Y_2}(\eta_1,\eta_2) = \frac{\eta_1}{2\pi u_x^2}\exp\left(-\frac{\eta_1^2}{2u_x^2}\right),$$

and it follows that Y_1 and Y_2 are mutually independent with distributions

$$g_{Y_1}(\eta_1) = \frac{\eta_1}{u_x^2}\exp\left(-\frac{\eta_1^2}{2u_x^2}\right),$$

a Rayleigh distribution with parameter u_x, and

$$g_{Y_2}(\eta_2) = \frac{1}{2\pi},$$

a rectangular distribution between $-\pi$ and π.

C.3 Application of the GUM uncertainty framework

C.3.1 For the co-ordinate system transformation problem considered in 9.3, the measurement model can be written as the bivariate measurement model

$$Y_1 = f_1(X_1, X_2) = \sqrt{X_1^2 + X_2^2}, \qquad Y_2 = f_2(X_1, X_2) = \tan^{-1}(X_2/X_1),$$

where it is understood that $Y_1 \geq 0$ and $-\pi < Y_2 \leq \pi$. The input quantities X_1 and X_2 have estimates x_1 and x_2 and associated uncertainties $u(x_1)$ and $u(x_2)$, respectively, and associated covariance $u(x_1, x_2)$.

C.3.2 The application of 6.2.1.2 gives

$$y_1 = \sqrt{x_1^2 + x_2^2}, \qquad y_2 = \tan^{-1}(x_2/x_1),$$

as the estimates of Y_1 and Y_2.

C.3.3 The sensitivity matrix $\boldsymbol{C_x}$ of dimension 2×2 is given by evaluating

$$\boldsymbol{C_X} = \begin{bmatrix} \dfrac{\partial f_1}{\partial X_1} & \dfrac{\partial f_1}{\partial X_2} \\ \dfrac{\partial f_2}{\partial X_1} & \dfrac{\partial f_2}{\partial X_2} \end{bmatrix} = \begin{bmatrix} \dfrac{X_1}{\sqrt{X_1^2 + X_2^2}} & \dfrac{X_2}{\sqrt{X_1^2 + X_2^2}} \\ \dfrac{-X_2}{X_1^2 + X_2^2} & \dfrac{X_1}{X_1^2 + X_2^2} \end{bmatrix}$$

at $X_1 = x_1$ and $X_2 = x_2$. Therefore, provided $y_1 = \sqrt{x_1^2 + x_2^2} > 0$,

$$\boldsymbol{C_x} = \begin{bmatrix} \dfrac{x_1}{\sqrt{x_1^2 + x_2^2}} & \dfrac{x_2}{\sqrt{x_1^2 + x_2^2}} \\ \dfrac{-x_2}{x_1^2 + x_2^2} & \dfrac{x_1}{x_1^2 + x_2^2} \end{bmatrix} = \begin{bmatrix} \cos y_2 & \sin y_2 \\ -(\sin y_2)/y_1 & (\cos y_2)/y_1 \end{bmatrix}.$$

C.3.4 The application of 6.2.1.3 gives

$$\boldsymbol{U_y} = \begin{bmatrix} u^2(y_1) & u(y_1, y_2) \\ u(y_2, y_1) & u^2(y_2) \end{bmatrix}$$

as the covariance matrix associated with the estimates $\boldsymbol{y} = (y_1, y_2)^\top$, with $u(y_2, y_1) = u(y_1, y_2)$ and

$$\begin{aligned} u^2(y_1) &= u^2(x_1)\cos^2 y_2 + u^2(x_2)\sin^2 y_2 + 2u(x_1, x_2)\cos y_2 \sin y_2, \\ u(y_1, y_2) &= (u^2(x_2) - u^2(x_1))(\sin y_2 \cos y_2)/y_1 + u(x_1, x_2)(\cos^2 y_2 - \sin^2 y_2)/y_1, \\ u^2(y_2) &= u^2(x_1)(\sin^2 y_2)/y_1^2 + u^2(x_2)(\cos^2 y_2)/y_1^2 - 2u(x_1, x_2)(\sin y_2 \cos y_2)/y_1^2. \end{aligned}$$

C.3.5 In the context of the GUM uncertainty framework, $\boldsymbol{Y}$ is characterized by the bivariate Gaussian distribution $\mathrm{N}(\boldsymbol{y}, \boldsymbol{U_y})$, which can be used as the basis of determining coverage regions for $\boldsymbol{Y}$ corresponding to a prescribed coverage probability p (see 6.5).

C.3.6 Consider the case that $u(x_1) = u(x_2) = u_x$ and $u(x_1, x_2) = 0$ (see C.2.3). Then,

$$u^2(y_1) = u_x^2, \qquad u(y_1, y_2) = 0, \qquad u^2(y_2) = u_x^2/y_1^2,$$

with $\boldsymbol{Y}$ characterized by a bivariate Gaussian distribution as in C.3.5. It follows that, in this special circumstance of uncorrelated quantities assigned a bivariate Gaussian distribution, Y_1 and Y_2 are mutually independent [19, theorem 3.1.3]. Consequently, Y_1 and Y_2 are characterized by univariate Gaussian distributions $\mathrm{N}(y_1, u^2(y_1))$ and $\mathrm{N}(y_2, u^2(y_2))$, respectively.

NOTE In contrast, in the analytical treatment C.2, where $\boldsymbol{Y}$ is not characterized by a bivariate Gaussian distribution, the conditions $u(x_1) = u(x_2)$ and $u(x_1, x_2) = 0$ are not sufficient for Y_1 and Y_2 to be independent. An additional condition, viz. $x_1 = x_2 = 0$, is required (see C.2.6).

Annex D
(informative)
Glossary of principal symbols

$\boldsymbol{C_x}$	sensitivity matrix of dimension $m \times N$ associated with $\boldsymbol{x}$
$\boldsymbol{C_y}$	sensitivity matrix of dimension $m \times m$ associated with $\boldsymbol{y}$
c	n_{dig}-decimal digit integer
$\text{Corr}(X_i, X_j)$	correlation for two random variables X_i and X_j
$\text{Cov}(X_i, X_j)$	covariance for two random variables X_i and X_j
$\det(\boldsymbol{J})$	Jacobian determinant
$E(X_i)$	expectation of random variable X_i
$\boldsymbol{E}(\boldsymbol{X})$	expectation of random variable $\boldsymbol{X}$
$F_{m,n}$	Fisher-Snedecor distribution with m and $n - m$ degrees of freedom
f	univariate measurement function depending on input quantities $\boldsymbol{X}$
$\boldsymbol{f}$	multivariate measurement function depending on input quantities $\boldsymbol{X}$
$\boldsymbol{G}$	discrete representation of distribution function $G_{\boldsymbol{Y}}(\boldsymbol{\eta})$ for output quantity $\boldsymbol{Y}$ from a Monte Carlo procedure
$G_{\boldsymbol{X}}(\boldsymbol{\xi})$	distribution function with variable $\boldsymbol{\xi}$ for input quantity $\boldsymbol{X}$
$g_{X_i}(\xi_i)$	probability density function with variable ξ_i for input quantity X_i
$g_{\boldsymbol{X}}(\boldsymbol{\xi})$	joint (multivariate) probability density function with variable $\boldsymbol{\xi}$ for input quantity $\boldsymbol{X}$
$G_{\boldsymbol{Y}}(\boldsymbol{\eta})$	distribution function with variable $\boldsymbol{\eta}$ for output quantity $\boldsymbol{Y}$
$g_{\boldsymbol{Y}}(\boldsymbol{\eta})$	joint (multivariate) probability density function with variable $\boldsymbol{\eta}$ for output quantity $\boldsymbol{Y}$
h	univariate measurement model expressed as a relationship between output quantity Y and input quantities $\boldsymbol{X}$ on which Y depends
$\boldsymbol{h}$	multivariate measurement model expressed as a relationship between output quantities $\boldsymbol{Y}$ and input quantities $\boldsymbol{X}$ on which $\boldsymbol{Y}$ depends
i	imaginary unit given by $\text{i}^2 = -1$
$\boldsymbol{J}$	Jacobian matrix
k_p	coverage factor for a coverage region in the form of a hyper-ellipsoid corresponding to coverage probability p
k_q	coverage factor for a coverage region in the form of a hyper-rectangle corresponding to coverage probability p
$\boldsymbol{L}$	lower triangular matrix

ℓ	integer in the representation $c \times 10^{\ell}$ of a numerical value, where c is an n_{dig}-decimal digit integer
m	number of output quantities $Y_1, \ldots, Y_m$
M	number of Monte Carlo trials
$\boldsymbol{M}$	matrix of sums of squares and products
N	number of input quantities $X_1, \ldots, X_N$
$\mathrm{N}(0, 1)$	standard Gaussian distribution
$\mathrm{N}(\mu, \sigma^2)$	Gaussian distribution with parameters μ and σ^2
$\mathrm{N}(\boldsymbol{\mu}, \boldsymbol{V})$	multivariate Gaussian distribution with parameters $\boldsymbol{\mu}$ and $\boldsymbol{V}$
n	number of indication values in a series
n_{dig}	number of significant decimal digits regarded as meaningful in a numerical value
$\Pr(z)$	probability of event z
p	coverage probability
$R_{\boldsymbol{Y}}$	coverage region in m dimensions for $\boldsymbol{Y}$
$\boldsymbol{R}_{\boldsymbol{y}}$	correlation matrix of dimension $m \times m$ associated with $\boldsymbol{y}$
$\mathrm{R}(0, 1)$	standard rectangular distribution over the interval $[0,\ 1]$
$\mathrm{R}(a, b)$	rectangular distribution over the interval $[a,\ b]$
$r(x_i, x_j)$	correlation coefficient associated with estimates x_i and x_j of input quantities X_i and X_j
s	standard deviation of a series of n indication values $x_1, \ldots, x_n$
s_z	standard deviation associated with average z of values $z^{(1)}, \ldots, z^{(h)}$ in adaptive Monte Carlo procedure, where z may denote estimate y_j of output quantity Y_j, standard uncertainty $u(y_j)$ associated with y_j, maximum eigenvalue $\lambda_{\max}$ of correlation matrix $\boldsymbol{R}_{\boldsymbol{y}}$, or coverage factor k_p of coverage region for $\boldsymbol{Y}$
$\top$	superscript denoting matrix transpose
$t_{\nu}(\boldsymbol{\mu}, \boldsymbol{S})$	multivariate t-distribution with parameters $\boldsymbol{\mu}$ and $\boldsymbol{S}$, and ν degrees of freedom
U_p	expanded uncertainty corresponding to coverage probability p
$\boldsymbol{U}_{\boldsymbol{x}}$	covariance matrix associated with estimate $\boldsymbol{x}$ of input quantity $\boldsymbol{X}$
$\boldsymbol{U}_{\boldsymbol{y}}$	covariance matrix associated with estimate $\boldsymbol{y}$ of output quantity $\boldsymbol{Y}$
$u_x,\ u(x)$	standard uncertainty associated with estimate x of input quantity X
$u(x_i)$	standard uncertainty associated with estimate x_i of input quantity X_i
$u(x_i, x_j)$	covariance associated with estimates x_i and x_j of input quantities X_i and X_j

$\boldsymbol{u}(\boldsymbol{x})$	vector $(u(x_1), \ldots, u(x_N))^\top$ of standard uncertainties associated with estimate $\boldsymbol{x}$ of input quantity $\boldsymbol{X}$
$V(X_i)$	variance of random variable X_i
$\boldsymbol{V}$	covariance (variance-covariance) matrix
$\boldsymbol{V}(\boldsymbol{X})$	covariance matrix of random variable $\boldsymbol{X}$
X_i	ith input quantity, regarded as a random variable
$\boldsymbol{X}$	vector $(X_1, \ldots, X_N)^\top$ of input quantities
$\bar{x}$	average of series of n indication values $x_1, \ldots, x_n$
x_i	estimate (expectation) of X_i, or ith indication value in series
$\boldsymbol{x}$	estimate (expectation) $(x_1, \ldots, x_N)^\top$ of $\boldsymbol{X}$
$x_{i,r}$	rth Monte Carlo draw from probability density function for X_i
$\boldsymbol{x}_r$	rth Monte Carlo draw, containing values $x_{1,r}, \ldots, x_{N,r}$, drawn from probability density functions for N input quantities $X_1, \ldots, X_N$ or from joint probability density function for $\boldsymbol{X}$
Y_j	jth output quantity, regarded as a random variable
$\boldsymbol{Y}$	vector $(Y_1, \ldots, Y_m)^\top$ of output quantities, regarded as random variables
y_j	estimate (expectation) of Y_j
$\boldsymbol{y}$	estimate (expectation) $(y_1, \ldots, y_m)^\top$ of $\boldsymbol{Y}$
$\widetilde{\boldsymbol{y}}$	estimate of $\boldsymbol{Y}$, obtained as average of M model values $\boldsymbol{y}_r$ from a Monte Carlo run
$\boldsymbol{y}_r$	rth model value $\boldsymbol{f}(\boldsymbol{x}_r)$
$\mathring{\boldsymbol{y}}_r$	rth model value $\boldsymbol{f}(\boldsymbol{x}_r)$ suitably transformed
$z^{(h)}$	hth value in adaptive Monte Carlo procedure, where z may denote estimate y_j of output quantity Y_j, standard uncertainty $u(y_j)$ associated with y_j, maximum eigenvalue $\lambda_{\max}$ of correlation matrix $\boldsymbol{R}_{\boldsymbol{y}}$, or coverage factor k_p for a coverage region for $\boldsymbol{Y}$
α	probability value
$\Gamma(z)$	gamma function with variable z
δ	numerical tolerance associated with numerical value
$\boldsymbol{\eta}$	variable describing possible values of output quantity $\boldsymbol{Y}$
κ_p	numerical tolerance associated with coverage factor k_p for a hyper-ellipsoidal coverage region
κ_q	numerical tolerance associated with coverage factor k_q for a hyper-rectangular coverage region
$\lambda_{\max}$	largest eigenvalue of correlation matrix
$\lambda_{\min}$	smallest eigenvalue of correlation matrix

μ	expectation of quantity characterized by probability distribution
$\boldsymbol{\mu}$	expectation of quantity characterized by joint probability distribution
ν	degrees of freedom of t-distribution or chi-squared distribution
ν_{eff}	effective degrees of freedom associated with standard uncertainty $u(y)$
ξ_i	variable describing possible values of input quantity X_i
$\boldsymbol{\xi}$	variable $(\xi_1, \ldots, \xi_N)^\top$ describing possible values of input quantity $\boldsymbol{X}$
ρ	numerical tolerance associated with largest eigenvalue $\lambda_{\max}$ of a correlation matrix
σ	standard deviation of quantity characterized by probability distribution
σ^2	variance (squared standard deviation) of quantity characterized by probability distribution
$\boldsymbol{\Sigma}$	covariance matrix of vector quantity characterized by joint probability distribution
χ^2_ν	chi-squared distribution with ν degrees of freedom

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