Guide to the Expression of Uncertainty in Measurement
Supplement 1
Numerical Methods for the Propagation of Distributions

This version is intended for circulation to the member organizations of the JCGM and National Measurement Institutes for review.

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Foreword

This Supplement is concerned with the concept of the propagation of distributions as a basis for the evaluation of uncertainty of measurement. This concept constitutes a generalization of the law of propagation of uncertainty given in the Guide to the Expression of Uncertainty in Measurement (GUM) [3]. It thus facilitates the provision of uncertainty evaluations that are more valid than those provided by the use of the law of propagation of uncertainty in circumstances where the conditions for the application of that law are not fulfilled. The propagation of distributions is consistent with the general principles on which the GUM is based. An implementation of the propagation of distributions is given that uses Monte Carlo simulation.

In 1997 a Joint Committee for Guides in Metrology (JCGM), chaired by the Director of the BIPM, was created by the seven International Organizations that had prepared the original versions of the GUM and the International Vocabulary of Basic and General Terms in Metrology (VIM). The Committee had the task of the ISO Technical Advisory Group 4 (TAG4), which had developed the GUM and the VIM. The Joint Committee, as was the TAG4, is formed by the BIPM with the International Electrotechnical Commission (IEC), the International Federation of Clinical Chemistry and Laboratory Medicine (IFCC), 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). A further organization joined these seven international organizations, namely, the International Laboratory Accreditation Cooperation (ILAC). Within JCGM two Working Groups have been established. Working Group 1, “Expression of Uncertainty in Measurement”, has the task to promote the use of the GUM and to prepare supplements 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. The present Guide has been prepared by Working Group 1 of the JCGM.

Introduction

This Supplement is concerned with the concept of the propagation of probability distributions through a model of measurement as a basis for the evaluation of uncertainty of measurement, and its implementation by Monte Carlo simulation. The treatment applies to a model having any number of input quantities, and a single (scalar-valued) output quantity (sometimes known as the measurand). A second Supplement, in preparation, is concerned with arbitrary numbers of output quantities. In particular, the provision of the probability density function for the output quantity value permits the determination of a coverage interval for that value corresponding to a prescribed coverage probability. The Monte Carlo simulation technique in general provides a practical solution for complicated models or models with input quantities having “large” uncertainties or asymmetric probability density functions. The evaluation procedure based on probability distributions is entirely consistent with the GUM, which states in Subclause 3.3.5 that “...a Type A standard uncertainty is obtained from a probability density function derived from an observed frequency distribution, while a Type B standard uncertainty is obtained from an assumed probability density function based on the degree of belief that an event will occur ...”. It is also consistent in the sense that it falls in the category of the “other analytical or numerical methods” [GUM Subclause G.1.5] permitted by the GUM. Indeed, the law of propagation of uncertainty can be derived from the propagation of distributions. Thus, the propagation of distributions is a generalization of the approach predominantly advocated in the GUM, in that it works with richer information than that conveyed by best estimates and the associated standard uncertainties alone.

This supplement also provides a procedure for the validation, in any particular case, of the use of the law of propagation of uncertainty.

This document is a supplement to the use of the GUM and is to be used in conjunction with it.
1 Scope

This Supplement provides guidance on the evaluation of measurement uncertainty in situations where the conditions for the applicability of the law of propagation of uncertainty and related concepts are not fulfilled or it is unclear whether they are fulfilled. It can also be used in circumstances where there are difficulties in applying the law of propagation of uncertainty, because of the complexity of the model, for example. This guidance includes a general alternative procedure, consistent with the GUM, for the numerical evaluation of measurement uncertainty, suitable for implementation by computer.

In particular, this Supplement provides a procedure for determining a coverage interval for an output quantity value corresponding to a specified coverage probability. The intent is to determine this coverage interval to a prescribed degree of approximation. This degree of approximation is relative to the realism of the model and the quality of the information on which the probability density functions for the model input quantities are based.

It is usually sufficient to report the measurement uncertainty to one or perhaps two significant decimal digits. Further digits would normally be spurious, because the information provided for the uncertainty evaluation is typically inaccurate, involving estimates and judgements. The calculation should be carried out in a way to give a reasonable assurance that in terms of this information these digits are correct. Guidance is given on this aspect.

NOTE — This attitude compares with that in mathematical physics where a model (e.g., a partial differential equation) is constructed and then solved numerically. The construction involves idealizations and inexactly known values for geometric quantities and material constants, for instance. The solution process should involve the application of suitable numerical methods in order to make supported statements about the quality of the solution obtained to the posed problem.

This Supplement provides a general numerical procedure, consistent with the broad principles of the GUM [GUM G.1.5], for carrying out the calculations required as part of an evaluation of measurement uncertainty. The procedure applies to arbitrary models having a single output quantity where the values of the input quantities are assigned any specified probability density functions, including asymmetric probability density functions [GUM G.5.3].

The approach operates with the probability density functions for the values of the input quantities in order to determine the probability density function for the output quantity value. This is the reason for the description of the approach as the propagation of distributions. Unlike the GUM, it does not make use of the law of propagation of uncertainty. That approach operates with the best estimates (expectations) of the values of the input quantities and the associated standard uncertainties (and where appropriate the corresponding degrees of freedom) in order to determine an estimate of the output quantity value, the associated standard uncertainty, and a coverage interval for the output quantity value. Whereas there are some limitations to that approach, (a sound implementation of) the propagation of distributions will always provide a probability density function for the output quantity value that is consistent with the probability density functions for the values of the input quantities. Once the probability density function for the output quantity value is available, its expectation is taken as an estimate of the output quantity value, its standard deviation is used as the associated standard uncertainty, and a 95 % coverage interval for the output quantity value is obtained from it.

NOTE — Some distributions, such as the Cauchy distribution, which arise exceptionally, have no expectation or standard deviation. A coverage interval can always be obtained, however.

The approach here obviates the need for “effective degrees of freedom” [GUM G.6.4] in the determination of the expanded uncertainty, so avoiding the use of the Welch-Satterthwaite formula [GUM G.4.2] and hence the approximation inherent in it.

The probability density function for the output quantity value is not in general symmetric. Consequently, a coverage interval for the output quantity value is not necessarily centred on the estimate of the output quantity value. There are many coverage intervals corresponding to a specified coverage probability. This Supplement can be used to provide the shortest coverage interval.

NOTE — Sensitivity coefficients [GUM 5.1.3] are not an inherent part of the approach and hence the calculation or approximation of the partial derivatives of the model with respect to the input quantities is not required. Values akin to sensitivity coefficients can, however, be provided using a variant of the approach (Appendix B).

Typical of the uncertainty evaluation problems to which this Supplement can be applied include

— those where the contributory uncertainties may be arbitrarily large, even comparable to the uncertainty associated with the estimate of the output quantity value;

— those where the contributions to the uncertainty associated with the estimate of the output quantity value are not necessarily comparable in magni-
tude [GUM G.2.2];

— those where the probability distribution for the output quantity value is not Gaussian, since reliance is not placed on the Central Limit Theorem [GUM G.2.1];

— those where the estimate of the output quantity value and the associated standard uncertainty are comparable in magnitude, as for measurements at or near the limit of detection;

— those in which the models have arbitrary degrees of non-linearity or complexity, since the determination of the terms in a Taylor series approximation is not required [GUM 5.1.2];

— those in which asymmetric distributions for the values of the input quantities arise, e.g., when dealing with the magnitudes of complex variables in acoustical, electrical and optical metrology;

— those in which it is difficult or inconvenient to provide the partial derivatives of the model (or approximations to these partial derivatives), as needed by the law of propagation of uncertainty (possibly with higher-order terms) [GUM 8].

This Supplement can be used in cases of doubt to check whether the law of propagation of uncertainty is applicable. A validation procedure is provided for this purpose. Thus, the considerable investment in this use of the GUM is respected: the law of propagation of uncertainty procedure remains the main approach to the calculation phase of uncertainty evaluation, certainly in circumstances where it is demonstrably applicable.

Guidance is given on the manner in which the propagation of distributions can be carried out, without making unquantified approximations.

This Supplement applies to mutually independent input quantities, where the value of each such quantity is assigned an appropriate probability density function, or mutually dependent input quantities, the values of which have been assigned a joint probability density function.

Models with more than one output quantity are the subject of a further Supplement to the GUM that is in preparation.

2 Notation and definitions

For the purposes of this Supplement the definitions of the GUM [3], the International Vocabulary of Basic and General Terms in Metrology (VIM) [4] and ISO 3534, Part 1 [20] apply.

JCGM-WG1 has decided that the subscript “c” [GUM 2.3.4, 5.1.1] for the combined standard uncertainty is redundant. The standard uncertainty associated with an estimate $y$ of an output quantity value $Y$ can therefore be written simply as $u(y)$, but the use of $u_c(y)$ remains acceptable if it is helpful to emphasize the fact that it represents a combined standard uncertainty. Moreover, the qualifier “combined” in “combined standard uncertainty” is also regarded as superfluous and may be omitted. One reason for the decision is that the argument (here $y$) already indicates the estimate of the output quantity value with which the standard uncertainty is associated. Another reason is that frequently the results of one or more uncertainty evaluations become the inputs to a subsequent uncertainty evaluation. The use of the subscript “c” and the qualifier “combined” are inappropriate in this regard.

This Supplement departs from the symbols often used for probability density function and distribution function. The GUM uses the generic symbol $f$ to refer to a model and a probability density function. Little confusion arises in the GUM as a consequence of this usage. The situation in this Supplement is different. The concepts of model, probability density function and distribution function are central to following and implementing the procedure provided. Therefore, in place of the symbols $f$ and $F$ to denote a probability density function and a distribution function, the symbols $g$ and $G$, respectively, are used. The symbol $f$ is reserved for the model.

Citations of the form [GUM 4.1.4] are to the indicated (sub)clauses of the GUM.

The decimal point is used as the symbol to separate the integer part of a decimal number from its fractional part. A decimal comma is used for this purpose in continental Europe.

In this Supplement the term law of propagation of uncertainty applies to the use of a first-order Taylor series approximation to the model. The term is qualified accordingly when a higher-order approximation is used. Sometimes the term is extended to apply also to the assumption of the applicability of the Central Limit Theorem as a basis for providing coverage intervals. The context makes clear the usage in any particular case.
3 Concepts

A model of measurement having any number of input quantities and a single (scalar-valued) output quantity is considered. For this case, the main stages in the determination of an estimate of the output quantity value, the associated standard uncertainty, and a coverage interval for the output quantity value are as follows.

a) Define the output quantity, the quantity required to be measured.

b) Decide the input quantities upon which the output quantity depends.

c) Develop a model relating the output quantity to these input quantities.

d) On the basis of available knowledge assign probability density functions —Gaussian (normal), rectangular (uniform), etc.— to the values of the input quantities.

NOTES

1 Assign instead a joint probability density function to the values of those input quantities that are mutually dependent.

2 A probability density function for the values of more than one input quantity is commonly called “joint” even if the probability density functions for the values of all the input quantities are mutually independent.

e) Propagate the probability density functions for the values of the input quantities through the model to obtain the probability density function for the output quantity value.

f) Obtain from the probability density function for the output quantity value

1) its expectation, taken as the estimate of the output quantity value;

NOTE — The expectation may not be appropriate for all applications (Clause 6.1, [GUM 4.1.4]).

2) its standard deviation, taken as the standard uncertainty associated with the estimate of the output quantity value [GUM E.3.2];

3) an interval (the coverage interval) containing the unknown output quantity value with a specified probability (the coverage probability).

Stages a)–d) are regarded in this Supplement as formulation, and Stages e) and f) as calculation. The formulation stages are carried out by the metrologist, perhaps with expert support. (Advice on formulation stages a)–c) will be provided in a further Supplement to the GUM on modelling that is under development.) Guidance on the assignment of probability density functions (Stage d) above) is given in this Supplement for some common cases. The calculation stages, e) and f), for which detailed guidance is provided here, require no further metrological information, and in principle can be carried out to any required degree of approximation, relative to how well the formulation stages have been undertaken.

A measurement model [GUM 4.1] is expressed by a functional relationship

\[ Y = f(X), \]  

where \( Y \) is a single (scalar) output quantity (the output quantity) and \( X \) represents the \( N \) input quantities \((X_1, \ldots, X_N)^T\).

NOTES

1 It is not necessary that \( Y \) is given explicitly in terms of \( X \), i.e., \( f \) constitutes a formula. It is only necessary that a prescription is available for determining \( Y \) given \( X \) [GUM 4.1.2].

2 In this Supplement, \( T \) in the superscript position denotes “transpose”, and thus \( X \) represents \( X_1, \ldots, X_N \) arranged as a column (vector) of values.

The GUM provides general guidance on many aspects of the above stages. It also contains a specific procedure, the law of propagation of uncertainty [GUM 5.1, 5.2], for the calculation phase of uncertainty evaluation.

The law of propagation of uncertainty has been adopted by many organizations, is widely used and has been implemented in standards and guides on measurement uncertainty and also in computer packages. In order to apply this law, the values of the model input quantities are summarized by the expectations and standard deviations of the probability density functions for these values. This information is “propagated” through a first-order Taylor series approximation to the model to provide an estimate of the output quantity value and the associated standard uncertainty. That estimate of the output quantity value is given by evaluating the model at the best estimates of the values of the input quantities. A coverage interval for the output quantity value is provided based on taking the probability density function for the output quantity value as Gaussian.

The intent of the GUM is to derive the expectation and standard deviation of the probability density function for the output quantity value, having first determined the expectations and standard deviations of the probability density functions for the values of the input quan-
NOTES

1 The best estimates of the values of the input quantities are taken as the expectations of the corresponding probability density functions [GUM 4.1.6].

2 The summaries of values of the input quantities also include, where appropriate, the degrees of freedom of the standard uncertainties associated with the estimates of the values of the input quantities [GUM 4.2.6].

3 The summaries of the values of the input quantities also include, where appropriate, covariances associated with the estimates of the values of input quantities [GUM 5.2.5].

4 The GUM [Note to GUM Subclause 5.1.2] states that if the non-linearity of the model is significant, higher-order terms in the Taylor series expansion must be included in the expressions for the standard uncertainty associated with the estimate of the output quantity value.

5 If the analytic determination of the higher derivatives, required when the non-linearity of the model is significant, is difficult or error-prone, suitable software systems for automatic differentiation can be used. Alternatively, these derivatives can be calculated numerically using finite differences [GUM 5.1.3]. Care should be taken, however, because of the effects of subtractive cancellation when forming differences in values of the model for close values of the input quantities.

6 The most important terms of next highest order to be added to those of the formula in GUM Subclause 5.1.2 for the standard uncertainty are given in the Note to this subclause. Although not stated in the GUM, this formula applies when the values of $X_i$ are Gaussian. In general, it would not apply for other probability density functions.

7 The statement in the GUM [Note to GUM Subclause 5.1.2] concerning significant model non-linearity relates to input quantities that are mutually independent. No guidance is given in the GUM if they are mutually dependent, but it is taken that the same statement would apply.

8 A probability density function related to a $t$-distribution is used instead of a Gaussian probability density function if the effective degrees of freedom associated with the estimate of the standard deviation of the probability density function for the output quantity value is finite [GUM C].

The calculation stages (Stages e) and f) above) of the GUM that use the law of propagation of uncertainty and the abovementioned concepts can be summarized as the following computational steps. Also see Figure 1.

a) Obtain from the probability density functions for the values of the input quantities $X_1, \ldots, X_N$, respectively, the expectation $x = (x_1, \ldots, x_N)^T$ and the standard deviations (standard uncertainties) $u(x) = (u(x_1), \ldots, u(x_N))^T$. Use the joint probability density function for the value of $X$ instead if the $X_i$ are mutually dependent.

b) Take the covariances (mutual uncertainties) [GUM C] $u(x_i, x_j)$ as $\text{Cov}(X_i, X_j)$, the covariances of mutually dependent pairs $(X_i, X_j)$ of input quantities.

c) Form the partial derivatives of first order of $f$ with respect to the input quantities.

d) Calculate the estimate $y$ of the output quantity value by evaluating the model at $x$.

e) Calculate the model sensitivity coefficients [GUM 5.1] as the above partial derivatives evaluated at $x$.

f) Determine the standard uncertainty $u(y)$ by combining $u(x)$, the $u(x_i, x_j)$ and the model sensitivity coefficients [GUM Formulae (10) and (13)].

g) Calculate $\nu$, the effective degrees of freedom of $y$, using the Welch-Satterthwaite formula [GUM Formula (G.2b)].

h) Compute the expanded uncertainty $U_p$, and hence a coverage interval for the output quantity value (having a stipulated coverage probability $p$), by forming the appropriate multiple of $u(y)$ through taking the probability distribution of $(y - Y)/u(y)$ as a standard Gaussian distribution ($\nu = \infty$) or $t$-distribution ($\nu < \infty$).

![Figure 1](image-url) — Illustration of the law of propagation of uncertainty. The model has mutually independent input quantities $X = (X_1, X_2, X_3)^T$, whose values are estimated by $x_i$ with associated standard uncertainties $u(x_i)$, for $i = 1, 2, 3$. The value of the output quantity $Y$ is estimated by $y$, with associated standard uncertainty $u(y)$.

The computational steps above require the following conditions to hold:

a) the non-linearity of $f$ to be insignificant [Note to GUM 5.1.2];
b) the Central Limit Theorem [GUM G.2.1, G.6.6] to apply, implying the representativeness of the probability density function for the output quantity value by a Gaussian distribution or in terms of a t-distribution;

c) the adequacy of the Welch-Satterthwaite formula for calculating the effective degrees of freedom [GUM G.4.2].

NOTE — The last two conditions are required for computational steps g) and h) above.

When these three conditions hold, the results from the sound application of the law of propagation of uncertainty are valid. These conditions apply in many circumstances. The approach is not always applicable, however. This Supplement provides a more general approach that does not require these conditions to hold.

4 Assignment of probability density functions to the values of the input quantities

In the first phase—formulation—of uncertainty evaluation, the probability density functions for the values of the input quantities of the model are assigned [GUM 2.3.2, 3.3.5] based on an analysis of series of observations or based on scientific judgement [GUM 2.3.3, 3.3.5] using all the relevant information [38], such as historical data, calibrations and expert judgement.

The probability density function for the possible values $\xi_i$ of the $i$th input quantity $X_i$ is denoted by $g_i(\xi_i)$ and that for the possible values of the output quantity value $Y$ by $g(\eta)$. The distribution function for $X_i$ is denoted by $G_i(\xi_i)$ and that for $Y$ by $G(\eta)$. The probability density functions and the distribution functions are related by $g_i(\xi_i) = G_i'(\xi_i)$ and $g(\eta) = G'(\eta)$.

When the input quantities are mutually dependent, in place of the $N$ individual probability density functions $g_i(\xi_i)$, $i = 1, \ldots, N$, there is a joint probability density function $g(\xi)$. See Notes 1 and 2 at the end of Section 5. Intermediate to these extremes, groups of the input quantities may have values with joint probability density functions.

Clauses 4.2 and 4.3 of the GUM contain much relevant information on the assignment of probability density functions.

NOTES
1 The Principle of Maximum Information Entropy can be applied to assist in the assignment [7, 39, 40].

2 It may be possible to remove some mutual dependencies by re-expressing some or all of the input quantities in terms of more fundamental mutually independent input quantities on which the original input quantities depend [GUM F1.2.4, GUM H.1]. Such changes can simplify both the application of the law of propagation of uncertainty and the propagation of distributions. Details and examples are available [13].

4.1 Probability density function assignment for some common circumstances

Assignments of probability density functions to the input quantities are given in Table 1 for some common circumstances.

<table>
<thead>
<tr>
<th>All available information concerning quantity $X$</th>
<th>Probability density function (PDF) assigned to the value of $X$</th>
</tr>
</thead>
<tbody>
<tr>
<td>The estimate $x$ and the associated standard uncertainty $u(x)$</td>
<td>The Gaussian PDF $N(x, u^2(x))$</td>
</tr>
<tr>
<td>The estimate $x$ ($&gt;0$), and $X$ is known to be nonnegative</td>
<td>The exponential PDF with expectation $x$, viz., $\exp(-\xi/x)/x$, for $\xi \geq 0$, and zero otherwise.</td>
</tr>
<tr>
<td>Independent observations of a quantity value taken to follow a normal law with unknown expectation equal to the value of $X$. From a sample of size $n$, an arithmetic mean $\bar{x}$ and a standard deviation $s$ have been calculated</td>
<td>Product of $\sqrt{n}/s$ and the $t$-distribution with argument $(\xi - \bar{x})/(s/\sqrt{n})$ and $n-1$ degrees of freedom and where $\bar{x}$ and $s$ are known constants</td>
</tr>
<tr>
<td>The estimate $x$ of the value of a multivariate quantity $X$ and the corresponding uncertainty matrix (covariance matrix) $V$</td>
<td>The multivariate Gaussian PDF $N(x, V)$ is assigned to the value of $X$ (Section 5, Note 2)</td>
</tr>
<tr>
<td>The endpoints $a_-$ and $a_+$ of an interval containing the value of $X$</td>
<td>The rectangular PDF with endpoints $a_-$ and $a_+$</td>
</tr>
<tr>
<td>The lower and upper limits $a_-$ and $a_+$ of an interval within which the value of $X$ is known to cycle sinusoidally</td>
<td>The scaled and shifted arcsine PDF with endpoints $a_-$ and $a_+$, viz., $(2/\pi){(a_+ - a_-)/2 - (2\xi - a_+ - a_-)/2}^{1/2}$, for $a_- &lt; \xi &lt; a_+$, and zero otherwise [14, 17, Section 3.5]</td>
</tr>
</tbody>
</table>

Table 1 — The assignment of a probability density function to the value of an input quantity $X$ based on available information for some common circumstances.
4.2 Probability distributions from previous uncertainty calculations

A previous uncertainty calculation may have provided a probability distribution for the value of an output quantity that is to become an input quantity for a further uncertainty calculation. This probability distribution may be available analytically in a recognized form, e.g., as a Gaussian probability density function, with values for its expectation and standard deviation. It may be available as an approximation to the distribution function for a quantity value obtained from a previous application of Monte Carlo simulation, for example. A means for describing such a distribution function for a quantity value is given in Clause 6.5.

5 The propagation of distributions

Several approaches can be used for the second phase — calculation — of uncertainty evaluation:

a) analytical methods;

b) uncertainty propagation based on replacing the model by a first-order Taylor series approximation [GUM 5.1.2] — the law of propagation of uncertainty;

c) as b), except that contributions derived from higher-order terms in the Taylor series approximation are included [Note to GUM 5.1.2];

d) numerical methods [GUM G.1.5] that implement the propagation of distributions, specifically Monte Carlo simulation (Section 6).

NOTE — Analytical methods are ideal in that they do not introduce any approximation. They are applicable in simple cases only, however. A treatment and examples are available [7, 12]. These methods are not considered further in this Supplement, apart from in the examples section (Section 8.1.1) for comparison purposes.

Techniques other than the law of propagation of uncertainty are permitted by the GUM [GUM G.1.5]. The approach advocated in this Supplement, based on the propagation of distributions, is general. For linear or linearized models and input quantities with values for which the probability density functions are Gaussian, the approach yields results consistent with the law of propagation of uncertainty. But in cases where the law of propagation of uncertainty cannot be applied the advocated approach still gives correct uncertainty statements.

In terms of the calculations required, there are three classes of uncertainty evaluation problem:

a) those for which a general approach is needed;

b) those for which uncertainty propagation based on a first-order Taylor series approximation is applicable;

c) those for which it is unclear which approach should be followed.

For Class a), this Supplement provides a generic, broadly applicable approach based on the propagation of distributions. With respect to Class b), this Supplement does not provide new material. For Class c), this Supplement provides a procedure for validating in any particular circumstance the use of the law of propagation of uncertainty (possibly based on a higher-order Taylor series approximation).

The propagation of the probability density functions $g_i(\xi_i), i = 1, \ldots, N$, for the values of the input quantities through the model to provide the probability density function $g(\eta)$ for the output quantity value is illustrated in Figure 2 for the case $N = 3$. This figure is the counterpart of Figure 1 for the law of propagation of uncertainty. Like the GUM, this Supplement is concerned with models having a single output quantity.

![Figure 2 — Illustration of the propagation of distributions. The model input quantities are $X = (X_1, X_2, X_3)^T$. The probability density functions $g_i(\xi_i)$, for $X_i, i = 1, 2, 3$, are Gaussian, triangular and Gaussian, respectively. The probability density function $g(\eta)$ for the value of the output quantity $Y$ is indicated as being asymmetric, as can arise for nonlinear models. (An asymmetric $g(\eta)$ can also arise when the probability density functions for the values of the input quantities are asymmetric.)](image)

NOTES

1 The only joint probability density functions considered in this Supplement are multivariate Gaussian.

2 A multivariate Gaussian probability density function with expectation $\mathbf{x} = (x_1, \ldots, x_N)^T$ and uncertainty matrix $V$ is given by

$$g(\xi) = \frac{1}{((2\pi)^N \det V)^{1/2}} \exp \left\{ -\frac{1}{2} (\xi - \mathbf{x})^T V^{-1} (\xi - \mathbf{x}) \right\}.$$
This probability density function reduces to the product of \( N \) univariate Gaussian probability density functions when there are no covariance effects, for the following reason. In that case

\[
V = \text{diag}(u^2(x_1), \ldots, u^2(x_N)),
\]

whence

\[
g(\xi) = \frac{1}{(2\pi)^{N/2}u(x_1) \cdots u(x_N)} \exp \left\{ -\frac{1}{2} \sum_{i=1}^{N} \frac{(\xi_i - x_i)^2}{u^2(x_i)} \right\}
\]

\[
= \prod_{i=1}^{N} g_i(\xi_i),
\]

with

\[
g_i(\xi_i) = \frac{1}{\sqrt{2\pi}u(x_i)} \exp \left\{ -\frac{(\xi_i - x_i)^2}{2u^2(x_i)} \right\}.
\]

### 6 Calculation using Monte Carlo simulation

#### 6.1 Rationale and overview

Monte Carlo simulation provides a general approach to numerically approximating the distribution function \( G(\eta) \) for the value of the output quantity \( Y = f(X) \). The following GUM Subclause is relevant to the concept embodied in Monte Carlo simulation:

An estimate of the measurand \( Y \), denoted by \( y \), is obtained from equation (1) [identical to expression (1) of this [Supplement]] using input estimates \( x_1, x_2, \ldots, x_N \) for the values of the \( N \) quantities \( X_1, X_2, \ldots, X_N \). Thus the output estimate \( y \), which is the result of the measurement, is given by

\[
y = f(x_1, x_2, \ldots, x_N) \quad \ldots (2)
\]

**NOTE** – In some cases the estimate \( y \) may be obtained from

\[
y = Y = \frac{1}{n} \sum_{k=1}^{n} Y_k = \frac{1}{n} \sum_{k=1}^{n} f(X_{1,k}, X_{2,k}, \ldots, X_{N,k})
\]

That is, \( y \) is taken as the arithmetic mean or average (see 4.2.1) of \( n \) independent determinations \( Y_k \) of \( Y \), each determination having the same uncertainty and each being based on a complete set of observed values of the \( N \) input quantities \( X_k \) obtained at the same time. This way of averaging, rather than \( y = f(X_1, X_2, \ldots, X_N) \), where \( X_i = (\sum_{k=1}^{n} X_{i,k})/n \) is the arithmetic mean of the individual observations \( X_{i,k} \), may be preferable when \( f \) is a nonlinear function of the input quantities \( X_1, X_2, \ldots, X_N \), but the two approaches are identical if \( f \) is a linear function of the \( X_i \) (see H.2 and H.4).

Although the GUM formula (2) need not provide the most meaningful estimate of the output quantity value, as stated in the note to GUM Subclause 4.1.4, repeated above, it plays a relevant role within Monte Carlo simulation as an implementation of the propagation of distributions.

Monte Carlo simulation for uncertainty calculations [7, 9] is based on the premise that any value drawn at random from the distribution of possible values of an input quantity is as legitimate as any other such value. Thus, by drawing for each input quantity a value according to its assigned probability density function, the resulting set of values is a legitimate set of values of these quantities. The value of the model corresponding to this set of values constitutes a possible value of the output quantity \( Y \). Figure 3 is similar to Figure 2 except that it shows a value sampled from each of the three probability density functions for the input quantities and the resulting value of the output quantity.

![Figure 3 — As Figure 2 except that what is shown is a value sampled from each of the three probability density functions for the values of the input quantities, and the resulting output quantity value.](image)

Consequently, a large set of model values so obtained can be used to provide an approximation to the distribution of possible values for the output quantity. Monte Carlo simulation can be regarded as a generalization of GUM 4.1.4 (above) to obtain the distribution for \( Y \), rather than the expectation of \( Y \). In particular, the above drawing of a value from the probability density function for each input quantity corresponds to “a complete set of observed values of the \( N \) input quantities \( X_i \) obtained at the same time” in GUM 4.1.4.

Monte Carlo simulation operates as follows:

1. Generate a sample of size \( N \) by independently sampling at random from the probability density function for each \( X_i, i = 1, \ldots, N \) (or in the case of mutually dependent input quantities, from the joint probability density function for \( X \)). Repeat this procedure a large number, \( M \), say, of times to yield \( M \) independent samples of size \( N \) of the set of input quantities. For each such independent sample of size \( N \), calculate the resulting model value of \( Y \), yielding \( M \)
values of $Y$ in all.

NOTES

1 Appendix C provides information on sampling from probability distributions.

2 Clause 6.4 gives more explicit information concerning the sample taken.

3 According to the Central Limit Theorem [30, p169], the arithmetic mean of the $M$ values of the output quantity obtained in this manner converges as $1/M^{1/2}$ to the expectation of the probability density function for the value of $Y = f(X)$.

— Use these $M$ values of $Y$ to provide $\hat{G}(\eta)$, an approximation to the distribution function $G(\eta)$ for the value of $Y$.

— Produce any required statistical quantity from $\hat{G}(\eta)$. Particularly relevant quantities are (a) the expectation of $\hat{G}(\eta)$ as the estimate $\hat{y}$ of the output quantity value, (b) the standard deviation of $\hat{G}(\eta)$ as the associated standard uncertainty $u(\hat{y})$, and (c) two quantiles of $\hat{G}(\eta)$ as the endpoints of a coverage interval $I_p(Y)$ for a stipulated coverage probability $p$ [7]. For further details see Clause 6.7.

The effectiveness of Monte Carlo simulation to determine a coverage interval for the output quantity value depends on the use of an adequately large value of $M$. Guidance on obtaining such a value and generally on implementing Monte Carlo simulation is available [7, 8]. Also see Clauses 6.2 and 6.10.

The inputs to the Monte Carlo simulation procedure for the calculation stage are

— the model $Y = f(X)$ (provided at the formulation stage of uncertainty evaluation);

— the joint probability density function for the values of $X$ (provided at the formulation stage also see Section 4);

NOTE — This joint probability density function reduces to the collection of the individual probability density functions for $X_1, \ldots, X_N$ in the case of $N$ mutually independent input quantities.

— the required coverage probability $p$ (e.g., 0.95, or 95 %);

— the number $M$ of Monte Carlo trials.

The primary output from the Monte Carlo simulation procedure is a numerical approximation $\hat{G}(\eta)$ to the distribution function $G(\eta)$ for the output quantity value, from which the required quantities can be determined.

Monte Carlo simulation as an implementation of the propagation of distributions is shown diagrammatically in Figure 4 and can conveniently be stated as a step-by-step procedure:

a) Select the number $M$ of Monte Carlo trials to be made. See Clause 6.2.

b) Generate $M$ samples of the (set of $N$) input quantities. See Clause 6.3.

c) For each sample, evaluate the model to give the corresponding output quantity value. See Clause 6.4.

d) Sort these values of the output quantity into non-decreasing order, using the sorted values to approximate the distribution function for the output quantity value. See Clause 6.5.

e) Form the estimate of the output quantity value and the associated standard uncertainty from this distribution function (or directly from the set of values of the output quantity). See Clause 6.6.

f) Form the shortest 95 % coverage interval for the output quantity value from this distribution function. See Clause 6.7.
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Coverage interval \([y_{\text{low}}, y_{\text{high}}]\) for the output quantity value

Clause 6.7

Estimate \(y\) of the output quantity value and associated standard uncertainty \(u(y)\)

Clause 6.6

Approximate distribution function \(\hat{G}(\eta)\)

Clause 6.5

M samples \(x_1, \ldots, x_M\) of \(X\) from \(g(\xi)\)

Clause 6.3

Number \(M\) of Monte Carlo trials

Clause 6.2

M samples \(x_1, \ldots, x_M\) of \(X\) from \(g(\xi)\)

Clause 6.3

M model values
\(y = (y_1, \ldots, y_M) = (f(x_1), \ldots, f(x_M))\)

Clause 6.4

Approximate distribution function \(\hat{G}(\eta)\)

Clause 6.5

MCS INPUTS

Model \(Y = f(X)\)

Concepts

Probability density functions \(g(\xi)\)

Section 4

Number \(M\) of Monte Carlo trials

Coverage probability \(p\)

MCS INPUTS

MCS samples \(x_1, \ldots, x_M\) of \(X\) from \(g(\xi)\)

MCS samples \(x_1, \ldots, x_M\) of \(X\) from \(g(\xi)\)

MCS samples \(x_1, \ldots, x_M\) of \(X\) from \(g(\xi)\)

MCS samples \(x_1, \ldots, x_M\) of \(X\) from \(g(\xi)\)

MCS samples \(x_1, \ldots, x_M\) of \(X\) from \(g(\xi)\)

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MCS samples \(x_1, \ldots, x_M\) of \(X\) from \(g(\xi)\)

MCS samples \(x_1, \ldots, x_M\) of \(X\) from \(g(\xi)\)

Figure 4 — The calculation phase of uncertainty evaluation using Monte Carlo simulation (MCS) to implement the propagation of distributions.
6.2 The number of Monte Carlo trials

A value of $M$, the number of Monte Carlo trials to be made, needs to be selected. It can be chosen a priori, in which case there will be no direct control over the degree of approximation delivered by the Monte Carlo procedure. The reason is that the number needed to provide a prescribed degree of approximation will depend on the “shape” of the probability density function for the output quantity value and on the coverage probability required. Also, the calculations are stochastic in nature, being based on random sampling. However, a value of $M = 10^6$ can often be expected to deliver a 95% coverage interval for the output quantity value, such that this length has a degree of approximation of one or two significant decimal digits.

Because there is no guarantee that this or any specific number will suffice, it is recommended to use a process that selects $M$ adaptively, i.e., as the trials progress. Some guidance in this regard is available [2, 7]. Also see Clause 6.10. A property of such a process is that it takes a number of trials that is economically consistent with the requirement to achieve the required degree of approximation [7].

NOTE — If the model is complicated, e.g., involving the solution of a finite-element model or a non-linear least-squares problem, because of the consequently prohibitive computing time, it may not be possible to use a sufficiently large value of $M$ to obtain adequate distributional knowledge of the output quantity value. In such a case one approach could be as follows. A relatively small value of $M$, 10 or 20, perhaps, would be used. The arithmetic mean and standard deviation of the resulting $M$ values of $Y$ would be taken as $\bar{y}$ and $\sigma(y)$, respectively, and a coverage interval for the output quantity value obtained by regarding $Y$ to be distributed as $y + Tu(y)$, where $T$ denotes the $t$-distribution with $M - 1$ degrees of freedom.

6.3 Sampling from probability distributions

In an implementation of the Monte Carlo procedure, $M$ samples $x_i$, $i = 1, \ldots, M$ (Clause 6.2), are obtained from the probability density functions for the values of the input quantities $X$. Samples would be obtained from a joint (multivariate) Gaussian probability density function when appropriate. Recommendations [8] concerning the manner in which this sampling can be carried out are given in Appendix C for the commonest distributions, viz., the rectangular, Gaussian, $t$ and multivariate Gaussian. It is possible to sample from any other distribution [7]. Some such distributions would be those based on Monte Carlo results from a previous uncertainty calculation (Clauses 4.2 and 6.5).

NOTE — For the results of Monte Carlo simulation to be statistically valid it is necessary that the pseudorandom number generators used to sample from the distributions required have appropriate properties. Tests of randomness of the numbers produced by a generator are indicated in Appendix C.

6.4 Evaluation of the model

The model is evaluated for each of the $M$ samples from each of the probability density functions for the values of the $N$ input quantities. Specifically, denote the $M$ samples by $x_1, \ldots, x_M$, where the $r$th sample $x_r$ contains values $x_{1,r}, \ldots, x_{N,r}$, with $x_{i,r}$ a “draw” from the probability density function for $X_i$. Then, the model values are

$$y_r = f(x_r), \ r = 1, \ldots, M.$$  

NOTE — In Monte Carlo simulation the model is evaluated for each sample of the input quantities and hence for values that may be distanced by “several standard deviations” from the estimates of the values of the input quantities. For this reason some issues may arise regarding the numerical procedure used to evaluate the model, e.g., ensuring its convergence (where iterative schemes are used) and numerical stability. When applying the law of propagation of uncertainty, the model is evaluated only at the estimates of the values of the input quantities or, if finite-difference approximations are used [GUM 5.1.3, Note 2], also at points perturbed by ± one standard deviation from the estimate of the value of each input quantity in turn. The user should ensure that, where appropriate, the numerical methods used to evaluate $f$ are valid for a sufficiently large region centred on these estimates.

6.5 Distribution function for the output quantity value

An approximation $\hat{G}(\eta)$ to the distribution function $G(\eta)$ for the output quantity value $Y$ can be obtained as follows. Sort the values $y_r, \ r = 1, \ldots, M$, of the output quantity provided by Monte Carlo simulation into non-decreasing order. Denote the sorted values by $y_r(r), \ r = 1, \ldots, M$. Assign uniformly spaced cumulative probabilities $p_r = (r - 1/2)/M, \ r = 1, \ldots, M$, to the ordered values [7].

NOTES

1 The term “non-decreasing” rather than “increasing” is used because of possible equalities among the values of $y_r$.

2 A sorting algorithm taking a number of operations proportional to $M \log M$ should be used [36]. A naive algorithm would take a time proportional to $M^2$, making the computation time unnecessarily long. See Clause 6.9.

3 The values $p_r, \ r = 1, \ldots, M$, are the midpoints of $M$ contiguous probability intervals of width $1/M$ between zero and one.
Form $\hat{G}(\eta)$ as the piecewise-linear function joining the $M$ points $(y(r), p_r)$, $r = 1, \ldots, M$:

$$\hat{G}(\eta) = \frac{r - 1/2}{M} + \frac{\eta - y(r)}{M(y(r+1) - y(r))},$$

$$y(r) \leq \eta \leq y(r+1), \quad r = 1, \ldots, M - 1.$$  \hspace{1cm} (2)

Figure 5 illustrates $\hat{G}(\eta)$ from a Monte Carlo simulation based on $M = 50$ trials.

Figure 5 — The piecewise-linear function, forming an approximation $\hat{G}(\eta)$ to the distribution function $G(\eta)$, derived from 50 sampled values from a Gaussian probability density function $g(\eta)$ with expectation 10 and standard deviation 1.

NOTES

1 $\hat{G}(\eta)$ is defined only for values of $\eta$ corresponding to values of probability $p$ in the interval $1/(2M) \leq p \leq 1 - 1/(2M)$. Indeed, it should not be used near the endpoints of this interval, e.g., for very large coverage probabilities in the case of a symmetric or approximately symmetric distribution, because it is less reliable there.

2 The values of $y(r)$ (or $y_r$), when assembled into a histogram (with suitable cell widths) form a frequency distribution that, when normalized to have unit area, provides an approximation $\hat{g}(\eta)$ to the probability density function $g(\eta)$ for $Y$. Calculations are not generally carried out in terms of this histogram, the resolution of which depends on the choice of cell size, but in terms of the approximation $\hat{G}(\eta)$ to the distribution function $G(\eta)$. The histogram can, however, be useful as an aid to understanding the nature of the probability density function, e.g., the extent of its asymmetry.

3 The very small value of $M$ used to provide $\hat{G}(\eta)$ in Figure 5 is for purposes of illustration only.

6.6 The estimate of the output quantity value and the associated standard uncertainty

The expectation $\hat{y}$ of the function $\hat{G}(\eta)$ (Expression (2)) approximates the expectation of the probability density function $g(\eta)$ for the value of $Y$ and is taken as the estimate $y$ of the output quantity value. The standard deviation $u(\hat{y})$ of $\hat{G}(\eta)$ approximates the standard deviation of $g(\eta)$ and is taken as the standard uncertainty $u(y)$ associated with $y$. $\hat{y}$ can be taken as the arithmetic mean

$$\hat{y} = \frac{1}{M} \sum_{r=1}^{M} y_r,$$  \hspace{1cm} (3)

formed from the $M$ values $y_1, \ldots, y_M$, and the standard deviation $u(\hat{y})$ determined from

$$u^2(\hat{y}) = \frac{1}{M-1} \sum_{r=1}^{M} (y_r - \hat{y})^2.$$  \hspace{1cm} (4)

NOTES

1 Formulae (3) and (4) do not in general provide values that are identical to the expectation and standard deviation, respectively, of $\hat{G}(\eta)$. The latter values are given by

$$\hat{y} = \frac{1}{M} \sum_{r=1}^{M} y_r$$  \hspace{1cm} (5)

and

$$u^2(\hat{y}) = \frac{1}{M} \left( \sum_{r=1}^{M} y_r^2 - y^2 \right) - \frac{1}{M-1} \sum_{r=1}^{M-1} (y_{r+1} - y_r)^2.$$  \hspace{1cm} (6)

where the double prime on the summation in Expression (5) and on the first summation in Expression (6) indicates that the first and the last terms are to be taken with weight one half. For a sufficiently large value of $M$ (104, say, or greater), the values obtained using Formulae (3) and (4) would generally be indistinguishable for practical purposes from those given by (5) and (6).

2 If the standard deviation is formed directly from the $M$ values $y_1, \ldots, y_M$, it is important to use Formula (4) rather than the mathematically equivalent formula

$$u^2(\hat{y}) = \frac{1}{M-1} \left( \frac{1}{M} \sum_{r=1}^{M} y_r^2 - y^2 \right).$$

For cases in which $u(y)$ is much smaller than $|y|$ (in which case the $y_r$ have a number of leading digits in common) the latter formula suffers numerically from subtractive cancellation (involving a mean square less a squared mean). This effect can be so severe that the resulting value may have too few correct significant decimal digits for the uncertainty evaluation to be valid [6].

3 In some special circumstances, such as when one of the input quantities has been assigned a probability density function based on the $t$-distribution with fewer than three degrees of freedom, and that input quantity has a dominant effect, the expectation and the standard deviation of $g(\eta)$ may not exist. Formulae (5) and (6) (or Formulae (3) and (4)) will not then provide meaningful results. A coverage interval for the output quantity value (Clause 6.7) can, however, be formed. See also the second Note in Section 1.
4. The value of $y$ so obtained yields the smallest mean squared deviation over all possible estimates of the output quantity value. However, the value will not in general agree with the model evaluated at the estimates of the values of the input quantities [GUM 4.1.4]. When the model is linear in the input quantities, agreement (in a practical sense) will be achieved for a large value of $M$. Whether this general lack of agreement is important depends on the application. The value of $y$, even in the limit as $M \to \infty$, is not in general equal to the model evaluated at the expectations of the probability density functions for the input quantities, unless the model is linear [GUM 4.1.4].

6.7 Coverage interval for the output quantity value

Let $\alpha$ denote any value between zero and $1 - p$, where $p$ is the required coverage probability. The endpoints of a $100p\%$ coverage interval $I_p(Y)$ for the output quantity value are $G^{-1}(\alpha) = G^{-1}(\alpha; \mu) = G^{-1}(\alpha; \mu)$ and $G^{-1}(p + \alpha)$, i.e., the $\alpha$- and $(p + \alpha)$-quantiles of $G(\eta)$. The $\beta$-quantile is the value of $\eta$ such that $G(\eta) = \beta$. The choice $\alpha = 0.025$ gives the coverage interval defined by the 0.025- and 0.975-quantiles, providing an $I_{0.95}(Y)$ that is probabilistically symmetric. The probability is 2.5% that the value of $Y$ is smaller than the left-hand endpoint of the interval and 2.5% that it is larger than the right-hand endpoint. If $g(\eta)$ is symmetric about its expectation, $I_p(Y)$ is symmetric about the estimate of the output quantity value, and the left-hand and right-hand endpoints of $I_p(Y)$ are equidistant from $y$.

NOTE — For a symmetric probability density function for the output quantity value $Y$, the procedure would, for a sufficiently large value of $M$, give the same coverage interval for practical purposes as taking the product of the standard uncertainty and the coverage factor that is appropriate for that probability density function. This probability density function is generally not known analytically.

A value of $\alpha$ different from 0.025 would generally be appropriate were the probability density function asymmetric. Usually the shortest $I_p(Y)$ is required, because it corresponds to the best possible location of the value of the output quantity $Y$ within a specified probability. It is given by the value of $\alpha$ satisfying $g(G^{-1}(\alpha)) = g(G^{-1}(p + \alpha)), g(\eta)$ is single-peaked, and in general by the value of $\alpha$ such that $G^{-1}(p + \alpha) - G^{-1}(\alpha)$ is a minimum. If $g(\eta)$ is symmetric, the shortest $I_p(Y)$ is given by taking $\alpha = (1 - p)/2$.

The shortest $I_p(Y)$ can generally be obtained computationally from $G(\eta)$ by determining $\alpha$ such that $G^{-1}(p + \alpha) - G^{-1}(\alpha)$ is a minimum.

Henceforth $I_p(Y)$ will denote the shortest $100p\%$ coverage interval. The law of propagation of uncertainty, as in the GUM [3], provides the shortest such interval for the Gaussian (or scaled and shifted $t$-) distribution assigned to the output quantity value. Therefore, it is appropriate in contrasting this approach with other approaches to use the shortest $100p\%$ coverage interval for the distributions they provide.

Figure 6 shows a distribution function $G(\eta)$ for an asymmetric probability density function.

![Figure 6 — A distribution function $G(\eta)$ corresponding to an asymmetric probability density function. Broken lines mark the endpoints of the probabilistically symmetric 95% coverage interval and the corresponding probability points, viz., 0.025 and 0.975. Full lines mark the endpoints of the shortest 95% coverage interval and the corresponding probability points, which are 0.006 and 0.956 in this case. The lengths of the 95% coverage intervals in the two cases are 1.76 units and 1.69 units, respectively.]

6.8 Reporting the results

The estimate $y$ of the output quantity value and the endpoints $y_{\text{low}}$ and $y_{\text{high}}$ of the coverage interval $I_p(Y) = [y_{\text{low}}, y_{\text{high}}]$ corresponding to the coverage probability $p$ for the output quantity value should be reported to a number of decimal digits such that the least significant digit is in the same position with respect to the decimal point as that for the standard uncertainty $u(y)$ [GUM 7.2.6].

NOTES

1 One significant digit or two significant digits would be adequate to represent $u(y)$ in many cases.

2 A factor influencing the choice of one or two significant digits is the leading significant digit of $u(y)$. If this digit is 1, the relative accuracy to which $u(y)$ is reported is low if one digit is used. If the leading significant digit is 9, the relative accuracy is almost an order of magnitude greater.

3 If the results are to be used within further calculations,
Consider an artificial problem with a model consisting of the sum of five terms:

$$Y = \cos X_1 + \sin X_2 + \tan^{-1} X_3 + e^{X_4} + X_5^{1/2}. \quad (7)$$

Assign a Gaussian probability density function to each of the input quantities $X_i$. Make $M = 10^6$ Monte Carlo trials. Computation times observed for a 1 GHz Pentium 3 PC using MATLAB \[27\] are summarized in Table 2. This information provides a simple basis for estimating the computation time for other models, other values of $M$ and other PCs. The times quoted apply to a particular PC, a particular implementation, and the version of MATLAB used, and are therefore only indicative. They do not necessarily scale well to other configurations.

<table>
<thead>
<tr>
<th>Operation</th>
<th>Time/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Generate $5M$ random Gaussian numbers</td>
<td>1</td>
</tr>
<tr>
<td>Form $M$ model values</td>
<td>1</td>
</tr>
<tr>
<td>Sort the $M$ model values</td>
<td>3</td>
</tr>
<tr>
<td>Total</td>
<td>5</td>
</tr>
</tbody>
</table>

Table 2 — Computation times for the main steps in Monte Carlo simulation applied to the model (7), where each $X_i$ is assigned a Gaussian probability density function and $M = 10^6$ Monte Carlo trials are taken.

### 6.10 Adaptive Monte Carlo procedure

A basic implementation of an adaptive Monte Carlo procedure can be described as follows. It is based on carrying out an increasing number of Monte Carlo trials until the various quantities of interest have stabilized in a statistical sense. A quantity is deemed to have stabilized if twice the standard deviation associated with the estimate of its value is less than the degree of approximation required in the standard uncertainty $u(y)$.

**NOTE** — Typically, the more sensitive quantities are the endpoints of the coverage interval for the value of the output quantity $Y$. The expectation and the standard deviation as the estimate $y$ of the output quantity value and the associated standard uncertainty $u(y)$, respectively, generally “converge” considerably faster.

A practical approach consists of carrying out a sequence of Monte Carlo calculations, each containing a relatively small number, say, $M = 10^4$ trials. For each Monte Carlo calculation in the sequence, $y$, $u(y)$ and $I_{0.95}(Y)$ are formed from the results obtained, as in Clauses 6.6 and 6.7. Denote by $y^{(h)}$, $u(y^{(h)})$, $y_{low}^{(h)}$ and $y_{high}^{(h)}$ the values of $y$, $u(y)$ and the left- and right-hand endpoints of $I_{0.95}(Y)$ for the $h$th member of the sequence.

After the $h$th Monte Carlo calculation (apart from the first) in the sequence, the arithmetic mean $y$
of the values \( y^{(1)}, \ldots, y^{(4)} \) and the standard deviation \( s_y \) associated with this arithmetic mean are formed. The counterparts of these statistics for \( y \) are determined for \( u(y) \), \( y_{\text{low}} \) and \( y_{\text{high}} \). If the largest of \( 2s_y, 2s_{u(y)}, 2s_{y_{\text{low}}} \) and \( 2s_{y_{\text{high}}} \) does not exceed the degree of approximation required in \( u(y) \), the overall computation is regarded as having stabilized. The results from the total number of Monte Carlo trials taken are then used to provide the estimate of the output quantity value, the associated standard uncertainty and the coverage interval for the output quantity value.

7 Validation of the law of propagation of uncertainty using Monte Carlo simulation

The law of propagation of uncertainty can be expected to work well in many circumstances. However, it is generally difficult to quantify the effects of the approximations involved, viz., linearization [GUM 5.1.2], the Welch-Satterthwaite formula for the effective degrees of freedom [GUM G.4.2] and the assumption that the probability distribution for the output quantity value is Gaussian (i.e., that the Central Limit Theorem is applicable) [GUM G.2.1, G.6.6]. Indeed, the degree of difficulty of doing so would typically be considerably greater than that required to apply Monte Carlo simulation (assuming suitable software were available [8]). Therefore, since these circumstances cannot readily be tested, any cases of doubt should be validated. To this end, since the propagation of distributions is more general, it is recommended that both the law of propagation of uncertainty and Monte Carlo simulation be applied and the results compared. Should the comparison be favourable, the law of propagation of uncertainty could be used on this occasion and for sufficiently similar problems in the future. Otherwise, consideration could be given to using Monte Carlo simulation instead.

Specifically, it is recommended that the two steps below and the following comparison process be carried out.

a) Apply the law of propagation of uncertainty (possibly based on a higher-order Taylor series approximation) [GUM 5] to yield a 95 % coverage interval \( y \pm U_{0.95}(y) \) for the output quantity value.

b) Apply Monte Carlo simulation (Section 6) to provide values for the standard uncertainty \( u(y) \) and the endpoints \( y_{\text{low}} \) and \( y_{\text{high}} \) of a 95 % coverage interval for the output quantity value.

NOTE — The process is described here in terms of a 95 % coverage interval, but other coverage intervals can be used.

A comparison procedure is based on the following objective: determine whether the coverage intervals obtained by the law of propagation of uncertainty and Monte Carlo simulation agree to a stipulated degree of approximation. This degree of approximation is assessed in terms of the endpoints of the coverage intervals and corresponds to that given by expressing the standard uncertainty \( u(y) \) to what is regarded as a meaningful number of significant decimal digits (cf. Clause 6.10). The procedure is as follows:

a) Let \( n_{\text{dig}} \) denote the number of significant digits regarded as meaningful in the numerical value of \( u(y) \). Usually, \( n_{\text{dig}} = 1 \) or \( n_{\text{dig}} = 2 \) (Clause 6.8). Express the value of \( u(y) \) in the form \( a \times 10^r \), where \( a \) is an \( n_{\text{dig}} \)-digit integer and \( r \) an integer. The comparison accuracy is

\[
\delta = \frac{1}{2} 10^{-r}. \tag{8}
\]

EXAMPLES

1 — The estimate of the output quantity value for a nominally 100 g measurement standard of mass [GUM 7.2.2] is \( y = 100.021 \) g. The standard uncertainty \( u(y) = 0.000 \) 35 g. Thus, \( n_{\text{dig}} = 2 \) and \( u(y) \) can be expressed as \( 35 \times 10^{-3} \) g, and so \( a = 35 \) and \( r = -3 \). Take \( \delta = \frac{1}{2} \times 10^{-3} g = 0.000 \) 005 g.

2 — As Example 1 except that only one significant digit in \( u(y) \) is regarded as meaningful. Thus, \( n_{\text{dig}} = 1 \) and \( u(y) = 0.000 \) 4 g = \( 4 \times 10^{-3} \) g. giving \( a = 4 \) and \( r = -4 \). Thus, \( \delta = \frac{1}{2} \times 10^{-4} g = 0.000 \) 005 g.

3 — \( u(y) = 2 \) K. Then, \( n_{\text{dig}} = 1 \) and \( u(y) = 2 \times 10^0 \) K, giving \( a = 2 \) K and \( r = 0 \). Thus, \( \delta = \frac{1}{2} \times 10^0 \) K = 0.5 K.

b) Compare the coverage intervals obtained by the law of propagation of uncertainty and Monte Carlo simulation to determine whether the required number of correct digits in the coverage interval provided by the law of propagation of uncertainty has been obtained. Specifically, determine the quantities

\[
|y - U_{0.95}(y) - y_{\text{low}}|, \quad |y + U_{0.95}(y) - y_{\text{high}}|, \tag{9}
\]

viz., the absolute values of the differences of the respective endpoints of the two coverage intervals. Then, if both these quantities are no larger than \( \delta \), the comparison is successful and the law of propagation of uncertainty has been validated in this instance.

NOTES

1 The validation applies for the specified coverage probability only.

2 The choice of 95 % coverage interval will influence the comparison. The shortest 95 % coverage interval should generally be taken, for consistency with the shortest (probabilistically symmetric) coverage interval determined following the application of the law of propagation of uncertainty.
8 Examples

The examples given illustrate various aspects of this Supplement. They show the application of the law of propagation of uncertainty with and without contributions derived from higher-order terms in the Taylor series approximation of the model function. They also show the corresponding results provided by Monte Carlo simulation, and the use of the validation procedure of Section 7. In some instances, solutions are obtained analytically for further comparison.

The first example (simple additive model) demonstrates that the results from Monte Carlo simulation agree with those from the application of the law of propagation of uncertainty when the conditions hold for the latter to apply. The same model, but with changes to the probability density functions assigned to the values of the input quantities, is also considered to demonstrate some departures when the conditions do not hold. In the second example (mass calibration) the law of propagation of uncertainty is shown to be valid only if the contribution derived from higher-order terms in the Taylor series approximation of the model function are included. In the third example (electrical measurement), the law of propagation of uncertainty is shown to yield invalid results, even if all higher-order terms are taken into account. Instances where the input quantities are uncorrelated and correlated are treated.

NOTE — Although it is generally recommended that a final statement of the uncertainty be made to no more than one or two significant decimal digits (Clause 6.8), more than two digits are reported in this section so as to highlight differences between the results obtained from the various approaches.

8.1 Simple additive model

This example considers the simple additive model

$$ Y = X_1 + X_2 + X_3 + X_4 $$

(10)

for three different sets of probability density functions $g_i(\xi_i)$ assigned to the $X_i$. The $X_i$ and $Y$ are expressed in (common) arbitrary units. For the first set each $g_i(\xi_i)$ is a standard Gaussian probability density function (expectation zero and standard deviation unity). For the second set each $g_i(\xi_i)$ is a rectangular probability density function with zero expectation and unit standard deviation. The third set consists of three identical rectangular probability density functions and a fourth rectangular probability density function with a standard deviation ten times as large.

Further information concerning additive models such as (10), where the probability density functions are Gaussian or rectangular or a combination of both, is available [12].

8.1.1 Normally distributed input quantities

Assign a standard Gaussian probability density function to the value of each $X_i$. The best estimates of the values of the input quantities are $x_i = 0, i = 1, 2, 3, 4$, with associated standard uncertainties $u(x_i) = 1$.

The law of propagation of uncertainty [GUM 5] gives the estimate $y = 0.0$ of the output quantity and the associated standard uncertainty $u(y) = 2.0$, using a degree of approximation of two significant decimal digits in $u(y)$ (Clause 6.8). A 95 % coverage interval for the value of $Y$ [GUM 6], based on a coverage factor of 1.96, is $[-3.9, 3.9]$.

The application of the Monte Carlo procedure (Section 6) with $M = 10^5$ trials gives $y = 0.0, u(y) = 2.0$ and the coverage interval $[-3.9, 3.9]$. Repetition with $M = 10^6$ trials confirms these results to the number of decimal digits reported. The latter case was re-run (different random samplings being made from the probability density functions) to show the variability in the results obtained.

The results are summarized in the first four columns of Table 3. Figure 7 shows some of the corresponding approximations obtained to the probability density function for the output quantity value. For this example, such agreement would be expected for a sufficiently large value of $M$, because all the conditions hold for the applicability of the law of propagation of uncertainty.

![](table3.png)

Table 3 — The application to the model (10), with each $X_i$ assigned a standard Gaussian probability density function (arbitrary units), of (a) the law of propagation of uncertainty (LPU) and (b) Monte Carlo simulation (MCS). MCS1 and MCS2 denote MCS with $10^5$ and $10^6$ trials, respectively. $y$ denotes the estimate of the value of the output quantity $Y$, $u(y)$ the standard uncertainty associated with $y$, 95 % CI the 95 % coverage interval for the output quantity value, $d_{low}$ and $d_{high}$ the magnitudes of the endpoint differences (9), and $V$ whether the results were validated to two significant digits.

Table 3 also shows the results of applying the comparison procedure of Section 7. Using the terminology of that section, $n_{dig} = 2$, since two significant digits
Approximations for the model (10), with each $X_i$ assigned a standard Gaussian probability density function, to the probability density function for the output quantity value provided by (a) the law of propagation of uncertainty and (b) Monte Carlo simulation. For (b) the approximation constitutes a scaled frequency distribution (histogram) of the $M = 10^6$ values of $Y$. The endpoints of the 95% coverage interval provided by both methods are shown as vertical lines. The approximations to the probability density function are visually indistinguishable, as are those of the coverage intervals.

\[
u(y)\text{ are sought. Hence, } u(y) = 2.0 = 20 \times 10^{-1}, \text{ and so } a = 20 \text{ and } r = -1. \text{ Thus the comparison accuracy is}
\[
\delta = \frac{1}{2} \times 10^{-1} = 0.05.
\]

The magnitudes of the endpoint differences (Expressions (9)), and whether the law of propagation of uncertainty has been validated, are shown in the right-most two columns of Table 3.

Figure 8 shows the length of the 95% coverage interval (Clause 6.7), as a function of the probability value at its left-hand endpoint, for the approximation to the distribution function provided by Monte Carlo simulation. As expected for a symmetric probability density function, the interval takes its shortest length when symmetrically disposed with respect to the expectation.

In contrast, Figure 9 shows the comparable figure for the asymmetric probability density function given in Figure 16 (Clause 8.3), relating to a model of comparison loss in power meter calibration. The 95% coverage interval does not take its shortest length when symmetrically disposed with respect to the expectation in this case. Indeed, the shortest 95% coverage interval is as far-removed as possible from an equiprobabilistic coverage interval, the left and right tail probabilities being 5% and 0%, respectively, as opposed to 2.5% and 2.5%. The length of the equiprobabilistic coverage interval is 50% greater than that of the shortest coverage interval.

Assign a rectangular probability density function having an expectation of zero and a standard deviation of unity (cf. Subclause 8.1.1) to the value of each $X_i$. Again, the best estimates of the values of the input quantities...
are \( x_i = 0 \), \( i = 1, 2, 3, 4 \), with associated standard uncertainties \( u(x_i) = 1 \).

By following the analogous steps of Subclause 8.1.1, the results in Table 4 were obtained. In addition, the analytic solution for the endpoints of the coverage interval, viz., \( \pm 2\sqrt{3(2 - (3/5)^{1/4})} \approx \pm 3.88 \), was determined by a simple calculation.

<table>
<thead>
<tr>
<th>Method</th>
<th>( y )</th>
<th>( u(y) )</th>
<th>95 % CI</th>
<th>( d_{low}, d_{high} )</th>
<th>( V )</th>
</tr>
</thead>
<tbody>
<tr>
<td>LPU</td>
<td>0.00</td>
<td>2.00</td>
<td>[-3.92, 3.92]</td>
<td>0.04, 0.07</td>
<td>No</td>
</tr>
<tr>
<td>MCS1</td>
<td>0.00</td>
<td>2.00</td>
<td>[-3.88, 3.85]</td>
<td>0.03, 0.05</td>
<td>Yes</td>
</tr>
<tr>
<td>MCS2</td>
<td>0.00</td>
<td>2.00</td>
<td>[-3.89, 3.87]</td>
<td>0.07, 0.02</td>
<td>No</td>
</tr>
<tr>
<td>Analytic</td>
<td>0.00</td>
<td>2.00</td>
<td>[-3.88, 3.88]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Table 4 — As Table 3, but for rectangular probability density functions having the same expectations and standard deviations, and with the analytic solution.**

Figure 10 shows the counterpart of Figure 7 in this case. By comparison with Figure 7, some modest differences between the approximations to the probability density functions can be seen. The use of the law of propagation of uncertainty overestimates the value of the probability density function in the neighbourhood of the expectation and to a lesser extent in the tails. It underestimates its value in the flanks. The endpoints of the coverage intervals provided are again almost visually indistinguishable, but Table 4 shows there are small differences.

The coverage interval determined on the basis of the law of propagation of uncertainty is in this case slightly more conservative than that obtained analytically. As for the previous example, the comparison procedure of Section 7 was applied (Columns 5 and 6 of Table 4). As before, \( n_{dig} = 2 \), \( u(y) = 20 \times 10^{-1} \), \( a = 20 \), \( r = -1 \) and \( \delta = 0.05 \). For Monte Carlo simulation with \( M = 10^5 \), the law of propagation of uncertainty is not validated. For one of the Monte Carlo simulations with \( M = 10^6 \), this law is validated and for the other it is not. These results emphasize the difficulty of making an absolute decision automatically when a stochastic process is involved. The user should take account of such results to decide whether they are fit for purpose. For a degree of approximation of one significant digit in \( u(y) \), for which \( \delta = 0.5 \), the validation status is positive in all three cases.

8.1.3 Rectangularly distributed input quantities with different widths

Consider the same example as in the previous section, except that the fourth probability density function has a standard deviation of ten rather than unity. Table 5 contains the results obtained.

![Figure 10](Image 339x590 to 565x760)

**Figure 10 — The counterpart of Figure 7 for rectangular probability density functions having the same expectations and standard deviations.**

<table>
<thead>
<tr>
<th>Method</th>
<th>( y )</th>
<th>( u(y) )</th>
<th>95 % CI</th>
<th>( d_{low}, d_{high} )</th>
<th>( V )</th>
</tr>
</thead>
<tbody>
<tr>
<td>LPU</td>
<td>0.0</td>
<td>10.1</td>
<td>[-19.9, 19.9]</td>
<td>2.8, 3.1</td>
<td>No</td>
</tr>
<tr>
<td>MCS1</td>
<td>0.0</td>
<td>10.1</td>
<td>[-17.1, 16.8]</td>
<td>2.9, 2.9</td>
<td>No</td>
</tr>
<tr>
<td>MCS2</td>
<td>0.0</td>
<td>10.1</td>
<td>[-17.0, 17.0]</td>
<td>2.9, 2.9</td>
<td>No</td>
</tr>
<tr>
<td>LPU</td>
<td>0.0</td>
<td>10.2</td>
<td>[-19.9, 19.9]</td>
<td>2.8, 3.1</td>
<td>No</td>
</tr>
</tbody>
</table>

**Table 5 — As Table 4, except that the probability density function for the value of the fourth input quantity has a standard deviation of ten rather than unity.**

Figure 11 shows the approximations obtained to the probability density function for the output quantity value and of the endpoints of the shortest 95 % coverage interval for the output quantity value. The approximations have very different appearance. The dominance of the probability density function for the fourth input quantity is evident. To a first approximation the probability density function for the output quantity value resembles that of the fourth input quantity. There is, however, an effect in the flanks resulting from the probability density functions for the other input quantities.

The coverage interval determined on the basis of the law of propagation of uncertainty in this case is more conservative than that obtained using Monte Carlo simulation. Again, the comparison procedure of Section 7 was applied (Columns 5 and 6 of Table 5). Now, \( n_{dig} = 2 \), \( u(y) = 10 = 10 \times 10^0 \), \( a = 10 \), \( r = 0 \) and \( \delta = 1/2 \times 10^0 = 0.5 \). In all three cases the law of propagation of uncertainty is not validated. For a degree of approximation of one significant digit in \( u(y) \), for which \( \delta = 5 \), the validation status would be positive in all three cases, the 95 % coverage intervals all being \([-2 \times 10^1, 2 \times 10^1] \).

NOTES
Figure 11 — As Figure 10, except that the probability density function for the fourth input quantity has a standard deviation of ten rather than unity. The inner pair of vertical lines indicates the endpoints of the shortest 95% for the output quantity value determined by Monte Carlo simulation. The outer pair is those from the law of propagation of uncertainty and the assignment of a Gaussian probability density function, with a coverage factor of $k = 2$.

1 The conditions for the Central Limit Theorem to apply are not well met in this circumstance [GUM G.6.5], because of the dominance of the fourth probability density function. However, because these conditions are often in practice assumed to hold, especially when using proprietary software for uncertainty evaluation (cf. the Note in Subclause 8.3.2), the Gaussian probability density function assigned on the assumption of the applicability of this theorem is made in this subclause for comparison purposes.

2 The coverage interval is expressed as $[-2 \times 10^3, 2 \times 10^3]$ because the form $[-20, 20]$ would imply that its endpoints were given to two significant decimal digits rather than one.

8.2 Mass calibration

8.2.1 Formulation

Consider the calibration of a weight $W$ of mass density $\rho_W$ against a reference weight $R$ of mass density $\rho_R$ having the same nominal mass using a balance operating in air of mass density $\rho_0$ [29]. Since $\rho_W$ and $\rho_R$ are generally different it is necessary to account for buoyancy effects. Applying Archimedes’ Principle, the model takes the form

$$m_W \left( 1 - \frac{a}{\rho_W} \right) = (m_R + \delta m_R) \left( 1 - \frac{a}{\rho_R} \right), \tag{11}$$

where $\delta m_R$ is the mass of a small weight of density $\rho_R$ added to $R$ to balance it with $W$.

Since weights are generally used in air at a density close to a particular value, it is usual to work in terms of “conventional” values. The conventional mass $m_{W,c}$ of $W$ is the mass of a (hypothetical) weight of density $\rho_0 = 8 \ 000 \ \text{kg/m}^3$ that balances $W$ in air at density $\rho_0 = 1.2 \ \text{kg/m}^3$. Thus,

$$m_W \left( 1 - \frac{a}{\rho_W} \right) = m_{W,c} \left( 1 - \frac{a}{\rho_0} \right).$$

In terms of conventional values $m_{W,c}$, $m_{R,c}$ and $\delta m_{R,c}$, the model (11) becomes

$$m_{W,c} \left( 1 - \frac{a}{\rho_W} \right) \left( 1 - \frac{a}{\rho_W} \right)^{-1} = (m_{R,c} + \delta m_{R,c}) \left( 1 - \frac{a}{\rho_R} \right) \left( 1 - \frac{a}{\rho_R} \right)^{-1}, \tag{12}$$

from which, approximately,

$$m_{W,c} = (m_{R,c} + \delta m_{R,c}) \left( 1 + (a - a_0) \left( \frac{1}{\rho_W} - \frac{1}{\rho_R} \right) \right). \tag{13}$$

Table 6 lists the input quantities and the probability density functions assigned to their values for the model (13).

<table>
<thead>
<tr>
<th>$X_i$</th>
<th>PDF</th>
<th>Parameter values</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m_{R,c}$</td>
<td>Gaussian</td>
<td>100 g, 0.050 mg</td>
</tr>
<tr>
<td>$\delta m_{R,c}$</td>
<td>Gaussian</td>
<td>1.234 mg, 0.020 mg</td>
</tr>
<tr>
<td>$a$</td>
<td>Rectangular</td>
<td>1.20 kg/m$^3$, 0.10 kg/m$^3$</td>
</tr>
<tr>
<td>$\rho_W$</td>
<td>Rectangular</td>
<td>8 000 kg/m$^3$, 1 000 kg/m$^3$</td>
</tr>
<tr>
<td>$\rho_R$</td>
<td>Rectangular</td>
<td>8 000 kg/m$^3$, 50 kg/m$^3$</td>
</tr>
</tbody>
</table>

Table 6 — The mutually independent input quantities $X_i$ and the probability density functions (PDFs) assigned to their values for the mass calibration model (13). A Gaussian distribution is described by its expectation and standard deviation, and a rectangular distribution by its expectation and semi-width.

8.2.2 Calculation

Let $\delta m = m_{W,c} - m_{\text{nom}}$ be the deviation of $m_{W,c}$ from the nominal value of $m_{\text{nom}} = 100$ g. The law of propagation of uncertainty [GUM 5] and Monte Carlo simulation (Section 6), with $M = 10^5$ trials, were each used to obtain an estimate $\delta m$ of the output quantity value, the associated standard uncertainty $u(\delta m)$, and a 95% coverage interval for the output quantity value. The results obtained from these approaches are shown in rows 2 and 3 of Table 7. Figure 12 shows the approximations to the probability density function for $\delta m$ obtained from the two approaches.

The results show that, although the law of propagation of uncertainty (first order) and Monte Carlo simulation give estimates of the output quantity values in good agreement, the values for the associated standard uncertainty are noticeably different. The value (0.075 5 mg)
\[ \delta m \text{ associated with put quantity value, } u \text{ value, of the 95 \% coverage interval for the output quantity } \]

\[ \text{Table 7 — Results of the calculation phase for the mass calibration model (13) from (a) the law of propagation of uncertainty (LPU1), (b) Monte Carlo simulation (MCS) with } 10^5 \text{ trials, and (c) the law of propagation of uncertainty with second order terms (LPU2). } \delta m \text{ denotes the estimate of the output quantity value, } u(\delta m) \text{ the standard uncertainty associated with } \delta m, \text{ 95 \% CI endpoints the endpoints of the 95 \% coverage interval for the output quantity value, } d_{\text{low}} \text{ and } d_{\text{high}}, \text{ the magnitudes of the endpoint differences (9), and } V \text{ whether the results were validated to two significant digits.} \]

\[
\begin{array}{cccccc}
\text{Method} & \delta m \text{, } u(\delta m) & 95 \% \text{ CI endpoints} & d_{\text{low}}, d_{\text{high}} & V \\
LPU1 & 1.234 0, 0.053 9 & 1.128 4, 1.339 6 & 0.043 9, 0.044 6 & \text{No} \\
MCS & 1.234 0, 0.075 5 & 1.084 5, 1.384 2 & \text{Yes} \\
LPU2 & 1.234 0, 0.075 0 & 1.087 0, 1.381 0 & 0.002 5, 0.002 2 & \text{Yes} \\
\end{array}
\]

Table 8 lists the partial derivatives of first order for the model (13) with respect to the values of the input quantities together with the model sensitivity coefficients, viz., these derivatives evaluated at the estimates of the values of the input quantities. These derivatives indicate that for the purposes of the law of propagation of uncertainty the model for this example can be considered as being replaced by the simple additive model

\[ m_{W,c} = m_{R,c} + \delta m_{R,c}. \]

Monte Carlo simulation makes no such (implied) approximation to the model.

Table 7 also shows in the right-most two columns the results of applying the comparison procedure of Section 7 in the case where one significant digit in \( u(y) \) is regarded as meaningful. Using the terminology of that section, \( n_{\text{dig}} = 1 \), since a degree of approximation of one significant digit in \( u(y) \) is required. Hence, \( u(\delta m) = 0.08 = 8 \times 10^{-2} \), and so \( a = 8 \) and \( r = -2 \). Thus \( \delta = 1/2 \times 10^{-2} = 0.005 \). The magnitudes of the endpoint differences (Expressions (9)) are shown, and whether the law of propagation of uncertainty has been validated. If only first-order terms are accounted for, the application of the law of propagation of uncertainty is not validated. If second-order terms are accounted for [GUM 5.1.2], the law of propagation of uncertainty is validated.

NOTES

1. Applying the law of propagation of uncertainty to the “exact” model (12) is made difficult by the algebraic complexity of the partial derivatives. Applying Monte Carlo simulation is no more complicated, because only model values need be evaluated.

2. Results obtained from applying the law of propagation of uncertainty and Monte Carlo simulation procedures using the “exact model” (12) indicate that the approximation (13) is very good.

\[ X_i \] Partial derivative \[ \text{Sensitivity coefficient} \]

\[
\begin{array}{ccc}
\text{model} & m_{R,c} & \text{1} \\
\text{LPU1} & 1 + (a - a_0) \left( \frac{1}{r_W - \frac{1}{r_R}} \right) & 1 \\
\text{MCS} & 1 + (a - a_0) \left( \frac{1}{r_W - \frac{1}{r_R}} \right) & 1 \\
\text{LPU2} & \frac{2}{a} \frac{1}{r_W - \frac{1}{r_R}} & 0 \\
\text{MCS} & \frac{2}{a} \frac{1}{r_W - \frac{1}{r_R}} & 0 \\
\text{LPU2} & \frac{2}{a} \frac{1}{r_W - \frac{1}{r_R}} & 0 \\
\text{MCS} & \frac{2}{a} \frac{1}{r_W - \frac{1}{r_R}} & 0 \\
\end{array}
\]

\[ \text{Table 8 — Model sensitivity coefficients for the mass calibration model (13).} \]
8.3 Comparison loss in microwave power meter calibration

8.3.1 Formulation

During the calibration of a microwave power meter, the power meter and a standard power meter are connected in turn to a stable signal generator. The power absorbed by each power meter will in general be different because their complex-valued input voltage reflection coefficients are not identical. The ratio $Y$ of the power $P_M$ absorbed by the power meter being calibrated and that, $P_S$, absorbed by the standard power meter is [31]

$$ Y = \frac{P_M}{P_S} = \frac{1 - |\Gamma_M|^2}{1 - |\Gamma_S|^2} \times \frac{|1 - \Gamma_S \Gamma_G|^2}{|1 - \Gamma_M \Gamma_G|^2}, \quad (14) $$

where $\Gamma_G$ is the voltage reflection coefficient of the signal generator, $\Gamma_M$ that of the power meter being calibrated and $\Gamma_S$ that of the standard power meter. This power ratio is an instance of "comparison loss" [1, 21]. For physical reasons, $0 \leq Y \leq 1$.

Consider the case where the standard and the signal generator are reflectionless, i.e., $\Gamma_S = \Gamma_G = 0$, and measurements are made of the real and imaginary parts $X_1$ and $X_2$ of $\Gamma_M = X_1 + jX_2$, where $j^2 = -1$. Since $|\Gamma_M|^2 = X_1^2 + X_2^2$, Formula (14) becomes

$$ Y = 1 - X_1^2 - X_2^2. \quad (15) $$

The evaluation of uncertainty for this model can be treated (a) analytically (at least in one instance), (b) by applying the law of propagation of uncertainty [GUM 5], or (c) by using Monte Carlo simulation as an implementation of the propagation of distributions (Section 6).

NOTE — All three approaches presented do not constrain the probability density function for $Y$ to take positive values. However, for sufficiently small uncertainties associated with the estimates of the values of $X_1$ and $X_2$, the probability density function for $Y$ may adequately be approximated by a simpler probability density function defined over all values less than unity. A rigorous treatment, using Bayesian inference [39], that applies regardless of the magnitudes of the uncertainties, is possible, but beyond the scope of this Supplement.

Given estimates $x_1$ and $x_2$, respectively, of the values of $X_1$ and $X_2$ from measurement, the corresponding value

$$ y = 1 - x_1^2 - x_2^2 $$

of $Y$ is formed [GUM 4.1.4] as the estimate of the output quantity value. $x_1$ and $x_2$ are often correlated in practice, with an associated covariance $u(x_1, x_2)$. Equivalently [GUM 5.2.2], this covariance is $u(x_1, x_2) = r(x_1, x_2)u(x_1)u(x_2)$, where $r(x_1, x_2)$ denotes the associated correlation coefficient [GUM 5.2.2]. The measurements are such that the value of $\Gamma_M$ is assigned a bivariate Gaussian probability density function in $X_1$ and $X_2$ with expectation $(x_1, x_2)^T$ and uncertainty matrix [7, p49]

$$ \begin{bmatrix} u^2(x_1) & r(x_1, x_2)u(x_1)u(x_2) \\ r(x_1, x_2)u(x_1)u(x_2) & u^2(x_2) \end{bmatrix}. \quad (16) $$

The evaluation of $y$, the associated standard uncertainty $u(y)$, and a coverage interval for the value of $Y$ will be considered for choices of $x_1$, $x_2$, $u(x_1)$, $u(x_2)$ and $r(x_1, x_2)$.

NOTE — An alternative way of evaluating $y$ (as in Monte Carlo simulation) may be preferable [GUM 4.1.4] (cf. Clause 6.1).

8.3.2 Calculation: uncorrelated input quantities

Consider first measurements $x_1 = x_2 = 0$, with $u(x_1) = u(x_2) = 0.005$ and $r(x_1, x_2) = 0$. All quantities are of dimension one The uncertainty matrix (16) reduces to diag($u^2(x_1), u^2(x_2)$) and the corresponding distribution to the product of two univariate Gaussian distributions for the value of $X_i$, with expectation $x_i$ and standard deviation $u(x_i)$, for $i = 1, 2$. The probability density function $g(y)$ for the value of $Y$ can be obtained (a) analytically, (b) using the law of propagation of uncertainty with second-order terms, and (c) by Monte Carlo simulation. The reason that the law of propagation of uncertainty with second-order terms must be used is that the partial derivatives $\partial Y/\partial X_1$ and $\partial Y/\partial X_2$ evaluated at $X_1 = x_1$ and $X_2 = x_2$ are identically zero when $x_1 = x_2 = 0$. Thus, if the law of propagation of uncertainty with first-order terms only were applied, the resulting standard uncertainty would incorrectly be computed as zero.

The analytic derivation (a) is given in Appendix D.1. The application of the law of propagation of uncertainty (b) is given in Appendix D.2.1. For (c), $M = 10^5$ trials were made. Figure 13 shows the probability density functions provided by (a), (b) and (c).

It is seen in the figure that the use of the law of propagation of uncertainty with second-order terms to assign a Gaussian distribution for the output quantity value yields a probability density function that is very different from the analytic solution. The latter in fact takes the form of a particular $\chi^2$-distribution—the sum of squares of two Gaussian variables (Appendix D.1). The Gaussian distribution so determined is in a sense the best in this case that is possible using the law of propagation of uncertainty to assign such a distribution to the output quantity value: since the partial derivatives of order higher than two are all identically zero,
the solution obtained essentially corresponds to taking all Taylor-series terms into account, i.e., the “full non-linearity” of the problem. It can therefore be concluded that the reason for the departure from the analytical solution of the results of the use of the approach based on the law of propagation of uncertainty is that a Gaussian probability density function is assigned to the output quantity value. Evidently, no Gaussian probability density function, however it is obtained, could adequately represent the analytical solution in this case.

Figure 13 — Results for the model of comparison loss in power meter calibration in the case $x_1 = x_2 = 0$, with $u(x_1) = u(x_2) = 0.005$ and $r(x_1, x_2) = 0$. The probability density functions shown are (a) determined analytically (the exponentially increasing curve for $Y < 1$ and zero for $Y \geq 1$), (b) provided by the law of propagation of uncertainty with second-order terms to assign a Gaussian probability density function to the output quantity value (bell-shaped curve), and (c) provided by Monte Carlo simulation (scaled frequency distribution) using $10^5$ trials. The broken vertical lines denote the endpoints of the shortest 95% coverage interval $I_{0.95}(y)$ as derived from the Gaussian probability density function provided by the law of propagation of uncertainty. The solid vertical lines are those derived from the analytical solution, as described in Appendix D.1. The endpoints of $I_{0.95}(y)$ determined from Monte Carlo simulation are indistinguishable to graphical accuracy from those for the analytical solution.

It is also seen in Figure 13 that the solution provided by Monte Carlo simulation is consistent with the analytical solution, at least to visual accuracy.

The estimate $y$ of the output quantity value obtained from the expectation of the $X^2$-distribution, the law of propagation of uncertainty as above, and Monte Carlo simulation are the second, third and fourth entries of the row immediately below the heading in Table 9. Values in this table relate to $1 - Y$ rather than $Y$ in order to show better their departures from unity. Clearly the value of $1 - y = 0$ obtained by evaluating the model at the input estimates is invalid: the correct (analytic) $g(\eta)$ is identically zero for $Y > 1$; this value lies on the boundary of the nonzero part of that function. The value from Monte Carlo simulation agrees with that obtained analytically. The remaining four entries in the row are values for $u(y)$ obtained analytically, from the law of propagation of uncertainty based on linear and on linear plus higher-order terms, and from Monte Carlo simulation. The law of propagation of uncertainty based on linear terms gives the wrong, zero, value already noted. The value (500) from the law of propagation of uncertainty based on higher-order terms agrees with that obtained analytically. The value (502) provided by Monte Carlo simulation agrees closely with the analytical value (500). When the Monte Carlo simulation was repeated several times the values obtained were scattered about 500. When Monte Carlo simulation was repeated a number of times with a larger value of $M$ the values were again scattered about 500, but with a reduced dispersion. (Such dispersion effects are expected from theoretical considerations (Clause 6.1) and were seen for the other Monte Carlo simulation calculations made.)

Figure 13 also shows the coverage intervals $I_{0.95}(Y)$ for the corresponding approximations to $g(\eta)$. Clearly, $I_{0.95}(Y)$ (indicated by broken vertical lines) as provided by the law of propagation of uncertainty is unreasonable: it is symmetric about $Y = 1$ and therefore erroneously implies there is a 50% probability that the output quantity value is greater than unity.

The above calculations were then repeated, but with (a) $x_1 = 0.01$ (Figure 14) and (b) $x_1 = 0.05$ (Figure 15), in order to investigate the manner in which the solution obtained using the law of propagation of uncertainty departs from that provided by the propagation of distributions (through Monte Carlo simulation) when $x_1$ deviates (a) a little and (b) appreciably from zero. The two figures show the results obtained using the law of propagation of uncertainty with first-order terms only and with higher-order terms.

As $x_1$ becomes increasingly removed from zero, the results given by the law of propagation of uncertainty, with first-order and with higher-order terms, and those for Monte Carlo simulation become closer to each other. Because of the symmetry of the model in $X_1$ and $X_2$, exactly the same effect would occur were $x_2$ used in place of $x_1$. For $x_1 = 0.01$ the probability density function provided by Monte Carlo simulation is starting to exhibit a right-hand tail, although it is “truncated” at unity, the largest possible value of the output quantity. Further, it is closer in form to the Gaussian probability
Table 9 — Comparison loss results for a standard and a signal generator that are reflectionless obtained analytically, and using the law of propagation of uncertainty (LPU) and Monte Carlo simulation (MCS). Column 1 shows values $x_1$ of the real part $X_1$ of the voltage reflection coefficient $\Gamma_M = X_1 + jX_2$ of the power meter being calibrated, for the case where the value $x_2$ of the imaginary part $X_2$ is taken as zero. Columns 2–4 are output estimates of the value of $1 - Y$. Column 2 shows (only for $x_1 = 0$) the expectation of $1 - Y$ obtained from the probability density function for the value of $Y$ obtained analytically (Appendix D.1). The values in Column 3 are the output estimates obtained by evaluating the model at the input estimates $X_1 = x_1$ and $X_2 = x_2$. Those in Column 4 are the expectations of the probability density functions determined for the value of $Y$ using MCS. Columns 5–8 contain values of $u(y)$. The values in Column 5 are formed from the probability density function for the value of $Y$ obtained analytically (Appendix D.1). Those in Column 6 are obtained using the law of propagation of uncertainty based on linear terms in the Taylor series expansion of $f$ (LPU1). Those in Column 7 are as for Column 6 except that higher-order terms in the Taylor series expansion are additionally used (LPU2). Those in Column 8 are obtained as the standard deviations of the probability density functions determined for the value of $Y$ using MCS. All quantities are of dimension one.

Figure 14 — As for Figure 13 except that $x_1 = 0.01$, and the probability density functions resulting from the law of propagation of uncertainty with first-order (higher-peaked curve) and with higher-order terms (lower-peaked curve). The analytic solution was not obtained. The solid vertical lines denote the endpoints of the 95% coverage interval provided by Monte Carlo simulation, the broken vertical lines those resulting from the law of propagation of uncertainty with first-order terms, and the dot-dashed vertical lines from the law of propagation of uncertainty with higher-order terms.

Figure 15 — As for Figure 14 except that $x_1 = 0.05$. 

<table>
<thead>
<tr>
<th>$x_1$</th>
<th>$(1 - y)/10^{-7}$</th>
<th>Stnd uncertainty $u(y)/10^{-7}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Anal</td>
<td>Input</td>
<td>MCS</td>
</tr>
<tr>
<td>0.00</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0.01</td>
<td>1 000</td>
<td>1 507</td>
</tr>
<tr>
<td>0.05</td>
<td>25 000</td>
<td>25 506</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>5 000</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>5 025</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>5 012</td>
</tr>
<tr>
<td>Anal</td>
<td>LPU1</td>
<td>LPU2</td>
</tr>
<tr>
<td>0.00</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0.01</td>
<td>1 000</td>
<td>1 118</td>
</tr>
<tr>
<td>0.05</td>
<td>25 000</td>
<td>5 025</td>
</tr>
</tbody>
</table>
density functions provided by the law of propagation of uncertainty. These Gaussian probability density functions are in turn reasonably close to each other, having expectations of $1 - 1.0 \times 10^{-4}$ and $1 - 1.5 \times 10^{-4}$ and standard deviations of $1.0 \times 10^{-4}$ and $1.1 \times 10^{-4}$.

Figure 14, for $x_1 = 0.01$, also shows the endpoints of $I_{0.95}(Y)$ as obtained by the three approaches. The intervals provided by the law of propagation of uncertainty are shifted to the right compared with $I_{0.95}(Y)$ for Monte Carlo simulation. As a consequence they again include infeasible values of $Y$. The shift is about $70\%$ of the standard uncertainty. The interval provided by Monte Carlo simulation has its right-hand endpoint at unity, the largest feasible value.

Figure 15, for $x_1 = 0.05$, shows similar information. Now, however, the probability density functions provided by both implementations of the law of propagation of uncertainty are virtually indistinguishable from each other (a slight “thickening of the curve” at the peak is indicative of a region where visually there is a discernible difference). Further, they are now much closer to the approximation to the probability density function provided by Monte Carlo simulation. The latter exhibits a slight skewness, as evidenced in the tail regions. The coverage intervals provided by the two variants of the law of propagation of uncertainty are visually almost identical, but still shifted from those for Monte Carlo simulation. The shift is now about $10\%$ of the standard uncertainty. The intervals provided by the law of propagation of uncertainty are now feasible.

NOTES

1 One reason why the law of propagation of uncertainty with first-order terms (only) might be used in practice is that software for its implementation is readily available: results obtained from it might sometimes be accepted without question. For the case where $x_1 = x_2 = 0$ (Figure 13), the danger would be apparent because the standard uncertainty $u(y)$ was computed as zero, and consequently any coverage interval for $Y$ would be of zero length for any coverage probability. For $x_1 \neq 0$ (or $x_2 \neq 0$), $u(y)$ and the length of the coverage interval for $Y$ are both finite, so no such warning would be available without prior knowledge of likely values. Thus, a danger in implementing software based on the law of propagation of uncertainty for these calculations is that checks of the software for $x_1$ or $x_2$ sufficiently far from zero would not indicate obvious problems, although when used subsequently in practice for small values of these quantities the results would be invalid, but conceivably unwittingly accepted.

2 The values $x_1 = x_2 = 0$ lie in the centre of the region of interest to the electrical engineer and thus in no sense constitute an “extreme case” in practice.

The last two rows of Table 9 show the counterparts of the quantities in the previous row that apply for the above values $x_1 = 0.01$ and $x_1 = 0.05$, except that an analytic solution was not attempted for $x_1 > 0$.

8.3.3 Calculation: correlated input quantities

Consider measurements $x_1 = 0$, $0.01$ and $0.05$, $x_2 = 0$, with $u(x_1) = u(x_2) = 0.005$ and $r(x_1, x_2) = 0.9$. $\Gamma_M$, the voltage reflection coefficient of the power meter being calibrated, is assigned a bivariate Gaussian probability density function for the values of $X_1$ and $X_2$ with expectation $(x_1, 0)^T$ and uncertainty matrix (16)

$$
\begin{bmatrix}
 0.005^2 & 0.9 \times 0.005^2 \\
0.9 \times 0.005^2 & 0.005^2
\end{bmatrix}.
$$

(17)

The probability density function $g(y)$ for the value of $Y$ can be obtained (a) using the law of propagation of uncertainty with first-order terms, and (b) by Monte Carlo simulation. The law of propagation of uncertainty with second-order terms for the case of mutually dependent input quantities is not treated in the GUM and is not considered here.

The basis of the calculations required to implement for the model (15) the law of propagation of uncertainty with first-order terms and mutually dependent input quantities is given in Appendix D.2.1. The standard uncertainty $u(y)$ is evaluated from Expression (21) which, since $x_2 = 0$, reduces to

$$
u^2(y) = 4 x_1^2 u^2(x_1).
$$

Consequently, the standard uncertainty does not depend on the value of $r(x_1, x_2)$ and the law of propagation of uncertainty with first-order terms gives identical results to those presented in Appendix D.2.1. In particular, for the case $x_1 = 0$, the standard uncertainty $u(y)$ is computed as zero, as in Subclause 8.3.2.

To implement Monte Carlo simulation (b) it is necessary to sample randomly from a bivariate Gaussian probability density function with given expectation and uncertainty matrix. The procedure in Appendix C.5 was used. Results are obtained here for $M = 10^5$ trials.

NOTE — Apart from the requirement to sample from a multivariate distribution, the implementation of Monte Carlo simulation for mutually dependent input quantities is no more complicated than when the input quantities are mutually independent (Subclause 8.3.2).

Table 10 contains the results obtained from the two approaches in the cases $x_1 = 0$, $0.01$ and $0.05$. The results obtained from the law of propagation of uncertainty using first-order terms are identical to those given in Table 9. The results obtained from Monte Carlo simulation indicate that although the output estimate $y$ is unaffected by the correlation between input quantities,
the standard uncertainty \( u(y) \) is influenced by the correlation, especially for small \( x_1 \).

\[
\begin{array}{cccc}
\hline
x_1 & \text{Output quantity value (1 - y)/10}^{-7} & u(y)/10^{-7} \\
\text{From input estimates} & \text{MCS} & \text{LPU1} & \text{MCS} \\
0.00 & 0 & 499 & 0 & 672 \\
0.01 & 1,000 & 1,501 & 1,000 & 1,207 \\
0.05 & 25,000 & 25,530 & 5,000 & 5,047 \\
\hline
\end{array}
\]

Table 10 — As Table 9 but with the following differences. Columns 2 and 3 are output estimates of the value of \((1 - Y)/10^{-7}\). The values in Column 2 are the output estimates obtained by evaluating the model at the input estimates \( X_1 = x_1 \) and \( X_2 = x_2 \). Those in Column 3 are the expectations of the probability density functions determined for \( Y \) using MCS. Columns 4 and 5 contain values for the standard uncertainties \( u(y)/10^{-7} \). The values in Column 4 are obtained using LPU1. Those in Column 5 are obtained as the standard deviations of the distributions determined for the value of \( Y \) using MCS.

Figures 16 and 17 show the probability density functions provided by the law of propagation of uncertainty with first-order terms (bell-shaped curve) and approximated by Monte Carlo simulation (scaled frequency distributions) in the cases \( x = 0.01 \) and \( x = 0.05 \), respectively. The endpoints of the shortest 95 % coverage interval \( I_{0.95}(Y) \) provided by the two approaches are also shown, as “dash-dot” vertical lines for the law of propagation of uncertainty and solid vertical lines for Monte Carlo simulation.

NOTE — Strictly, the conditions under which a Gaussian probability density function can be assigned do not hold following an application of the law of propagation of uncertainty in this circumstance [GUM 6.2.3]. However, this probability density function and the endpoints of the corresponding 95 % coverage interval are shown because such an assignment is commonly practised.

In the case \( x_1 = 0.01 \) (Figure 16) the effect of the correlation of the input quantities has been to change noticeably the results returned by Monte Carlo simulation (compare with Figure 14). Not only has the “shape” of (the approximation to) the probability density function changed, but the corresponding coverage interval no longer has its right-hand endpoint at \( Y = 1 \). In the case \( x = 0.05 \), the differences between the results for the correlated and uncorrelated cases (compare with Figure 15) are less obvious.

Figure 16 — Results for the model of comparison loss in power meter calibration in the case \( x_1 = 0.01 \), \( x_2 = 0 \), with \( u(x_1) = u(x_2) = 0.005 \) and \( r(x_1, x_2) = 0.9 \). The figure shows the probability density function (a) provided by the use of the law of propagation of uncertainty with first-order terms to assign a Gaussian probability density function to the output quantity value (bell-shaped curve), and (b) provided by Monte Carlo simulation (scaled frequency distribution) with \( 10^5 \) trials. The “dash-dot” vertical lines denote the endpoints of the shortest 95 % coverage interval \( I_{0.95}(Y) \) as derived from the Gaussian probability density function provided by the law of propagation of uncertainty. The solid vertical lines are those derived from Monte Carlo simulation.

Figure 17 — As for Figure 16 except that \( x_1 = 0.05 \).
References


A  Historical perspective

The GUM is a rich document, covering many aspects of uncertainty evaluation. Although it does not refer explicitly to the use of Monte Carlo simulation, this option was recognized during the drafting of the GUM. The ISO/IEC/OIML/BIPM draft (First Edition) of June 1992, produced by ISO/TAG 4/WG 3, states, as Subclause G.1.5:

If the relationship between $Y$ [the output measurand] and its input quantities is non-linear, or if the values available for the parameters characterizing the probabilities of the $X_i$ [the input quantities] (expectation, variance, higher moments) are only estimates and are themselves characterized by probability distributions, and a first order Taylor expansion is not an acceptable approximation, the distribution of $Y$ cannot be expressed as a convolution. In this case, numerical methods (such as Monte Carlo calculations) will generally be required and the evaluation is computationally more difficult.

In the published version of the GUM [3], this subclause had been modified to read:

If the functional relationship between $Y$ and its input quantities is non-linear and a first-order Taylor expansion is not an acceptable approximation (see 5.1.2 and 5.1.5), then the probability distribution of $Y$ cannot be obtained by convolving the distributions of the input quantities. In such cases, other analytical or numerical methods are required.

The interpretation made here of this re-wording is that “other analytical or numerical methods” cover any other appropriate approach. This interpretation is consistent with that of the National Institute of Standards and Technology of the United States [38]:

[Clause 6.6] The NIST policy provides for exceptions as follows (see Appendix C):

It is understood that any valid statistical method that is technically justified under the existing circumstances may be used to determine the equivalent of $u_i$ [the standard deviation of the $i$th input quantity], $u_c$ [the standard deviation of the output quantity], or $U_p$ [the half-width of a coverage interval for the output measurand value, under a Gaussian assumption]. Further, it is recognized that international, national, or contractual agreements to which NIST is a party may occasionally require deviation from NIST policy. In both cases, the report of uncertainty must document what was done and why.

Further, within the context of statistical modelling in analyzing the homogeneity of reference materials, it is stated within ISO Guide 35 [19]:

[Subclause 9.2.3] ... where lack of a normal distribution is a problem, robust or non-parametric statistical procedures may be used to obtain a valid confidence interval for the quantity of interest.
B Sensitivity coefficients

Neither the propagation of distributions nor its implementation using Monte Carlo simulation provides sensitivity coefficients [GUM 5.1.3], for two reasons. First, sensitivity coefficients are not an inherent part of the propagation of distributions. Second, for a non-linear model, sensitivity coefficients are in general approximate. However, simply by holding all input quantities but one fixed at their best estimates, Monte Carlo simulation can be used to provide the probability density function for the output quantity value for the model having just that input quantity as a variable [7]. The ratio of the standard deviation of this probability density function and that of the relevant input quantity can be taken as a sensitivity coefficient. This value corresponds to that which would be obtained by taking all higher-order terms in the Taylor series expansion of the model into account. In the case of complicated models this approach can be used as a practical alternative to the “tedious analysis” required to provide sensitivity coefficients [16].

The sensitivity coefficients so obtained must not generally be taken in conjunction with the standard uncertainties associated with the best estimates of the input quantities as the only contributions to the standard uncertainty associated with the output quantity value. There will be further contributions arising from any interaction (i.e., non-additive) terms in the model.
C Sampling from probability distributions

This appendix provides some technical information concerning sampling from probability distributions. Such sampling forms a central part of the use of Monte Carlo simulation as an implementation of the propagation of distributions for uncertainty evaluation.

C.1 General distributions

It is possible to provide a sample \( z \) from any continuous distribution function \( G(\eta) \) by transforming a sample from a rectangular distribution:

a) Sample a random number \( \psi \) from the rectangular distribution \( U[0, \ 1] \).

b) Find the value \( z \) satisfying \( G(z) = \psi \).

NOTES

1 The “inversion” required in Step b), i.e., forming \( z = G^{-1}(\psi) \), may be possible analytically. Otherwise it can be carried out numerically.

2 As an example of an analytic inversion, consider the exponential probability density function with expectation \( x \), viz., \( g(\xi) = \exp(-\xi/x)/x \), for \( \xi \geq 0 \), and zero otherwise (Clause 4.1). Then \( G(\xi) = 1 - \exp(\xi/x) \), for \( \xi \geq 0 \), and zero otherwise. Hence \( z = -x \log(1 - \psi) \).

3 Numerically, \( z \) can generally be determined by solving the “zero-of-a-function” problem \( G(z) - \psi = 0 \). Upper and lower bounds for \( z \) are typically easily found, in which case a recognised “bracketing” algorithm such as bisection or, more efficiently, a combination of linear interpolation and bisection [10], for example, can be used to determine \( z \).

Emphasis is given here to the commonest distributions.

C.2 Rectangular distribution

The ability to generate pseudo-random numbers from a (continuous) rectangular distribution is fundamental in its own right, and also as the basis for generating pseudo-random numbers from any distribution (above and Appendices C.3 and C.4), using an appropriate algorithm or formula. In the latter regard, the quality of the numbers generated from a non-rectangular distribution depends on that of the rectangular generator and on the properties of the algorithm employed. The quality of the non-rectangular generator can therefore be expected to be correlated with that of the rectangular generator. Only a good rectangular generator and a good algorithm can be expected to provide a good non-rectangular generator. It is thus important that the underlying rectangular generator is sound (cf. [24]). Unless the user is sure of the pedigree of a rectangular generator it should not be used until adequate testing has been carried out. Invalid results can otherwise be obtained. Some of the “tests for randomness” that should be undertaken are indicated below. A recommended rectangular generator, that has been shown to perform well in these tests and that is straightforward to implement, is given in this appendix.

Table C.1 defines relevant aspects of the functioning of a procedure for generating rectangular pseudo-random numbers in the interval \([0, \ 1]\), specifying the input, input-output and output parameters associated with their determination.

<table>
<thead>
<tr>
<th>Input parameters</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>( q )</td>
<td>Number of rectangular pseudo-random numbers to be generated</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Input-output parameters</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>( t )</td>
<td>Column vector of parameters required as input quantities and that may be changed as part of the computation. The subsequent values of these quantities are not usually of immediate concern to the user. The parameters are needed to help control the process by which the pseudo-random numbers are produced. The parameters may be realized as global variables and thus not explicitly appear as parameters of the procedure. One or more of these parameters may be a seed, used to initiate the sequence of random numbers produced by successive calls of the procedure. By setting the seeds to values previously used, the same sequence of random numbers can be produced. Doing so is important as part of software regression testing, used to verify the consistency of results produced using the software with those from previous versions</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Output parameters</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>( z )</td>
<td>( q ) “draws” from a variable rectangularly distributed between zero and one</td>
</tr>
</tbody>
</table>

Table C.1 — Rectangular pseudo-random number generation.

A rectangular pseudo-random number \( x \) in the interval \([a, \ b]\) can be formed by determining \( a + (b - a)z \), where \( z \) is a rectangular pseudo-random number in the interval \([0, \ 1]\).

C.2.1 Randomness tests

A review [28] has been carried out of the use of random numbers in solving problems using Monte Carlo simulation. It draws conclusions concerning, in particular, the best methods to employ for generating rectangular pseudo-random numbers. The so-called “combination generators” are recommended and are reported as being favoured by experts as fulfilling the requirements of possessing the longest periods and passing a set of statistical tests for randomness.

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NOTES

1 A pseudo-random number generator of necessity provides a sequence of numbers. The period of the sequence is the number of consecutive values in the sequence before they are repeated.

2 The tests include the so-called standard tests [23], viz., the $\chi^2$ test, the Kolmogorov-Smirnov test, the frequency test, the serial test, the gap test, the coupon collector’s test, and the more stringent Die Hard tests [25], which include the overlapping $M$-tuple test, the overlapping permutation test, the parking lot and lattice test and the birthday-spacing test.

A combination generator simultaneously uses more than one generator. Each such generator is typically a member of the class of congruential generators or the class of shift register generators, both of which are widely discussed in the literature [15, 23, 32, 34]. The KISS generator [26] is a combination of a congruential generator and two shift register generators. A version in the C programming language is available [33, p42] and in Fortran [26].

NOTE — KISS is an acronym for Keep It Simple, Stupid!

The Hill-Wichmann generator [18] is a combination of three congruential generators. It and the KISS generator satisfy the above standard and Die Hard tests [28], [33, p41] and are recommended.

C.2.2 A recommended rectangular random number generator

Table C.2 defines the Hill-Wichmann generator for generating rectangular pseudo-random numbers in the interval $[0, 1]$.

C.3 Gaussian distribution

The procedure in Table C.3 provides a straightforwardly implementable approach [5] to generate values from the standard Gaussian distribution $N(0, 1)$ using the Box-Muller transform.

To sample from the Gaussian distribution $N(\mu, \sigma^2)$, take $X = \mu + \sigma Z$, where $Z$ is a standard Gaussian variable.

C.4 $t$–distribution

...The probability distribution of the variable $(\bar{Z} - \mu_c)/s(\bar{Z})$ is the $t$–distribution if the random variable $\bar{Z}$ is normally distributed with expectation $\mu_c$, where $\bar{Z}$ is the arithmetic mean of $n$ in-

---

<table>
<thead>
<tr>
<th>Input parameters</th>
<th>None</th>
</tr>
</thead>
<tbody>
<tr>
<td>Input-output parameters</td>
<td>$i_A, i_B, i_C$</td>
</tr>
<tr>
<td>Integer parameters required as input quantities and that are changed by the procedure. Set to integer values between 1 and 30000 before the first call. Do not disturb between calls. Subsequent values of these quantities are not usually of concern to the user. The parameters provide the basis by which the pseudo-random numbers are produced. They may be realised as global variables and thus not appear explicitly as parameters of the procedure.</td>
<td></td>
</tr>
<tr>
<td>Output parameters</td>
<td>$Z$</td>
</tr>
<tr>
<td>Rectangular random number between zero and one</td>
<td></td>
</tr>
<tr>
<td>Computation</td>
<td></td>
</tr>
<tr>
<td>a) Form $i_A = 171i_A \mod 30269$</td>
<td></td>
</tr>
<tr>
<td>b) Form $i_B = 172i_B \mod 30307$</td>
<td></td>
</tr>
<tr>
<td>c) Form $i_C = 170i_C \mod 30323$</td>
<td></td>
</tr>
<tr>
<td>d) Form $Z = (i_A/30269 + i_B/30307 + i_C/30323) \mod 1$</td>
<td></td>
</tr>
</tbody>
</table>

Table C.2 — The Hill-Wichmann rectangular pseudo-random number generator.

---

<table>
<thead>
<tr>
<th>Input parameters</th>
<th>None</th>
</tr>
</thead>
<tbody>
<tr>
<td>Output parameters</td>
<td>$Z_1, Z_2$</td>
</tr>
<tr>
<td>Two draws from a Gaussian variable with zero expectation and unit standard deviation</td>
<td></td>
</tr>
<tr>
<td>Computation</td>
<td></td>
</tr>
<tr>
<td>a) Generate rectangular random variates $V_1$ and $V_2$ between zero and one</td>
<td></td>
</tr>
<tr>
<td>b) Form $Z_1 = \sqrt{-2\log V_1} \cos 2\pi V_2$ and $Z_2 = \sqrt{-2\log V_1} \sin 2\pi V_2$</td>
<td></td>
</tr>
<tr>
<td>c) Take $Z_1$ and $Z_2$ as two standard Gaussian variates</td>
<td></td>
</tr>
</tbody>
</table>

Table C.3 — The Box-Muller Gaussian pseudo-random number generator.
dependent observations $\zeta_i$ of $\zeta$, $s(\zeta_i)$ is the experimental standard deviation of the $n$ observations, and $s(\zeta) = s(\zeta_i)/\sqrt{n}$ is the experimental standard deviation of the arithmetic mean $\bar{\zeta}$ with $\nu = n - 1$ degrees of freedom. [GUM C.3.8]

The procedure in Table C.4 provides an approach [22], [33, p63] to generate values from the $t$-distribution with $\nu$ degrees of freedom, which is also straightforward to implement. Full details are available [22].

<table>
<thead>
<tr>
<th>Input parameters</th>
<th>Output parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu$ Degrees of freedom</td>
<td>$Z$ Draw from a $t$-distribution with $\nu$ degrees of freedom</td>
</tr>
</tbody>
</table>

Table C.4 — A $t$-distribution pseudo-random number generator.

For an expectation $\mu$ and standard deviation $\sigma$ and $\nu$ degrees of freedom, take $X = \mu + \sigma T$, where $T$ is a variable having a $t$-distribution with $\nu$ degrees of freedom.

Sampling from the $t$-distribution can be used in Monte Carlo simulation when synthesizing probability density functions assigned to input quantities represented by repeated observations that can be regarded as drawn from a Gaussian distribution.

NOTE — This use has been criticized in some quarters in that coverage intervals determined for the output quantity value can be pessimistically long. Conversely, were a Gaussian probability density function assigned, i.e., with no account taken of the degrees of freedom that the $t$-distribution is intended to accommodate, the resulting coverage intervals could be optimistically short. This matter remains a research topic. It is recommended that a decision is agreed and recorded with the details of the uncertainty evaluation in any one instance. In particular, despite the statement in the GUM that uncertainty evaluations should be realistic, if in doubt it might be wiser and certainly cautious to use the $t$-distribution, accompanying the results of uncertainty evaluation by a suitable qualifying statement.

C.5 Multivariate Gaussian distribution

The most important multivariate distribution is the multivariate Gaussian distribution. An $n \times 1$ vector of expectations $\mu$ and an uncertainty matrix $V$ of order $n$ define the parameters of the $n$-dimensional Gaussian distribution.

Values can be sampled from this multivariate (or joint) Gaussian distribution [35, 37] using the procedure in Table C.5.

<table>
<thead>
<tr>
<th>Input parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n$ Dimension of the multivariate Gaussian distribution</td>
</tr>
<tr>
<td>$\mu$ $n \times 1$ vector of expectations</td>
</tr>
<tr>
<td>$V$ Uncertainty matrix of order $n$</td>
</tr>
<tr>
<td>$q$ Number of multivariate Gaussian pseudo-random numbers to be generated</td>
</tr>
</tbody>
</table>

Table C.5 — A multivariate Gaussian random number generator.

Figure C.1 shows 200 points generated from a bivariate Gaussian distribution, using the MULTNORM generator [35], with expectation $\mu = (2, 3)^T$ and uncertainty matrix

$$V = \begin{bmatrix} 2.0 & 1.9 \\ 1.9 & 2.0 \end{bmatrix}.$$  

Similar generators are available elsewhere [11].

In this figure the points “span” an elongated angled ellipse. Were the off-diagonal elements of $V$ to be replaced by zero, the points would span a circle. Were the diagonal elements made unequal, and the off-diagonal elements kept at zero, the points would span an ellipse.
Figure C.1 — Points sampled from a bivariate Gaussian distribution with positive correlation.

whose axes were parallel to the axes of the graph.
D The comparison loss problem

D.1 The analytic solution for a zero value of the voltage reflection coefficient

For the case \(x_1 = x_2 = r(x_1, x_2) = 0\) and \(u(x_1) = u(x_2)\), the probability density function \(g(\eta)\) (Subclause 8.3.1) can be obtained analytically. It is valuable to have such a solution for validation purposes, even though in other cases this may not be possible. The model \(Y = 1 - X_1^2 - X_2^2\) can be expressed in the above circumstances as

\[
Y = 1 - u^2(x_1)\{X_1^2/u^2(x_1) + X_2^2/u^2(x_2)\}.
\]

The term in braces is the sum, \(Z\), say, of the squares of two mutually independent standard normal probability density functions, and is therefore distributed as \(\chi^2\) with two degrees of freedom [30, p177]. Thus,

\[
Y = 1 - u^2(x_1)Z.
\]

\(Y\) is a differentiable and strictly monotonic function of \(Z\). The application of a general formula [7, Formula (5.1)], [30, pp57–61] for the probability density function \(g(\eta)\) of a function of a variable with a specified probability density function hence yields

\[
g(\eta) = \chi^2(Z)/u^2(x_1),
\]

where \(\chi^2(Z)\) is \(\chi^2\) in \(Z\) with \(\nu\) degrees of freedom. Since \([30, pp177-178]\)

\[
\chi^2(Z) = Z^{\nu/2 - 1}e^{-Z/2}/2^{\nu/2} \Gamma(\nu/2),
\]

where here, as opposed to Clause 8.3, \(\Gamma\) denotes the gamma function, the required probability density function is

\[
g(\eta) = \exp(-((1 - \eta)/(2u^2(x_1)))/(2u^2(x_1))), \quad \eta \leq 1.
\]

The expectation is straightforwardly shown to be

\[
E(\eta) = \int_{-\infty}^{1} \eta g(\eta)d\eta = 1 - 2u^2(x_1)
\]

and the variance

\[
\int_{-\infty}^{1} (\eta - E(\eta))^2 g(\eta)d\eta = 4u^4(x_1),
\]

i.e., the standard deviation is \(2u^2(x_1)\).

The corresponding distribution function is given by integration as

\[
G(\eta) = \exp(-((1 - \eta)/(2u^2(x_1)))) , \quad \eta \leq 1. \quad (18)
\]

A 95 % coverage interval \(I_{0.95}(Y)\) for the output quantity value is then (Clause 6.7)

\[
[G^{-1}(p), \; G^{-1}(p + 0.95)],
\]

for any \(p\) satisfying \(0 \leq p \leq 0.05\). The shortest \(I_{0.95}(Y)\) is given by the value of \(p\) that minimizes \(H(p) \equiv G^{-1}(p + 0.95) - G^{-1}(p)\). Let \(y_p\) be the value of \(Y\) in (18) corresponding to \(G(\eta) = p\). Simple algebra gives

\[
y_p = 1 + 2u^2(x_1)\log p.
\]

Hence

\[
I_{0.95}(Y) = [1 + 2u^2(x_1)\log p, \; 1 + 2u^2(x_1)\log(p + 0.95)]
\]

and

\[
H(p) = 1 + 2u^2(x_1)\log(p + 0.95) - (1 + 2u^2(x_1)\log p),
\]

which simplifies to

\[
H(p) = 2u^2(x_1)\log(1 + 0.95/p),
\]

a decreasing function of \(p\). Since \(p\) is to satisfy \(0 \leq p \leq 0.05\), \(H(p)\) is minimized when \(p = 0.05\). Thus,

\[
I_{0.95}(Y) = [1 + 2u^2(x_1)\log 0.05, \; 1]
\]

which, expressed as a coverage interval for \(1 - Y\), is

\[
I_{0.95}(1 - Y) = [0, -2u^2(x_1)\log 0.05].
\]

For the above value of \(u(x_1) = 0.005\), \(I_{0.95}(1 - Y) = [0, 0.0001498]\).

For comparison, the 95 % coverage interval that is symmetric with respect to probability (Clause 6.7) is

\[
I_{0.95}(1 - Y) = [-2u^2(x_1)\log(p + 0.975), \; -2u^2(x_1)\log(p + 0.025)]
\]

\[
= [0.0000039, \; 0.0001844],
\]

which is 20 % longer than the shortest interval.

NOTE — The above analysis is indicative of an analytic approach that can be applied to some problems of this type. In this particular case, the results could in fact have been obtained more directly, based on the observation that \(g(\eta)\) is monotonically increasing and using the fact that the shortest coverage interval is always in the region of highest density.

D.2 The law of propagation of uncertainty applied to the comparison loss problem

D.2.1 Uncorrelated input quantities

The comparison loss problem considered in Clause 8.3 has as the mathematical model of measurement

\[
Y = f(X) = f(X_1, X_2) = 1 - X_1^2 - X_2^2,
\]

where the values of \(X_1\) and \(X_2\) are assigned Gaussian probability density functions with expectations \(x_1\) and \(x_2\) and variances \(u^2(x_1)\) and \(u^2(x_2)\), respectively.
The application of GUM Subclause 5.1.1 gives

\[ y = 1 - x_1^2 - x_2^2 \]
as the estimate of the output quantity value. The only non-trivially nonzero partial derivatives of the model are, for \( i = 1, 2 \),

\[ \frac{\partial f}{\partial X_i} = -2x_i, \quad \frac{\partial^2 f}{\partial X_i^2} = -2. \]

Hence the application of GUM Subclause 5.1.2 gives, as the standard uncertainty \( u(y) \),

\[ u^2(y) = \left( \frac{\partial f}{\partial X_1} \right)^2 \bigg|_{X=x} u^2(x_1) \]
\[ + \left( \frac{\partial f}{\partial X_2} \right)^2 \bigg|_{X=x} u^2(x_2) \]
\[ = 4x_1^2 u^2(x_1) + 4x_2^2 u^2(x_2), \quad (19) \]
based on a first-order Taylor series approximation of \( f(X) \). If the non-linearity of \( f \) is significant, the term

\[ \frac{1}{2} \left\{ \left( \frac{\partial^2 f}{\partial X_1^2} \right)^2 + \left( \frac{\partial^2 f}{\partial X_2^2} \right)^2 \right\} \bigg|_{X=x} u^2(x_1) u^2(x_2) \]

must be appended to Formula (19), in which case Formula (19) becomes

\[ u^2(y) = 4x_1^2 u^2(x_1) + 4x_2^2 u^2(x_2) + 4u^2(x_1) u^2(x_2). \quad (20) \]

A 95% coverage interval for \( Y \) is then given by

\[ y \pm 2u(y), \]
as a consequence of the assumption that \( Y \) has a Gaussian probability density function.

### D.2.2 Correlated input quantities

The extension of the comparison loss problem to mutually dependent input quantities is considered. The changes necessary to the above treatment are given. The uncertainty matrix for the input quantities is given in Formula (16), where the correlation coefficient \( r(x_1, x_2) \) is specified and in general takes a nonzero value.

The application of GUM Subclause 5.2.2 gives

\[ u^2(y) = (\frac{\partial f}{\partial X_1})^2 u^2(x_1) + (\frac{\partial f}{\partial X_2})^2 u^2(x_2) \]
\[ + 2(\frac{\partial f}{\partial X_1})(\frac{\partial f}{\partial X_2}) r(x_1, x_2) u(x_1) u(x_2) \]
\[ = 4x_1^2 u^2(x_1) + 4x_2^2 u^2(x_2) \]
\[ + 8r(x_1, x_2)x_1x_2 u(x_1) u(x_2), \quad (21) \]
based on a first-order Taylor series approximation of \( f(X) \), where all derivatives are evaluated at \( X = x \).
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