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Guide to the expression of uncertainty in measurement (GUM) — Supplement 1: Numerical methods for the propagation of distributions

Guide pour l'expression de l'incertitude de mesure (GUM) — Supplément 1: Méthodes numériques pour la propagation de distribution

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Please see the administrative notes on page iii

In accordance with the ISO/IEC Directives, Part 1, 2001, Clause A.5, this draft is submitted to the ISO national bodies for approval.

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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.

Contents

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 magnitude [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 [GUM C.2.5] —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 f:

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

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

NOTES

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

2 In this *Supplement*, T in the superscript position denotes "transpose", and thus $\boldsymbol{X}$ 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 quantities.

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 G].

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 $\boldsymbol{x} = (x_1, \ldots, x_N)^{\mathrm{T}}$ and the standard deviations (standard uncertainties) $\boldsymbol{u}(\boldsymbol{x}) = (u(x_1), \ldots, u(x_N))^{\mathrm{T}}$. Use the joint probability density function for the value of $\boldsymbol{X}$ instead if the X_i are mutually dependent.

NOTE — The X_i are regarded as random variables with possible values ξ_i and expectations x_i.

b) Take the *covariances* (mutual uncertainties) [GUM C] $u(x_i, x_j)$ as $\mathrm{Cov}(X_i, X_j)$, 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 $\boldsymbol{x}$.

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

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

g) Calculate ν, 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 ($\nu < \infty$).

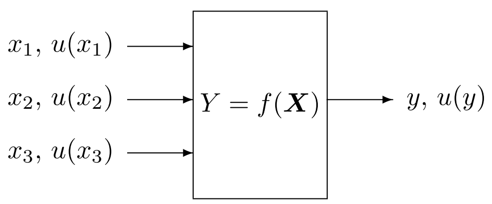

Figure 1 — Illustration of the law of propagation of uncertainty. The model has mutually independent input quantities $\boldsymbol{X} = (X_1, X_2, X_3)^{\mathrm{T}}$, whose values are estimated by x_i with associated standard uncertainties $u(x_i)$, for $i = 1, 2, 3$. The value of the output quantity 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 ξ_i of the ith 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 $g(\boldsymbol{\xi})$. 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.

All available information concerning quantity X	Probability density function (PDF) assigned to the value of X
The estimate x and the associated standard uncertainty $u(x)$	The Gaussian PDF $N(x, u^2(x))$
The estimate x (> 0), and X is known to be nonnegative	The exponential PDF with expectation x, viz., $\exp(-\xi/x)/x$, for $\xi \geq 0$, and zero otherwise.
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	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
The estimate $\boldsymbol{x}$ of the value of a multivariate quantity $\boldsymbol{X}$ and the corresponding uncertainty matrix (covariance matrix) $\boldsymbol{V}$	The multivariate Gaussian PDF $N(\boldsymbol{x}, \boldsymbol{V})$ is assigned to the value of $\boldsymbol{X}$ (Section 5, Note 2)
The endpoints a_- and a_+ of an interval containing the value of X	The rectangular PDF with endpoints a_- and a_+
The lower and upper limits a_- and a_+ of an interval within which the value of X is known to cycle sinusoidally	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 $a_- < \xi < a_+$, and zero otherwise [14], [17, Section 3.5]

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.

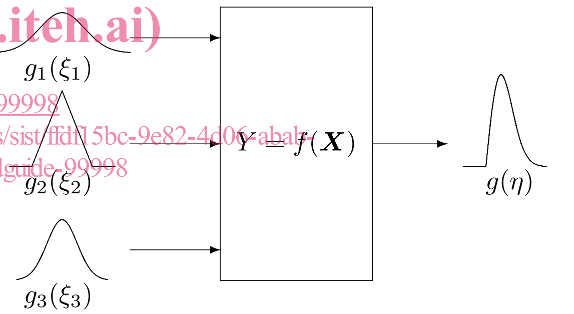

Figure 2 — Illustration of the propagation of distributions. The model input quantities are $\boldsymbol{X} = (X_1, X_2, X_3)^{\mathrm{T}}$. The probability density functions $g_i(\xi_i)$, for X_i, $i = 1, 2, 3$, are Gaussian, triangular and Gaussian, respectively. The probability density function $g(\eta)$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

NOTES

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

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

$$g(\boldsymbol{\xi}) = \frac{1}{((2\pi)^N \det \boldsymbol{V})^{1/2}} \exp\left\{-\frac{1}{2}(\boldsymbol{\xi} - \boldsymbol{x})^{\mathrm{T}} \boldsymbol{V}^{-1} (\boldsymbol{\xi} - \boldsymbol{x})\right\}.$$

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

$$\boldsymbol{V} = \mathrm{diag}(u^2(x_1), \ldots, u^2(x_N)),$$

whence

$$\begin{aligned} g(\boldsymbol{\xi}) &= \frac{1}{(2\pi)^{N/2} u(x_1) \cdots u(x_N)} \exp\left\{-\frac{1}{2}\sum_{i=1}^{N} \frac{(\xi_i - x_i)^2}{u^2(x_i)}\right\} \\ &= \prod_{i=1}^{N} g_i(\xi_i), \end{aligned}$$

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 $Y = f(\boldsymbol{X})$. 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
>
> $$y = f(x_1, x_2, \ldots, x_N) \qquad \ldots (2)$$
>
> NOTE – In some cases the estimate y may be obtained from
>
> $$y = \bar{Y} = \frac{1}{n}\sum_{k=1}^{n} Y_k = \frac{1}{n}\sum_{k=1}^{n} f(X_{1,k}, X_{2,k}, \ldots, X_{N,k})$$
>
> 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_i obtained at the same time. This way of averaging, rather than $y = f(\bar{X}_1, \bar{X}_2, \ldots, \bar{X}_N)$, where $\bar{X}_i = (\sum_{k=1}^{n} X_{i,k})/n$ 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). [GUM 4.1.4]

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.

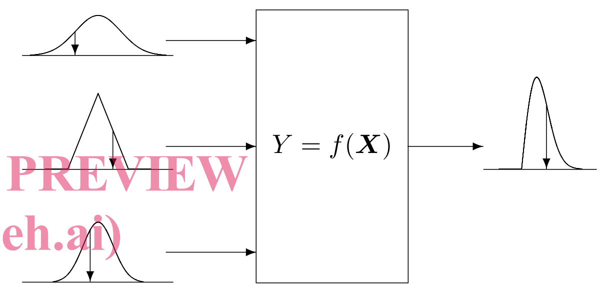

Figure 3 — As Figure 2 except that what is shown is a value sampled from each of the three probability density functions for the values of the input quantities, and the resulting output quantity value.

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:

— 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 $\boldsymbol{X}$). 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