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Part 6:
Developing and using measurement models

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Partie 6: Élaboration et utilisation de modèles de mesure

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This document was prepared by Working Group 1 of the Joint Committee for Guides in Metrology (as JCGM GUM-6:2020), and was adopted by the national bodies of ISO and IEC.

A list of all parts in the ISO/IEC Guide 98 series can be found on the ISO and IEC websites.

Given that ISO/IEC Guide 98-6 is identical in content to JCGM GUM-6, the decimal symbol is a point on the line in the English version.

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

Any feedback or questions on this document should be directed to the user's national standards body. A complete listing of these bodies can be found at www.iso.org/members.html and www.iec.ch/national-committees.

Joint Committee for Guides in Metrology

Guide to the expression of uncertainty in measurement — Part 6: Developing and using measurement models

Guide pour l'expression de l'incertitude de mesure — Partie 6: Élaboration et utilisation des modèles de mesure

JCGM GUM-6:2020

Contents

Foreword

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

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

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

In 2008 the JCGM made available a slightly revised version (mainly correcting minor errors) of the 'Guide to the expression of uncertainty in measurement', labelling the document 'JCGM 100:2008'. In 2017 the JCGM rebranded the documents in its portfolio that have been produced by Working Group 1 or are to be developed by that Group: the whole suite of documents became known as the 'Guide to the expression of uncertainty in measurement' or 'GUM'. This document, previously known as JCGM 103, Supplement 3 to the GUM, is the first to be published as a part of that portfolio, and is entitled and numbered accordingly.

The present guide is concerned with the development and use of measurement models, and supports the documents in the entire suite of JCGM documents concerned with uncertainty in measurement. The guide has been prepared by Working Group 1 of the JCGM, and has benefited from detailed reviews undertaken by member organizations of the JCGM and National Metrology Institutes.

Introduction

A measurement model constitutes a relationship between the output quantities or measurands (the quantities intended to be measured) and the input quantities known to be involved in the measurement. There are several reasons for modelling a measurement. Models assist in developing a quantitative understanding of the measurement and in improving the measurement. A model enables values of the output quantities to be obtained given the values of the input quantities. Additionally, a model not only allows propagation of uncertainty from the input quantities to the output quantities; it also provides an understanding of the principal contributions to uncertainty. This document is accordingly concerned with the development of a measurement model and the practical use of the model.

One of the purposes of measurement is to assist in making decisions. The reliability of these decisions and the related risks depend on the values obtained for the output quantities and the associated uncertainties. In turn, these decisions depend on a suitable measurement model and the quality of information about the input quantities.

Although the development of a measurement model crucially depends on the nature of the measurement, some generic guidance on aspects of modelling is possible. A measurement model might be a straightforward mathematical relationship, such as the ideal gas law, or, at the other extreme, involve a sophisticated numerical algorithm for its evaluation, such as the detection of peaks in a signal and the determination of peak parameters.

A measurement model may take various forms: theoretical, empirical or hybrid (part-theoretical, part-empirical). It might have a single output quantity or more than one output quantity. The output quantity may or may not be expressed directly in terms of the input quantities. The quantities in the measurement model may be real-valued or complex-valued. Measurement models may be nested or multi-stage, in the sense that input quantities in one stage are output quantities from a previous stage, as occurs, for instance, in the dissemination of measurement standards or in calibration. Measurement models might describe time series of observations, including drift, and dynamic measurement. A measurement model may also take the form of a statistical model. In this document the concept 'measurement model' is intended in this broader meaning.

In developing or using a measurement model there are important choices to be made. The selection of a model that is adequate or fit for purpose is a key issue. Particularly for empirical models, there is choice of representation (or parametrization) of the families of functions concerned (polynomials, polynomial splines or rational functions, etc.). Certain choices can be far superior to others in their numerical behaviour when the model is implemented on a computer. The uncertainty arising from the choice of model is a necessary consideration.

In many disciplines, a basic measurement model requires extension to incorporate effects such as temperature corrections arising from the measurement to enable values for output quantities and the associated uncertainties to be obtained reliably.

Following the introduction in 1993 of the Guide to the expression of uncertainty in measurement, or GUM (also known as JCGM 100:2008), the practice of uncertainty evaluation has broadened to use a wider variety of models and methods. To reflect this, this Guide includes an introduction to statistical models for measurement modelling (clause 11) and additional guidance on modelling random variation in Annex C.

Guide to the expression of uncertainty in measurement — Part 6: Developing and using measurement models

1 Scope

This document provides guidance on developing and using a measurement model and also covers the assessment of the adequacy of a measurement model. The document is of particular interest to developers of measurement procedures, working instructions and documentary standards. The model describes the relationship between the output quantity (the measurand) and the input quantities known to be involved in the measurement. The model is used to obtain a value for the measurand and an associated uncertainty. Measurement models are also used in, for example, design studies, simulation of processes, and in engineering, research and development.

This document explains how to accommodate in a measurement model the quantities involved. These quantities relate i) to the phenomenon or phenomena on which the measurement is based, that is, the measurement principle, ii) to effects arising in the specific measurement, and iii) to the interaction with the artefact or sample subject to measurement.

The guidance provided is organised in accordance with a work flow that could be contemplated when developing a measurement model from the beginning. This work flow starts with the specification of the measurand (clause 6). Then the measurement principle is modelled (clause 7) and an appropriate form of the model is chosen (clause 8). The basic model thus obtained is extended by identifying (clause 9) and adding (clause 10) effects arising from the measurement and the artefact or sample subject to measurement. Guidance on assessing the adequacy of the resulting measurement model is given in clause 12. The distinction between the basic model and the (complete) measurement model in the work flow should be helpful to those readers who already have a substantial part of the measurement model in place, but would like to verify that it contains all effects arising from the measurement so that it is fit for purpose.

Guidance on the assignment of probability distributions to the quantities appearing in the measurement model is given in JCGM 100:2008 and JCGM 101:2008. In clause 11, this guidance is supplemented by describing how statistical models can be developed and used for this purpose.

When using a measurement model, numerical problems can arise including computational effects such as rounding and numerical overflow. It is demonstrated how such problems can often be alleviated by expressing a model differently so that it performs well in calculations. It is also shown how a reformulation of the model can sometimes be used to eliminate some correlation effects among the input quantities when such dependencies exist.

Examples from a number of metrology disciplines illustrate the guidance provided in this document.

2 Normative references

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP, and OIML. Evaluation of measurement data — Guide to the expression of uncertainty in measurement. Joint Committee for Guides in Metrology, JCGM 100:2008.

BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP, and OIML. Evaluation of measurement data — Supplement 1 to the 'Guide to the expression of uncertainty in measurement' — Propagation of distributions using a Monte Carlo method. Joint Committee for Guides in Metrology, JCGM 101:2008.

BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP, and OIML. Evaluation of measurement data — Supplement 2 to the 'Guide to the expression of uncertainty in measurement' — Extension to any number of output quantities. Joint Committee for Guides in Metrology, JCGM 102:2011.

BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP, and OIML. International vocabulary of metrology — Basic and general concepts and associated terms. Joint Committee for Guides in Metrology, JCGM 200:2012.

3 Terms and definitions

The terms and definitions of JCGM 100:2008, JCGM 101:2008, JCGM 102:2011 and JCGM 200:2012 apply.

ISO, IEC and IUPAC maintain terminological databases for use in standardization at the following addresses:

- IEC Electropedia: available at `http://www.electropedia.org`
- ISO Online Browsing Platform: available at `http://www.iso.org/obp`
- IUPAC Gold Book: available at `http://www.goldbook.iupac.org`

4 Conventions and notation

4.1 The conventions and notation in JCGM 100:2008, JCGM 101:2008 and JCGM 102:2011 are adopted. Principal symbols used throughout the document are explained in annex A. Other symbols and those appearing in examples are explained at first occurrence.

4.2 Most examples in this document contain numerical values rounded to a number of decimal digits appropriate to the application. Because of rounding there are often numerical inconsistencies among the values presented. An instance is the correlation coefficient of −0.817 in the example in 8.1.6. It is obtained from the *computer-held values* of two standard uncertainties and a covariance. If it were computed from the three presented values (three significant decimal digits), its value correct to three decimal digits would be −0.822.

4.3 Links to numbered subclauses are indicated by underlining.

5 Basic principles

5.1 A *measurand* (see JCGM 200:2012, 2.3) is in many cases not measured directly, but is indirectly determined from other *quantities* (see JCGM 200:2012, 1.1) to which it is related by a *measurement model* (see JCGM 200:2012, 2.48) such as formula (1) in 5.2. The measurement model is a mathematical expression or a set of such expressions (see JCGM 100:2008, 4.1.2), comprising all the quantities known to be involved in a measurement. It enables a value (see JCGM 200:2012, 1.19) of the measurand to be provided and an associated standard uncertainty to be evaluated. The measurement model may be specified wholly or partly in the form of an algorithm. The quantities to which the measurand is related constitute the *input quantities* (see JCGM 200:2012, 2.50) in the measurement model. The measurand constitutes the *output quantity* (see JCGM 200:2012, 2.51).

5.2 Many measurements are modelled by a real functional relationship f between N real-valued input quantities $X_1, \ldots, X_N$ and a single real-valued output quantity (or measurand) Y in the form

$$Y = f(X_1, \ldots, X_N). \quad (1)$$

This simple form is called a real explicit univariate measurement model; real since all quantities involved take real (rather than complex) values, explicit because a value for Y can be computed directly given values of $X_1, \ldots, X_N$, and univariate since Y is a single, scalar quantity. However, it does not apply for all measurements. A measurement model can be complex, involving *complex-valued quantities* (see JCGM 102:2011, 3.2). It can be *implicit* where a value for Y cannot be determined directly given values of $X_1, \ldots, X_N$ (see 13.5). The measurement model can be *multivariate* where there is more than one measurand, denoted by $Y_1, \ldots, Y_m$; for further information, see 13.4 and JCGM 102:2011.

EXAMPLE *Volume of a cylinder*

The volume of a cylinder is given by the measurement model

$$V = \frac{\pi}{4} L d^2$$

in which cylinder length L and diameter d are the $N = 2$ input quantities, corresponding to X_1 and X_2, and an output quantity V corresponding to Y.

5.3 The process of building a measurement model can be subdivided into the following steps, each step being described in the indicated clause:

a) Select and specify the measurand (see clause 6).

b) Model the measurement principle, thus providing a basic model for this purpose (see clause 7), choosing an appropriate mathematical form (see clauses 8 and 11).
c) Identify effects involved in the measurement (see clause 9).
d) Extend the basic model as necessary to include terms accounting for these effects (see clauses 10 and 11).
e) Assess the resulting measurement model for adequacy (see clause 12).

In any one instance, a number of passes through the process may be required, especially following step c). It may be more efficient or effective to take the steps as listed in a different order.

5.4 The manner in which a measurement model is used to obtain a value for the measurand (or values for the measurands) and evaluate the associated standard uncertainty (or covariance matrix) depends on its mathematical form (see clause 13). JCGM 100:2008 mainly considers explicit univariate models and applies the law of propagation of uncertainty (LPU). JCGM 102:2011 gives guidance on the use of generalizations of LPU for multivariate models and implicit models. For non-linear models, the use of the Monte Carlo method of JCGM 101:2008 (univariate measurement models) and JCGM 102:2011 (multivariate models) is often more appropriate (see clause 13).

5.5 The measurement model is a mathematical relationship among quantities, and as such it is subject to the rules of quantity calculus [20]. The same symbols used for the quantities are also used for the corresponding *random variables* (see JCGM 100:2008, C.2.2), whose *probability distributions* (see JCGM 101:2008, 3.1) describe the available knowledge about the quantities. Therefore, the measurement model can also be considered to be a model involving random variables, subject to the rules of mathematical statistics. The law of propagation of uncertainty as described in JCGM 100:2008, 5.1 and 5.2 uses a simple property of the transformation of *random variables* when only expectations and variances (and, perhaps, covariances) are used, rather than the whole distributions.

EXAMPLE *Mass of a spherical weight*

The mass of a weight that has been machined in the form of a sphere from a block of material is given by

$$m = \frac{\pi}{6} d^3 \rho, \tag{2}$$

where d is the diameter of the weight and ρ is the density of the material.

Expression (2) is a simple, well-known physical model that is idealized, applying to a perfect sphere and relating the output quantity mass to the input quantities diameter and density. At the same time, d and ρ can be considered as random variables describing the available information on the corresponding physical quantities obtained, for instance, from a dimensional measurement made with a vernier caliper and from a table of reference data, respectively. Thus, expression (2) also describes how to transform this information about the input physical quantities to the mass m of the weight (the measurand).

5.6 When building a measurement model that is fit for purpose, all effects known to affect the measurement result should be considered. The omission of a contribution can lead to an unrealistically small uncertainty associated with a value of the measurand [156], and even to a wrong value of the measurand.

Considerations when building a measurement model are given in 9.3. Also see JCGM 100:2008, 3.4.

5.7 The fitness for purpose of a measurement model can encompass considerations made before measurement. Such aspects include the measurement capability [85] (see JCGM 200, 2.6) in the case of a laboratory routinely performing calibrations. Fitness for purpose can also encompass the cost of measurement at a given level of uncertainty compared with the consequent costs of incorrect decisions of conformity (see also JCGM 106:2012 [21]). The measurand, which in the terminology of conformity assessment is a 'quality characteristic of the entity', can be, as in statistics, either

- a measure of 'location', for instance, a quantity relating to an entity such as the mass of a single object, an error in mass (deviation from a nominal value), or an average mass of a batch of objects, or
- a measure of 'dispersion', for instance, the standard deviation in mass amongst a batch of objects in a manufacturing process.

5.8 When developing a measurement model, the ranges of possible values of the input quantities and output quantities should be considered. The model should be capable of providing credible estimates and associated uncertainties for all output quantities over the required ranges of the input quantities, which should be specified as appropriate. The measurement model should only be used within the ranges of all quantities for which it has been developed and assessed for adequacy. See 13.2.

5.9 One aspect of specifying the domain of validity of the measurement model (see also 5.8) is to identify any restrictions on the domains of the quantities involved in the measurement model. Some quantities are necessarily positive (or at least non-negative). Some quantities might have lower and upper limits. There can be interrelationships between two or more quantities that need to be included in the measurement model.

EXAMPLE *Quantities having restrictions*

- Positive quantities, for instance, mass and volume.
- Quantity with limits, for instance, a mass fraction can only take values between zero and one.
- Quantities having interrelationships, for instance, the relative proportions (fractions) of all components (hydrocarbons and other molecules) of a natural gas sum to a constant.

Such quantities can sometimes be re-expressed by applying transformations. For instance, denoting by θ a new real quantity that is unconstrained:

- a quantity q is positive if re-expressed as $q = \theta^2$,
- a quantity q lies between a and b if re-expressed as $q = a + (b - a)\sin^2\theta$, and
- quantities q_1 and q_2 sum to unity by the transformation $q_1 = \sin^2\theta$, $q_2 = \cos^2\theta$.

6 Specifying the measurand

6.1 The choice of the measurand depends on the purpose of the measurement and may take account of the *target measurement uncertainty* (see JCGM 200, 2.34). Other processes and measurands are possible and the appropriate choice depends on the application of the measurement result.