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CHARACTERISTIC VALUES IN MEASUREMENT OF IONIZING RADIATION – MATERIAL FOR A CRITICAL DISCUSSION ON FUNDAMENTALS AND ALTERNATIVES

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CHARACTERISTIC VALUES IN MEASUREMENT OF IONIZING RADIATION — MATERIAL FOR A CRITICAL DISCUSSION ON FUNDAMENTALS AND ALTERNATIVES

CHARAKTERISTISCHE WERTE BEI DER MESSUNG IONISIERENDER STRAHLUNG — MATERIAL FÜR EINE KRITISCHE DISKUSSION ÜBER GRUNDLAGEN UND ALTERNATIVEN

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Summary — *The new international standard ISO 11929:2010 and a recent, more general publication by the authors of the present paper provide for a non-negative radiation measurand definitions of the best estimate, the associated standard uncertainty of measurement, limits of coverage intervals, the decision threshold and the detection limit, here summarized by the term characteristic values. These values are based on Bayesian statistics and the ISO Guide to the Expression of Uncertainty in Measurement (GUM) and are mathematically defined by means of moments and quantiles of probability distributions of the possible measurand values. During the preparation of the documents, some criticisms were already expressed and alternatives proposed. These are described and discussed in order to achieve agreement between the experts which can be used for a future revision of ISO 11929:2010.*

Zusammenfassung — *Die neue internationale Norm ISO 11929:2010 und eine jüngere, allgemeinere Publikation der Autoren des vorliegenden Papiers stellen für eine nichtnegative Strahlungs-Messgröße Definitionen bereit für den besten Schätzwert, der beigeordneten Standard-Messunsicherheit, die Grenzen von Überdeckungsintervallen, die Erkennungsgrenze und die Nachweisgrenze, hier summarisch charakteristische Werte genannt. Diese Werte basieren auf der Bayes-Statistik und dem ISO Guide to the Expression of Uncertainty in Measurement (GUM) und sind mathematisch definiert durch Momente und Quantile von Wahrscheinlichkeits-Verteilungen der möglichen Werte der Messgröße. Schon während der Ausarbeitung der Dokumente wurden Kritik geäußert und Alternativen vorgeschlagen. Diese werden beschrieben und diskutiert, um zwischen den Experten Übereinkunft zu erzielen, die für eine künftige Revision von ISO 11929:2010 verwendet werden kann.*

Keywords — *Measurement result, measurement uncertainty, coverage interval, decision threshold, detection limit*
Schlüsselwörter — *Messergebnis, Messunsicherheit, Überdeckungsintervall, Erkennungsgrenze, Nachweisgrenze*

Contents

Page

Summary i
Zusammenfassung i

1. Introduction 1

2. Distributions 3
2.1 Denotations and nomenclature 3
2.2 Distributions for estimating physical quantities 4
2.3 Distribution propagation 5
2.4 Information modification 6

3. Establishing distributions 8
3.1 PME and Bayes and expansion theorems 8
3.2 Additional remarks 10

4. Definitions of the characteristic values 11
4.1 Preliminary remarks 11
4.2 Best estimate and standard uncertainty 12
4.3 Coverage intervals 13
4.4 Decision threshold and detection limit 14

5. Justifications against criticisms 16
5.1 Denoting distributions 16
5.2 Applying Bayesian statistics 17
5.3 Using Gaussian distributions 17
5.4 Using Dirac and Heaviside functions 18
5.5 PME and Bernoulli principle 19
5.6 Using second-order loss functions, consistency 20
5.7 Counting measurement 21
5.8 Random influences by sample treatment 24
5.9 Treating a single spectral line 27
5.10 Exceptional values of the detection limit 28

6. Proposed alternatives 29
6.1 Distributions 29
6.2 Final measurement result 30
6.3 Coverage intervals 31
6.4 Decisions 31
6.5 Recommendations for computing 33
6.6 Naming of terms 34

7. Conclusions 34

Appendix A: More about PME 36
A.1 Priors from the Bernoulli principle 36
A.2 A derivation of the PME 36
A.3 PME versus Bayes theorem 38

Appendix B: The shortest coverage interval **39**
B.1 General case 39
B.2 Gaussian case 41
B.3 Monte Carlo application 41

Appendix C: Uncertainty calculation in the case of random influences by sample treatment **42**
C.1 Approach without counting uncertainties 42
C.2 Including counting uncertainties 44

Appendix D: Glossary of some important terms and symbols **47**

Acknowledgements **48**

References **48**

1. Introduction

The recognition and detection of ionizing radiation are indispensable basic prerequisites for radiation protection. For this purpose, the new standard ISO 11929:2010 [1] provides *characteristic limits*, i.e. decision threshold, detection limit and limits of a coverage interval, for a diversity of application fields. The *decision threshold* allows a decision to be made for a measurement on whether or not, for instance, radiation of a possibly radioactive sample is present. The *detection limit* allows a decision to be made on whether or not the measurement procedure intended for application to the measurement meets the requirements to be fulfilled and is, therefore, appropriate for the measurement purpose. The *limits of a coverage interval*—formerly called the *confidence limits*, also in ISO 11929—include with a specified probability the *true value* of the *measurand*, i.e. the physical quantity to be measured. In addition, the *best estimate* of the measurand and the associated *standard uncertainty* are of interest, together called the *(complete) measurement result*. In the following, the characteristic limits and the measurement result are summarized by the term *characteristic values*. The best estimate, the standard uncertainty, and the limits of a coverage interval are characteristic values appertaining to a particular sample whereas the decision threshold and the detection limit characterize the measurement procedure.

Because of developments in metrology concerning measurement uncertainty, laid down in the ISO *Guide to the Expression of Uncertainty in Measurement* (GUM) [2], the new ISO 11929:2010 [1] was drawn up by the authors of the present paper and others on the basis of GUM, but using *Bayesian statistics* (BSt) [3–13] and the Bayesian theory of measurement uncertainty [14–18]. This theory provides a Bayesian foundation for GUM. Moreover, ISO 11929:2010 [1] is based on the definitions of the characteristic limits [19], the standard proposal [20], the introducing article [21], and the precursory ISO 11929-7:2005 [22]. It unifies and replaces all old parts of ISO 11929 and is applicable not only to a large variety of particular measurements of ionizing radiation but also, in analogy, to other measurement procedures.

The new standard ISO 11929:2010 [1] has a history of many years. It is itself a revised version of the precursory ISO 11929-7:2005 [22] and ...-8:2005, DIN 25482-10:2000 [23], ...-12:2003 and ...-13:2003. These standards already provide the general procedure stipulated in sections 5 and 6 of ISO 11929:2010 for the determination of the characteristic values on the basis of Bayesian statistics (BSt) and the concept of measurement uncertainty according to GUM (1993) [2] and DIN 1319-3:1996 and ...-4:1999 [24]. All earlier published parts ISO 11929-1:2000 to ...-6:2005 and DIN 25482-1:1989 to ...-6:1997 are founded on conventional, frequency-based statistics (CSt), as far as applicable. The general procedure was first published in 1998 [19] and first stipulated by DIN 25482-10:2000 [23]. The new ISO 11929:2010 now merely unifies, generalizes and replaces on the basis of BSt all the mentioned standard parts, which had been prepared since 1989 and earlier for particular applications to various radiation measurements. These applications now occur as examples in annexes B to D of ISO 11929:2010. The present paper and reference [25] now take a step beyond the present state of standardization represented by ISO 11929:2010 by considering not only Gaussian normal probability distributions (GD) but also other arbitrary ones. This history should make clear that the characteristic values and the general procedure to obtain them are well defined and well established and seem to have been successfully applied in practice during the past twelve years since

no major criticism of the procedure has been received. But nothing is perfect. Thus, a future revision of the new ISO 11929:2010 [1] may be justified.

Recently, a supplement [26] to GUM [2] has been published, dealing comprehensively with the treatment of measurement uncertainty using the Monte Carlo (MC) method in complex measurement evaluations. This provided an incentive for writing a corresponding MC supplement [25] to ISO 11929 [1]. The paper is also essentially founded on Bayesian statistics and can serve as a bridge between documents [1] and [26]. Moreover, more general definitions (see section 4) and the MC computation of the characteristic values make it possible to go a step beyond the present state of standardization laid down in ISO 11929 since probability distributions rather than uncertainties can be propagated. It is thus more comprehensive and promising.

Nevertheless, during the preparation of ISO 11929 [1] and its MC supplement [25], the general fundamentals and definitions of the characteristic values were already criticized and alternatives proposed. This requires a future discussion between the experts concerned. Some material for such a discussion is presented in the present paper. A satisfying consensus of opinion or at least a practicable compromise should be the aim of the discussion on a future revision of ISO 11929 between the users of the standard and experts in Bayesian statistics and decision theory. An attempt should also be made to reconcile diverging Bayesian schools, called schools A and B in the following (see subsection 5.5).

Applying Bayesian statistics (BSt) together with the *principle of maximum (information) entropy* (PME) [10–16] and the *Bernoulli principle* in reference [25] and the present paper (see subsections 3.1 and 5.5 and appendix A) makes it possible to also take into account non-statistical information, for instance, of uncertain physical quantities and influences, which do not behave randomly in repeated or counting measurements and thus cannot be treated by conventional, frequency-based statistics (CSt). BSt and CSt are both based on probability theory but differ essentially in their understanding of the probability $\Pr(A)$ of a random event A. In CSt, the probability is the limit of the relative frequency with which the event happens randomly in measurements repeated independently more and more frequently under identical nominal conditions. In contrast, the probability in BSt expresses the degree of belief, based on information actually available, that the event will happen in a measurement, e.g., *before* the measurement is carried out. An example is the probability $1/2$ reasonably assigned to each side of a coin before tossing the coin. This meaning of probability is in fact the classical one introduced by Bernoulli and Laplace. BSt and CSt are asymptotically equivalent on the same basis of data, conditions, assumptions and other information if both statistics are applicable. But there are cases, for example, of non-statistical information where CSt cannot be applied. For a comprehensive comparison of BSt and CSt in repeated measurements, see reference [27].

The present paper serves to improve and generalize ISO 11929 [1]. It is written mainly for experts, tutors, and developers of procedures and programs in the field of characteristic values. Basic tools are stated in sections 2 and 3. Several probability distributions are first formally introduced in section 2. In particular, these are distributions of the measurand Y, which depends by a *model equation* $Y = G(X_1, X_2, \ldots)$ on *input quantities* X_i with their joint distribution also needed to perform a *distribution propagation*

from X_i to Y. The way to establish distributions in general from available information by using the PME or other methods such as the Bayes theorem is shown in section 3. Then the characteristic values are mathematically stipulated in section 4 by means of integrals, i.e. moments and quantiles, of the distributions of Y. Metrological and practical demands are observed. Sections 1 to 4 are taken in essence from the authors' publication [25], but are revised, updated and supplemented. ISO 11929 [1] and reference [25] are justified against criticisms in section 5. Proposed alternatives of the characteristic values are discussed in section 6. The conclusions of section 7 comprise proposals for a revision of ISO 11929. A derivation of the PME is given in appendix A. The mathematics of the shortest coverage interval is treated in appendix B. The uncertainty caused by influences of sample treatment is calculated in appendix C.

For the definitions of the metrological terms used see references [1, 2, 26, 28], for statistical terms and symbols see, for example, references [29–31]. A glossary of some important terms and symbols is given in appendix D.

There are problems in this respect between BSt and CSt, between BSt without and with PME (schools A and B, respectively), and in nomenclature and notation (see subsections 2.1, 5.1 and 6.6). To avoid misunderstandings in such cases, it is attempted, if necessary, to clearly and exactly define the concepts in question where they are introduced and to designate and denote them in conformity with other usages as far as is suitable and possible.

2. Distributions

2.1 Denotations and nomenclature

In the following, if not otherwise stated, an upper-case letter, say Z, is used to denote some random variable and (preferably corresponding) lower-case letters z or ζ are used for values of the random variable. The distinct meanings of the random variable and its values should always be kept in mind. Bold-face symbols are used for sets of related entities. For instance, a set of quantities or values $\{v_1, v_2, \ldots\}$ is abbreviated by the corresponding symbol $\mathbf{v}$ used as a column matrix (or vector) $(v_1,\, v_2,\, \ldots)^\top$. The corresponding $\mathbf{v}$-space volume element $\mathrm{d}\mathbf{v}$ is applied in multiple integrals. The *(probability) density (function)*, also called the *density* for short, of a random variable Z is denoted by $f_Z(z \mid \mathbf{a})$ (similar to DIN 13303-1 [30] and to the symbol $\{z \mid \mathbf{a}\}$ for a set of elements z with a property described by $\mathbf{a}$). The set $\mathbf{a}$ summarily represents all the information taken into account, i.e. data, conditions, assumptions, functional relations, and other relevant information given or obtained from measurements and other sources. The data can also comprise values of other random variables as statistical information, e.g., a value v of a random variable V, if needed, written as $V = v$. Other information may be non-statistical such as functional relations. Particular fixed values of a random variable are marked by suitable affixes.

As in common practice and in ISO 11929 [1], the general symbol f is used for probability densities and F for the corresponding *(cumulative) (probability) distribution functions*, for instance, $F_Z(z \mid \mathbf{a}) = \Pr(Z \le z \mid \mathbf{a}) = \int_{-\infty}^{z} f_Z(\zeta \mid \mathbf{a})\,\mathrm{d}\zeta$ or, conversely, $f_Z(z \mid \mathbf{a}) = \mathrm{d}F_Z(z \mid \mathbf{a})/\mathrm{d}z$. The joint density of a set $\mathbf{Z}$ of random variables Z_i with values $\mathbf{z}$ is denoted by $f_{\mathbf{Z}}(\mathbf{z} \mid \mathbf{a})$. Notice that the random variable Z or $\mathbf{Z}$ as a subscript of the

distribution symbols f and F is not dropped [30]. This avoids mistakes, which can be caused easily by the less informative, but simpler, bare symbols usually preferred in the literature for brevity and convenience. Nevertheless, abbreviations such as f or f_Z or $f(z)$ for $f_Z(z \mid \mathbf{a})$ are also sometimes well defined and are then used in the following if there is no danger of misunderstanding. See also subsections 5.1 and 6.6.

According to ISO 3534-1 [29], *(probability) distribution (of a random variable)* is used in the present paper as a general, generic term comprising the *(cumulative) (probability) distribution function* F for a general random variable, the *(probability) density (function)* f for a continuous random variable, and the *probability function* p for a discrete random variable. The words in brackets are often dropped for brevity and convenience if there is no danger of misunderstanding. *(Probability) density (function)* is the most frequently used term. The word *function* is here always dropped since any density in physics is a function in the space just in question (e.g., mass density, neutron flux density). The common abbreviation *pdf* is not used since it can easily be misunderstood as an operator symbol like *sin* or *lim*. The *probability density function of the Gaussian normal probability distribution* is abbreviated by *Gaussian density* or simply by GD. The functions F_Z, f_Z and p_Z of the same random variable Z are taken as alternative, equivalent representations of the (generic) distribution of Z (see also subsection 5.4).

2.2 Distributions for estimating physical quantities

A random variable Z, called an *estimator*, is assigned to every particular physical quantity involved. Its values z (or ζ) are *estimates* of the physical quantity. Only for brevity and convenience, the quantity and its estimator are denoted by the same symbol Z if suitable and not otherwise stated, although they are not identical and should be distinguished as corresponding physical and mathematical entities, respectively. In this way, for instance, "estimator R of the count rate" can be shortened to "count rate R" although the count rate is not a random variable if the count rate is taken as a physical quantity with a fixed *true value* to be determined.

The symbol $f = f_Z(z \mid \mathbf{a})$ of the estimator Z represents the probability density of an estimate z as the true value of the physical quantity on the information $\mathbf{a}$. The estimate z is therefore also taken as a *possible true value* if $f > 0$ for z. An already known or assumed f used as a computation input is called a *prior*. It is stressed again that in BSt applied here to metrology, a distribution is in most cases a probability density f in a degree-of-belief sense and represents the information about the physical quantity actually present and taken into account. Such a distribution is not that of values which occur in measurements repeated many times under identical or similar nominal conditions as in CSt. However, CSt frequency distributions may also be involved, for instance, the Poisson distribution in counting measurements.

In order to define the characteristic values in measurements of ionizing radiation, a non-negative particular physical quantity Y, called the *measurand*, is considered that quantifies the radiation effect of interest and assumes the true value 0 if the effect is not present. This measurand is the very quantity for which the true value and the characteristic values are to be determined. An estimator, also denoted by Y, with values y (or η) and with a density $f_Y = f_Y(y \mid \mathbf{a})$ is assigned to the measurand. The characteristic values are based on this density (see section 4). The measurand Y depends on several

input quantities $\mathbf{X}$. This is expressed by the model equation $Y = G(\mathbf{X})$. The joint input density $f_{\mathbf{X}} = f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{a})$ is needed to form f_Y by *distribution propagation* treated in subsection 2.3. It is established by methods described in section 3.

2.3 Distribution propagation

Estimator sets $\mathbf{X}$ and $\mathbf{Y}$ of the physical *input* and *output quantities* involved are considered together with their values $\boldsymbol{\xi}$ and $\boldsymbol{\eta}$, respectively. Their joint densities based on information sets $\mathbf{a}$ and $\mathbf{a}'$, respectively, meet the product rule

$$f_{\mathbf{X},\mathbf{Y}}(\boldsymbol{\xi}, \boldsymbol{\eta} \mid \mathbf{a}, \mathbf{a}') = f_{\mathbf{Y}}(\boldsymbol{\eta} \mid \mathbf{X} = \boldsymbol{\xi}, \mathbf{a}')\, f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{a})\,. \tag{1}$$

This rule follows from the first equation of the general probability product rule $\Pr(A \cap B) = \Pr(A \mid B)\Pr(B) = \Pr(B \mid A)\Pr(A)$ for random events (sets) A and B. In many cases, the set $\mathbf{a}$ mainly contains the input data information and the set $\mathbf{a}'$ the relations between $\mathbf{X}$ and $\mathbf{Y}$, i.e. the model information, and further, updating data. The first density on the right-hand side of equation (1) is therefore sometimes called the *model prior* and the second one the *(data) prior* or *input density* although the different kinds of information cannot always be strictly separated. The sets $\mathbf{a}$ and $\mathbf{a}'$ need not be disjoint. The *output density* of $\mathbf{Y}$ on the combined information $\mathbf{a}$ and $\mathbf{a}'$ is the density of interest. It is also called the *posterior* and is obtained from equation (1) by a *marginalization*:

$$f_{\mathbf{Y}}(\boldsymbol{\eta} \mid \mathbf{a}, \mathbf{a}') = \int f_{\mathbf{X},\mathbf{Y}}(\boldsymbol{\xi}, \boldsymbol{\eta} \mid \mathbf{a}, \mathbf{a}')\, \mathrm{d}\boldsymbol{\xi} = \int f_{\mathbf{Y}}(\boldsymbol{\eta} \mid \mathbf{X} = \boldsymbol{\xi}, \mathbf{a}')\, f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{a})\, \mathrm{d}\boldsymbol{\xi}\ . \tag{2}$$

Some important required formulas are derived in the following from the posterior by application, together with equation (1), to some particular model priors $f_{\mathbf{Y}}(\boldsymbol{\eta} \mid \mathbf{X} = \boldsymbol{\xi},\ \mathbf{a}')$ in the integrand. These densities represent the *model relations*, which form $\mathbf{a}'$ and have to be observed between the physical quantities involved (and the corresponding estimators). Model relations $M_i(\mathbf{X}, \mathbf{Y}) = 0$ or ≥ 0 are considered. They may also depend on data contained in the information sets. The model priors are expressed by $C_i\, \delta(M_i)$ for $M_i(\boldsymbol{\xi}, \boldsymbol{\eta}) = 0$ or $C_i\, H(M_i)$ for $M_i \geq 0$ with suitable constants C_i. If there are several model relations to be observed in a particular case, then the corresponding priors must be multiplied to form the total model prior. The priors considered are based on the *Heaviside unit step function* $H(t) = 1$ $(t \geq 0)$ and $H(t) = 0$ $(t < 0)$. The derivative $\delta(t) = \mathrm{d}H(t)/\mathrm{d}t$ is called the *Dirac delta function*. It has the properties $\delta(t) = 0$ $(t \neq 0)$ and $\int_{\mathbf{R}} \delta(t) g(t)\, \mathrm{d}t = g(0)$ or $= 0$ for any function $g(t)$ and any region $\mathbf{R}$ if $0 \in \mathbf{R}$ or $0 \notin \mathbf{R}$, respectively. $\delta(t)$ and $H(t)$ are the density and the distribution function of a random variable, respectively, which can only apply the value $t = 0$ with the probability 1. t may also be a vector. See also subsection 5.4.

The dependence of the measurand Y on several input quantities $\mathbf{X}$ is expressed by the model equation $M = Y - G(\mathbf{X}) = 0$ or $Y = G(\mathbf{X})$. The input density $f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{a})$ together with the model prior $f_Y(y \mid \mathbf{X} = \boldsymbol{\xi}, y = G(\boldsymbol{\xi})) = C\, \delta(y - G(\boldsymbol{\xi}))$, where the information $\mathbf{a}'$ is formed by the relation $y = G(\boldsymbol{\xi})$, then yield according to equations (1) and (2) the posterior

$$f_Y(y \mid \mathbf{a}) = \int \delta(y - G(\boldsymbol{\xi}))\, f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{a})\, \mathrm{d}\boldsymbol{\xi}\ ;\ \ F_Y(y \mid \mathbf{a}) = \int H(y - G(\boldsymbol{\xi}))\, f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{a})\, \mathrm{d}\boldsymbol{\xi}\ . \tag{3}$$

$C = 1$ is obtained by normalization. The model function G may also depend on the information $\mathbf{a}$, for instance, on the uncertainties involved in spectrum unfolding. Equation (3) is called the *Markov formula*. It is the well-known, basic equation of *distribution propagation* [26] or transformation from $\mathbf{X}$ to Y in probability theory.

Particular estimates y of the measurand Y may be negative when obtained from measurement data or generated by MC, but only the estimates $y \geq 0$ are possible true values of the non-negative measurand. In most cases, this knowledge is not taken into account in $\mathbf{a}$ and, thus, then requires an update. This is done by introducing the additional model relation $M' = Y \geq 0$ and the corresponding model prior $f_Y(y \mid y \geq 0) = C\,H(y)$, which has to be multiplied by the delta function in equation (3) to form the total model prior. However, $H(y)$ does not depend on $\boldsymbol{\xi}$ and can thus be moved to the front of the integral. In this way, the posterior

$$f_Y(y \mid \mathbf{a}, y \geq 0) = H(y)\, f_Y(y \mid \mathbf{a}) \,/\, I_0 \;\; ; \quad I_0 = \int_0^\infty f_Y(y \mid \mathbf{a})\, \mathrm{d}y = 1 - F_Y(0 \mid \mathbf{a}) \tag{4}$$

of the possible true measurand values on the combined information easily follows from equation (3). The normalization constant $C = 1/I_0$ is obtained. See also the paragraph between equations (8) and (9) for a derivation of equation (4) from the *principle of maximum entropy* (PME).

Other formulas, better suited for MC application than equation (3), follow from equations (3) and (4), for example,

$$F_Y(y \mid \mathbf{a}, y \geq 0) = \frac{1}{I_0} \int_{\mathbf{R}} f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{a})\, \mathrm{d}\boldsymbol{\xi} \;\; ;$$

$$\mathbf{R} = \{\boldsymbol{\xi} \mid 0 \leq G(\boldsymbol{\xi}) \leq y\} \;\; ; \quad I_0 = \int_{G(\boldsymbol{\xi}) \geq 0} f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{a})\, \mathrm{d}\boldsymbol{\xi} \;\; . \tag{5}$$

2.4 Information modification

It may be asked why the condition $y \geq 0$ is not taken as included in the information set $\mathbf{a}$ from the beginning but is later added to form $f_Y(y \mid \mathbf{a}, y \geq 0)$. The reason is that $\mathbf{a}$ may or should contain a primary estimate y_0 of the measurand and the associated standard uncertainty $u(y_0)$, both are obtained, as a first step towards the characteristic values, from an evaluation of measurements according to GUM [2] where the condition $y \geq 0$ is in most cases not taken into account and y_0 may become negative. Then (and only then), the condition must subsequently be observed. The model function G can be used to determine the primary estimate $y_0 = G(\mathbf{x}_0)$ from the available data $\mathbf{x}_0$ of the input quantities $\mathbf{X}$. A primary estimate y_0 is also needed for the decision on whether or not the radiation effect in question, quantified by the measurand Y, is recognized as present, for instance, the radiation of a measured, possibly radioactive sample. This decision has to be made by comparing y_0 with the decision threshold y^* (see subsection 4.4).

Unfortunately, not all the necessary elements of the set $\mathbf{a}$ are available in the situation where the decision threshold and the detection limit are to be determined. For instance,

the result of a gross-effect radiation measurement is missing in this case since the decision threshold and the detection limit, as characteristics of the measurement procedure, should be known *before* the first gross-effect measurement is carried out. A suitable true measurand value $\widetilde{y} \geq 0$ is then assumed for an indirect compensation, and $\mathbf{a}$ is replaced by $\widetilde{\mathbf{a}}(\widetilde{y})$. This function transforms the present information for a chosen $\widetilde{y}$. Thus this means a modified $\mathbf{a}$, which would be *obtained from the measurement to be carried out* if the true measurand value $\widetilde{y}$ is assumed. This *assumed true measurand value* $\widetilde{y}$ is neither the true measurand value itself nor an estimate of it but can freely be chosen. The function $\widetilde{\mathbf{a}}(\widetilde{y})$ is a generalization of the uncertainty function $\widetilde{u}(\widetilde{y})$ introduced in ISO 11929 [1]. At least a reasonable approximation of $\widetilde{\mathbf{a}}(\widetilde{y})$ must be available, but it is not easy to establish this function in practice.

If the gross-effect value, say x_1, of a radiation measurement is not available, y is replaced by $\widetilde{y}$ in the model equation $y = G(\mathbf{x})$ and this equation is solved for x_1 resulting in $x_1 = L(\widetilde{y}, x_2, \ldots)$ with some function L. This x_1 is then used to form $\widetilde{\mathbf{a}}(\widetilde{y})$ and the density $f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y}))$ in analogy to $\mathbf{a}$ and $f_Y(y \mid \mathbf{a})$, respectively. For instance, if $\mathbf{a} = \{x_1, x_2, \ldots\}$, then $\widetilde{\mathbf{a}}(\widetilde{y}) = \{L(\widetilde{y}, x_2, \ldots), x_2, \ldots\}$. Or $\mathbf{a} = \{y_0, u(y_0)\}$ in ISO 11929 [1], with y_0 not yet available, becomes $\widetilde{\mathbf{a}}(\widetilde{y}) = \{\widetilde{y}, \widetilde{u}(\widetilde{y})\}$. Not only x_1 but also the whole $\mathbf{x}$ can be influenced by $\widetilde{y}$ as in the case of spectrum unfolding. For more examples, see reference [25]. Alternatively, x_1 can be obtained more easily without the function L by varying x_1 until $G(\mathbf{x}) = \widetilde{y}$ with an assumed $\widetilde{y}$ (for instance, $\widetilde{y} = 0$ for the decision threshold). This can be carried out iteratively, e.g., by the regula falsi.

The measurand of one of the simplest realistic radiation measurements is a net count rate $Y = R_\mathrm{n} = G(X_1, X_2) = X_1 - X_2$ given as the difference of a gross count rate $X_1 = R_\mathrm{g}$ with the estimate $x_1 = n_\mathrm{g}/t_\mathrm{g}$ and a background count rate $X_2 = R_0$ with the estimate $x_2 = n_0/t_0$ (see also subsection 5.7). Independent Poisson processes are assumed for counting n_g and n_0 pulses during the measuring times t_g and t_0, respectively. Then, $y_0 = x_1 - x_2 = n_\mathrm{g}/t_\mathrm{g} - n_0/t_0$ and $u^2(y_0) = u^2(x_1) + u^2(x_2) = x_1/t_\mathrm{g} + x_2/t_0 = n_\mathrm{g}/t_\mathrm{g}^2 + n_0/t_0^2$ are obtained. However, n_g is not available before the gross effect measurement is carried out. Instead, y_0 is replaced by the assumed $\widetilde{y}$ and the expression for y_0 is solved for x_1 leading to $x_1 = \widetilde{y} + n_0/t_0$ and, finally, by inserting x_1 into the expression for $u^2(y_0)$ to

$$\widetilde{u}^2(\widetilde{y}) = \frac{\widetilde{y} + n_0/t_0}{t_\mathrm{g}} + \frac{n_0}{t_0^2} \quad . \tag{6}$$

Accordingly, $\widetilde{u}^2(\widetilde{y})$ is a linear function of $\widetilde{y}$. In other cases often encountered, also terms with $\widetilde{y}^2$ occur which are caused by calibration or similar influence factors [1].

It is often sufficient to use as an approximation of the function $\widetilde{\mathbf{a}}(\widetilde{y})$ an interpolation of the sets $\mathbf{a}_j$ belonging to the results y_j from some previous measurements of the same kind carried out on samples with differing activities, but in other respects as far as possible under similar conditions. One of these measurements can be a background or blank measurement with $y_j = 0$. The measurement just carried out can be taken as another one with $y_j = y_0$. The values y_j serve as the interpolation abscissas of the variable $\widetilde{y}$. Since $\widetilde{u}^2(\widetilde{y})$ is often a second-order polynomial of $\widetilde{y}$, three interpolation abscissas will be sufficient in such cases.

3. Establishing distributions

3.1 PME and Bayes and expansion theorems

In order to establish the posterior of Y needed for the calculation of the characteristic values, the input density $f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{a})$ according to equations (3) to (5) has to be formed. This task is described in detail in the GUM supplement [26] and in the Bayesian theory of measurement uncertainty [14, 15]. A short introduction will thus suffice here.

The density $f = f_{\mathbf{Z}}(\boldsymbol{\zeta} \mid \mathbf{a})$ of any random variables $\mathbf{Z}$ can in general be obtained from any actually available information $\mathbf{a}$ by using the *principle of maximum (information) entropy* (PME) [10–15] or other tools of probability theory such as the *Bayes theorem* or the *expansion theorem*. For a derivation of the PME, see appendix A.2. The PME is a fundamental principle added to BSt. It plays a part similar to other famous variational principles in physics such as that of extremal action. Its importance should therefore not be underestimated. The Bayes and expansion theorems can be applied to include known frequency or parameter distributions, respectively. If possible and suitable, the above-mentioned methods can be applied alternatively, in combination, or in succession. If two of them are in fact alternatively applicable in a particular case, then their results f must be identical provided that equivalent information is analogously and correctly taken into account (see appendix A.3).

The PME consists in choosing as $f = f_{\mathbf{Z}}(\boldsymbol{\zeta} \mid \mathbf{a})$ the most likely density by taking into account relevant information available as so-called *constraints* and maximizing the entropy

$$S = -\int_{\mathbf{R}} f \, \ln(f/f_0) \, \mathrm{d}\boldsymbol{\zeta} = \max \tag{7}$$

by applying a variational method. $\mathbf{R}$ is the region of all possible values $\boldsymbol{\zeta}$ of $\mathbf{Z}$ (where $f_0 > 0$). The function $f_0 = f_{0,\mathbf{Z}}(\boldsymbol{\zeta})$ is the *prior*, the density of $\mathbf{Z}$ based on the information already known and included before the new information $\mathbf{a}$, represented by the constraints, became available. If nothing was known before, then the prior is uniform according to the *Bernoulli principle* (see subsection 5.5). Only this case is assumed by the PME application of the GUM supplement [26 (6.3.2)]. It is stressed once more that this solution of the PME depends essentially on the—nearly always incomplete—information available and taken into account. There is thus no "true" distribution in BSt.

If constraints $\mathrm{E}\,(g_i(\mathbf{Z})) = d_i$ have to be met by given, linearly independent functions $g_i(\mathbf{Z})$ and data d_i, then the maximization can be carried out by the Lagrange method (see any textbook on variational methods, e.g., reference [32]) and results for $\boldsymbol{\zeta} \in \mathbf{R}$ in

$$f_{\mathbf{Z}}(\boldsymbol{\zeta} \mid \mathbf{a}) = C \, f_{0,\mathbf{Z}}(\boldsymbol{\zeta}) \, \exp\Big(-\sum_i \mu_i g_i(\boldsymbol{\zeta}) \Big) \ . \tag{8}$$

The density $f = f_{\mathbf{Z}}(\boldsymbol{\zeta} \mid \mathbf{a})$ vanishes outside $\mathbf{R}$. The normalization constant C and the *Lagrange multipliers* μ_i have to be determined from the normalization condition

of a density and the constraints. The normalization condition can also be taken as a constraint with $i = 0$; $g_0(\mathbf{Z}) = 1$; $d_0 = 1$ and $C = \exp(-\mu_0)$.

If there are no constraints, then $f = Cf_0$ inside $\mathbf{R}$ and $f = 0$ outside $\mathbf{R}$. This leads to equation (4) with $\mathbf{Z} = Y$; $\boldsymbol{\zeta} = y$; $\mathbf{R} = \{y \mid y \geq 0\}$; $f = f_Y(y \mid \mathbf{a}, y \geq 0)$, and the prior $f_0 = f_Y(y \mid \mathbf{a})$, which is taken as already known and updated by equation (4) for the condition $y \geq 0$.

If, in particular, $\mathbf{Z} = \mathbf{X}$ and only the expectation $\mathrm{E}(\mathbf{X}) = \mathbf{x}$ and the non-singular (positive definite) uncertainty (covariance) matrix $\mathbf{U_x}$ associated with $\mathbf{x}$ are known and taken into account such that $\mathbf{a} = \{\mathbf{x}, \mathbf{U_x}\}$ and, moreover, the prior is uniform and $\mathbf{R}$ is the whole ν-dimensional $\mathbf{X}$-space, then a Gaussian density (GD) f is obtained:

$$f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{x}, \mathbf{U_x}) = \frac{\exp\left(-\frac{1}{2}(\boldsymbol{\xi}-\mathbf{x})^\top \mathbf{U_x}^{-1}(\boldsymbol{\xi}-\mathbf{x})\right)}{\sqrt{(2\pi)^\nu \det \mathbf{U_x}}} \quad . \tag{9}$$

In this case, $f_Y(y \mid \mathbf{a})$ according to equation (3) is also a GD if $G(\mathbf{X})$ is a linear function.

The also important Bayes theorem in the form

$$f_{\mathbf{Z}}(\boldsymbol{\zeta} \mid \mathbf{v})\, f_{\mathbf{V}}(\mathbf{v}) = f_{\mathbf{V}}(\mathbf{v} \mid \boldsymbol{\zeta})\, f_{1,\mathbf{Z}}(\boldsymbol{\zeta}) \tag{10}$$

follows from the second equation of the general product rule below equation (1) and can be applied if a (frequency) density $f_{\mathbf{V}}(\mathbf{v} \mid \boldsymbol{\zeta})$ of random variables $\mathbf{V}$ with values $\mathbf{v}$, being parts of the information $\mathbf{a}$, and the prior $f_1 = f_{1,\mathbf{Z}}(\boldsymbol{\zeta})$ are available from previous measurements, experience, or reasonable assumptions. Since $\mathbf{v}$ is fixed, $f_{\mathbf{V}}(\mathbf{v})$ is a constant $1/C$. The subscript 1 in equation (10) only indicates that the prior f_1 can differ from f_0 in the PME according to equations (7) and (8). Hence it follows

$$f_{\mathbf{Z}}(\boldsymbol{\zeta} \mid \mathbf{v}) = C\, f_{\mathbf{V}}(\mathbf{v} \mid \boldsymbol{\zeta})\, f_{1,\mathbf{Z}}(\boldsymbol{\zeta}) \tag{11}$$

where C acts as the normalization constant. This density can be taken as the final f if no further information such as $\mathbf{R}$ or constraints has to be included. Otherwise, it must be used as the prior f_0 of the PME. In equation (11), the factor $C\, f_{\mathbf{V}}(\mathbf{v} \mid \boldsymbol{\zeta})$, taken as a function of $\boldsymbol{\zeta}$ but not as a density of $\mathbf{V}$, is called the *likelihood*. It is an analogue to the factor $C\exp(\ldots)$ of equation (8).

An example of the likelihood is C times the Poisson frequency distribution $f_{\mathbf{V}}(\mathbf{v} \mid \boldsymbol{\zeta}) = p_N(n \mid \varrho)$, taken as a function of ϱ, with the counting variable $\mathbf{V} = N$, its recorded value $\mathbf{v} = n$, and the expectation $\mathrm{E}(N) = \varrho t$. Here, $\boldsymbol{\zeta} = \varrho$ is the possible true value of the count rate $\mathbf{Z} = R$ to be determined and t is the duration of the measurement. The density $f_{\mathbf{Z}}(\boldsymbol{\zeta} \mid \mathbf{v}) = f_R(\varrho \mid n)$ becomes a gamma density if, for instance, the prior $f_{1,\mathbf{Z}}(\boldsymbol{\zeta}) = f_R(\varrho) = H(\varrho)$ is applied since $\varrho \geq 0$ (see also equation (4) and subsection 5.7). Although $p_N(n \mid \varrho) = \Pr(N = n \mid R = \varrho)$ is not a probability density but a probability function since N is a discrete random variable, this does not matter in the Bayes theorem.

The expansion theorem, also called the *theorem of total probability*, reads

$$f_{2,\mathbf{Z}}(\boldsymbol{\zeta}) = \int f_{\mathbf{Z}}(\boldsymbol{\zeta} \mid \mathbf{w})\, f_{\mathbf{W}}(\mathbf{w})\, \mathrm{d}\mathbf{w} \quad . \tag{12}$$

It follows from the general probability expansion rule $\Pr(A) = \sum_i \Pr(A \mid B_i)$ for random events (sets) A and alternative events B_i if exactly one of the B_i occurs in each trial. Its output density f_2 can be taken as the final f if the densities of the integrand, which depend on values $\mathbf{w}$ of parameters $\mathbf{W}$, are given, for instance, as results from the PME or as priors. $f_{\mathbf{W}}(\mathbf{w})$ can also express a density of weights assigned to the values $\mathbf{w}$. The expansion theorem can be obtained by a marginalization similar to equations (1) and (2).

3.2 Additional remarks

There are cases where an update has to be made for new, additional information on the measurand. This can be done in several ways depending on the kind of information:

(a) The model equations can be refined by introducing new input quantities X_i. e.g., influence quantities, if the information refers to these quantities.

(b) The PME can be applied if the new information refers to the region $\mathbf{R}$ of the possible true values of the measurand or to the constraints. Then, the old density f has to be used as the prior f_0.

(c) A distribution of a quantity Z, e.g., a prior, which will be more reasonable than a first one assumed such as a uniform prior over an interval, can be established by *Bayesian updating* [12] if a pool of comparable data z_k $(k = 1, \ldots, M)$ from previous, similar measurements is available. The improved distribution is then obtained, for instance, by fitting a suitably assumed function to the data [33]. These data, ordered by magnitude and renumbered as $z^{(k)}$, can also be used like MC samples $y^{(k)}$ [25]. A suitably assumed inverse distribution function fitted to the M points $(k/M, z^{(k)})$ can be advantageous (see appendix B).

(d) If a new prior, possibly improved according to (c), of the measurand or of a parameter or a distribution of weights has to be taken into account, then either the product rule according to equation (1) or the Bayes or expansion theorems according to equations (11) and (12) can be applied.

If the ν input components X_i of $\mathbf{X}$ are known to be independent random variables or if nothing is known about their mutual dependence, then $f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{a}) = \prod_{i=1}^{\nu} f_{X_i}(\xi_i \mid \mathbf{a}_i)$ with $\mathbf{a} = \{\mathbf{a}_1, \ldots, \mathbf{a}_\nu\}$. In multi-channel spectrum unfolding, all the $f_{X_i}(\xi_i \mid \mathbf{a}_i)$ are gamma distribution densities of the count rates $X_i = R_i$ and $\xi_i = \varrho_i$ with $\mathbf{a}_i = n_i$.

According to the *central limit theorem* of probability theory, the posterior $f_Y(y \mid \mathbf{a})$ becomes in most cases, but with some exceptions, an approximation of a GD even if $f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{a})$ is non-Gaussian. But the expectations $\mathbf{x}$ and the uncertainty matrix $\mathbf{U}_{\mathbf{x}}$ of $\mathbf{X}$ must exist and none of the ν input quantities X_i should strongly dominate by uncertainty. There should be more than only a few dimensions ν, but ν need not necessarily be a large number. However, if ν tends to infinity as in multi-channel spectrum unfolding, then the expectation $\mathrm{E}(Y)$ and the variance $\mathrm{Var}(Y)$ should remain finite. Otherwise, if $\mathrm{E}(Y) \to \infty$ or $\mathrm{Var}(Y) \to \infty$ or 0, then a standardization by the substitution $Y' = (Y - \mathrm{E}(Y))/\sqrt{\mathrm{Var}(Y)}$ can help to see whether or not an approximation of a standardized GD is involved. Moreover, the model function $G(\mathbf{X})$ must be sufficiently

linear in a neighbourhood of $\mathbf{x}$ determined by the condition $(\boldsymbol{\xi} - \mathbf{x})^\top \mathbf{U}_\mathbf{x}^{-1} (\boldsymbol{\xi} - \mathbf{x}) <\approx \nu$ (second-order loss function, see subsection 5.6). If all these conditions are (nearly) met and, accordingly, $f_Y(y \mid \mathbf{a})$ is (approximately) a GD, then ISO 11929 can be applied directly. This is an important result for many cases, especially for spectrum unfolding. It also shows the prominence of the GD in measurement evaluation (see also subsection 5.3).

Nevertheless, one should be cautious. If $f_Y(y \mid \mathbf{a})$ can indeed be well approximated by a GD, this applies mainly to the bulk of the density, but not necessarily to the tails, which play a prominent part in the important integrals I_4 to I_7 used for the definitions of the characteristic values since the probabilities α, β, and γ are commonly specified as small numbers. The same applies to the integral I_3 if $\widehat{y} \gg u(\widehat{y})$. (For the integrals, see also subsection 5.7 below equation (34). The quantities used in the present paragraph are introduced in section 4.)

There are cases where the PME seems to have no solution [34]. Let, for instance, an estimate x (expectation) and the associated standard uncertainty $u(x)$ (standard deviation) be given for a measurand X known to be valued in some interval between a and $b > a$. If x is not contained in the interval or $u(x) > b - a$, then, indeed, there is no solution from the PME for the density $f = f_X(\xi \mid x, u(x), a, b)$ to be determined. What does this mean? It merely indicates that there is something wrong with the information. The information is contradictory or badly interpreted. This should give an incentive to carefully inspect the measurement and the data evaluation in order to find the reason for the inconsistency. The first question should be: How are x and $u(x)$ obtained from what information? Suppose, for instance, that x and $u(x)$ are determined from measurement data v_i according to GUM [2] as the arithmetic mean and the empirical standard deviation (type-A evaluation of measurement uncertainty [28 (2.28)]), respectively. The interval information a and b has not yet been used. Thus, x and $u(x)$ do *not* belong to the density f but to a density $f_0 = f_X(\xi \mid x, u(x))$! GUM does not provide this density but f_0 can be reconstructed by the PME with a uniform prior and turns out to be the GD $f_0 = \exp(-(\xi - x)^2/(2u^2(x)))/\sqrt{2\pi u^2(x)}$. This density must now be subsequently updated for the additional interval information to form the final density f. This can again be done by the PME, but f_0 must now act as the prior since it represents the knowledge already taken into account. Then, equation (7) has to be solved for f with $\mathbf{Z} = X$; $\boldsymbol{\zeta} = \xi$ and $\mathbf{R} = \{\xi \mid a \leq \xi \leq b\}$ and with the normalization condition only. Equation (8), where the sum now vanishes, yields $f = Cf_0$ for $\xi \in \mathbf{R}$ and $f = 0$ elsewhere. Thus, f_0 is truncated at a and b and renormalized to form f. There is always a solution f. Naturally, with f and according to section 4, the "best" estimate now turns out to be $\widehat{x} = \mathrm{E}(X) \neq x$ with $a \leq \widehat{x} \leq b$ and $u(\widehat{x}) = \sqrt{\mathrm{Var}(X)} \leq \min(u(x), b-a)$. All possible coverage intervals are contained in the interval between a and b. The prior f_0 introduced in the PME here reasonably eliminates the difficulty. The example treated here is similar to subsequently taking into account the condition $y \geq 0$ for a non-negative measurand Y as is shown below equation (8). In this case, $a = 0$ and $b = \infty$.

4. Definitions of the characteristic values

4.1 Preliminary remarks

In many cases, the functional values of the estimator densities cannot be explicitly calculated for particular argument values y, since the analytic formulas or algorithms

required for solving the complicated integrals in equation (3) are often missing. Only argument values can be obtained by MC sampling from a preceding probability analysis according to references [14, 15, 26]. This is the reason why the following integrals of the densities then need to be calculated by MC and not more easily by the Simpson or similar numerical integration methods [35, 36] (see also subsection 6.5).

The preceding paragraph does not apply to ISO 11929 [1], where the estimator densities are taken as Gaussian ones and thus MC need not be used. However, the following more general mathematical definitions of the characteristic values are stipulated in accordance with ISO 11929.

The best estimate of the measurand, the standard uncertainty associated with this best estimate, and the lower and upper limits of the coverage interval are defined in the following by means of moments and quantiles of the densities $f_Y(y \mid \mathbf{a})$ and $f_Y(y \mid \mathbf{a}, y \geq 0)$. The definitions of the decision threshold and the detection limit are similarly based on the density $f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y}))$ with different assumed true measurand values $\widetilde{y}$. The *p-quantile* of a density $f_Z(\zeta)$ is the upper integral limit q in the equation $\int_{-\infty}^{q} f_Z(\zeta)\,\mathrm{d}\zeta = F_Z(q) = \Pr(Z \leq q) = p$ with the given probability p. The particular probabilities α and β of the *false positive and negative decisions*, respectively,—formerly called the *errors of the first and second kind*—and the *coverage probability* $(1 - \gamma)$ used in the following have to be specified. For I_0, see equation (4). For illustrations of the densities and the characteristic limits, see figures 1 and 2.

Although the integrals of equations (4) and (13) to (16) refer to the density $f_Y(y \mid \mathbf{a}, y \geq 0)$, only the function $f_Y(y \mid \mathbf{a})$ is needed for numerical calculations.

It is pointed out again that the best estimate, the standard uncertainty and the limits of a coverage interval are characteristic values of a possibly radioactive sample whereas the decision threshold and the detection limit are those of the measurement procedure and do not depend on the sample radiation.

4.2 Best estimate and standard uncertainty

The *best estimate* $\widehat{y}$ of the measurand Y is the expectation of the density $f_Y(y \mid \mathbf{a}, y \geq 0)$:

$$\widehat{y} = \mathrm{E}(Y \mid \mathbf{a}, y \geq 0) = I_1 / I_0 \;\; ; \quad I_1 = \int_0^\infty y\, f_Y(y \mid \mathbf{a})\,\mathrm{d}y \;\; . \tag{13}$$

The *standard uncertainty* $u(\widehat{y})$ of the measurand associated with $\widehat{y}$ is the standard deviation of the density $f_Y(y \mid \mathbf{a}, y \geq 0)$:

$$u(\widehat{y}) = \sqrt{\mathrm{Var}(Y \mid \mathbf{a}, y \geq 0)} = \sqrt{I_2 / I_0 - \widehat{y}^2} \;\; ; \quad I_2 = \int_0^\infty y^2\, f_Y(y \mid \mathbf{a})\,\mathrm{d}y \;\; . \tag{14}$$

The measurement uncertainty $u(y)$ associated with an arbitrary estimate y is in general given by $u(y) = \sqrt{\mathrm{E}((Y - y)^2)}$ [14, 15] where $\mathrm{E}((Y - y)^2)$ is the non-central second-order moment with respect to y. Accordingly, $u(y)$ assumes with $y = \mathrm{E}(Y)$ its minimum value, the standard deviation $\sqrt{\mathrm{Var}(Y)}$ of Y, also called the *standard uncertainty* [28 (2.30)]. The expectation $\mathrm{E}(Y)$ is therefore taken as the "best" estimate $\widehat{y}$

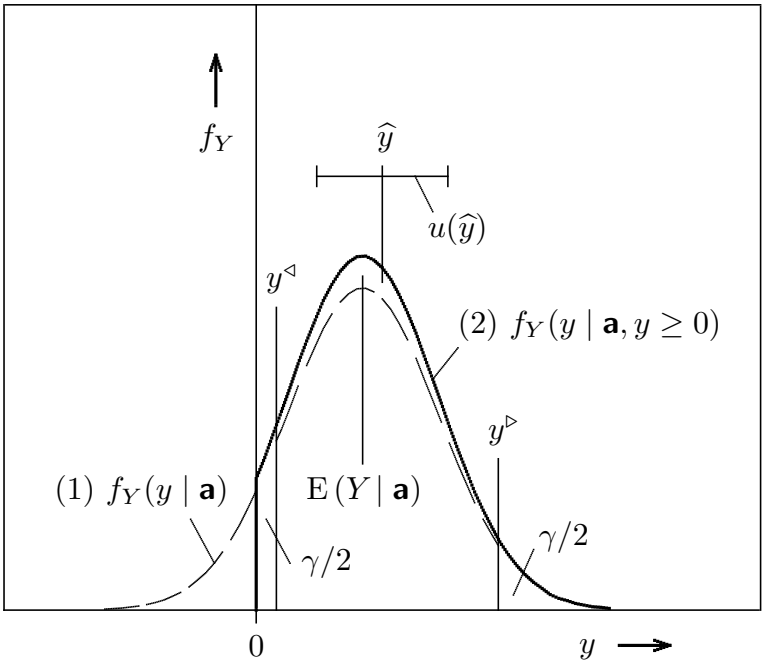

Figure 1: Illustration of the best estimate $\widehat{y}$ (expectation of density (2)) of a non-negative measurand Y with the associated standard uncertainty $u(\widehat{y})$ (standard deviation), and the limits $y^{\triangleleft}$ and $y^{\triangleright}$ of the probabilistically symmetric coverage interval that covers the true measurand value with the probability $1-\gamma$. The dashed line represents the density (1) of the possible true measurand values y, based on the available information **a** *(from the measurement evaluated according to GUM [2]). By adding the condition $y \geq 0$ to* **a**, *the density (1) is truncated at $y = 0$ and renormalized to form the bold-face density (2). This leads to $y^{\triangleleft} \geq 0$.*

of the measurand Y and, together with the associated standard uncertainty $u(\widehat{y})$, as the *(complete) measurement result* [28 (2.9)]. For other proposals of the best estimate, see subsection 6.2. For the reason why uncertainty is defined by a second-order loss function, see subsection 5.6.

4.3 Coverage intervals

The *lower limit $y^{\triangleleft}$ of the coverage interval* is the $(\gamma/2)$-quantile of the density $f_Y(y \mid \mathbf{a}, y \geq 0)$:

$$F_Y(y^{\triangleleft} \mid \mathbf{a},\, y \geq 0) = \gamma/2 = I_3 \,/\, I_0 \;\; ;$$

$$I_3 = \int_0^{y^{\triangleleft}} f_Y(y \mid \mathbf{a})\,\mathrm{d}y = F_Y(y^{\triangleleft} \mid \mathbf{a}) - F_Y(0 \mid \mathbf{a}) \;\; . \tag{15}$$

The *upper limit $y^{\triangleright}$ of the coverage interval* is the $(1-\gamma/2)$-quantile of the density $f_Y(y \mid \mathbf{a}, y \geq 0)$:

$$1 - F_Y(y^{\triangleright} \mid \mathbf{a}, y \geq 0) = \gamma/2 = I_4 \,/\, I_0 \;\; ;$$

$$I_4 = \int_{y^{\triangleright}}^{\infty} f_Y(y \mid \mathbf{a})\,\mathrm{d}y = 1 - F_Y(y^{\triangleright} \mid \mathbf{a}) \;\; . \tag{16}$$

The *coverage interval* [26 (3.12), 28 (2.36)] between the limits according to equations (15) and (16) contains the true value of the measurand with the specified *coverage probability* $(1-\gamma)$ [26 (3.13), 28 (2.37)]. It is identical with the *(Bayesian) confidence interval* of the references cited. However, there is a great contrast to the merely analogous *confidence interval* in CSt where, for example, the *confidence level*, which corresponds to the coverage probability in BSt, cannot be understood as a probability. The limits of the coverage interval are sometimes also called the *credible limits*. The coverage interval as defined above is *probabilistically symmetric* [26 (3.15)] as in common practice and ISO 11929 [1] for historical and practical demands. Other stipulations are possible. For the shortest coverage interval, see subsection 6.3 and appendix B. If, for instance, $\widehat{y}$ in rare cases happens not to be contained in the coverage interval, then the median m, defined by $F_Y(m \mid \mathbf{a}, y \geq 0) = 1/2$ and, thus, always contained in the coverage interval, may be taken as a reasonable estimate of the measurand, but with a larger associated uncertainty $u(m) = \sqrt{\mathrm{E}\left((Y-m)^2\right)} > u(\widehat{y})$ and other shortcomings (see subsection 6.2). If the true value 0 of the measurand is required to be contained in the coverage interval if y_0 is small, then $y^{\triangleleft} = 0$ and $y^{\triangleright}$ defined by $F_Y(y^{\triangleright} \mid \mathbf{a}, y \geq 0) = 1-\gamma$ could be stipulated (but see subsection 6.3 and appendix B). However the coverage interval is stipulated, it does not enlarge the knowledge of the measurand since all the information available and taken into account is already represented by the density $f_Y(y \mid \mathbf{a}, y \geq 0)$.

4.4 Decision threshold and detection limit

The *decision threshold* y^* is the $(1-\alpha)$-quantile of the density $f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y}=0))$ for the assumed true value $\widetilde{y} = 0$ of the measurand:

$$1 - F_Y(y^* \mid \widetilde{\mathbf{a}}(\widetilde{y}=0)) = I_5 = \int_{y^*}^{\infty} f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y}=0))\,\mathrm{d}y = \alpha \ . \tag{17}$$

The *detection limit* $y^\sharp$ is the assumed true value of the measurand if the decision threshold y^* is the β-quantile of the density $f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y}=y^\sharp))$:

$$F_Y(y^* \mid \widetilde{\mathbf{a}}(\widetilde{y}=y^\sharp)) = I_6 = \int_{-\infty}^{y^*} f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y}=y^\sharp))\,\mathrm{d}y = \beta \ . \tag{18}$$

Equations (17) and (18) also read $I_5 = 1 - P(0) = \alpha$ and $I_6 = P(y^\sharp) = \beta$, respectively, with the function $P(\widetilde{y}) = F_Y(y^* \mid \widetilde{\mathbf{a}}(\widetilde{y})) = \int_{-\infty}^{y^*} f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y}))\,\mathrm{d}y$. Possibly, equation (18) has no unique solution $y^\sharp$ or even no solution at all. Therefore, a more general mathematical definition of the detection limit is needed and could read as follows: The detection limit is the minimum true value $y^\sharp$ for which the *suitability condition* $P(\widetilde{y}) \leq \beta$ is met for all $\widetilde{y} \geq y^\sharp$. If there is no solution, then, formally, $y^\sharp = \infty$ is set. In this case, the measurement procedure needs to be improved or modified. $P(\widetilde{y})$ is assumed to be a continuous function. For more about this function, see the paragraph of equation (19).

The decision threshold y^* and the detection limit $y^\sharp$ should be known before a measurement is carried out on a sample to be tested for ionizing radiation. Thus, they are characteristics of the measurement procedure and do not depend on the particular sample. If $y_0 > y^*$ for a primary estimate y_0 from a measurement, then it is decided that the radiation effect in question, quantified by the measurand Y, is recognized as

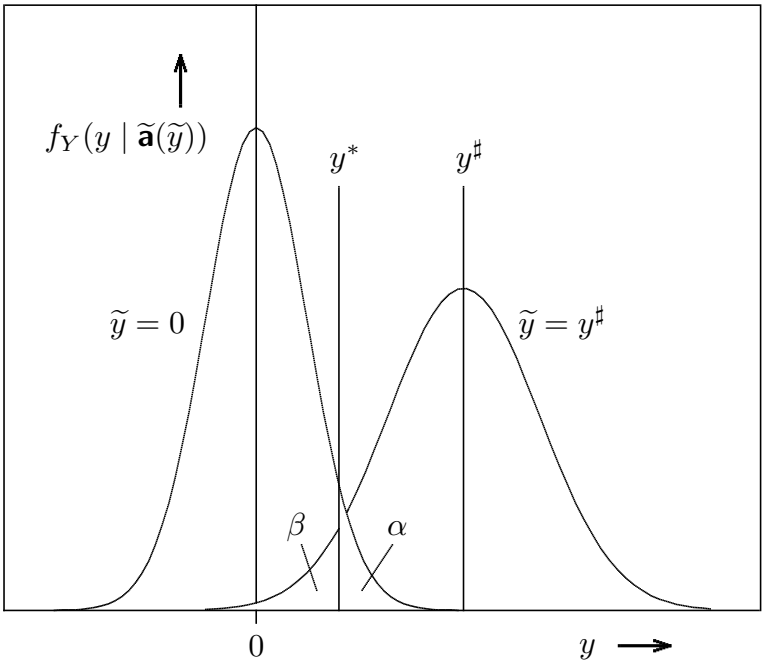

Figure 2: Illustration of the decision threshold y^* and the detection limit $y^\sharp$ of a non-negative measurand Y. The figure shows the densities $f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y}))$ of possible measurand estimates y from a measurement if the true values (expectations and parameter values) $\widetilde{y} = 0$ and $\widetilde{y} = y^\sharp$ of Y are assumed. If $y_0 > y^*$ for a particular primary estimate y_0 from a measurement, then it is decided that the radiation effect quantified by Y is recognized as present. The areas α and β below the densities on the right-hand and left-hand side of the abscissa y^* are the probabilities of false positive and negative decisions, respectively. The area α "covers" a piece of the line for $\widetilde{y} = y^\sharp$.

present. This decision is wrong and called a *false positive decision* if the radiation effect is actually absent. This case is assumed by choosing the true measurand value $\widetilde{y} = 0$. Its probability α is expressed by equation (17) (see figure 2). ISO 11929 [1] requires the best estimate $\widehat{y}$, the associated standard uncertainty $u(\widehat{y})$, and the limits $y^\triangleleft$ and $y^\triangleright$ of the coverage interval to be determined only if $y_0 > y^*$.

Notice that the condition $y \geq 0$ is not involved in the definitions of the decision threshold y^* and the detection limit $y^\sharp$ according to equations (17) and (18), respectively, since y_0, which has to be compared with y^*, is taken as obtained directly from the measurement data evaluation according to GUM [2] where the condition is ignored. Therefore, y^* must also be defined without the condition. This also applies to $y^\sharp$ since it depends on y^*. For a possible, alternatively defined decision threshold y^{**}, see subsection 6.4.

If $y^\sharp \leq y_\mathrm{r}$ with a guideline value y_r specified for scientific, legal or other demands, then it is decided that the measurement procedure is suitable for the intended measurement purpose. (For exceptional values of $y^\sharp$, see subsection 5.10.)

Assume a present radiation effect by choosing any true measurand value $\widetilde{y} > 0$. Then the decision that the radiation effect is recognized as absent—because of $y_0 \leq y^*$ —is wrong and called a *false negative decision*. The function $P(\widetilde{y})$ defined below equation

(18) is the probability of this wrong decision. It must meet the suitability condition $P(\widetilde{y}) \leq \beta$ for all $\widetilde{y} \geq y^\sharp$ (see figure 2) if $y_0 > y^*$, i.e. in the case of the decision that the radiation effect is recognized as present. For $\widetilde{y} = y_\mathrm{r} \geq y^\sharp$, in particular,

$$I_7 = P(y_\mathrm{r}) = \int_{-\infty}^{y^*} f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y} = y_\mathrm{r}))\,\mathrm{d}y \leq \beta \ . \tag{19}$$

Vice versa, if $P(\widetilde{y}) \leq \beta$ for all $\widetilde{y} \geq y_\mathrm{r}$, then $y^\sharp \leq y_\mathrm{r}$ since $y^\sharp$ is a minimum value with respect to the suitability condition. Hence it follows that the detection limit $y^\sharp$ is not needed if only the suitability decision has to be made with a given y_r. If $P(\widetilde{y})$ is known to decrease monotonely, then the condition $P(y_\mathrm{r}) \leq \beta$ is easier to test than $y^\sharp \leq y_\mathrm{r}$ and is sufficient for the suitability decision.

Since $\widetilde{y}$ is an assumed true measurand value, the expectation of the density $f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y}))$ should meet the condition

$$\mathrm{E}\,(Y \mid \widetilde{\mathbf{a}}(\widetilde{y})) = \widetilde{y} \tag{20}$$

in analogy to equation (13). Moreover, $\mathrm{Var}\,(Y \mid \widetilde{\mathbf{a}}(\widetilde{y})) = \widetilde{u}^2(\widetilde{y})$ is the squared uncertainty function $\widetilde{u}(\widetilde{y})$ used in ISO 11929 [1] and similar to equation (14).

The definitions given in equations (13) to (18) are in accordance with ISO 11929 [1], where only Gaussian densities are used for $f_Y(y \mid \mathbf{a})$ and $f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y}))$. These densities follow exactly from the PME (see section 3) if, according to GUM [2], only their expectations y_0 and $\widetilde{y}$ and standard deviations $u(y_0)$ and $\widetilde{u}(\widetilde{y})$, respectively, are taken into account as constraints and form the information sets $\mathbf{a} = \{y_0, u(y_0)\}$ and $\widetilde{\mathbf{a}}(\widetilde{y}) = \{\widetilde{y}, \widetilde{u}(\widetilde{y})\}$.

5. Justifications against criticisms

5.1 Denoting distributions

The probability density of any random variable Z is denoted by $f_Z(z)$ according to DIN 13303 [30] in reference [25] and in the present paper, but not by $f(z)$ as usually preferred. This has been criticized, but it arises from a simple reason. In fact, the more informative symbol $f_Z(z)$ for a density of a random variable Z is often abbreviated by the simpler symbol $f(z)$ in the literature for brevity and convenience. But $f(z)$ is a dangerous symbol. It is useless in general since Z and its value z are identified. Consequently, $f(t)$ would be the density of a second random variable T but not $f_Z(t)$ where the functional argument z is merely replaced by t. This has to be done, for instance, in integrals such as $F_Z(z) = \int_{-\infty}^{z} f_Z(t)\,\mathrm{d}t$. By dropping Z, the result $F(z) = \int_{-\infty}^{z} f(t)\,\mathrm{d}t$ would become erroneous. Thus, if one uses $f(z)$ as a convenient abbreviation—as is also sometimes done in the present paper—then one must explicitly explain the exact meaning of this symbol.

The more general symbol $f_Z(z \mid \mathbf{a})$ is introduced for the (conditional) probability density of any random variable Z with values z and, as the condition, with the information $\mathbf{a}$ taken into account. The information set $\mathbf{a}$ summarizes all the data, conditions, assumptions, and other relevant information given or obtained from measurements and other sources. Naturally, the data can also include values of any other random variables,

for instance, in the form $V = v$ or, for short, v alone as is usual in probability theory. This form is explicitly required in the Bayes theorem according to equation (11).

5.2 Applying Bayesian statistics

Why is Bayesian statistics (BSt) exclusively used as a basis in uncertainty theory and in the field of characteristic values in radiation measurement, particularly, in ISO 11929? Several attempts were made in the past before 1990 to apply conventional, frequency-based statistics (CSt) to measurement uncertainty, but in vain. Finally, the ISO committee working on this task was disbanded. The reason is that there are nearly always uncertain physical quantities which must be taken into account, however, do not behave randomly in repeated or counting (radiation) measurements and thus cannot be treated by CSt, for instance, influence quantities causing systematic deviations. In parallel, GUM was prepared, adopted, and first published in 1993 although it offers a theoretically unsatisfying, but practical mixture of type-A (CSt) and type-B (BSt) methods to obtain uncertainty components. The theory of measurement uncertainty [14] based entirely on BSt was published in 1992, but was too late to be included in GUM. However, BSt is used throughout as a unique statistical basis in the current revision of GUM.

5.3 Using Gaussian distributions

It was said that using the (truncated) Gaussian density (GD) nearly exclusively in ISO 11929 is not general enough. This may hold true in rare cases. But the GD plays an exceptional, dominant part since it is exact according to the PME if, as is often the case, only y_0 and $u(y_0)$ are available from GUM as input information. In many other cases, GD is the limiting distribution for long durations of measurement (see below equation (34) and reference [25]). And it is nearly always a good and very practical approximation which requires only a minimum of computational effort to obtain the characteristic values. In a revised ISO 11929, general distributions could also be treated according to reference [25] and section 4, if really necessary in practice. However, this would require a considerably greater modelling and computing effort by applying the Monte Carlo method (MC).

Another reason for the great importance of the GD is the *central limit theorem* of probability theory. This theorem states that the measurand can in most cases be assessed, at least approximately, by using a GD if the measurand depends sufficiently linearly on several input quantities in the data region of interest. The parameters of the GD can be obtained already by the methods provided by GUM. The truncated GD can be accepted as a suitable approximation even in cases of poor measurement, for instance, in the simplest case of radiation measurement under low-level circumstances where the measurand Y is a net count rate R_n to be obtained as the difference of a gross count rate R_g and a background count rate R_0 and if only very small numbers n_g and n_0 of radiation events were recorded from assumed Poisson distributions (see subsection 5.7 and reference [25]).

Finally, it is stressed that using the GD throughout in ISO 11929 is in any case not an inadmissible simplification but a suitable, pragmatic approximation for practice.

5.4 Using Dirac and Heaviside functions

The usage of the Dirac delta function $\delta(t)$ and the Heaviside unit step function $H(t)$ in the Bayesian theory of measurement uncertainty [14–18], in reference [25] and in the present paper, has been criticized. However, they are convenient auxiliary functions and suitable tools often applied in theoretical physics. They are used to express and introduce constraints, for instance, model relations. Their main properties and usage are described in subsection 2.3.

They can also be taken as densities of a random variable which can assume the value $t = 0$ only or the values $t \geq 0$ only with a uniform density, respectively. Thus, they are used and treated like other densities, for instance, as model priors in equations (2) and (3). They can also help to change the representation of a distribution since there are, for instance, the relations

$$f_Z(z) = \sum_i p_Z(z_i)\,\delta(z - z_i) \;\; ; \tag{21}$$

$$F_Z(z) = \sum_i p_Z(z_i)\,H(z - z_i) \tag{22}$$

for a discrete random variable Z, which can only assume the values z_i with the probabilities $p_Z(z_i)$.

Moreover, these tools are applied to conveniently represent alternative notations if suitable. For instance, if some function $L(t)$, given by a particular arithmetic expression $g(t)$, is known to vanish for negative t, i.e. $L(t) = 0$ for $t < 0$, then the following notations are equivalent:

$$L(t) = \left\{ \begin{array}{rl} g(t) \;\; ; & (t \geq 0) \\ 0 \;\; ; & (t < 0) \end{array} \right\} = H(t)\,g(t) \;\; ; \tag{23}$$

$$\int_{-\infty}^{\infty} L(t)\,\mathrm{d}t = \int_{0}^{\infty} L(t)\,\mathrm{d}t = \int_{-\infty}^{\infty} H(t)\,g(t)\,\mathrm{d}t \;\; ; \tag{24}$$

$$L(t') = \int_{-\infty}^{\infty} \delta(t - t')\,L(t)\,\mathrm{d}t \;\; . \tag{25}$$

Another auxiliary function $U(\mathbf{t}; \mathbf{R}) = 1$ for $\mathbf{t} \in \mathbf{R}$ and $= 0$ for $\mathbf{t} \notin \mathbf{R}$, which is uniform in a region $\mathbf{R}$, can formally be used for any function $L(\mathbf{t})$ as a tool to avoid integral limits since

$$\int_{\mathbf{R}} L(\mathbf{t})\,\mathrm{d}\mathbf{t} = \int U(\mathbf{t}; \mathbf{R})\,L(\mathbf{t})\,\mathrm{d}\mathbf{t} \;\; . \tag{26}$$

If $L(\mathbf{t}) = f_{\mathbf{T}}(\mathbf{t})$ is the density of a random variable $\mathbf{T}$, then the integrals in equation (26) are the probability of $\mathbf{T} \in \mathbf{R}$ or the expectation $\mathrm{E}\,(U(\mathbf{T}; \mathbf{R}))$.

5.5 PME and Bernoulli principle

ISO 11929 [1], reference [25] and the present paper are based on the well established Bayesian statistics in combination with the PME [10, 11], which is used for obtaining probability distributions. Bayesian statistics and PME were first applied in combination to measurement uncertainty in reference [14] in order to form a unique theoretical basis for GUM [2].

The PME is used as a necessary supplement to other methods such as the Bayes theorem. It is taken as a fundamental principle although it can also be derived (or, at least, made plausible) by limiting processes via the multinomial distribution by using the deeper *Bernoulli principle*: "Assign same probabilities to equally likely states of the physical system in question" (for instance, probability 1/2 to both sides of a coin to be tossed) (see reference [15] and appendix A.1). This is the classical understanding of probability as introduced by Bernoulli and Laplace. The Bernoulli principle can help to form the necessary prior f_0 in equation (7) at the beginning with a minimum of primary physical information about the system, e.g., natural laws, geometry, invariances and other circumstances. "Equally likely" should be understood in a very wide sense as a symmetry of the system. Symmetries are very important in theoretical physics. Accordingly, two different states of the system should be taken as equally likely if there is a physical operation which transfers one of the states to the other state without any essential physical change (for instance, a 180° rotation around an axis in the plane of the coin to be tossed). For "non-informative" priors, see references [37] and [38].

One can say that there are two schools using Bayesian methods:

School A very strictly and exclusively uses the Bayes theorem according to equations (10) and (11) for establishing probability distributions by trying to obtain the likelihood $C\, f_V(v \mid \zeta)$ (as a function of ζ) and the prior $f_{1,Z}(\zeta)$ on the right-hand sides of these equations from available or assumed information. That is acceptable if sufficient information is present, for instance, from a pool of statistical data from previous measurements. However, that is by no means always the case. Likelihood or prior are often missing.

School B uses the same Bayesian methods as school A but also the PME according to equation (7) as an essential additive to pure Bayesian statistics. Strict statisticians of school A sometimes call school B "non-Bayesian" and use the adjectives "speculative" and "highly questionable" for the PME.

The PME is indeed a more pragmatic, more physical tool than a mathematical or statistical means to establish probability distributions. It is taken as a fundamental principle or a postulate such as the famous principle of extremal action in physics. It is well-established and has been successfully applied in many fields of statistical physics such as quantum statistics, statistical thermodynamics (by Gibbs even in the 19th century) and image processing [12]. Moreover, some presently and formerly valid (inter)national standards, e.g., GUM [2], its supplement 1 [26], ISO 11929-7 [22] and DIN 25482-10 [23] are in effect based on the PME.

If there is enough information at hand, then the Bayes theorem may be sufficient to establish probability densities, for instance, by "Bayesian updating" [12] or other methods [33]. But in general cases, especially in those of poor or non-statistical information as often encountered in a single radiation measurement, the PME of school B and the Bernoully principle are valuable, indispensable tools for the determination of distributions and characteristic values.

The PME is used in combination with the well-known Bayesian statistics as a necessary supplement to other methods such as the Bayes theorem. The PME and Bayes theorem according to equations (7) and (11), respectively, complete one another. The PME is indispensable if the likelihood needed in the Bayes theorem is not available, as often happens, or information of uncertain quantities must be taken into account if these quantities do not behave randomly in repeated or counting measurements or if constraints are to be met or only poor or non-statistical information is available. Naturally, the PME and Bayes theorem must yield the same results if both are really alternatively applicable in a particular case and equivalent information and conditions are in analogy and correctly taken into account (see appendix A.3).

5.6 Using second-order loss functions, consistency

A selection of the "best" alternative out of a number of others is often carried out by extremizing a suitably chosen, problem-dependent *loss function*, which is a concept of decision theory [3]. For uncertainty, second-order (quadratic, binomial) loss functions are used in order to obey *consistency* in metrology, as is explained in the following.

An example is the selection of the best estimate $\widehat{y}$ of a measurand with an estimator Y by minimizing the squared uncertainty $u^2(y) = \mathrm{E}\left((Y-y)^2\right)$ associated with some possible estimate y and taken as the loss function $L(y)$. This minimization $L(y) = \min$ leads to the best estimate $\widehat{y} = \mathrm{E}\,(Y)$ of the measurand with the associated squared standard uncertainty $u^2(\widehat{y}) = \mathrm{Var}\,(Y)$, which is the minimum of the chosen loss function (see also subsection 4.2). Another example is $L(\mathbf{y}) = \chi^2 = (\mathbf{x} - \mathbf{A}\mathbf{y})^\top \mathbf{U}_\mathbf{x}^{-1} (\mathbf{x} - \mathbf{A}\mathbf{y}) = \min$ for linear fits such as spectrum unfolding. $\mathbf{y}$ represents the fit parameter estimates and $\mathbf{x}$, $\mathbf{U}_\mathbf{x}$ and $\mathbf{A}$ are given data matrices (see, e.g., references [1, 25]).

It was asked why both the above-mentioned loss functions and others in uncertainty theory, including linear fits, are of second order in y or $\mathbf{y}$, respectively, but not, for instance, of the form $L(y) = \mathrm{E}\,(|Y-y|)$ for selecting a "best" estimate and defining the associated uncertainty. The answer to this question is not easy, but is comprehensively described in reference [39]. Only a short review is given in the following.

Any uncertainty theory should meet at least the following six metrological requirements: (1) generality, (2) consistency (information conservation), (3) unique statistical basis, (4) possibility of a critical comparison of different measurement results of the same measurand, (5) protection against large possible measurement deviations, and (6) simplicity, transparency, practicability, small computing effort.

It appears that only second-order loss functions used to define uncertainty or in fits including an uncertainty treatment can meet, at least in a linear model approximation in the data range of interest, the most stringent requirement (2) of consistency. All other

uncertainty theories proposed in the past came to grief on this very important, but nearly always disregarded metrological requirement. Consistency means: Let estimates $\mathbf{x}$ and the associated uncertainty matrix $\mathbf{U_x}$ of quantities $\mathbf{X}$ be used to calculate those of $\mathbf{Y}$ with the model function $\mathbf{Y} = \mathbf{F}(\mathbf{X})$ and then those of $\mathbf{Z}$ with the model function $\mathbf{Z} = \mathbf{G}(\mathbf{Y})$. The results for $\mathbf{Z}$ must then be identical to those obtained in a different way, for instance, directly from the data of $\mathbf{X}$ with the model function $\mathbf{Z} = \mathbf{H}(\mathbf{X}) = \mathbf{G}(\mathbf{F}(\mathbf{X}))$. If, in particular, $\mathbf{G}$ is the inverse function of $\mathbf{F}$ and, thus, $\mathbf{Z} = \mathbf{X}$, then the original data $\mathbf{x}$ and $\mathbf{U_x}$ of $\mathbf{X}$ must be conserved when calculated via $\mathbf{Y}$ to $\mathbf{Z}$ [39].

The PME and Bayes theorem are also consistent when connected with independence as a precondition. This is shown in the following.

If the set $\mathbf{V}$ of random variables in the Bayes theorem according to equation (11) consists of mutually independent subsets $\mathbf{V}_1$ and $\mathbf{V}_2$, then $Cf_{\mathbf{V}}(\mathbf{v} \mid \boldsymbol{\zeta}) = C_1 f_{\mathbf{V}_1}(\mathbf{v}_1 \mid \boldsymbol{\zeta}) \cdot C_2 f_{\mathbf{V}_2}(\mathbf{v}_2 \mid \boldsymbol{\zeta})$ and equation (11) can be split into two similar steps:

$$f_{\mathbf{Z}}^{(1)}(\boldsymbol{\zeta} \mid \mathbf{v}_1) = C_1 \, f_{\mathbf{V}_1}(\mathbf{v}_1 \mid \boldsymbol{\zeta}) \, f_{1,\mathbf{Z}}(\boldsymbol{\zeta}) \ ;$$

$$f_{\mathbf{Z}}(\boldsymbol{\zeta} \mid \mathbf{v}_1, \mathbf{v}_2) = C_2 \, f_{\mathbf{V}_2}(\mathbf{v}_2 \mid \boldsymbol{\zeta}) \, f_{\mathbf{Z}}^{(1)}(\boldsymbol{\zeta} \mid \mathbf{v}_1) \ . \tag{27}$$

The outcome of the first step of the split serves as the prior of the second step, which can also be taken as an update of the first step for new information $\mathbf{v}_2$.

Similarly, the PME according to equation (8) allows an analogous split by

$$f_{\mathbf{Z}}^{(1)}(\boldsymbol{\zeta} \mid \mathbf{a}_1) = C_1 \exp\left(-\sum\nolimits_i \mu_i^{(1)} g_i^{(1)}(\boldsymbol{\zeta})\right) f_{0,\mathbf{Z}}(\boldsymbol{\zeta}) \ ;$$

$$f_{\mathbf{Z}}(\boldsymbol{\zeta} \mid \mathbf{a}_1, \mathbf{a}_2) = C_2 \exp\left(-\sum\nolimits_i \mu_i^{(2)} g_i^{(2)}(\boldsymbol{\zeta})\right) f_{\mathbf{Z}}^{(1)}(\boldsymbol{\zeta} \mid \mathbf{a}_1) \ . \tag{28}$$

Here, for independence, the multipliers $\mu_i^{(1)}$ and functions $g_i^{(1)}(\boldsymbol{\zeta})$ must only refer to the density $f_{\mathbf{Z}}^{(1)}$, and $\mu_i^{(2)}$ and $g_i^{(2)}(\boldsymbol{\zeta})$ only to the final density $f_{\mathbf{Z}}$.

A crosswise application of equations (27) and (28) is also possible, e.g., in order to form $f_{\mathbf{Z}}(\boldsymbol{\zeta} \mid \mathbf{v}_1, \mathbf{a}_2)$.

5.7 Counting measurement

The present subsection first deals with a direct counting measurement of a single count rate measurand. This is then applied to one of the simplest non-trivial, realistic measurements of ionizing radiation where the measurand of interest is a net count rate, given as the difference of a gross count rate and a background count rate, both measured by counting radiation events from assumed stationary Poisson processes of pulses. The truncated GD of the measurand can be accepted as a reasonable approximation in such cases, even in cases of poor measurement, e.g., under low-level circumstances when only a few radiation events were recorded.

Let n ionizing-radiation events be recorded in a counting measurement of a fixed duration t. The number n of counts is assumed to be drawn from an underlying Poisson

frequency distribution of a random variable N with an unknown parameter $\varrho t \geq 0$. Here, ϱ is a value of the count rate $Y = R$ of interest, the measurand. For N, a Poisson probability function

$$p_N(n \mid \varrho, t) = \frac{\mathrm{e}^{-\varrho t}(\varrho t)^n}{n!} \quad ; \quad (n = 0, 1, \ldots) \tag{29}$$

with $\mathrm{E}(N) = \mathrm{Var}(N) = \varrho t$ can in most cases be assumed for physical reasons because nuclear events are physically independent and mean-life and dead-time effects, pile-up of pulses, and instrumental instabilities can often be neglected except, for instance, when short-lived radionuclides or very high count rates are involved or, in multi-channel spectrum measurement, in channels at the slopes of strong spectral lines.

In order to establish the density of the count rate measurand R, the Bayes theorem $f_R(\varrho \mid n, t) = C\, p_N(n \mid \varrho, t)\, f_R(\varrho \mid t)$ similar to equation (11) is applied. The prior $f_R(\varrho \mid t)$ is the density of R before the measurement is performed. Jaynes [37] obtained it by a scaling consideration similar to the following one. Assuming a stationary Poisson process of the radiation measured, the prior of the count rate R cannot depend on the arbitrary measurement duration t, i.e. $f_R(\varrho \mid t) = f_R(\varrho) = tg(\varrho t)$, where the function $g(\varrho t)$ expresses the density of the transformed random variable $V = Rt$ with the value $v = \varrho t$. Differentiation with respect to t yields the differential equation $\partial(tg(\varrho t))/\partial t = g(v) + vg'(v) = 0$ with the solution $g(v) = C/v$ ($v > 0$; C is the integration constant) finally leading to the prior $f_R(\varrho \mid t) = C/\varrho$ ($\varrho > 0$). The fact that this prior is not normalizable is due to the neglect of short-term and long-term influences on the measurement. Accordingly, the prior must be taken as an approximation of a more realistic, normalizable one. By inserting $f_R(\varrho \mid t) = C/\varrho$ into the Bayes theorem considered above and normalizing yields with equation (29) the *gamma density*

$$f_R(\varrho \mid n, t) = \frac{t\mathrm{e}^{-\varrho t}(\varrho t)^{n-1}}{(n-1)!} \quad ; \quad (\varrho \geq 0) \tag{30}$$

which is set to zero for $\varrho < 0$. The expectation $\mathrm{E}(R) = r = n/t$ is the measurement result. The variance $\mathrm{Var}(R) = r/t = n/t^2$ leads to the associated standard uncertainty $u(r) = \sqrt{r/t} = \sqrt{n}/t$.

The particular case $n = 0$ must be treated separately: $\mathrm{E}(R)$ and $\mathrm{Var}(R)$ vanish, and $f_R(\varrho \mid n, t) = \delta(\varrho)$ and a zero uncertainty follow. This is not reasonable in practice since one can never be sure that exactly $R = 0$ if no event happens to be recorded in a measurement of finite duration. Thus, no reasonable statement can be made on the count rate R if $n = 0$. With any more realistic prior $f_R(\varrho \mid t)$, one should always obtain $\mathrm{E}(R) > 0$ and $\mathrm{Var}(R) > 0$. In CSt, N itself is commonly used as an *unbiased* estimator of Rt since $\mathrm{E}(N) = \varrho t$. Thus, the number n of events counted is an estimate of Rt. With $\mathrm{Var}(N)$ also estimated by n, the standard uncertainty $u(r) = \sqrt{n}/t$ of the measurand R follows and also turns out to be unreasonable for $n = 0$.

To avoid this shortcoming, which can lead to severe difficulties [19], it is assumed that the counting measurement is carried out with a duration t chosen suitably large according to the experience of former, similar measurements, so that for any reasonable $\varrho > 0$ at least a few counts can be expected. The duration t is therefore no longer arbitrary. This

knowledge can justify a prior $f_R(\varrho \mid t) = C/\varrho^\nu$ with $0 \leq \nu < 1$, e.g., the Jeffreys prior with $\nu = 1/2$ [38]. This reduces the prior for small ϱ significantly, makes it integrable and removes the shortcoming, but requires a reasonable, physically motivated choice of ν. Moreover, R will be bounded for physical or experimental reasons, although a sufficiently large upper bound need not be specified explicitly. This knowledge is represented by an equally likely R between zero and the upper bound, thus, by a uniform prior $f_R(\varrho \mid t)$ —i.e. $\nu = 0$—similar to other physical quantities in practice. The Bayes theorem and normalization then yield the gamma density

$$f_R = f_R(\varrho \mid n, t) = H(\varrho) \cdot t\mathrm{e}^{-\varrho t}(\varrho t)^n/n! \ . \tag{31}$$

The Heaviside unit step function $H(\varrho)$ here formally indicates that $f_R = 0$ for $\varrho < 0$. According to equation (31), $\mathrm{E}\,(R) = r = (n+1)/t$ and $\mathrm{Var}\,(R) = r/t = (n+1)/t^2$. This result is more reasonable for $n = 0$ since the standard uncertainty $u(r) = \sqrt{n+1}/t$ does not vanish, and the interval with limits $r \pm u(r)$ of reasonable estimates of the measurand (according to GUM [2]) turns out to also contain the estimate $\varrho = 0$. Asymptotically for large n, both approaches discussed lead to the same results. The main differences only occur for very small n.

The following subscripts g and 0 refer to independent counting radiation measurements of gross and background effects, respectively [25]. The model $Y = G(\mathbf{X}) = X_1 - X_2 = R_\mathrm{g} - R_0$ is introduced where the measurand $Y = R_\mathrm{n}$ is the net count rate and $X_1 = R_\mathrm{g}$ and $X_2 = R_0$. It is one of the simplest possible non-trivial models in measurement of ionizing radiation. The information set $\mathbf{a}$ consists of the recorded counts n_g and n_0 and of the measurement durations t_g and t_0, i.e., $\mathbf{a} = \{n_\mathrm{g}, n_0, t_\mathrm{g}, t_0\}$. The due rate values are $x_1 = \mathrm{E}\,(R_\mathrm{g} \mid n_\mathrm{g}, t_\mathrm{g}) = r_\mathrm{g} = (n_\mathrm{g} + 1)/t_\mathrm{g}$ and $x_2 = \mathrm{E}\,(R_0 \mid n_0, t_0) = r_0 = (n_0 + 1)/t_0$. Uniform priors are used as above equation (31). A primary estimate of the measurand is $y_0 = x_1 - x_2 = r_\mathrm{g} - r_0$ with the associated squared standard uncertainty $u^2(y_0) = x_1/t_\mathrm{g} + x_2/t_0$. According to equation (3), all this yields

$$\begin{aligned} f_Y(y \mid \mathbf{a}) &= \int \delta(y - \xi_1 + \xi_2)\, f_{X_1}(\xi_1 \mid n_\mathrm{g}, t_\mathrm{g})\, f_{X_2}(\xi_2 \mid n_0, t_0)\, \mathrm{d}\xi_1\, \mathrm{d}\xi_2 \\ &= \int_0^\infty f_{X_1}(y + \xi \mid n_\mathrm{g}, t_\mathrm{g})\, f_{X_2}(\xi \mid n_0, t_0)\, \mathrm{d}\xi \ . \end{aligned} \tag{32}$$

This density $f_Y(y \mid \mathbf{a})$ is thus obtained by folding two gamma densities. It also becomes a GD for large $n_\mathrm{g}, n_0, t_\mathrm{g}, t_0$ when standardized, since folding two GD again yields such a density. It remains to be truncated at $y = 0$ and renormalized to finally form the density $f_Y(y \mid \mathbf{a}, y \geq 0) = C\, H(y)\, f_Y(y \mid \mathbf{a})$. The truncation is criticized by reference [40] but can alternatively be replaced by also observing the condition $\xi_1 \geq \xi_2$ in the integration of equation (32). This additional integration condition is equivalent to $y = \xi_1 - \xi_2 \geq 0$ because of the model equation and yields the same result.

In order to obtain $\widetilde{\mathbf{a}}(\widetilde{y})$ if n_g is missing before the gross-effect measurement is carried out, the model equation $\widetilde{y} = x_1 - x_2 = r_\mathrm{g} - r_0$ is solved for $x_1 = r_\mathrm{g} = \widetilde{y} + r_0$. This leads to $\widetilde{\mathbf{a}}(\widetilde{y})$ and to $f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y}))$ by replacing n_g in $\mathbf{a}$ and in equation (32) by $(\widetilde{y} + r_0)t_\mathrm{g} - 1$. The gamma density of $X_1 = R_\mathrm{g}$ accordingly changes, but the new value n_g is no longer necessarily a natural number. Then, $n!$ must be replaced by the gamma function $\Gamma(n+1)$.

The density $f = f_Y(y \mid \mathbf{a})$ according to equation (32) can be analytically calculated [7, 19, 25]. Its expansion in terms of *Hermite polynomials* $\mathrm{He}_i(\eta)$ [25, 36] reads

$$f_Y(y \mid \mathbf{a}) = \frac{\exp(-\eta^2/2)}{\sigma\sqrt{2\pi}} \left(1 + \frac{a_3}{3!}\mathrm{He}_3(\eta) + \frac{a_4}{4!}\mathrm{He}_4(\eta) + \dots\right) \; ; \quad \eta = \frac{y-\mu}{\sigma} \tag{33}$$

with $\mathrm{He}_3(\eta) = \eta^3 - 3\eta$ and $\mathrm{He}_4(\eta) = \eta^4 - 6\eta^2 + 3$. The *cumulants*

$$\kappa_i = (i-1)! \left(\frac{r_\mathrm{g}}{t_\mathrm{g}^{i-1}} + \frac{(-1)^i r_0}{t_0^{i-1}}\right) \tag{34}$$

provide the expectation $\mu = \kappa_1 = r_\mathrm{g} - r_0$, the variance $\sigma^2 = \kappa_2 = r_\mathrm{g}/t_\mathrm{g} + r_0/t_0$, the skewness $a_3 = \kappa_3/\sigma^3$ and the excess $a_4 = \kappa_4/\sigma^4$ [25, 36]. If the measurement durations t_g and t_0 are enlarged by a factor τ, then $\sigma^2 \sim 1/\tau$ and $a_3 \sim 1/\sqrt{\tau}$ and $a_4 \sim 1/\tau$. Accordingly, the density f converges for $\tau \to \infty$ (in distribution) via the GD to the Dirac delta function $\delta(y - \mu)$. This convergence *in distribution* is important for the characteristic values since it means, if some conditions are met, not only the pointwise convergence of a distribution to a limiting one, but also that any intergral of a function formed with respect to the distribution converges to the corresponding integral with respect to the limiting distribution [19]. If r_g is replaced by $\widetilde{y} + r_0$ for $\widetilde{\mathbf{a}}(\widetilde{y})$, then $\mu = \widetilde{y}$. This meets the condition according to equation (20).

The density f and the corresponding GD, which is the leading fraction of equation (33), differ visibly but not too greatly in cases of only a few recorded events. The differences vanish by enlarging the measurement durations and keeping the count rates constant. In view of a considerable number of disregarded possible influences in practice, it can therefore be stated that the Gaussian approach is always a reasonable approximation. If this statement is not regarded as satisfactory then either MC should be applied according to reference [25] or a poor measurement improved by analysing the influences and by repeating it with greater durations.

5.8 Random influences by sample treatment

Equation (B.7) in annex B.4.1 of ISO 11929 [1] deals with a series of counting measurements on some comparable, randomly influenced, radioactive samples with the same nominal activity quantified by the measurand Y. It is criticized by reference [41] that equation (B.7)
(a) does not take into account the standard uncertainties $u(x_i) = \sqrt{n_i}$ $(i = 1, \dots, m)$ associated with the results $x_i = n_i$ of m individual counting measurements and
(b) leads to too small a coverage interval.

The criticism seems to be justified since equation (B.7) of ISO 11929 is indeed a CSt relic. Therefore, this equation is reconsidered. Problems (a) and (b) turn out to be largely independent since (b) can already be understood and removed without using the uncertainties $u(x_i)$. This is shown by the analytical BSt approach of appendix C, which solves both problems on the basis of an assumed Gaussian density (GD) of deviations caused by sample treatment and of Poisson counting distributions. See also references [15, 27].

There are several ways to approach problems (a) and (b). It is therefore stressed that reasonable, possibly improved equations similar to equation (B.7) can differ slightly not only because of applying either BSt or CSt, but also because of using different approximations, assumptions or information sets such as known or unknown distributions or uncertainties or different models such as arithmetic, weighted or harmonic means or different methods such as minimum chi-square or maximum likelihood.

Let random input variables X_i be assigned to the individual radioactivities of m comparable samples of the same nominal activity quantified by the measurand Y. This can be achieved, for instance, by homogenizing the possibly radioactive material to be investigated before the samples are taken from the material. Then, a sufficiently well-defined true value of the measurand can be assumed. The X_i differ because of sample treatment, the contribution of which can be expressed by individual unknown deviations d_i of other random input variables D_i. This means $X_i = Y + D_i$ or $Y = X_i - D_i$. If the radiation measurements on the samples and the sample treatments are independently carried out, then the variables X_i and D_i can be taken as being altogether independent or at least uncorrelated. The D_i are assumed to follow the same GD. If the expectations $x_i = \mathrm{E}\, X_i$ are given as the numbers n_i of events recorded from Poisson counting measurements of the same duration t on the samples, then $u^2(x_i) = \mathrm{Var}\,(X_i) = n_i$ (for simplicity; or $= n_i + 1$. See subsection 5.7).

The recommendation to improve equation (B.7) of ISO 11929 consists simply in replacing the second part of this equation by

$$u^2(\overline{n}) = \frac{1}{m}\left(\overline{n} + \frac{m-1}{m-3}\,\overline{n} + \frac{A}{m-3}\right) \;; \quad A = \sum_{i=1}^{m}(n_i - \overline{n})^2 \tag{35}$$

and s^2/m everywhere in annex B.4 of ISO 11929 by $u^2(\overline{n})$, which is the variance $\mathrm{Var}\,(Y)$ and the squared standard uncertainty of the measurand Y associated with the expectation $\mathrm{E}\,(Y) = \overline{n}$. Obviously, $m > 3$ is required. If the two terms with $m-3$ are abbreviated by u^2 and if equation (B.12) of ISO 11929 is also observed, then

$$u^2(\overline{n}) = \frac{\overline{n} + u^2}{m} = \frac{\overline{n} + \vartheta^2\overline{n}^2}{m} \quad \text{or} \quad \vartheta = u/\overline{n}\ . \tag{36}$$

The somewhat surprising result of equation (35) is derived in appendix C. It requires some explanation. The denominator $m-3$ comes from BSt and replaces $m-1$ from CSt. It has nothing to do with the counting uncertainties $\sqrt{n_i}$, which give rise to the first term $\overline{n}$ between the brackets. Similar to CSt, the third term is a part of the estimation of the variance of the underlying GD. The unexpected second term, also proportional to $\overline{n}$, represents some "cross effect" due to the influence of the counting uncertainties on the variance estimation.

Other proposed changes are:
(a) The unsubscripted ϑ is used in annex B.4.3 of ISO 11929 in order to convey information from measurements of a larger number of reference samples to measurements of a small number of comparable samples. Otherwise, ϑ should be suitably replaced by

ϑ_g, ϑ_0, and ϑ_r. The results $\vartheta_\mathrm{g} = 0.2022$, $\vartheta_0 = 0.2379$, $\vartheta_\mathrm{r} = 0.1457$ are already obtained with the input data from table D.2 of ISO 11929 where ϑ corresponds to $\vartheta_\mathrm{r} = 0.1377$.
(b) No need for the requirement $\vartheta < 0.2$ can be seen. It should either be deleted or 0.2 be enlarged to 0.25 since ϑ is always larger than the old ϑ.
(c) The symbol s^2 should no longer be used. Instead, s^2/m should be replaced by $u^2(\overline{n})$.
(d) The results presented in table D.2 of ISO 11929 must still be recalculated.

In cases of $m \leq 3$, infinite uncertainties are involved and the GD approximations of ISO 11929 are thus no longer suitable. Nevertheless, the quantiles of the density f_Y leading to equation (35) remain finite so that the more general approach of section 4 by MC [25] to the characteristic limits according to equations (15) to (18) remains applicable. However, an unsuitable, much greater computational effort will be necessary, possibly greater than the alternative effort for carrying out the required four sample measurements at least.

The assumption of Poisson counting distributions leading to Bayesian gamma distributions can be justified by physical considerations (see the paragraph of equation (29)). The assumption of a GD for the deviations D_i from the influence of the sample treatment is also criticized, but can be justified at least as a suitable approximation following from PME as long as only its expectation μ and variance σ^2 are of interest and need to be estimated, or by the central limit theorem of probability theory if the deviations are assumed to be caused in total by several superposed influences. The log-normal distribution may be preferred. However, this should only be done for multiplicative models in question such as $Y = \prod_{i=1}^{m} X_i^{\nu_i}$ (which can also read $\ln Y = \sum_{i=1}^{m} \nu_i \ln X_i$), but never for additive models, for instance, $Y = \overline{X} = (1/m) \sum_{i=1}^{m} X_i$ as in the present case. An empirical distribution replacing the GD could be constructed if, in rare cases or in MC, m is very large [25, 26]. The variance σ^2 (or standard deviation σ) is a scale parameter according to reference [15 (2.8.2)]. This justifies a prior for it proportional to $1/\sigma^2$ (or $1/\sigma$, respectively). The expectation μ is a location parameter for which a constant prior is suitable. A prior proportional to $1/\xi$ is assumed for the Poisson distribution parameter ξ (see subsection 5.7).

The density f_Y leading to equation (35) reads according to appendix C

$$f_Y = f_Y(y \mid \mathbf{n}) = C \int_0^\infty \left(A + m\,(y - \overline{\xi})^2\right)^{-m/2} \prod_{i=1}^{m} \xi_i^{n_i - 1} \exp(-\xi_i)\, \mathrm{d}\boldsymbol{\xi} \ . \tag{37}$$

For ξ_i fixed, f_Y is a Student density, which is proportional to $|y|^{-m}$ for $y \to \pm\infty$. It is thus normalizable only for $m > 1$. Its expectation $\mathrm{E}(Y) = \overline{n}$ exists only for $m > 2$ and, in addition, for $m = 2$ as the principal value $\lim_{\varepsilon\to\infty} \int_{-\varepsilon}^{\varepsilon} y f_Y \,\mathrm{d}y$. Its variance $\mathrm{Var}(Y) = u^2(\overline{n})$ according to equation (35) exists only for $m > 3$. The necessary integrations for C, $\mathrm{E}(Y)$ and $\mathrm{Var}(Y)$ can be carried out by elementary means (see appendix C). Only normalizable distributions can have quantiles and, thus, coverage intervals. Notice that the tails of f_Y are much more pronounced than those of a GD. This leads to coverage intervals of larger widths compared with the corresponding ones obtained from ISO 11929.

It should finally be pointed out that knowledge of the measurand Y to be non-negative is neglected. The lower tail of the GD to $-\infty$ is thus merely a convenient approximation.

This does not matter if x_i and n_i are sufficiently large. Otherwise, the density f_Y must be truncated at $y = 0$ and renormalized (see also subsection 6.1).

5.9 Treating a single spectral line

Annex C.2 of ISO 11929 [1] deals with the treatment of a single line expected to be present or not in a multi-channel spectrum on a linear or curved background. Denotations C.n in the following refer to this annex C.2. Equations (C.9) and (C.10) stipulate the width t_g of a suitable region B covering the line for the determination of the line intensity, which is the measurand Y (see figure C.1). It was said that these equations are not obvious enough because a derivation is missing, their application is questionable and equation (C.10) should be deleted. They are therefore reconsidered.

Equations (C.9) and (C.10) read $t_g = 2.5\,h$ and $t_g = 1.2\,h$ for a negligible or dominant background, respectively. Here, h is the full width at half-maximum (FWHM) of the line of interest. The equations can only be applied in a case where the line location and FWHM are already known sufficiently well from preceding line shape calibration using large, well defined lines and a Gaussian line shape with variance σ^2 can be assumed. Equation (C.10) was first stipulated in DIN 25482-2:1992 [42] by the working group AK SIGMA (see "Acknowledgements"). It is based on the unpublished derivation made 1986 by the group and is now given below. For a later, similar derivation, see reference [43]. Equation (C.10) is specific for the treatment of a small, but important line of interest on a high (dominant) background in order to minimize the measurand uncertainty. This can be important particularly when it has to be decided whether or not the line is recognized as present. Notice that the decision threshold $y^* = k_{1-\alpha}\widetilde{u}(\widetilde{y} = 0)$ according to equation (21) of ISO 11929 is proportional to the uncertainty in the case of an assumed dominant background. This uncertainty depends on the chosen width t_g of the line region B (see figure C.1) and has a minimum at t_g given by equation (C.10), which should therefore not be deleted.

If, in contrast, intensity, location, FWHM and shape of a line are unknown and must all be determined from the same measured multi-channel spectrum just at hand, then this case represents a quite different situation of information and task and requires its own model and a fit procedure. Therefore, the same corresponding characteristic values as above for the measurand Y cannot be expected. Corresponding characteristic values for the same measurand but from two different cases need not be comparable. Such values depend on the state of information just available but are not physical quantities with a true value to be determined. The two cases must be distinguished and never be mixed up.

Because of $h = 2\sqrt{2\ln 2}\,\sigma = 2.35\,\sigma$ for a Gaussian line shape, it is $t_g = 2.5\,h = 5.9\,\sigma \approx 6\,\sigma$ in equation (C.9). This means $3\,\sigma$ on each side of the line center. The value $3\,\sigma$ is sometimes used in statistics by agreement. Accordingly, region B covers with its agreed width $t_g = 2.5\,h$ nearly the whole line, whereas with $t_g = 1.2\,h = 2.8\,\sigma$ in equation (C.10), region B covers only 84 percent of the line. But it is outlined below that the choice of equation (C.10) approximately minimizes the standard uncertainty $u(y)$ of the measurand Y.

In order to obtain equation (C.10), a reasonable model for the measurand Y must first be established. Let a continuous variable ϑ be linearly assigned to the channel number

with $\vartheta = 0$ at the known line location and the line shape $g(\vartheta) \geq 0$ be given with $\int_{-\infty}^{\infty} g(\vartheta)\,\mathrm{d}\vartheta = 1$. The line portion of region B with full width t and centered on the line then is $L(t) = \int_{-t/2}^{t/2} g(\vartheta)\,\mathrm{d}\vartheta \leq 1$. The model equation $Y = (X_\mathrm{g} - Z_0)/L(t)$ now can be applied. Here, X_g estimates the gross portion of region B and Z_0 estimates the background contribution in region B, but determined from channel regions of a fixed total width t_0 outside region B. The estimators X_g and Z_0 are independent. Accordingly, the uncertainty equation $u^2(y) = (u^2(x_\mathrm{g}) + u^2(z_0))/L^2(t)$ applies with estimates x_g for X_g and z_0 for Z_0. Since X_g is an estimator of a Poisson distribution parameter, it has a gamma density and $x_\mathrm{g} = n_\mathrm{g}$ and $u^2(x_\mathrm{g}) = n_\mathrm{g}$ can be set with the number n_g of registered events in region B (see equation (C.4) and subsection 5.7). For a dominant background, the contribution of the line itself to n_g can be neglected. Then, $n_\mathrm{g} \sim t$, i.e. n_g is (nearly) proportional to the width t of the chosen region B. The contribution $u^2(z_0)$ of a linear or curved background from outside of region B is given in equations (C.11) or (C.12), respectively. It is rather complex in the latter case, but in both cases it has a leading factor $(t/t_0)^2$. Thus, if t_0 can be chosen large enough, then $(t/t_0)^2$ and the uncertainty contribution $u^2(z_0)$ are small and can be neglected. Finally, $u^2(y) \sim t/L^2(t) = \min$ (or $u(y) \sim \sqrt{t}/L(t) = \min$) remains to be solved for t. This can be done, e.g., by numerically varying t. For a Gaussian line shape $g(\vartheta) \sim \exp(-\vartheta^2/(2\sigma^2))$, in particular, the result $t = 2.800\,\sigma = 1.189\,h \approx 1.2\,h$ is obtained as is expected for equation (C.10).

The described assessment method can be applied to arbitrary line and background shapes. There is always an absolute minimum of $u(y)$. This follows from $u(y) \sim 1/\sqrt{t} \to \infty$ with $L(t) \approx tg(0)$ for $t \to 0$ and from $u(y) \to \infty$ with $L(t) \to 1$ for $t \to \infty$. However, there is no need to use the exact solution t of the minimum, e.g., $t = 1.189\,h$ as above for equation (C.10), since $u(y)$ does not depend considerably on t in a neighbourhood of the minimum. If a sufficiently large t_0 cannot be chosen, then $z_0 = (t/t_0)n_0 + \ldots$ and $u^2(z_0) \sim (t/t_0)^2 n_0 + \ldots$ must also be taken into account. Here, n_0 is the number of registered events in the involved regions outside region B, and the points $\ldots$ denote neglected terms of higher order in t/t_0. Then, $u^2(y) \sim (t + ct^2 + \ldots)/L^2(t)$ with a constant $c > 0$ has to be minimized. This shifts the solution t for $c = 0$ to a smaller value.

5.10 Exceptional values of the detection limit

The detection limit $y^\sharp$ serves for the decision on whether or not the measurement procedure intended for application is appropriate for the measurement purpose. The decision is made by comparing $y^\sharp$ with a specified guideline value y_r. If $y^\sharp \leq y_\mathrm{r}$, then it is decided that the procedure is appropriate (see subsection 4.4).

According to equations (21) and (22) of ISO 11929 [1], the condition $y^\sharp \geq y^* \geq 0$ must be met since there is no negative uncertainty and if $k_{1-\alpha}$, $k_{1-\beta} \geq 0$ ($\alpha, \beta \leq 1/2$) are specified as usual. However, $y^\sharp$ can apply infinite or negative values, which, for instance, follow from equation (28) of ISO 11929 if the denominator vanishes or is negative, respectively. This possibility of exceptional, physically meaningless values is criticized by reference [44] as an inacceptable shortcoming of the standard, but it should instead better be taken as a great advantage! The exceptional values provide a strong hint that the measurement procedure is unsuitable, even in a case where no guideline value y_r is specified. Then the procedure and the input information must be revised and

improved, e.g., by choosing longer measurement durations to reduce involved count rate uncertainties, by more realistically assessing uncertainties of calibration or influence factors, or by refining the model.

6. Proposed alternatives

6.1 Distributions

The present subsection deals with alternative distributions of the non-negative measurand Y with respect to knowledge of whether or not the condition $y \geq 0$ is observed or applied.

Any distribution in the Bayesian sense expresses the information just available and taken into account: neither more nor less. Let only a primary measurement result y_0 and the associated standard uncertainty $u(y_0)$ obtained from GUM be available as the expectation and the standard deviation, respectively, of an unknown primary density $f_0 = f_Y(y \mid y_0, u(y_0))$. Let it also be unknown whether or not the non-negativity of the measurand Y is taken into account. Then, f_0 can be reconstructed by the PME in a first step according to equation (28). With a uniform prior, the GD $f_0 = \exp(-(y - y_0)^2/(2u^2(y_0)))/(\sqrt{2\pi}u(y_0))$ for all y results.

In a second step, f_0 is updated for the non-negativity of the measurand Y to form the final density $f_Y = f_Y(y \mid y_0, u(y_0), y \geq 0)$. This f_Y becomes, according to the PME, equations (8) or (28), also a GD, but truncated at $y = 0$ and renormalized, i.e. $f_Y = C\,H(y)\exp(-(y - y_0)^2/(2u^2(y_0)))$. Truncation and renormalization are caused by the restriction to the region $\mathbf{R} = \{y \mid y \geq 0\}$. Since there are no further constraints for f_Y, the factor $\exp(\ldots) = 1$ is valid in equations (8) or (28). For another example, see below equation (32).

If it is, in contrast, definitely known that the condition $y \geq 0$ had already been taken into account when y_0 and $u(y_0)$ were determined, then these values are no longer the estimate and the standard deviation of f_0 but of the final (unknown) f_Y. In this case, f_Y is, according to equation (8), also a GD, truncated at $y = 0$ and renormalized. But now, $\mathrm{E}(Y) = \widehat{y} = y_0$ and $\sqrt{\mathrm{Var}(X)} = u(\widehat{y}) = u(y_0)$ for f_Y applies, i.e. the primary estimate y_0 and the best estimate $\widehat{y}$ are identical, and the respective uncertainties as well.

The authors of reference [40] and others wish to give more weight to the value $y = 0$ of the non-negative measurand Y by a modification of an arbitrary density $f(y) = f_Y(y \mid \mathbf{a})$, for instance, of $f(y) = f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y}))$, which is needed for the determination of the decision threshold y^* and the detection limit $y^\sharp$. They do this by truncating $f(y)$ at $y = 0$ and adding $Q\delta(y)$ with $Q = \int_{-\infty}^{0} f(y)\,\mathrm{d}y$. This yields the modified density $f'(y) = H(y)f(y) + Q\delta(y)$, which remains normalized. The authors have the "perception" that this would be an alternative better than the PME renormalization after the truncation which leads to $f'(y) = H(y)f(y)/(1 - Q)$. They are indeed free to do this in the framework of the present theory, but must have a reasonable motivation based on concrete physical information about the perception or use an accordingly refined model. Otherwise, the perception would merely act as an additional mathematical

postulate. In contrast, the PME approach only needs the knowledge that Y is a non-negative measurand and maximizes the due entropy $S = -\int_0^\infty f'(y) \ln(f'(y)/f(y)) \, \mathrm{d}y$. Here, $f(y)$ acts as the prior since it represents all the information already taken into account.

The density modification described above varies the characteristic values except y^* and $y^\sharp$. This exception is shown now. Equations (17) and (18) for the definition and determination of y^* and $y^\sharp$ can also read

$$\int_{y^*}^\infty f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y} = 0)) \, \mathrm{d}y = \alpha \ ; \quad \int_{y^*}^\infty f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y} = y^\sharp)) \, \mathrm{d}y = 1 - \beta \ . \tag{38}$$

The latter equation is obtained by subtracting equation (18) from the normalization condition $\int_{-\infty}^\infty f(y) \, \mathrm{d}y = 1$. Notice that $f(y)$ for $y < y^*$ and any $\widetilde{y}$ is not needed in equations (38) and can thus be arbitrarily deformed (while remaining a probability density) without any change of y^* and $y^\sharp$. The deformation proposed above is thus admissible if physically justified, but needless since $y^* > 0$.

6.2 Final measurement result

It is proposed to use the mode or the median of f_Y instead of the expectation as the "best estimate" of the true value of the measurand Y. This proposal should not be accepted, although in principle every possible value y of Y could be used as an estimate of Y and is associated with the uncertainty $u(y) = \sqrt{\mathrm{E}\,((Y - y)^2)}$. The expectation is thus associated with the minimum uncertainty, called the standard uncertainty (standard deviation, GUM), and is therefore taken as the best estimate. Another reason is consistency (see subsection 5.6), which can be achieved independently of any involved distributions only if expectations and uncertainty (covariance) matrices express complete measurement results. This also guarantees that such results can consistently be used as input data for a successive calculation.

As a simple example, consider the model equation $Y = X_1 + X_2$. Then, always $\mathrm{E}\,(Y) = \mathrm{E}\,(X_1) + \mathrm{E}\,(X_2)$ independently of the involved densities of the input estimators X_1 and X_2. But a similar equation is in general not valid either for modes or for medians as is shown below, except for particular, with respect to the expectation symmetric, single-mode densities such as (untruncated) Gaussian ones where expectation, mode and median are identical.

Numerically, let X_1 and X_2 be independent and non-negative and have the densities $f_{X_1}(\xi_1) = \exp(-\xi_1)$ and $f_{X_2}(\xi_2) = 2\exp(-2\xi_2)$; $(\xi_1, \xi_2 \geq 0)$, respectively, with the expectation sum $1 + 1/2 = 1.500$, mode sum $0 + 0 = 0$ and median sum $\ln 2 + (\ln 2)/2 = 1.040$. These sums should equal the respective expectation, mode and median of the estimator sum $Y = X_1 + X_2$, which is also non-negative. By folding the input densities according to equation (3), the density $f_Y(\eta) = 2(\exp(-\eta) - \exp(-2\eta))$; $(\eta \geq 0)$ results, indeed with the expectation 1.500. But its mode $\ln 2 = 0.693$ and median $-\ln(1 - 1/\sqrt{2}) = 1.228$ differ considerably from the respective sum values.

6.3 Coverage intervals

It is proposed to use the coverage interval of minimum width instead of the probabilistically symmetric coverage interval. This shortest coverage interval should be accepted in ISO 11929 at least as an alternative although in more general cases with MC application a considerably greater computational effort must be expected. However, it meets more of the metrological requirements described in the following. It includes, for instance, quite naturally the estimate $y = 0$ for small $y_0/u(y_0)$ as was demanded. See also appendix B, figure 3 and reference [45].

Every for practice reasonably stipulated coverage interval of a non-negative measurand, quantifying the physical effect in question, should meet as far as possible the following metrological demands:
(1) Its lower limit must be non-negative.
(2) It should cover the possible measurand value 0 if and only if this value is actually "highly probable".
(3) Its definition should not explicitly depend on the other characteristic values.
(4) Asymptotically for a large primary measurement result y_0 much greater than the associated standard uncertainty $u(y_0)$, it should become identical with the common symmetric coverage interval.
(5) The computing effort for its limits should not be much larger than that for the other characteristic values.

The probabilistically symmetric coverage interval meets the demands except (2), whereas the shortest coverage interval meets all of them, demand (5) at least in the Gaussian case of ISO 11929 (see also subsection 6.4, appendix B and figure 3).

The best estimate $\widehat{y} = \mathrm{E}(Y)$ can in rare cases be located outside the coverage interval. This can happen if the density $f_Y(y)$ has a pronounced tail as in the following illustrative example. Let $f_Y(y) = 1-\gamma$ for $0 \le y \le 1$ and $= \gamma/(c-1)$ for $1 < y \le c$ and $= 0$ elsewhere with $c > 1/(1-\gamma)$. Then, $y^{>} = 1$ is the upper limit of the shortest coverage interval for the coverage probability $1-\gamma$ (see appendix B). The best estimate $\widehat{y} = (1+c\gamma)/2$ is larger than $y^{>}$ and thus located outside the coverage interval if $c > 1/\gamma$, that is $c > 20$ for $\gamma = 0.05$. Replace γ by $\gamma/2$ in $f_Y(y)$ and $\widehat{y}$ for the probabilistically symmetric coverage interval. Then, $y^{\triangleright} = 1$ is the upper limit of this interval for the coverage probability $1-\gamma$ and it is $y^{\triangleright} < \widehat{y}$ and $\widehat{y}$ thus located outside the coverage interval if $c > 2/\gamma$, that is $c > 40$ for $\gamma = 0.05$.

6.4 Decisions

Decisions in ISO 11929:2010 are in general no longer made by testing hypotheses as in old parts of ISO 11929 and as is usual in CSt. Instead, they are based on decision theory [3] as advised by Bayesians, who pointed out that the common tests are only applicable in CSt and should therefore not be applied in BSt (see also subsection 6.6 (c) and (e)). Nevertheless, there are also Bayesian hypothesis tests [46].

If $y_0 > y^*$ with the decision threshold y^*, then it is decided that the radiation effect in question is recognized as present. Instead, the condition $\widehat{y} > y^{**}$ is proposed where y^{**} is defined similarly to y^* according to equation (17), but with the density $f_Y(y \mid$

$\widetilde{\mathbf{a}}(\widetilde{y}=0)$) replaced by $f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y}=0), y \geq 0)$. Such a definition could be possible but is it an improvement? Since $y_0 \leq \widehat{y}$ and also $y^* \leq y^{**}$, this question cannot easily be answered. Moreover, the proposal requires more computing effort. Nevertheless, a rough comparison of the two conditions can be made by the following considerations.

With ISO 11929, $f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y}=0))$ is a GD with expectation 0 and standard deviation $\widetilde{u}(0)$ and $f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y}=0), y \geq 0)$ is the same density, but truncated at $y=0$ and renormalized by a factor 2. This leads with the p-quantile k_p of the standardized Gaussian normal distribution function $\Phi(t)$ quite easily to $y^* = k_{1-\alpha}\widetilde{u}(0)$ [1] and, similarly, to $y^{**} = k_{1-\alpha/2}\widetilde{u}(0)$ because of the factor 2 (see figure 2). Moreover, the best estimate

$$\widehat{y} = y_0 + \frac{u(y_0)\exp\big(-y_0^2/(2u^2(y_0))\big)}{\Phi(y_0/u(y_0))\sqrt{2\pi}} \tag{39}$$

is given [1]. In many cases, the uncertainty function $\widetilde{u}(\widetilde{y})$ increases only slowly. The constant approximation $\widetilde{u}(\widetilde{y}) = u(y_0)$ is therefore used. The scaling $z = y/u(y_0)$ of all involved y values then leads to the decision thresholds $z^* = k_{1-\alpha}$ and $z^{**} = k_{1-\alpha/2}$, to the respective conditions $z_0 > k_{1-\alpha}$ and $\widehat{z} > k_{1-\alpha/2}$, and to

$$\widehat{z} = z_0 + \frac{\exp(-z_0^2/2)}{\Phi(z_0)\sqrt{2\pi}} \quad . \tag{40}$$

In order to compare the two conditions, $z_0 = k_{1-\alpha}$ is set identical to the decision threshold. What then happens with the second condition? Equation (40) yields with $\Phi(k_{1-\alpha}) = 1-\alpha$ the questionable condition

$$k_{1-\alpha} + \frac{\exp(-k_{1-\alpha}^2/2)}{(1-\alpha)\sqrt{2\pi}} \;><?\; k_{1-\alpha/2} \quad . \tag{41}$$

By varying α, it appears that the $<$ sign applies for $\alpha < 0.33$ and the $>$ sign otherwise. This result allows the following conclusion. If, for a commonly small α, the value z_0 is only slightly larger than the decision threshold $z^* = k_{1-\alpha}$ in this case, then it is decided that the radiation effect in question is recognized as present. But this decision can only be made with the condition $\widehat{y} > y^{**}$ if z_0 is considerably larger. This conclusion cannot please users of ISO 11929 in radiation protection, who are interested in measuring as small an effect as possible. Therefore, the proposal of using the condition $\widehat{y} > y^{**}$ should be rejected. Similarly, the detection limit $y^{\sharp\sharp}$ defined by using y^{**} instead of y^* according to equation (18) would become larger than $y^\sharp$. This would make the comparision of the detection limit with the guideline value y_r stronger and, thus, the measurement procedure to be tested less suitable.

The shortest coverage interval according to appendix B meets demand (2) of subsection 6.3. This could allow the following decision: "The radiation effect quantified by the measurand is recognized as present if the lower limit $y^<$ of the shortest coverage interval is greater than 0." Such a decision would not require the decision threshold y^* but a different decision philosophy depending on an already known primary complete measurement result y_0, $u(y_0)$ of an individual, possibly radioactive sample and on the coverage probability $1-\gamma$. This kind of decision would no longer characterize the measurement procedure but the sample itself and could therefore, in addition, be suitable for a single sample measurement. It should be considered and discussed.

If $y^\sharp \leq y_\mathrm{r}$, then it is decided that the measurement procedure is suitable. But in more general cases, the detection limit $y^\sharp$ needs a great deal of iterative MC computation. As shown in the text below equation (19), there is an equivalent condition $P(y_\mathrm{r}) \leq \beta$, which can be tested more easily since only a simple integral with fixed limits has to be calculated by MC. $y^\sharp$ is not needed in this case, but the decision threshold y^* as the upper integral limit of equation (19) must be known. It should be discussed whether or not the detection limit $y^\sharp$ is really needed.

6.5 Recommendations for computing

The model function $G(\mathbf{x})$ or an algorithm for calculating a measurand value y and the associated standard uncertainty $u(y)$ according to GUM should not be implemented as a single arithmetic expression but as a subroutine. This can considerably facilitate the numerical determination of the terms contributing to the uncertainty since, for instance, by replacing only x_i by $x_i \pm u(x_i)/2$,

$$\frac{\partial G}{\partial x_i}\, u(x_i) = G\big(x_1, \ldots, x_i + u(x_i)/2, \ldots\big) - G\big(x_1, \ldots, x_i - u(x_i)/2, \ldots\big) \tag{42}$$

for equation (3) of ISO 11929 [1]. This linear approximation of the partial derivatives is in most cases sufficient since uncertainty according to GUM already follows from a linear theory. People sometimes say that linear approximations for uncertainty calculations are not acceptable since models are often non-linear and MC must therefore used. That is wrong! Even a strongly non-linear model has to be approximately linear only *in the data region of interest*, determined by the uncertainties (see also subsection 3.2). This can easily be tested by slightly and suitably modifying the variation of x_i in equation (42) and observing what happens with the results. For instance, replace $x_i \pm u(x_i)/2$ by x_i and $x_i - u(x_i)$ or by $x_i + u(x_i)$ and x_i, respectively. For software, see references [15, 24].

A quantity A often has to be calculated from an arithmetic formula in terms of other quantities B_i, for instance, $A = \sqrt{B_1^2 + B_2^2}$. If the quantities B_i are themselves given by arithmetic expressions, then these expressions should never be inserted directly into the formula since this could enlarge the complexity and severely disturb the transparency. Instead, the B_i should first be calculated numerically from the expressions. Then the results should be inserted into the formula in order to finally obtain the numerical value of A.

Although the Monte Carlo (MC) method is proposed in the present paper and elsewhere as the method of first choice in more complex cases of numerical calculations of characteristic values, its application is not always inevitable. It is pointed out that there are also a lot of effective, sometimes simple numerical or analytical methods [35, 36] such as, for instance, (asymptotic) series expansions of distributions as already used in equation (33). These methods often furnish sufficient approximations, e.g., for quantiles since α, β and γ are usually small numbers. As an example, let a density $f(y)$ be truncated at $y = 0$ and have a value $f(0) > 0$ and an upper tail of the asymptotic form $f(y) \approx C/y^\nu$ ($\nu > 1$) or $f(y) \approx C\exp(-y/\lambda)$. The limits of the probabilistically symmetric coverage interval then are $y^\triangleleft \approx \gamma/(2f(0))$ and $y^\triangleright \approx (2C/((\nu-1)\gamma))^{1/(\nu-1)}$ or $y^\triangleright \approx \lambda \ln(2C\lambda/\gamma)$, respectively, obtained from $\gamma/2 = \int_0^{y^\triangleleft} f(y)\,\mathrm{d}y \approx f(0)y^\triangleleft$ and $\gamma/2 = \int_{y^\triangleright}^{\infty} f(y)\,\mathrm{d}y$.

6.6 Naming of terms

There is severe, long-lasting disagreement in understanding, nomenclature, and notation of concepts and methods between conventional, frequency-based statistics (CSt) and Bayesian statistics (BSt) and also between pure BSt (school A) and BSt including PME (school B). First of all, the different meanings of probability in BSt and CSt are mentioned (see section 1 and subsection 2.2). Other examples of such concepts are: confidence limits (coverage interval limits, credible limits) and errors of first and second kind. BSt including PME of school B is used as it is in ISO 11929 [1], reference [25], and the present paper since it seems to be the best method for proceeding successfully to the scope of characteristic values. However, this is not the place to discuss and justify the statistical directions, methods, and problems. Nevertheless, some proposals for changing terms, mainly relics of CSt, should be discussed:

(a) The term "confidence interval" in ISO 11929 should be changed to "coverage interval" according to references [26 (3.12), 28 (2.36)]. "Confidence interval" is a term from CSt.

(b) A proposal to replace the term "detection limit" by "minimum detectable activity" should not be accepted since "detection limit" is a term already well established in the older parts of ISO 11929 [22] and commonly applied. "Activity" is not general enough, but "measurand value" could instead be used. Detection limits can be determined for many physical or chemical quantities which are not activities.

(c) Proposals to replace the term "error of the first/second kind" of CSt by "false positive/negative decision" or "decision error of the first/second kind" have already been discussed. The first proposal is now used preliminarily in the present paper.

(d) A demand from purely Bayesian school A to use the term "likelihood" (originating from CSt) only for the function $C\, f_{\mathbf{V}}(\mathbf{v} \mid \boldsymbol{\zeta})$ of $\boldsymbol{\zeta}$ in the Bayes theorem according to equation (11) but never for the analogous function $C \exp(\ldots)$ from PME in equation (8) could be accepted. Then, annex F.2 of ISO 11929 [1] has to be revised accordingly. However, it is shown in appendix A.3 that both functions are identical for equivalent input information.

(e) The reading of decisions such as "It is decided that the physical effect quantified by the measurand is recognized as present" or, more general, "If <*conditions*>, then it is decided that <*statement*>." should be critically examined by experts in decision theory. A proposal of using "asserted" instead of "decided" does not seem to be strong enough for a radiation protection standard.

7. Conclusions

The characteristic values studied in the present paper are needed for the quantification, recognition and detection of ionizing radiation and allow decisions to be made for radiation protection purposes. They are defined quite generally in section 4 on Bayesian statistics (BSt) as closely as possible and in reasonable agreement with common practice and can be calculated in more complex and critical cases of radiation measurement by using Monte Carlo methods (MC). Moreover, the present approach to the characteristic

values makes it possible to go a step beyond the present state of standardization laid down in ISO 11929 [1] since distributions rather than uncertainties can be propagated. It is thus more comprehensive and promising.

ISO 11929 [1] mainly uses quite easy to handle (truncated) Gaussian probability distributions (GD). More general distributions representing all the available relevant knowledge on the radiation measurand in question can be obtained, for example, by the principle of maximum entropy (PME, subsection 3.1), but require in general the application of MC. The GD plays a dominant part since in very many cases distributions can be approximated by Gaussian ones if there is a parameter τ, for instance, the measurement duration, which can be made sufficiently large to improve the approximation. However, the convergence to the GD can be rather slow, i.e. only proportional to $1/\sqrt{\tau}$ [25]. For more reasons, see also subsection 5.3.

What should at least be improved in ISO 11929? First of all, the approach by means of the prominent GD should be retained and possibly supplemented by applications of more general distributions according to reference [25]. The latter and other reasons imply a revision of annexes B.4 and F.2 of the standard. The general definitions of the characteristic values according to section 4 of the present paper should be included and also the limits of the shortest coverage interval according to subsection 6.3 and appendix B as an alternative to the limits of the probabilistically symmetric coverage interval. Moreover, the way of expressing decisions (subsection 6.4) and of naming terms (subsection 6.6) should be revised. Demands for some simpler numerical examples of application worked out in detail should also be satisfied. Such examples are already available [47].

The present paper and reference [47] now provide all the material elaborated and collected until the end of 2012 for the planned revision of ISO 11929.

Finally, it should be understood that the matter of characteristic values is not a matter of right or wrong but a matter of knowledge, approximation, reasonableness, expenditure and agreement as is often the case in physics.

Appendix A: More about PME

A.1 Priors from the Bernoulli principle

A proponent of school A said that the PME according to equations (7) or (49) can never be used since the prior f_0 is not known from the first, i.e. at the beginning when no information at all is available and the probability of a random event is therefore completely arbitrary. That may hold true from a purely mathematical point of view. But the situation is quite different in physics. Some knowledge is nearly always present. Consider a coin to be tossed. The coin is a physical object with a symmetry of both its sides, and tossing is a physical process with an artificial arbitrariness. That is information enough to assign from the first the prior probability 1/2 to each of the two possible outcomes of tossing the coin. This is a simple example of the classical *Bernoulli principle* of assigning the same prior probability to equally possible random events. Since symmetry plays a prominent part in physics, "equally possible" should be understood in a very wide sense as "if there is any symmetry between possible events". In this way, the Bernoulli principle can help to establish the prior more from a physical than from a purely mathematical point of view. A prior is similarly needed in the Bayes theorem, which is preferred by school A. See also subsection 5.5.

A.2 A derivation of the PME

The following outline of a proof of the PME is based only on means common to both Bayesian schools A and B, i.e. on probability theory. It cannot really reconcile the schools but could show a possible direction to find a compromise between them.

In order to derive the PME, let each one of N real or abstract objects of the same kind be in one of n different possible states i $(i = 1, \ldots, n)$ with a given probability $p_i > 0$. Examples of such objects are bullets of the same volume and mass such as molecules of a substance or are independent trials under the same conditions. The states may be, for instance, boxes, quantum states or merely any alternative possibilities. The probability p_i may be, for instance, proportional to the opening area of a box i. The number $N_i \geq 0$ denotes the number of objects in the state i. It may be the number of hits of box i when tossing N bullets. The joint probability P (taken as a degree of belief) of a distribution $\{N_1, \ldots, N_n\}$ of all N_i with $\sum_{i=1}^{n} N_i = N$ is then given by the *multinomial distribution*, the probability function of which is

$$P = p(N_1, \ldots, N_n) = N! \prod_{i=1}^{n} p_i^{N_i}/N_i! \ . \tag{43}$$

P must not change if an arbitrary number of states with $p_i = 0$ is added. For these states, $N_i = 0$ with certainty, therefore, $p_i^{N_i} = 1$ must be set.

The Stirling formula [36]

$$\nu! = \sqrt{2\pi\nu} \cdot \nu^{\nu} \exp(-\nu + \theta/(12\nu)) \ ; \quad (\nu > 0 \ ; \ 0 < \theta < 1) \tag{44}$$

can with $\theta = 0$ or 1 also be written in the form

$$\ln \nu! = \nu \ln \nu - \nu + r(\nu) \ ;$$
$$\tfrac{1}{2} \ln(2\pi\nu) < r(\nu) < R(\nu) = \tfrac{1}{2} \ln(2\pi\nu) + 1/(12\nu) \ ; \quad (\nu > 0) \ ;$$
$$r(0) = R(0) = 0 \ ; \quad r(\nu) = O(\ln \nu) \ ; \quad R(\nu) - r(\nu) = O(1/\nu) \ . \tag{45}$$

The *order* $a_\nu = O(T(\nu))$ with $T(\nu) > 0$ means that there is a fixed number $\varepsilon > 0$ and a natural number ν_0 such that $|a_\nu| < \varepsilon T(\nu)$ for all $\nu > \nu_0$. Applying equation (45) to equation (43) results in

$$\frac{\ln P}{N} = -\sum_{i=1}^{n} \frac{N_i}{N} \ln \frac{N_i}{N p_i} + \frac{r(N)}{N} - \sum_{i=1}^{n} \frac{r(N_i)}{N}. \tag{46}$$

The function $R(\nu)$ increases monotonely for all natural numbers ν. Thus, $r(N_i) \leq R(N_i) \leq R(N)$ applies for the remainder r because of $N_i \leq N$. The sum of the third term on the right-hand side of equation (46) is thus $\leq nR(N)/N$ and of order $O((\ln N)/N)$ as well as the second term. Both these terms vanish with $N \to \infty$ independently of all N_i. Equation (46) now also reads with the relative numbers $y_i = N_i/N$

$$\frac{\ln P}{N} = S + O\Big(\frac{\ln N}{N}\Big) \ ; \quad S = -\sum_{i=1}^{n} y_i \ln \frac{y_i}{p_i} \ . \tag{47}$$

S is the *(information) entropy*, the limit of $(\ln P)/N$ for $N \to \infty$. Let S_0 be the absolute maximum of S with respect to some constraints and P_0 the probability belonging to S_0. Then,

$$P/P_0 = \exp\big(-N \cdot (S_0 - S) + O(\ln N)\big) < N^\varepsilon \exp(-\lambda N) \to 0 \ ; \ (N \to \infty) \tag{48}$$

follows for every distribution $\{y_1, \ldots, y_n\}$ kept fixed for $N \to \infty$ if $\lambda = S_0 - S > 0$, i.e. S does not absolutely maximize the entropy. The order $O(\ln N)$ means that the remainder is less than $\varepsilon \ln N$ with an existing fixed number $\varepsilon > 0$. For a very large number N of objects, every distribution with a non-maximum entropy with respect to the constraints therefore becomes extremely improbable when compared with the entropy-maximizing distribution. Although the probability P of a distribution loses its meaning for $N \to \infty$, the entropy remains as a measure of this probability.

Let a region $\mathbf{R}$ of the space of the values $\mathbf{x}$ of a random vector $\mathbf{X}$ be decomposed in n non-overlapping subregions $\mathbf{R}_i$ with the small volume elements $\Delta\mathbf{x}_i > 0$. The subregions $\mathbf{R}_i$ correspond to the states i. Then with $\mathbf{x} \in \mathbf{R}_i$, the normalized *density* $f(\mathbf{x})$ is introduced by $f(\mathbf{x})\Delta\mathbf{x}_i = N_i/N = y_i$ and, similarly, the *prior* by $f_0(\mathbf{x})\Delta\mathbf{x}_i = p_i$. If $p_i = 0$, then $N_i = 0$ and $f(\mathbf{x}) = 0$ and $f_0(\mathbf{x}) = 0$. A second limiting process (besides $N \to \infty$) with $n \to \infty$ and $\Delta\mathbf{x}_i \to 0$ transforms the entropy S according to equation (47) to the integral

$$S = -\int_{\mathbf{R}} f(\mathbf{x}) \ln\Big(\frac{f(\mathbf{x})}{f_0(\mathbf{x})}\Big) \, \mathrm{d}\mathbf{x} \ . \tag{49}$$

This entropy S as a function of P is a measure of the probability of the density $f(\mathbf{x})$, which itself may be a probability density of the random vector $\mathbf{X}$. An absolute maximum of entropy thus also means a maximum probability of $f(\mathbf{x})$. According to equation (48),

this density has an overwhelming probability in comparison to every other density. This explains the great importance of the PME. If the PME is applied to establish the density $f(\mathbf{x})$, the prior $f_0(\mathbf{x})$ must be known. The Bayes theorem also needs such a prior. To obtain the prior, the *Bernoulli principle* can be used, which assigns the same probabilities to states which are equally possible because of any known physical symmetry, e.g., to both sides of a coin (see appendix A.1).

A.3 PME versus Bayes theorem

It was doubted that the PME and the Bayes theorem furnish identical results f for equivalent input information (see subsection 3.1). Therefore, a proof is outlined here. Remember that any system of linear equations $\mathbf{Ax} = \mathbf{b}$ for unknowns $\mathbf{x}$ has a unique solution $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$ only if the coefficient matrix $\mathbf{A}$ is non-singular, i.e. its inverse matrix $\mathbf{A}^{-1}$ exists.

Consider a random variable Z with values z, density $f = f_Z(z \mid v)$ and prior $f_0 = f_{0,Z}(z)$. Moreover, let $l = l(z) = l_V(z, v) = f_V(v \mid z)$ with fixed v be the likelihood and $g_i = g_i(z)$ be a complete set of linearly independent functions with $g_0 = 1$. Every (to some extent well-behaved) function $h = h(z)$ then has a series expansion $h = \sum_i c_i g_i$ (e.g., a power series). The unknown coefficients c_i can uniquely be calculated by chosing n abscissas z_k such that the inverse matrix $(g_i(z_k))^{-1}$ exists. The series then becomes a system of n linear equations $h(z_k) = \sum_i c_i g_i(z_k)$ with a unique solution for n of the c_i. Since this solution is an approximation depending on the arbitrary n, the limit for $n \to \infty$ finally has to be formed.

If l and f_0 are known, then $f = C\, l\, f_0$ is directly obtained from the Bayes theorem according to equation (11). This f then leads to the integrals $d_i = \int g_i f \,\mathrm{d}z$. And with $h = \ln l$, the series expansion $\ln l = \sum_i c_i g_i$ follows. The normalization constant C is fused with l because of $g_0 = 1$. Then, $d_0 = 1$ and $l = f/f_0$.

If, vice versa, all d_i are known instead of the likelihood l, then the Riemann integral approximation $d_i = \sum_{k=1}^{n} g_i(z_k) f(z_k) \Delta z_k$ applies. With n chosen d_i, this is again a system of n linear equations with a unique solution for the n unknowns $f(z_k)\Delta z_k$. Hence it finally follows because of $l(z_k) = f(z_k)\Delta z_k / (f_0(z_k)\Delta z_k) = f(z_k)/f_0(z_k)$, that there is a one-to-one correspondence between the set of the $l(z_k)$ und the set of the d_i. These sets thus represent equivalent information. This holds true for an arbitrary n and for $n \to \infty$ with $\max \Delta z_k \to 0$.

It also follows that the factor $\exp(-\sum_i \mu_i g_i)$ (including C) from PME according to equation (8) based on the information d_i represents the likelihood $l = \exp(\sum_i c_i g_i)$. This means $\mu_i = -c_i$ because of the one-to-one correspondence. However, the linear independence of the g_i must be required to obtain unique solutions for the c_i and μ_i.

For example, let $l = \exp(-z)$; $f_0 = 1$; $g_0 = 1$ and $g_1 = z$ be given ($z \geq 0$). Then $f = l\, f_0 = \exp(-z)$ according to the Bayes theorem and $d_0 = d_1 = 1$. Vice versa with these d_i given instead of l, the density $f = \exp(-\mu_0 - \mu_1 z)$ follows from the PME according to equation (8). By inserting this f in the constraints $\int g_i f \,\mathrm{d}z = d_i$, at first $\exp(-\mu_0)/\mu_1 = 1$ and $\exp(-\mu_0)/\mu_1^2 = 1$ and then the solution $\mu_0 = 0$ and $\mu_1 = 1$ results. This finally leads to $f = \exp(-z)$ as must be expected.

There was another criticism concerning the input of observations v_i of the same measurand V obtained from independently repeated measurements under nominally identical conditions. The Bayes theorem leads with a known or assumed likelihood $l_V(z, v)$ for a single measurement and a prior f_0^* to $l = \prod_i l_V(z, v_i)$ and $f^* = C\, l\, f_0^*$. All this is known and can therefore be taken as the equivalent input information to obtain the corresponding PME solution f. This is quite trivial if f_0 in equation (49) is properly understood as the already known input density (not necessarily identical with f_0^*), that is, as the known f^* of the Bayes theorem. Without any further constraint, then $f = f^*$ readily follows from equation (8).

Although the PME and Bayes theorem yield identical densities f for equivalent input information, neither of these methods can be dispensed with. In contrast to the PME, the Bayes theorem requires the knowledge or assumption of the likelihood l, but represents, on the other hand, a quite general and powerful, formal probability relation.

Appendix B: The shortest coverage interval

The lower limit $y^<$ and upper limit $y^>$ of the shortest coverage interval of a non-negative measurand with a specified coverage probability $1 - \gamma$ are determined in this appendix B for
(a) known general distributions,
(b) the truncated GD of ISO 11929,
(c) not explicitly known general distributions by Monte Carlo (MC) application.

In figure 3, they are numerically compared in case (b) with the limits $y^\triangleleft$ and $y^\triangleright$ of the probabilistically symmetric coverage interval. The shortest coverage interval has interesting features for practical applications and meets all the metrological demands laid down in subsection 6.3. In particular, it covers the possible measurand value 0 if and only if this value 0 is actually "highly probable".

B.1 General case

In order to determine the limits $y^<$ and $y^>$ of the shortest coverage interval for the coverage probability $1 - \gamma$, let the density $f(y) = f_Y(y \mid \mathbf{a}, y \geq 0)$ of the estimator Y of the non-negative measurand and its distribution function $F(y) = F_Y(y \mid \mathbf{a}, y \geq 0) = \int_0^y f(\eta)\,\mathrm{d}\eta$ be given for $y > 0$. In addition, $F(y) = 0$ for $y \leq 0$ and $f(y) = 0$ for $y < 0$ and $a = f(0)$. The density $f(y)$ is thus discontinuous at $y = 0$. It jumps from 0 to a at this abscissa because of the truncation. This fact causes a difficulty which has to be removed without any consequences in integrals where $f(y)$ is involved. See the next paragraph.

The difference $y^> - y^<$ is now minimized with the constraint $F(y^>) - F(y^<) = 1 - \gamma$, which is multiplied by a Lagrange multiplier λ and added to the difference. This leads to

$$y^> - y^< + \lambda \cdot (F(y^>) - F(y^<)) = \min \quad . \tag{50}$$

If this expression is minimized instead of the limit difference itself, then the same solutions follow since the constraint is a constant. The partial derivatives of the expression with respect to the limits must be zero for the minimum. Thus,

$$1 + \lambda f(y^>) = 0 \;\; ; \quad 1 + \lambda f(y^<) = 0 \quad . \tag{51}$$

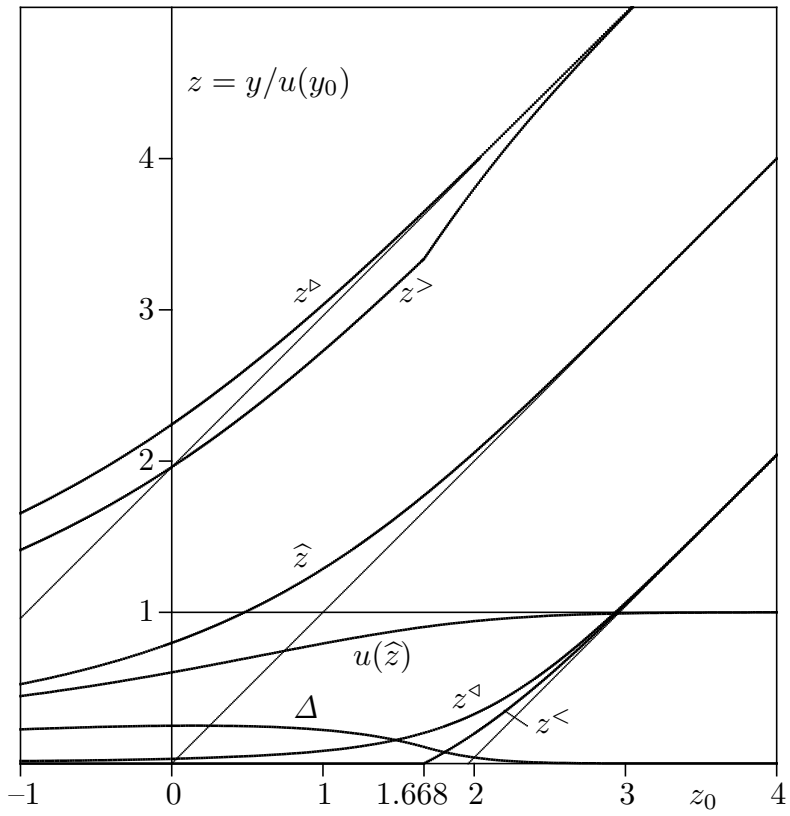

Figure 3: Best estimate $\widehat{z}$ and standard uncertainty $u(\widehat{z})$ of the scaled measurand $Z = Y/u(y_0)$, lower limit $z^{\triangleleft}$ and upper limit $z^{\triangleright}$ of the probabilistically symmetric coverage interval, and lower limit $z^{<}$ and upper limit $z^{>}$ of the shortest coverage interval. Δ is the difference of the widths of the two coverage intervals. All these characteristic values are shown as functions of the primary measurement result $z_0 = y_0/u(y_0)$, scaled with the standard uncertainty $u(y_0)$, and calculated with the truncated Gaussian density according to ISO 11929. The probability $\gamma = 0.05$ is chosen. It is $z^{<} = 0$ for abscissas $z_0 \leq 1.668$. Δ has a maximum 0.251 at $z_0 = 0.15$. The straight lines are asymptotes and show the usual symmetric coverage interval limits.

This means solving the two equations

$$f(y^{>}) = f(y^{<}) \ ; \tag{52}$$

$$F(y^{>}) - F(y^{<}) = 1 - \gamma \tag{53}$$

for the limits. Notice the lack of a solution in equation (52) if $f(y^{>}) < a$ due to the jump of $f(y)$ from 0 to a at $y = 0$. This difficulty is removed by explicitly stipulating $y^{<} = 0$ in this case.

In exceptional cases, a polymodal density can have several or even an infinity of possibly overlapping shortest coverage intervals for the same given γ. For instance, the rectangular density $f(y) = 1$ $(0 \leq y \leq 1)$ and $= 0$ (elsewhere) has an infinity of overlapping shortest coverage intervals of width $(1 - \gamma)$.

B.2 Gaussian case

In the case of ISO 11929 with a given primary measurement result y_0 with the associated standard uncertainty $u(y_0)$ according to GUM, $f(y)$ is a GD truncated at $y = 0$ and renormalized. By introducing the scaled random variable $Z = Y/u(y_0)$ with $z = y/u(y_0)$ and $z_0 = y_0/u(y_0)$ for more brevity and convenience, it reads

$$f_Z(z) = \frac{\exp\left(-(z - z_0)^2/2\right)}{\omega\sqrt{2\pi}} \quad ; \quad \omega = \Phi(z_0) \tag{54}$$

$$F_Z(z) = \frac{\Phi(z - z_0) - (1 - \omega)}{\omega} \tag{55}$$

for $z \geq 0$ and $f_Z(z) = F_Z(z) = 0$ for $z < 0$. Moreover, $a = f_Z(0) = \exp(-z_0^2/2)/(\omega\sqrt{2\pi})$. The standardized Gaussian distribution function $\Phi(t)$ is used with its property $\Phi(-t) = 1 - \Phi(t)$.

The density $f_Z(z)$ is symmetric with respect to z_0 in the range $0 < z < 2z_0$. Thus, according to equation (52), $z^{>,<} = z_0 \pm b$ with some b as long as $z^< > 0$. Equations (53) and (55) then lead to $\Phi(b) - \Phi(-b) = 2\Phi(b) - 1 = \omega \cdot (1 - \gamma)$. The solution is $b = k_p$ with $p = (1 + \omega \cdot (1 - \gamma))/2$. Here, k_p is the p-quantile of $\Phi(t)$, the solution of $\Phi(k_p) = p$. If $y^< < 0$ resulted, then $y^< = 0$ has to be set because of the truncation and jump of $f_Z(z)$ from 0 to a at $z = 0$. Hence it follows $F_Z(z^>) = 1 - \gamma$ according to equation (53) with $F(y^<) = 0$ and, moreover, $\Phi(b) = q = 1 - \omega\gamma$ with equation (55). Thus, $b = k_q$. The final complete result of the limits of the shortest coverage interval is either

$$z^{>,<} = z_0 \pm k_p \quad ; \quad p = (1 + \omega \cdot (1 - \gamma))/2 \tag{56}$$

or, if $z^< < 0$ were to result,

$$z^< = 0 \quad ; \quad z^> = z_0 + k_q \quad ; \quad q = 1 - \omega\gamma \quad . \tag{57}$$

Equation (56) shows the symmetry of $z^>$ and $z^<$ with respect to z_0. Identical results are obtained from equations (56) and (57) if $k_p = k_q = z_0$ or $p = q = \omega = 1/(1 + \gamma)$ and $z_0 = k_{1/(1+\gamma)} = 1.668$ for $\gamma = 0.05$. See figure 3 for numerical values as functions of z_0, also in comparision with the limits $z^\triangleleft$ and $z^\triangleright$ of the probabilistically symmetric coverage interval. The kinks of the curves of $z^>$ and $z^<$ are caused by the change between equations (56) and (57). The width difference $\Delta = (z^\triangleright - z^\triangleleft) - (z^> - z^<)$ of the two coverage intervals is also shown. It has a maximum 0.251 at $z_0 = 0.15$ for $\gamma = 0.05$ and disapears for large z_0. The computing efforts for each of the interval limits are fairly similar. Subroutines for $\Phi(t)$ and k_p are available or can easily be written according to ISO 11929 [1].

B.3 Monte Carlo application

In more general cases, $f(y)$ and $F(y)$ are often not explicitly known since the integrals according to equations (3) cannot be easily solved. A Monte Carlo (MC) method should then be applied [25, 26]. A large number N of MC samples $y^{(i)} \geq 0$ $(i = 1, \ldots, N)$ and, in addition, $y^{(0)} = 0$ are first sorted and renumbered by magnitude in a table

such that $y^{(i-1)} \le y^{(i)}$. A function $Q(p)$ is then defined in this table by $Q(i/N) = y^{(i)}$ $(i = 0, \ldots, N)$ and linear interpolation for real p with $0 \le p \le 1$. This function $Q(p)$ is unique, continuous, piecewise linear and non-decreasing. It is an approximation of the p-quantile of the measurand estimator, i.e. the solution y of $F(y) = p$. In particular, the coverage interval limits $y^{\triangleleft} = Q(\gamma/2)$ and $y^{\triangleright} = Q(1-\gamma/2)$ are obtained.

The determination of the limits $y^{<}$ and $y^{>}$ of the shortest coverage interval cannot easily be carried out by equations (52) and (53) since $f(y)$ is not available and cannot be approximated sufficiently well by MC as the derivative of $F(y)$. But the function $Q(p)$ can be used to directly minimize the interval width $w = y^{>} - y^{<}$ with $y^{<} = Q(p)$ and $y^{>} = Q(1-\gamma+p)$ according to equation (53) by systematically or randomly varying the probability p in a range $0 \le p' \le p \le p'' \le \gamma$. Here, p' and p'' are limits already known to enclose the p that minimizes the width w. At the beginning, $p' = 0$ and $p'' = \gamma$. Their difference can be made smaller and smaller during the iterative minimization until the p of the minimum w is caught with sufficient accuracy. $Q(p)$ is not needed in the range $\gamma < p < 1-\gamma$. Therefore, the values $y^{(i)}$ in a corresponding, large middle part of the table need not be sorted. This suggestion may possibly help to save considerable computing time since sorting is a time-consuming procedure if N is large. The computational MC effort was tested and found to be small and acceptable, compared with the effort for simulating N measurements.

Appendix C: Uncertainty calculation in the case of random influences by sample treatment

The following analytical BSt approach serves for the mathematical derivation of equation (35), recommended in subsection 5.8 to replace equation (B.7) of ISO 11929 [1]. Since the present appendix C describes a purely analytical calculation, subsection 5.8 should first be read as an introduction and as a justification of the Gaussian and gamma densities, and the Poisson probability functions used.

C.1 Approach without counting uncertainties

Let m data x_i be independently drawn from Gaussian densities (GD) of random variables X_i with the same, but unknown expectation μ and variance σ^2 to be determined. These parameters are values (estimates) of random variables (estimators) M and S^2, respectively, where M is assigned to the measurand Y in question ($M = Y$). The densities of X_i are

$$f_X(x \mid M = \mu, S^2 = \sigma^2) = \frac{\exp\big(-(x-\mu)^2/(2\sigma^2)\big)}{\sqrt{2\pi\sigma^2}} \quad ; \tag{58}$$

$$f_{\mathbf{X}}(\mathbf{x} \mid \mu, \sigma^2) = \prod_{i=1}^{m} f_{X_i}(x_i \mid \mu, \sigma^2) = \frac{\exp\big(-\sum_{i=1}^{m}(x_i-\mu)^2/(2\sigma^2)\big)}{(\sqrt{2\pi\sigma^2})^m} \quad . \tag{59}$$

The Bayes theorem and the PME as well (see appendix A.3) then lead to

$$\begin{aligned} f_{M,S^2}(\mu, \sigma^2 \mid \mathbf{x}) &= C\, f_{\mathbf{X}}(\mathbf{x} \mid \mu, \sigma^2)\, f_{M,S^2}(\mu, \sigma^2) = C\, f_{\mathbf{X}}(\mathbf{x} \mid \mu, \sigma^2)\,(1/\sigma^2) \\ &= C\, \frac{\exp\big(-\sum_{i=1}^{m}(x_i-\mu)^2/(2\sigma^2)\big)}{\sigma^{m+1}\sqrt{2\pi\sigma^2/m}} \quad . \end{aligned} \tag{60}$$

For convenience, the variance σ^2 is used as a quantity of interest instead of σ itself. Then, for the prior, $f_{M,S^2}(\mu,\sigma^2)\,\mathrm{d}\mu\,\mathrm{d}\sigma^2 = \mathrm{const}\,\mathrm{d}\mu\,\mathrm{d}\sigma^2/\sigma^2$ should be set since $\mathrm{d}\sigma^2/\sigma^2 = 2\,\mathrm{d}\sigma/\sigma$ [15 (2.8.2), 37]. See also subsection 5.8 for the prior $\sim 1/\sigma$ of the parameter σ. The constants $\sqrt{2\pi}$ are included in the normalization constant C. For convenience in the following, one of them is retained in the denominator and $\sqrt{m}$ is taken from C. The sum can be rearranged with $\sum_{i=1}^{m}(x_i-\overline{x}) = 0$. This yields $\sum_{i=1}^{m}(x_i-\mu)^2 = \sum_{i=1}^{m}((x_i-\overline{x})-(\mu-\overline{x}))^2 = \sum_{i=1}^{m}(x_i-\overline{x})^2 - 2\sum_{i=1}^{m}(x_i-\overline{x})(\mu-\overline{x}) + \sum_{i=1}^{m}(\mu-\overline{x})^2 = \sum_{i=1}^{m}(x_i-\overline{x})^2 + m\,(\mu-\overline{x})^2$ and, accordingly,

$$f_{M,S^2}(\mu,\sigma^2 \mid \mathbf{x}) = C\,\frac{\exp\big(-\big(A+m\,(\mu-\overline{x})^2\big)/(2\sigma^2)\big)}{\sigma^{m+1}\,\sqrt{2\pi\sigma^2/m}} \quad ; \quad A = \sum_{i=1}^{m}(x_i-\overline{x})^2 \quad . \tag{61}$$

For any fixed σ^2, this is a GD of M with expectation $\overline{x}$ and variance σ^2/m. Thus,

$$\mathrm{E}\,(M \mid \sigma^2,\mathbf{x}) = \mathrm{E}\,(M \mid \mathbf{x}) = \widehat{\mu} = \overline{x} \quad ; \quad \mathrm{Var}\,(M \mid \sigma^2,\mathbf{x}) = \sigma^2/m \quad . \tag{62}$$

The following integrals are needed for the best estimate $s^2 = \mathrm{E}\,(S^2 \mid \mathbf{x})$ of σ^2 and the squared standard uncertainty $u^2(\widehat{\mu}) = \mathrm{Var}\,(M \mid \mathbf{x})$ associated with the best estimate $\widehat{\mu} = \overline{x} = \mathrm{E}\,(M \mid \mathbf{x})$ of the measurand $M = Y$. The integrations over μ are carried out first and yield either 1 or σ^2/m.

$$s^2 = \mathrm{E}\,(S^2 \mid \mathbf{x}) = C\int_0^\infty\!\!\int_{-\infty}^\infty \sigma^2\,\frac{\exp\big(-\big(A+m\,(\mu-\overline{x})^2\big)/(2\sigma^2)\big)}{\sigma^{m+1}\,\sqrt{2\pi\sigma^2/m}}\,\mathrm{d}\mu\,\mathrm{d}\sigma^2$$

$$= C\int_0^\infty \sigma^2\,\frac{\exp\big(-A/(2\sigma^2)\big)}{\sigma^{m+1}}\,\mathrm{d}\sigma^2 \quad ; \tag{63}$$

$$u^2(\widehat{\mu}) = \mathrm{Var}\,(M \mid \mathbf{x}) = \mathrm{E}\,((M-\widehat{\mu})^2 \mid \mathbf{x}) = \mathrm{E}\,((M-\overline{x})^2 \mid \mathbf{x}) = \mathrm{E}\,(M^2 \mid \mathbf{x}) - \overline{x}^2$$

$$= C\int_0^\infty\!\!\int_{-\infty}^\infty (\mu-\overline{x})^2\,\frac{\exp\big(-\big(A+m\,(\mu-\overline{x})^2\big)/(2\sigma^2)\big)}{\sigma^{m+1}\sqrt{2\pi\sigma^2/m}}\,\mathrm{d}\mu\,\mathrm{d}\sigma^2$$

$$= C\int_0^\infty \frac{\sigma^2}{m}\,\frac{\exp\big(-A/(2\sigma^2)\big)}{\sigma^{m+1}}\,\mathrm{d}\sigma^2 = s^2/m \quad ; \tag{64}$$

$$1/C = \int_0^\infty\!\!\int_{-\infty}^\infty \frac{\exp\big(-\big(A+m\,(\mu-\overline{x})^2\big)/(2\sigma^2)\big)}{\sigma^{m+1}\sqrt{2\pi\sigma^2/m}}\,\mathrm{d}\mu\,\mathrm{d}\sigma^2$$

$$= \int_0^\infty \frac{\exp\big(-A/(2\sigma^2)\big)}{\sigma^{m+1}}\,\mathrm{d}\sigma^2 \quad . \tag{65}$$

Accordingly, $\mathrm{E}\,(M^2 \mid \mathbf{x}) = s^2/m + \overline{x}^2$ and $\mathrm{Var}\,(M \mid \mathbf{x}) = s^2/m$. Any integral

$$I_k = \int_0^\infty \frac{\exp\big(-A/(2\sigma^2)\big)}{\sigma^k}\,\mathrm{d}\sigma^2 \tag{66}$$

is carried out by substituting $A/(2\sigma^2) = t$ or $\sigma^2 = A/(2t)$ and $\mathrm{d}\sigma^2 = -(A/2)(\mathrm{d}t/t^2)$.

Then,

$$I_k = \int_0^\infty \frac{\exp(-t)}{(A/(2t))^{k/2}}(A/2)(\mathrm{d}t/t^2) = (2/A)^{k/2-1}\int_0^\infty t^{k/2-2}\,\exp(-t)\,\mathrm{d}t$$

$$= (2/A)^{k/2-1}\Gamma(k/2-1)\ . \tag{67}$$

With $k = m \pm 1$ and equations (63) and (65),

$$s^2 = \mathrm{E}\,(S^2 \mid \mathbf{x}) = \frac{I_{m-1}}{I_{m+1}} = \frac{A}{2}\cdot\frac{\Gamma((m-3)/2)}{\Gamma((m-1)/2)} = \frac{A}{m-3} = \frac{1}{m-3}\sum_{i=1}^{m}(x_i-\overline{x})^2 \tag{68}$$

is obtained since $\Gamma(z+1) = z\Gamma(z)$ or $\Gamma((m-1)/2) = ((m-3)/2)\Gamma((m-3)/2)$. This $s^2 = A/(m-3)$ has to be compared with the similar $s^2 = A/(m-1)$ according to equation (B.7) of ISO 11929. $m > 3$ is required. $u^2(\widehat{\mu}) = u^2(\widehat{y}) = s^2/m$ remains according to equation (64). It can easily be seen that $(m-3)$ does not come from counting uncertainties since these are not involved here.

By integrating equation (61) over σ^2 and using equations (66) and (67) with A replaced by $A + m(\mu-\overline{x})^2$, the density

$$f_M(\mu \mid \mathbf{x}) = \frac{C}{(A + m\,(\mu-\overline{x})^2)^{m/2}} \tag{69}$$

is obtained. The substitution $t = (\mu-\overline{x})/\sqrt{A/((m-1)m)}$ then leads to the Student density $f_T(t) = C\cdot(1+t^2/(m-1))^{-m/2}$ with $m-1$ degrees of freedom, $\mathrm{E}\,(T) = 0$ and $\mathrm{Var}\,(T) = (m-1)/(m-3)$. Hence it follows by reversing the substitution that $\widehat{\mu} = \mathrm{E}\,(M) = \overline{x}$ and $u^2(\widehat{\mu}) = \mathrm{Var}\,(M) = s^2/m$ with $s^2 = A/(m-3)$ as in equation (68).

C.2 Including counting uncertainties

Similarly to appendix C.1, let m data n_i be independently drawn from Poisson distributions of N_i with parameters ξ_i as values of random variables X_i.

According to the Bayes theorem, the density of X is proportional to the Poisson probability function of N, times the prior C/ξ of X (see subsection 5.7), i.e.

$$f_X(\xi \mid n) = C\,f_N(n \mid \xi)\,f_X(\xi) = \frac{\xi^n\,\exp(-\xi)}{n!}\cdot\frac{C}{\xi} = \frac{\xi^{n-1}\,\exp(-\xi)}{(n-1)!} \tag{70}$$

is a gamma density of X with $x = \mathrm{E}\,(X \mid n) = n$ and $u^2(x) = \mathrm{Var}\,(X \mid n) = n$.

$$f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{n}) = \prod_{i=1}^{m} f_{X_i}(\xi_i \mid n_i) = \prod_{i=1}^{m}\frac{\xi_i^{n_i-1}\,\exp(-\xi_i)}{(n_i-1)!}\ ; \tag{71}$$

$$f = f_{M,S^2,\mathbf{X}}(\mu,\sigma^2,\boldsymbol{\xi} \mid \mathbf{n}) = f_{M,S^2}(\mu,\sigma^2 \mid \boldsymbol{\xi})\,f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{n})$$

$$= C\,\frac{\exp\big(-\big(A + m\,(\mu-\overline{\xi})^2\big)/(2\sigma^2)\big)}{\sigma^{m+1}\sqrt{2\pi\sigma^2/m}}\cdot\prod_{i=1}^{m}\frac{\xi_i^{n_i-1}\,\exp(-\xi_i)}{(n_i-1)!} \tag{72}$$

according to equation (61) and with $\mathbf{x}$ replaced by $\boldsymbol{\xi}$, in particular, $A = \sum_{i=1}^{m} (\xi_i - \overline{\xi})^2$. By marginalization,

$$f_{M,S^2}(\mu, \sigma^2 \mid \mathbf{n}) = \int_0^\infty f_{M,S^2,\mathbf{X}}(\mu, \sigma^2, \boldsymbol{\xi} \mid \mathbf{n}) \, \mathrm{d}\boldsymbol{\xi} \tag{73}$$

is obtained, which leads with equations (72) and (73) for any function $h(M, S^2)$ to

$$\mathrm{E}\left(h(M, S^2) \mid \mathbf{n}\right) = \int_0^\infty \mathrm{E}\left(h(M, S^2) \mid \boldsymbol{\xi}\right) f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{n}) \, \mathrm{d}\boldsymbol{\xi} \ . \tag{74}$$

This is an important equation. It is first applied with $h = M$ to $\mathrm{E}\left(M \mid \boldsymbol{\xi}\right) = \overline{\xi}$ according to equation (62) and yields

$$\widehat{\mu} = \mathrm{E}\left(M \mid \mathbf{n}\right) = \int_0^\infty \overline{\xi} \, f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{n}) \, \mathrm{d}\boldsymbol{\xi} = \overline{n} \ . \tag{75}$$

It is similarly applied with $h = S^2$ to $\mathrm{E}\left(S^2 \mid \boldsymbol{\xi}\right) = A/(m-3)$ according to equation (68)

$$\begin{aligned} \mathrm{E}\left(S^2 \mid \mathbf{n}\right) &= \frac{1}{m-3} \int_0^\infty \sum_{i=1}^{m} \left(\xi_i - \overline{\xi}\right)^2 f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{n}) \, \mathrm{d}\boldsymbol{\xi} \\ &= \frac{1}{m-3} \left(\mathrm{E}\left(\sum_{i=1}^{m} X_i^2 \mid \mathbf{n} \right) - m \, \mathrm{E}\left(\overline{X}^2 \mid \mathbf{n} \right) \right) \ . \end{aligned} \tag{76}$$

With $\mathrm{E}\left(X \mid n\right) = n$; $\mathrm{E}\left(X^2 \mid n\right) = n(n+1)$; $\mathrm{Var}\left(X \mid n\right) = n$; $\mathrm{E}\left(\overline{X} \mid \mathbf{n}\right) = \overline{n}$; $\mathrm{Var}\left(\overline{X} \mid \mathbf{n}\right) = \overline{n}/m$ and $\overline{n^2} = \sum_{i=1}^{m} n_i^2 \, /m$, it follows from equation (76)

$$\mathrm{E}\left(\sum_{i=1}^{m} X_i^2 \mid \mathbf{n} \right) = \sum_{i=1}^{m} \mathrm{E}\left(X_i^2 \mid n_i\right) = m \cdot \overline{n(n+1)} = m \cdot \left(\overline{n^2} + \overline{n}\right) \ ; \tag{77}$$

$$\mathrm{E}\left(\overline{X}^2 \mid \mathbf{n}\right) = \mathrm{Var}\left(\overline{X} \mid \mathbf{n}\right) + \left(\mathrm{E}\left(\overline{X} \mid \mathbf{n}\right)\right)^2 = \overline{n}/m + \overline{n}^2 \ ; \tag{78}$$

$$\begin{aligned} \mathrm{E}\left(S^2 \mid \mathbf{n}\right) &= \frac{m\left(\overline{n^2} + \overline{n}\right) - \left(\overline{n} + m\,\overline{n}^2\right)}{m-3} = \frac{(m-1)\,\overline{n} + m\left(\overline{n^2} - \overline{n}^2\right)}{m-3} \\ &= \frac{m-1}{m-3}\,\overline{n} + \frac{1}{m-3} \sum_{i=1}^{m} (n_i - \overline{n})^2 = \frac{m-1}{m-3}\left(\overline{n} + s_0^2\right) \end{aligned} \tag{79}$$

where s_0^2 means s^2 according to equation (B.7) of ISO 11929. The first term is caused by the counting uncertainties. If these are set to zero, the term vanishes and equation (68) again follows since in this case $n = x$; $\mathrm{Var}\left(X \mid n\right) = n$ and $\mathrm{E}\left(X^2 \mid n\right) = n^2$ between equations (76) and (77).

$\mathrm{E}\left(S^2 \mid \mathbf{n}\right)$ is the best estimate of σ^2. Divided by m, it is used in form of s^2/m as a squared standard uncertainty needed in annex B.4 of ISO 11929. This is no longer possible here as is now shown. The squared standard uncertainty associated with $\widehat{y} = \widehat{\mu} = \mathrm{E}\left(M \mid \mathbf{n}\right) = \overline{n}$ according to equation (75) is $u^2(\overline{n}) = \mathrm{E}\left((M - \overline{n})^2 \mid \mathbf{n}\right)$, which differs

here from $\mathrm{E}\,(S^2 \mid \mathbf{n})/m$. This is an important statement. However, both expressions remain to be related to one another.

$$u^2(\overline{n}) = \mathrm{E}\,((M-\overline{n})^2 \mid \mathbf{n}) = \mathrm{E}\,(M^2 \mid \mathbf{n}) - \overline{n}^2 \;\; ; \tag{80}$$

$$\begin{aligned}\mathrm{E}\,(M^2 \mid \mathbf{n}) &= \int_0^\infty \mathrm{E}\,\big((M-\overline{\xi}+\overline{\xi})^2 \mid \boldsymbol{\xi}\big) f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{n})\,\mathrm{d}\boldsymbol{\xi} \\ &= \int_0^\infty\int_0^\infty\int_{-\infty}^\infty \big((\mu-\overline{\xi})^2 + 2(\mu-\overline{\xi})\overline{\xi} + \overline{\xi}^2\big)\, f\,\mathrm{d}\mu\,\mathrm{d}\sigma^2\,\mathrm{d}\boldsymbol{\xi}\end{aligned} \tag{81}$$

according to equation (74) with $h = M^2$ and with f from equation (72). The integration over μ yields σ^2/m similar to equation (64) for the first term and a vanishing second term. The third term does not depend on μ and σ^2. The integration over σ^2 then results in the continuation

$$= \int_0^\infty \big(\mathrm{E}\,(S^2 \mid \boldsymbol{\xi})/m + \overline{\xi}^2\big) f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{n})\,\mathrm{d}\boldsymbol{\xi} = \mathrm{E}\,(S^2 \mid \mathbf{n})/m + \mathrm{E}\,(\overline{X}^2 \mid \mathbf{n}) \;\; . \tag{82}$$

Equation (74) is used again with $h = S^2$. Finally, with equations (78) and (80),

$$\begin{aligned}u^2(\overline{n}) &= \mathrm{E}\,(M^2 \mid \mathbf{n}) - \overline{n}^2 = \mathrm{E}\,(S^2 \mid \mathbf{n})/m + \mathrm{E}\,(\overline{X}^2 \mid \mathbf{n}) - \overline{n}^2 = \frac{\mathrm{E}\,(S^2 \mid \mathbf{n}) + \overline{n}}{m} \\ &= \frac{1}{m}\Big(\overline{n} + \frac{m-1}{m-3}\,\overline{n} + \frac{1}{m-3}\sum_{i=1}^m (n_i - \overline{n})^2\Big)\end{aligned} \tag{83}$$

is obtained. This is the very formula that should replace equation (B.7) of ISO 11929.

The density $f_M(\mu \mid \mathbf{n})$ of the measurand $M = Y$ should be explicitly available for the determination of the characteristic limits, for instance, the limits of a coverage interval. This density follows by marginalization from f according to equation (72) similar to equation (73):

$$\begin{aligned}f_M(\mu \mid \mathbf{n}) &= \int_0^\infty\int_0^\infty f_{M,S^2,\mathbf{X}}(\mu,\sigma^2,\boldsymbol{\xi} \mid \mathbf{n})\,\mathrm{d}\sigma^2\,\mathrm{d}\boldsymbol{\xi} \\ &= C\int_0^\infty\int_0^\infty \frac{\exp\big(-\big(A + m\,(\mu-\overline{\xi})^2\big)/(2\sigma^2)\big)}{\sigma^{m+1}\,\sqrt{2\pi\sigma^2/m}} \cdot \prod_{i=1}^m \frac{\xi_i^{n_i-1}\,\exp(-\xi_i)}{(n_i-1)!}\,\mathrm{d}\sigma^2\,\mathrm{d}\boldsymbol{\xi} \;\; .\end{aligned} \tag{84}$$

The integration over σ^2 can be carried out by means of equations (66) and (67) with A replaced by $A + m\,(\mu-\overline{\xi})^2$ and $k = m+2$ and including constant factors into C as far as possible and appropriate. With $M = Y$ and $\mu = y$, this finally leads to

$$f_Y = f_Y(y \mid \mathbf{n}) = C\int_0^\infty \big(A + m\,(y-\overline{\xi})^2\big)^{-m/2} \cdot \prod_{i=1}^m \xi_i^{n_i-1}\,\exp(-\xi_i)\,\mathrm{d}\boldsymbol{\xi} \;\; . \tag{85}$$

The expectation $\overline{n}$ and the variance $u^2(\overline{n})$ of this distribution f_Y are known according to equations (75) and (83), respectively. However, the determination of the quantiles for the characteristic limits seems to require difficult, multidimensional, numerical integrations by MC. Other properties of f_Y are discussed below equation (37).

Appendix D: Glossary of some important terms and symbols

Z	general random variable; general estimator of a physical quantity or of the scaled measurand
z, ζ	values of Z; estimates of the physical quantity; particular values are marked by affixes
$u(z)$	measurement uncertainty of Z associated with z; standard uncertainty if z is the expectation of Z
Y	estimator assigned to the non-negative measurand; also used for the measurand itself
y	value of Y; general estimate of the true measurand value; possible true measurand value if $y \geq 0$
$u(y)$	measurement uncertainty of Y associated with y
$\mathbf{a}$	information set of data, conditions, assumptions, relations, and other relevant information
$f_Y(y \mid \mathbf{a})$	probability density of Y given the information $\mathbf{a}$
$F_Y(y \mid \mathbf{a}) = \Pr(Y \leq y \mid \mathbf{a}) = \int_{-\infty}^{y} f_Y(\eta \mid \mathbf{a})\,\mathrm{d}\eta$	distribution function of Y given the information $\mathbf{a}$
$\mathbf{X}$	vector of input quantity estimators X_i
$\boldsymbol{\xi}$	vector of general values ξ_i of X_i
$f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{a})$	probability density of $\mathbf{X}$ given the information $\mathbf{a}$
$G(\mathbf{X})$	model function, $Y = G(\mathbf{X})$ model equation
$\mathbf{x}$	vector of given particular values of $\mathbf{X}$
$\mathbf{U}_{\mathbf{x}}$	uncertainty (covariance) matrix associated with $\mathbf{x}$
$\widetilde{y}$	assumed true measurand value
$\widetilde{\mathbf{a}}(\widetilde{y})$	modification of $\mathbf{a}$ as a function of $\widetilde{y}$
y_0	primary estimate of the true measurand value
$u(y_0)$	standard uncertainty associated with y_0
$\widehat{y}$	best estimate of the true measurand value
$y^{\triangleleft}$, $y^{\triangleright}$	lower and upper limits of the probabilistically symmetric coverage interval
$y^{<}$, $y^{>}$	lower and upper limits of the shortest coverage interval
y^*	decision threshold
$y^\sharp$	detection limit
$y^{(k)}$	Monte Carlo samples sorted by magnitude ($k = 1, \ldots$)
α	probability of the physical effect being falsely recognized as present although $\widetilde{y} = 0$ (false positive decision)
β	probability of the physical effect being falsely recognized as absent although $\widetilde{y} > 0$ (false negative decision)
$1 - \gamma$	coverage probability; probability that the coverage interval contains the true measurand value
I_i	particular integrals ($i = 0, \ldots, 7$)
$H(t)$	Heaviside unit step function
$\delta(t)$	Dirac delta function
$\Phi(t)$	standardized Gaussian distribution function
k_p	quantile of $\Phi(t)$ for the probability p

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